Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:42 PM EDT

PDB ID	:	1JD2
Title	:	Crystal Structure of the yeast 20S Proteasome:TMC-95A complex: A non-covalent Proteasome Inhibitor
Authors	:	Groll, M.; Koguchi, Y.; Huber, R.; Kohno, J.
Deposited on	:	2001-06-12
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

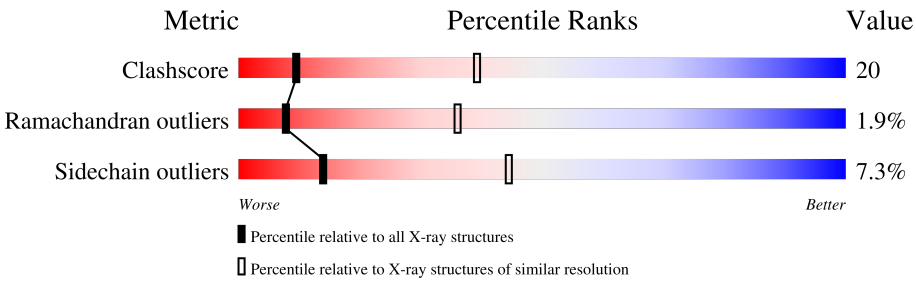
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	66% 32% •
1	V	250	66% 33% •
2	B	244	59% 38% •
2	W	244	61% 34% 5%
3	C	241	63% 33% •
3	X	241	56% 40% •
4	D	242	65% 31% •
4	Y	242	66% 31% •

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Mol	Chain	Length	Quality of chain
5	E	233	57% 38% 5%
5	Z	233	54% 40% 6%
6	1	244	48% 48% •
6	F	244	53% 44% •
7	2	243	51% 43% 6%
7	G	243	60% 35% 5%
8	H	222	61% 36% •
8	O	222	57% 37% 5%
9	I	204	67% 31% •
9	P	204	63% 33% •
10	J	198	63% 32% 6%
10	Q	198	62% 35% •
11	K	212	64% 32% •
11	R	212	70% 27% •
12	L	222	60% 37% •
12	S	222	66% 31% •
13	M	233	57% 40% •
13	T	233	55% 42% •
14	N	196	56% 42% •
14	U	196	53% 43% 5%
15	8	5	40% 20% 20% 20%
15	9	5	40% 20% 20% 20%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 52549 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	V	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called PROTEASOME COMPONENT Y13.

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

- Molecule 3 is a protein called PROTEASOME COMPONENT PRE6.

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

- Molecule 4 is a protein called PROTEASOME COMPONENT PUP2.

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

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	LEU	-	INSERTION	UNP P32379
D	122	ARG	-	INSERTION	UNP P32379
D	123	PHE	-	INSERTION	UNP P32379
D	123A	GLY	-	INSERTION	UNP P32379
D	123B	GLU	-	INSERTION	UNP P32379
D	123C	GLY	-	INSERTION	UNP P32379
D	123E	SER	-	INSERTION	UNP P32379
D	123F	GLY	-	INSERTION	UNP P32379
D	123G	GLU	-	INSERTION	UNP P32379
D	125	GLU	ALA	CONFLICT	UNP P32379
D	126	ARG	ALA	CONFLICT	UNP P32379
D	127	LEU	ALA	CONFLICT	UNP P32379
Y	121	LEU	-	INSERTION	UNP P32379
Y	122	ARG	-	INSERTION	UNP P32379
Y	123	PHE	-	INSERTION	UNP P32379
Y	123A	GLY	-	INSERTION	UNP P32379
Y	123B	GLU	-	INSERTION	UNP P32379
Y	123C	GLY	-	INSERTION	UNP P32379
Y	123E	SER	-	INSERTION	UNP P32379
Y	123F	GLY	-	INSERTION	UNP P32379
Y	123G	GLU	-	INSERTION	UNP P32379
Y	125	GLU	ALA	CONFLICT	UNP P32379
Y	126	ARG	ALA	CONFLICT	UNP P32379
Y	127	LEU	ALA	CONFLICT	UNP P32379

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE5.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	127	TYR	ALA	CONFLICT	UNP P40302
Z	127	TYR	ALA	CONFLICT	UNP P40302

- Molecule 6 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	1897	1205	330	358	4	0	0	0
6	1	244	1897	1205	330	358	4	0	0	0

- Molecule 7 is a protein called PROTEASOME COMPONENT C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	243	1921	1221	322	370	8	0	0	0
7	2	243	1921	1221	322	370	8	0	0	0

- Molecule 8 is a protein called PROTEASOME COMPONENT PUP1.

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

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP3.

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

- Molecule 10 is a protein called PROTEASOME COMPONENT C11.

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

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE2.

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

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

- Molecule 12 is a protein called PROTEASOME COMPONENT C5.

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

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE4.

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

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE3.

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

- Molecule 15 is a protein called TMC-95A inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	8	5	49	33	6	10	0	0	0
			Total	C	N	O			
15	9	5	49	33	6	10	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
16	D	1	1	1	0	0
			Total	Mg		
16	F	2	2	2	0	0

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	A	105	105	105	0	0
			Total	O		
17	B	80	80	80	0	0
			Total	O		
17	C	69	69	69	0	0
			Total	O		
17	D	90	90	90	0	0
			Total	O		
17	E	55	55	55	0	0
			Total	O		
17	F	99	99	99	0	0
			Total	O		
17	G	106	106	106	0	0
			Total	O		
17	H	114	114	114	0	0
			Total	O		
17	I	107	107	107	0	0
			Total	O		
17	J	116	116	116	0	0
			Total	O		
17	K	103	103	103	0	0
			Total	O		
17	L	140	140	140	0	0
			Total	O		
17	M	150	150	150	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	N	116	116	116	0	0
			Total	O		
17	O	121	121	121	0	0
			Total	O		
17	P	101	101	101	0	0
			Total	O		
17	Q	121	121	121	0	0
			Total	O		
17	R	107	107	107	0	0
			Total	O		
17	S	144	144	144	0	0
			Total	O		
17	T	142	142	142	0	0
			Total	O		
17	U	118	118	118	0	0
			Total	O		
17	V	104	104	104	0	0
			Total	O		
17	W	74	74	74	0	0
			Total	O		
17	X	70	70	70	0	0
			Total	O		
17	Y	89	89	89	0	0
			Total	O		
17	Z	53	53	53	0	0
			Total	O		
17	1	93	93	93	0	0
			Total	O		
17	2	103	103	103	0	0
			Total	O		
17	8	2	2	2	0	0
			Total	O		
17	9	1	1	1	0	0

3 Residue-property plots (i)

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

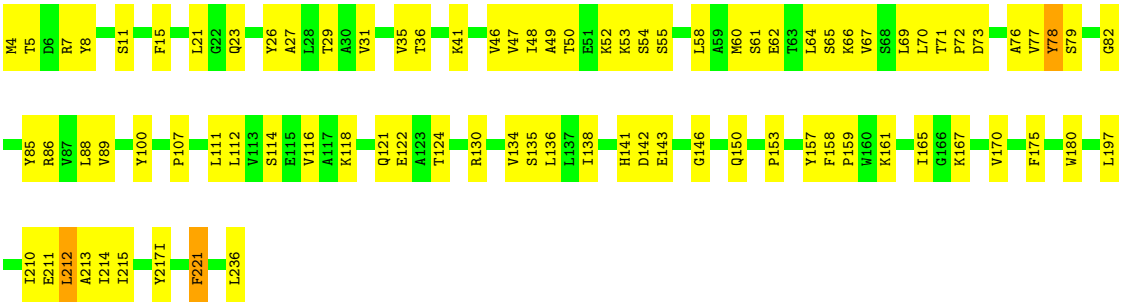
Note EDS was not executed.

• Molecule 1: PROTEASOME COMPONENT Y7

Chain A: 66% 32%

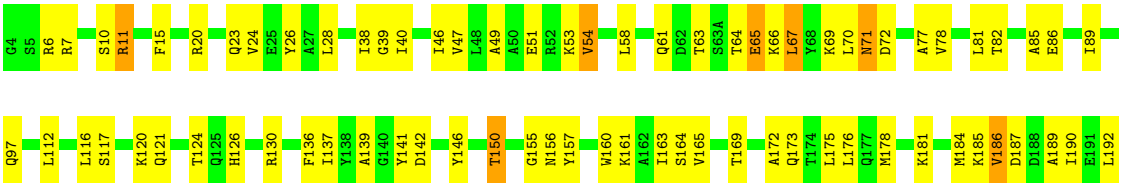
• Molecule 1: PROTEASOME COMPONENT Y7

Chain V: 66% 33%



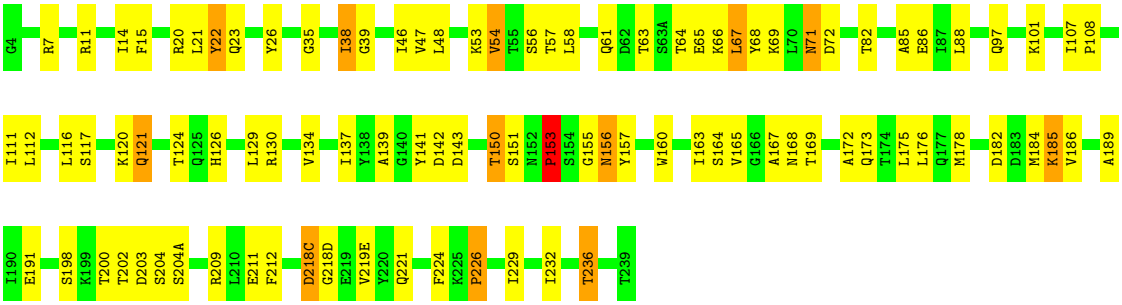
• Molecule 2: PROTEASOME COMPONENT Y13

Chain B: 59% 38%



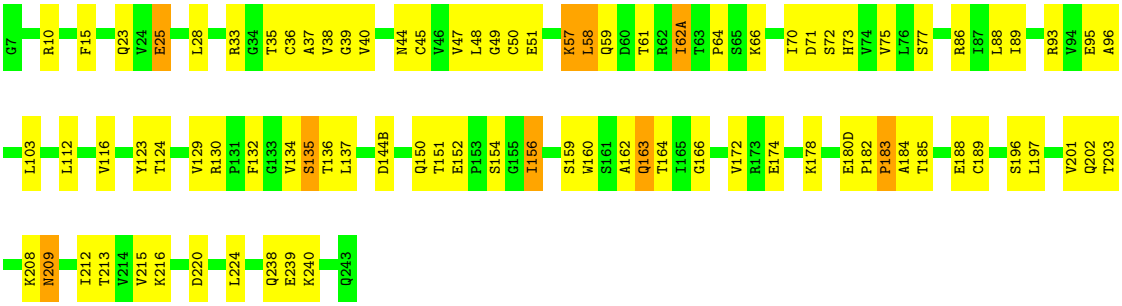
• Molecule 2: PROTEASOME COMPONENT Y13

Chain W:



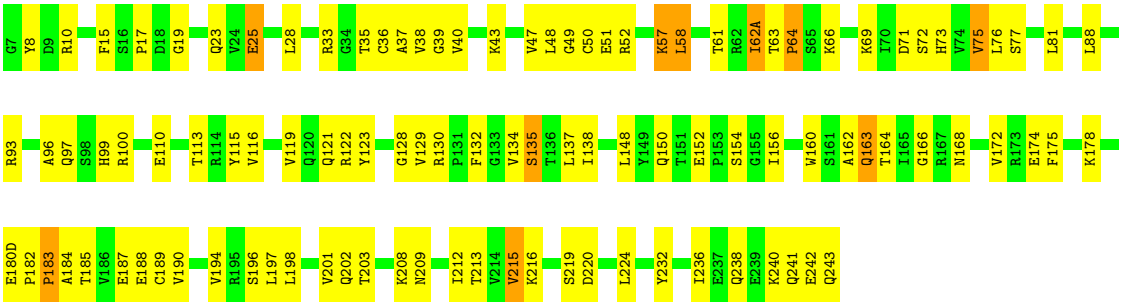
• Molecule 3: PROTEASOME COMPONENT PRE6

Chain C:



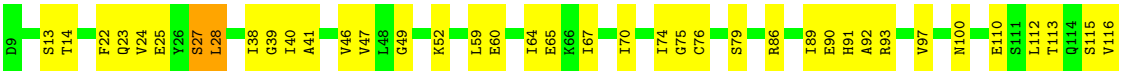
• Molecule 3: PROTEASOME COMPONENT PRE6

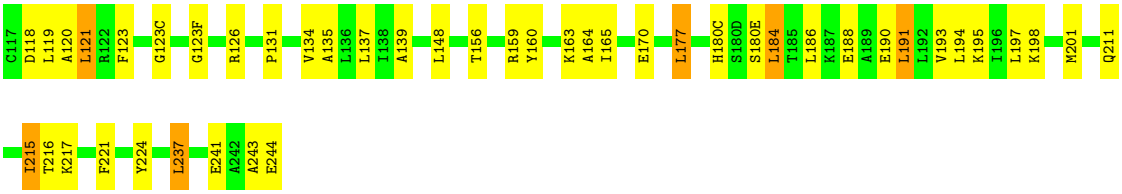
Chain X:



• Molecule 4: PROTEASOME COMPONENT PUP2

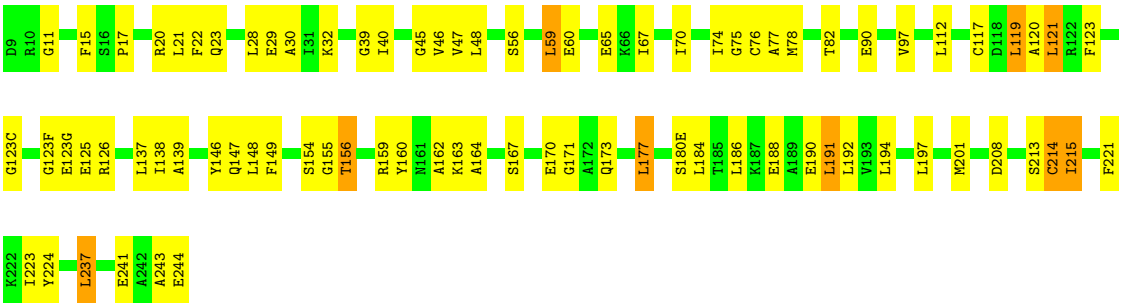
Chain D:





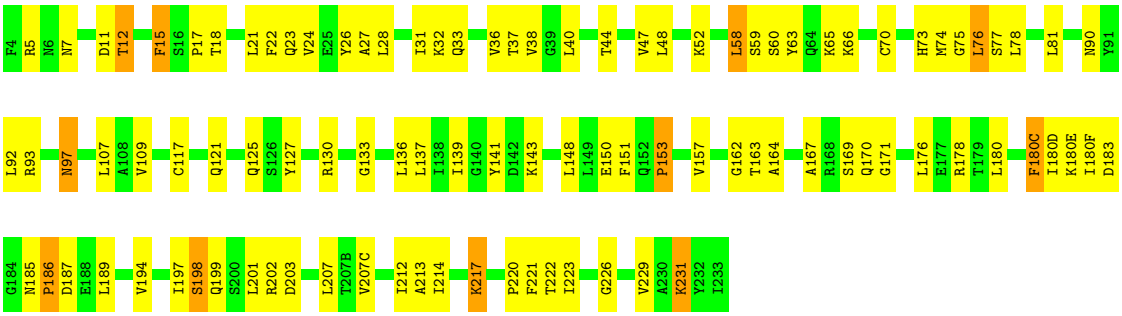
• Molecule 4: PROTEASOME COMPONENT PUP2

Chain Y:



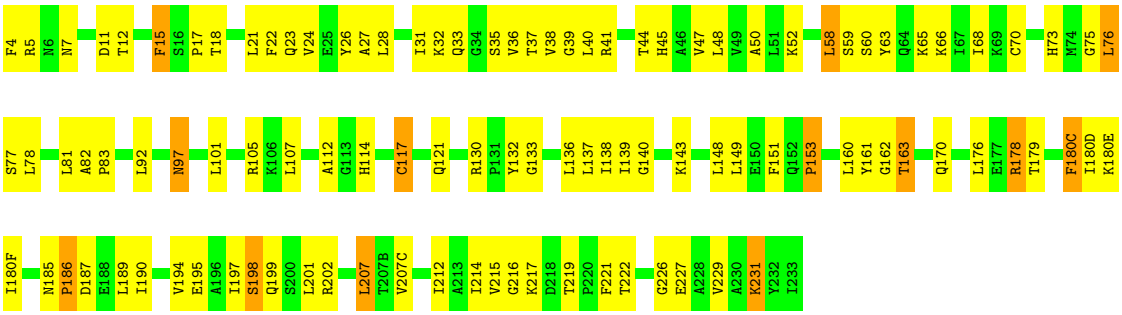
• Molecule 5: PROTEASOME COMPONENT PRE5

Chain E:



• Molecule 5: PROTEASOME COMPONENT PRE5

Chain Z:



• Molecule 6: PROTEASOME COMPONENT C1

Chain F:

G5 S11 N12 S13 V14 P17 D18 G19 R20 N21 F22 Q23 V24 E25 Y26 A27 V31 E32 N33 G34 T35 T36 S37 I38 C42 N43 V50 E51 K52 L53 I54 K66 I67 Q68 V69 V70 D71 R72 H73 I74 Y78 L81 I82 P83 D84 G85 R86 V89 I107 P108

I109 P110 A111 F112 A113 D114 R115 L116 Y119 V120 Q121 A122 L125 Y126 N127 R130 P131 F132 G133 V134 S135 T136 I137 V141 H147 L148 Y149 M150 L151 E152 P153 S154 G155 S156 Y157 W158 G159 Y160 K161 G162 A163 A164 T165 R169 Q170 S171 A172 K173 A174 E175 L176 E180E G180F

L184 S185 A186 R187 E188 A189 V190 K191 Q192 K195 I196 I197 Y198 L199 E203 D204 N205 K206 E206B K206C D207 F208 E209 L210 E211 I212 S213 W214 C215 S216 E218A T218B N218C H221 K222 F223 D227 I233 A236 Q237 K238 N241

- Molecule 6: PROTEASOME COMPONENT C1

Chain 1:

G5 T6 G7 Y8 D9 N12 S13 V14 F15 D18 G19 R20 Q23 V24 E25 Y26 A27 E32 N33 G34 T35 T36 S37 I38 C42 N43 V46 V47 F48 A49 V50 E51 K52 L53 I54 L59 V60 P61 Q62 K63 N64 V65 K66 I67 Q68 V69 V70 D71 R72 H73 I74 V77

L81 I82 P83 R86 H87 L88 V89 E95 A96 A97 S98 F99 L102 I107 P108 I109 P110 A111 R115 L116 Y119 V120 Q121 A122 L125 Y126 N127 R130 G133 V134 S135 T136 V141 D142 K143 M150 L151 E152 P153 S156 Y157 W158 G159 Y160 K161 G162 A163

A164 K167 G168 R169 Q170 S171 A172 K173 A174 E175 L176 E177 K178 L184 S185 A186 R187 E188 A189 V190 K191 Q192 A193 A194 K195 I196 I197 Y198 E203 D204 N205 K206 E206B K206C D207 F208 E211 I212 S213 W214 C215 N218C G219 L220 H221 K222 F223 V224 D227 L228 A232 I233 D234

F235 A236 Q237 K238 E239 I240 N241

- Molecule 7: PROTEASOME COMPONENT C7-ALPHA

Chain G:

A6 G7 Y8 D9 R10 H11 I12 T13 I14 F15 L21 Y26 A27 A30 I35 V40 C45 T46 V47 V48 I49 S50 Q51 P55 D56 L59 D60 P61 R72 T73 I74 G75 M76 V77 I82 P83 R86 N87 A88 A89 L90 R91 A96 F99 Y105 D106

M107 P108 C109 D110 V111 L112 R115 N118 L119 S120 Q121 T124 M129 R130 P131 T137 F138 P146 K150 T151 Y156 Y157 V158 G159 Q169 Q170 E171 I172 T173 T174 E177 S179D K179E I180A D180B H180C I180D N184 E184G E187 K188 E191 I194 I198

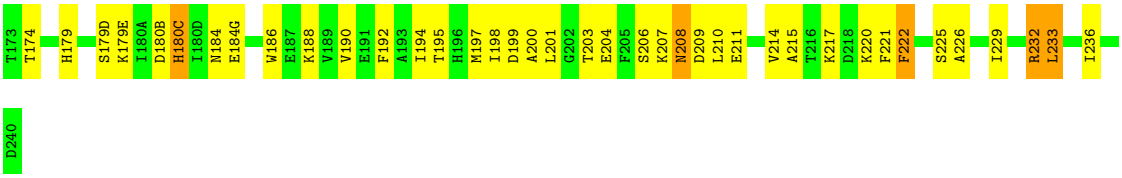
L201 G202 T203 E204 K207 N208 D209 L210 E211 V212 G213 V214 A215 T216 K217 D218 K220 F221 F222 S225 A226 I229 R232 L233 I236 A237 E238 Q239 D240

- Molecule 7: PROTEASOME COMPONENT C7-ALPHA

Chain 2:

A6 D9 I12 T13 I14 F15 S16 P17 E18 L21 E25 Y26 A27 F28 K29 L38 A39 V40 R41 T46 V47 V48 I49 S50 P55 D56 L59 D60 P61 T62 I67 F68 C69 R72 M76 V77 V78 I82 P83 D84 A85 R86 N87 R91 A92 K93

A96 F99 Y105 D106 M107 P108 C109 D110 V111 R115 N118 L119 S120 Q121 I122 Y123 T124 A127 Y128 M129 R130 P131 L132 L136 T137 F138 V139 S140 E143A P146 Y149 K150 T151 D152 P153 Y157 V158 G159 Y160 K161 A162 T165 G166 P167 K168 Q169 Q170 E171 I172

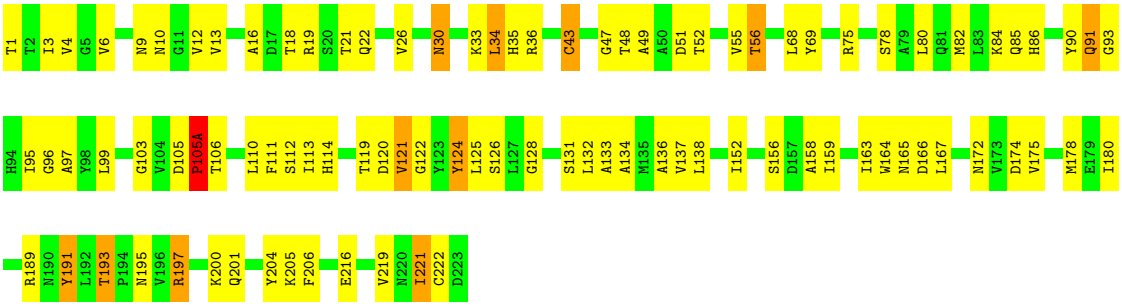


• Molecule 8: PROTEASOME COMPONENT PUP1

Chain H:

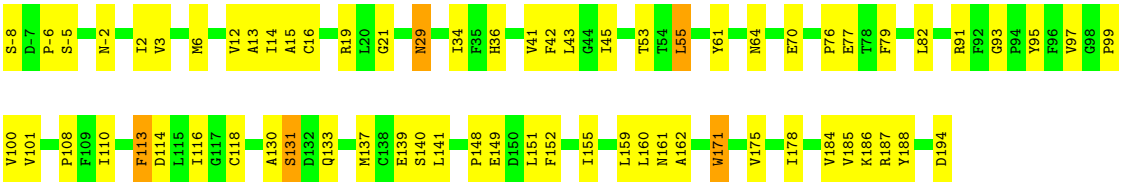
• Molecule 8: PROTEASOME COMPONENT PUP1

Chain O:



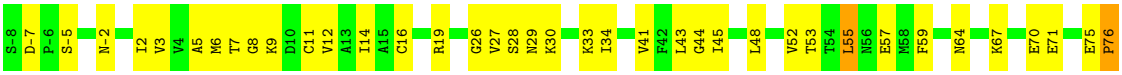
• Molecule 9: PROTEASOME COMPONENT PUP3

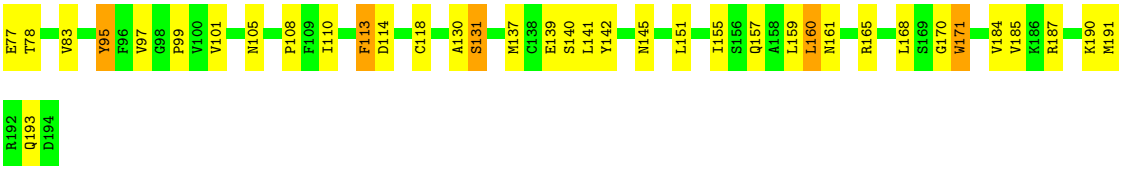
Chain I:



• Molecule 9: PROTEASOME COMPONENT PUP3

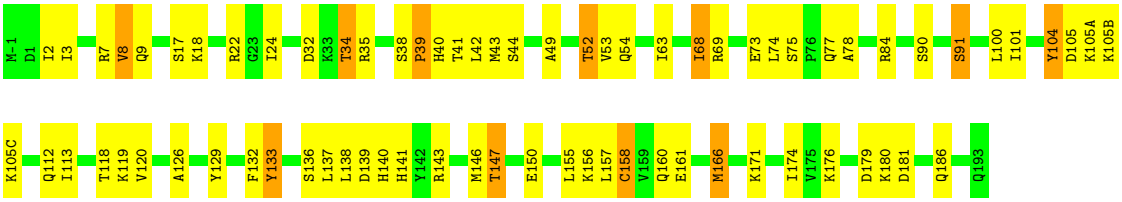
Chain P:





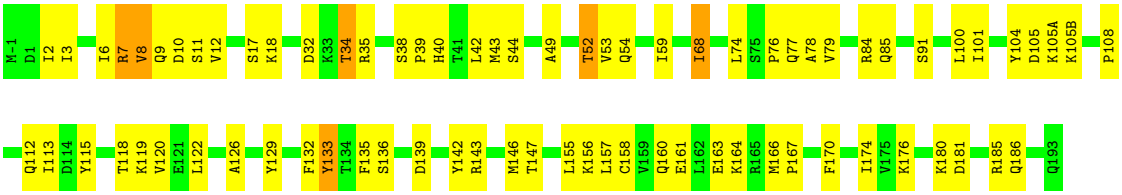
• Molecule 10: PROTEASOME COMPONENT C11

Chain J: 63% 32% 6%



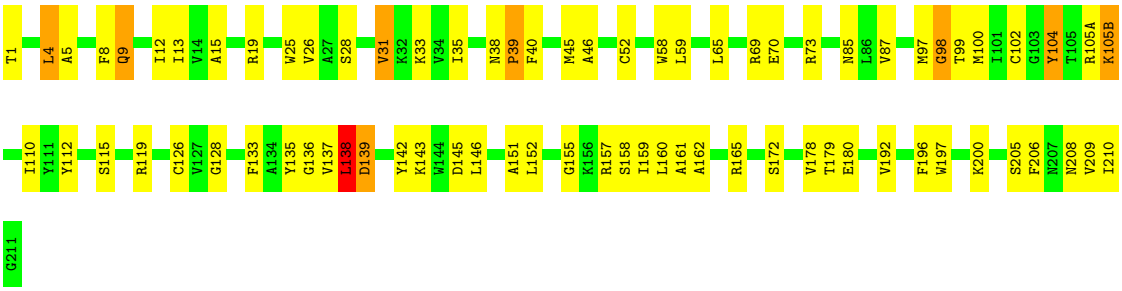
• Molecule 10: PROTEASOME COMPONENT C11

Chain Q: 62% 35% •



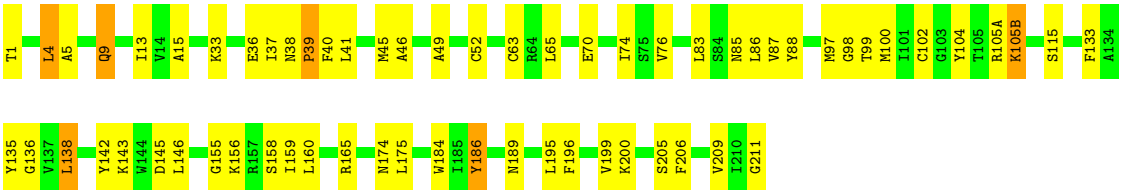
• Molecule 11: PROTEASOME COMPONENT PRE2

Chain K: 64% 32% •



• Molecule 11: PROTEASOME COMPONENT PRE2

Chain R: 70% 27% •

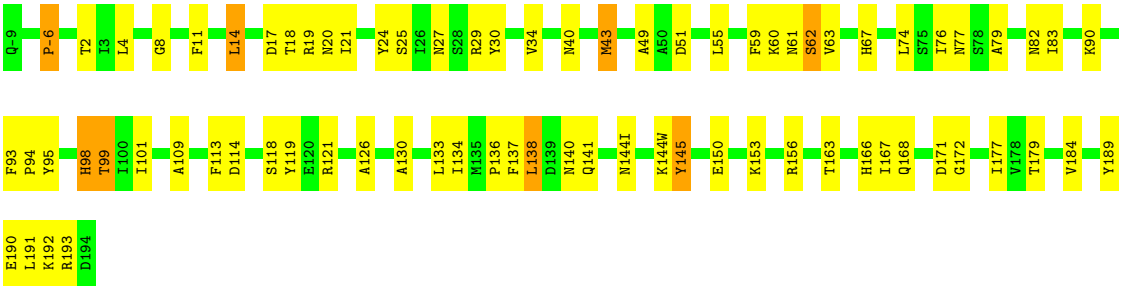


• Molecule 12: PROTEASOME COMPONENT C5

Chain L:

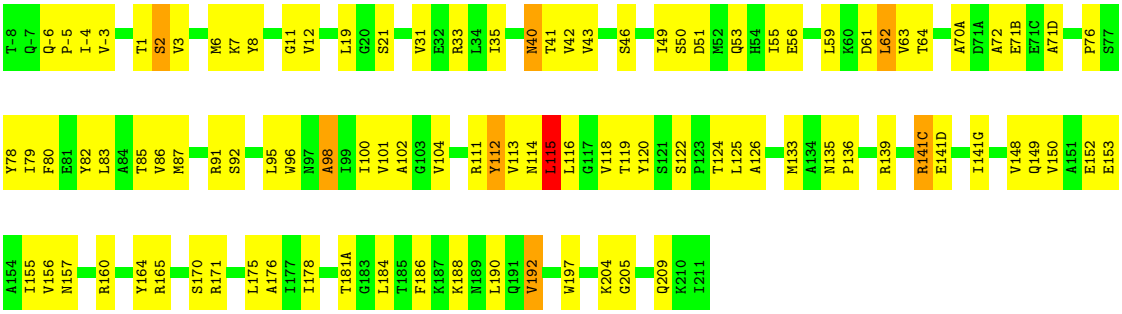
• Molecule 12: PROTEASOME COMPONENT C5

Chain S:



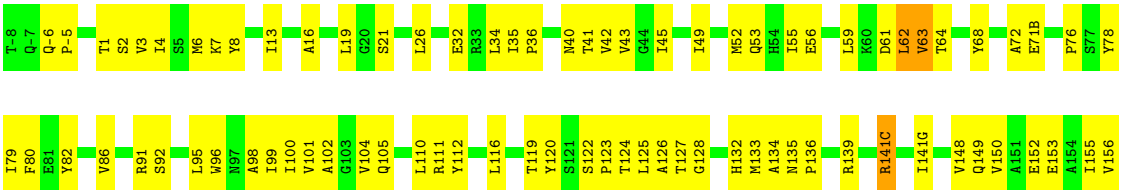
• Molecule 13: PROTEASOME COMPONENT PRE4

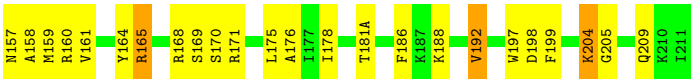
Chain M:



• Molecule 13: PROTEASOME COMPONENT PRE4

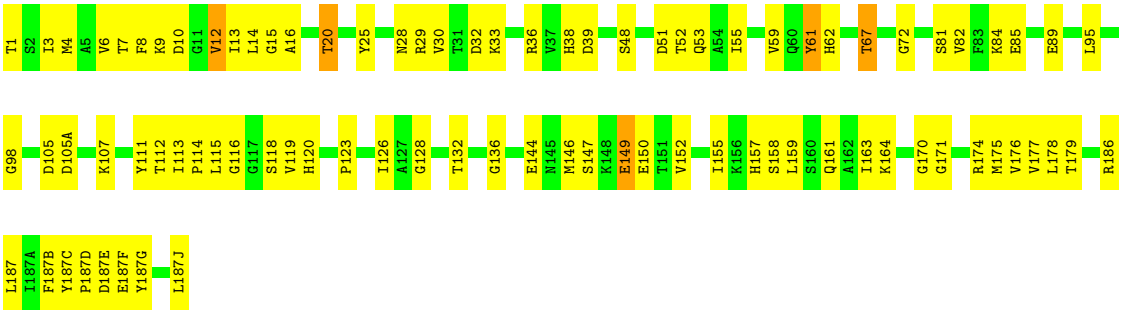
Chain T:





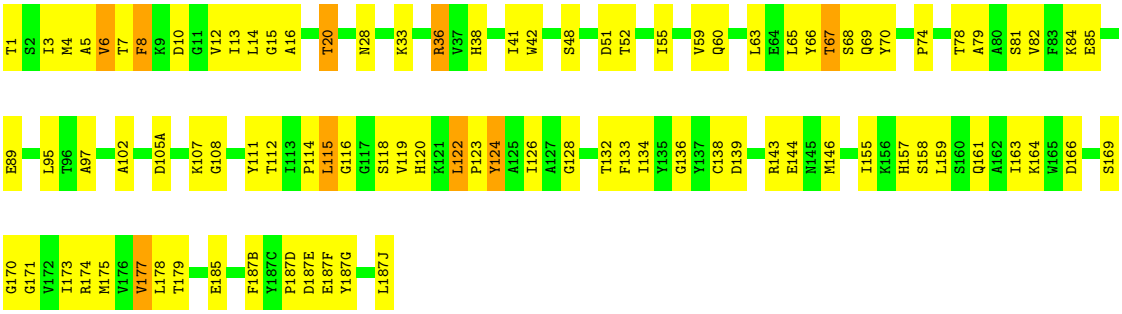
• Molecule 14: PROTEASOME COMPONENT PRE3

Chain N:



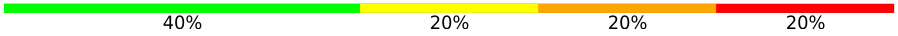
• Molecule 14: PROTEASOME COMPONENT PRE3

Chain U:



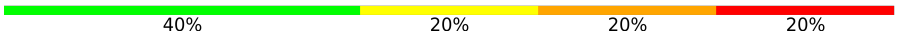
• Molecule 15: TMC-95A inhibitor

Chain 8:



• Molecule 15: TMC-95A inhibitor

Chain 9:



4 Data and refinement statistics (i)

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 301.30Å 144.80Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.251 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	52549	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AKK, R4K, 1QQ, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.65	0/1952	0.81	0/2642
1	V	0.62	0/1952	0.79	0/2642
2	B	0.65	0/1935	0.79	0/2618
2	W	0.62	0/1935	0.79	0/2618
3	C	0.65	0/1920	0.80	1/2598 (0.0%)
3	X	0.59	0/1920	0.78	0/2598
4	D	0.63	0/1887	0.78	1/2541 (0.0%)
4	Y	0.63	0/1887	0.78	2/2541 (0.1%)
5	E	0.57	0/1823	0.77	0/2463
5	Z	0.57	0/1823	0.78	0/2463
6	1	0.64	0/1937	0.79	0/2614
6	F	0.61	0/1937	0.78	1/2614 (0.0%)
7	2	0.71	0/1959	0.80	0/2652
7	G	0.65	0/1959	0.80	0/2652
8	H	0.72	0/1716	0.85	0/2326
8	O	0.69	1/1716 (0.1%)	0.81	0/2326
9	I	0.72	0/1611	0.84	0/2174
9	P	0.76	0/1611	0.85	2/2174 (0.1%)
10	J	0.70	1/1613 (0.1%)	0.82	0/2173
10	Q	0.69	0/1613	0.80	0/2173
11	K	0.71	0/1681	0.81	1/2274 (0.0%)
11	R	0.69	0/1681	0.80	0/2274
12	L	0.75	1/1795 (0.1%)	0.82	2/2420 (0.1%)
12	S	0.68	0/1795	0.83	1/2420 (0.0%)
13	M	0.68	0/1855	0.80	1/2514 (0.0%)
13	T	0.70	0/1855	0.84	3/2514 (0.1%)
14	N	0.75	0/1541	0.81	1/2087 (0.0%)
14	U	0.73	0/1541	0.78	1/2087 (0.0%)
15	8	1.96	0/20	2.20	2/26 (7.7%)
15	9	2.53	0/20	2.48	2/26 (7.7%)
All	All	0.67	3/50490 (0.0%)	0.81	21/68244 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	R	0	1
15	8	0	1
15	9	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	37	CYS	CB-SG	-5.27	1.73	1.81
8	O	43	CYS	CB-SG	-5.14	1.73	1.81
10	J	158	CYS	CB-SG	-5.06	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	9	3	ASN	CB-CG-OD1	-7.24	107.12	121.60
15	8	3	ASN	CB-CG-OD1	-7.21	107.18	121.60
13	T	98	ALA	N-CA-C	-6.22	94.20	111.00
15	9	3	ASN	OD1-CG-ND2	-6.11	107.85	121.90
9	P	95	TYR	N-CA-C	-6.02	94.74	111.00
12	L	98	HIS	N-CA-C	-5.80	95.34	111.00
3	C	103	LEU	CA-CB-CG	5.53	128.01	115.30
6	F	125	LEU	CA-CB-CG	5.49	127.94	115.30
13	M	98	ALA	N-CA-C	-5.45	96.28	111.00
15	8	3	ASN	OD1-CG-ND2	-5.40	109.49	121.90
14	U	122	LEU	CA-CB-CG	5.31	127.51	115.30
4	Y	214	CYS	CA-CB-SG	-5.25	104.55	114.00
4	Y	59	LEU	CA-CB-CG	5.21	127.27	115.30
13	T	116	LEU	CA-CB-CG	5.17	127.20	115.30
12	S	98	HIS	N-CA-C	-5.15	97.10	111.00
12	L	95	TYR	N-CA-C	-5.15	97.10	111.00
4	D	137	LEU	N-CA-C	-5.13	97.14	111.00
13	T	95	LEU	N-CA-C	-5.12	97.17	111.00
14	N	98	GLY	N-CA-C	-5.12	100.30	113.10
11	K	98	GLY	N-CA-C	-5.11	100.31	113.10
9	P	-7	ASP	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	8	3	ASN	Sidechain
15	9	3	ASN	Sidechain
11	R	186	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	59	0
1	V	1915	0	1926	71	0
2	B	1905	0	1901	75	0
2	W	1905	0	1901	75	0
3	C	1891	0	1900	68	0
3	X	1891	0	1900	92	0
4	D	1862	0	1836	75	0
4	Y	1862	0	1836	67	0
5	E	1795	0	1797	78	0
5	Z	1795	0	1797	111	0
6	1	1897	0	1886	111	0
6	F	1897	0	1886	101	0
7	2	1921	0	1910	95	0
7	G	1921	0	1910	83	0
8	H	1685	0	1688	75	0
8	O	1685	0	1688	83	0
9	I	1581	0	1574	56	0
9	P	1581	0	1574	67	0
10	J	1585	0	1590	55	0
10	Q	1585	0	1590	62	0
11	K	1644	0	1595	72	0
11	R	1644	0	1595	54	0
12	L	1757	0	1711	79	0
12	S	1757	0	1711	80	0
13	M	1824	0	1832	74	0
13	T	1824	0	1832	90	0
14	N	1512	0	1481	75	0
14	U	1512	0	1481	71	0
15	8	49	0	36	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	9	49	0	36	7	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	L	1	0	0	0	0
16	N	1	0	0	0	0
16	P	1	0	0	0	0
17	1	93	0	0	3	0
17	2	103	0	0	6	0
17	8	2	0	0	0	0
17	9	1	0	0	0	0
17	A	105	0	0	1	0
17	B	80	0	0	1	0
17	C	69	0	0	3	0
17	D	90	0	0	6	0
17	E	55	0	0	3	0
17	F	99	0	0	6	0
17	G	106	0	0	3	0
17	H	114	0	0	2	0
17	I	107	0	0	3	0
17	J	116	0	0	6	0
17	K	103	0	0	4	0
17	L	140	0	0	8	0
17	M	150	0	0	3	0
17	N	116	0	0	5	0
17	O	121	0	0	3	0
17	P	101	0	0	4	0
17	Q	121	0	0	5	0
17	R	107	0	0	4	0
17	S	144	0	0	6	0
17	T	142	0	0	8	0
17	U	118	0	0	1	0
17	V	104	0	0	2	0
17	W	74	0	0	2	0
17	X	70	0	0	4	0
17	Y	89	0	0	5	0
17	Z	53	0	0	2	0
All	All	52549	0	49326	1936	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 20.

All (1936) 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)
7:2:123:TYR:O	17:2:2009:HOH:O	1.54	1.25
14:N:136:GLY:HA2	14:U:161:GLN:HE21	1.13	1.10
8:H:21:THR:O	15:8:4:R4K:O33	1.75	1.05
14:N:161:GLN:HE21	14:U:136:GLY:HA2	1.21	1.05
8:O:21:THR:O	15:9:4:R4K:O33	1.75	1.04
3:C:15:PHE:H	4:D:23:GLN:HE22	1.13	0.97
3:C:185:THR:HB	3:C:188:GLU:HG2	1.46	0.96
2:W:202:THR:HG22	2:W:204:SER:H	1.31	0.96
5:Z:52:LYS:HB2	5:Z:63:TYR:HB3	1.45	0.96
7:G:96:ALA:HA	7:G:107:MET:HE2	1.48	0.95
9:P:114:ASP:HB3	15:9:3:ASN:ND2	1.80	0.95
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.48	0.94
6:1:81:LEU:HD12	6:1:133:GLY:HA3	1.45	0.94
8:O:166:ASP:O	17:O:2015:HOH:O	1.84	0.94
6:1:141:VAL:HG23	6:1:215:CYS:SG	2.09	0.93
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.33	0.92
9:I:114:ASP:HB3	15:8:3:ASN:HD21	1.35	0.92
5:Z:15:PHE:HB2	6:1:23:GLN:HE22	1.35	0.92
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.51	0.91
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.52	0.91
9:I:114:ASP:HB3	15:8:3:ASN:ND2	1.85	0.91
7:2:121:GLN:O	7:2:124:THR:HB	1.70	0.90
14:U:4:MET:HB3	14:U:126:ILE:HG22	1.54	0.90
6:F:141:VAL:HG23	6:F:215:CYS:SG	2.12	0.90
11:R:105(B):LYS:H	11:R:105(B):LYS:HD2	1.34	0.90
13:M:171:ARG:HG3	13:M:192:VAL:HG23	1.53	0.89
11:K:105(B):LYS:H	11:K:105(B):LYS:HD2	1.37	0.88
3:X:152:GLU:HG2	3:X:156:ILE:HG22	1.57	0.87
4:Y:177:LEU:HD22	5:Z:58:LEU:HD22	1.56	0.86
12:S:43:MET:HB2	12:S:101:ILE:HG22	1.55	0.86
13:T:157:ASN:ND2	13:T:160:ARG:HH11	1.73	0.86
13:M:41:THR:OG1	13:M:76:PRO:HG3	1.74	0.86
3:X:88:LEU:HD22	3:X:116:VAL:HG13	1.57	0.86
13:T:171:ARG:HG3	13:T:192:VAL:HG23	1.58	0.85
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.59	0.85
3:C:152:GLU:HG2	3:C:156:ILE:HG22	1.58	0.85
4:Y:214:CYS:HG	4:Y:224:TYR:HE2	0.88	0.84
3:X:185:THR:HB	3:X:188:GLU:HG2	1.55	0.84
6:1:186:ALA:O	6:1:190:VAL:HG23	1.77	0.84
7:G:76:MET:SD	7:G:138:PHE:CE2	2.70	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:37:SER:HB3	6:1:50:VAL:HG23	1.60	0.84
12:S:18:THR:HG22	12:S:30:TYR:HA	1.59	0.84
3:C:35:THR:HB	3:C:51:GLU:HG3	1.61	0.83
1:V:124:THR:HG22	2:W:130:ARG:HH21	1.41	0.83
10:Q:176:LYS:HE2	10:Q:186:GLN:HE21	1.44	0.82
5:E:194:VAL:O	5:E:197:ILE:HG22	1.79	0.82
8:H:21:THR:HG22	8:H:26:VAL:HA	1.62	0.81
10:Q:113:ILE:HG12	10:Q:119:LYS:HG3	1.60	0.81
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.62	0.81
14:N:136:GLY:HA2	14:U:161:GLN:NE2	1.94	0.81
10:Q:133:TYR:CZ	10:Q:166:MET:HG3	2.15	0.81
9:I:194:ASP:O	17:I:2016:HOH:O	1.99	0.81
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.63	0.80
11:K:142:TYR:O	11:K:143:LYS:HD2	1.82	0.79
6:F:81:LEU:HD12	6:F:133:GLY:HA3	1.62	0.79
3:X:163:GLN:HE21	3:X:164:THR:H	1.30	0.79
5:E:81:LEU:HB2	5:E:133:GLY:O	1.83	0.79
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.65	0.79
13:T:133:MET:O	13:T:136:PRO:HD2	1.81	0.79
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.17	0.79
14:U:157:HIS:CD2	14:U:187(J):LEU:HD13	2.18	0.79
3:X:163:GLN:NE2	3:X:164:THR:H	1.82	0.78
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.65	0.78
5:Z:81:LEU:HB2	5:Z:133:GLY:O	1.84	0.78
9:P:114:ASP:HB3	15:9:3:ASN:HD21	1.48	0.77
10:Q:32:ASP:OD2	10:Q:34:THR:HG22	1.84	0.77
5:Z:52:LYS:HD2	5:Z:63:TYR:O	1.84	0.77
2:B:202:THR:HG22	2:B:204:SER:H	1.48	0.77
5:E:176:LEU:HD22	5:E:180(C):PHE:HE2	1.50	0.77
10:Q:18:LYS:HD3	10:Q:174:ILE:HG13	1.63	0.77
12:S:190:GLU:O	12:S:191:LEU:HD23	1.85	0.77
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.67	0.77
13:T:41:THR:OG1	13:T:76:PRO:HG3	1.85	0.77
7:G:77:VAL:HG12	7:G:137:THR:HB	1.67	0.76
3:C:163:GLN:HE21	3:C:164:THR:H	1.32	0.76
10:J:90:SER:O	10:J:91:SER:HB3	1.85	0.76
11:R:143:LYS:O	11:R:146:LEU:HD13	1.86	0.76
7:2:96:ALA:HA	7:2:107:MET:HE2	1.67	0.75
5:E:143:LYS:HE3	13:M:78:TYR:OH	1.85	0.75
13:M:152:GLU:O	13:M:156:VAL:HG23	1.87	0.75
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:MET:SD	7:G:138:PHE:HE2	2.09	0.75
4:Y:70:ILE:HB	4:Y:74:ILE:HG22	1.68	0.75
3:C:57:LYS:HD2	3:C:58:LEU:N	2.02	0.75
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.69	0.74
7:2:198:ILE:HG23	7:2:203:THR:O	1.87	0.74
14:N:161:GLN:NE2	14:U:136:GLY:HA2	2.00	0.74
1:V:7:ARG:HH22	4:Y:123(C):GLY:HA3	1.52	0.74
9:I:41:VAL:HG22	9:I:76:PRO:HG3	1.67	0.74
5:E:198:SER:HA	5:E:201:LEU:HG	1.69	0.74
7:G:77:VAL:CG1	7:G:137:THR:HB	2.18	0.74
3:X:15:PHE:H	4:Y:23:GLN:HE22	1.36	0.73
5:Z:52:LYS:CB	5:Z:63:TYR:HB3	2.16	0.73
7:2:59:LEU:O	7:2:61:PRO:HD3	1.88	0.73
3:X:36:CYS:SG	3:X:37:ALA:N	2.61	0.73
7:G:220:LYS:HG2	7:G:221:PHE:H	1.52	0.73
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.71	0.73
14:U:157:HIS:HD2	14:U:187(J):LEU:HD13	1.51	0.73
5:Z:130:ARG:HH11	5:Z:130:ARG:HG3	1.52	0.73
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.24	0.73
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.52	0.73
12:S:8:GLY:HA3	12:S:11:PHE:CE2	2.23	0.73
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.03	0.73
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.72	0.72
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.71	0.72
12:S:18:THR:HG21	12:S:30:TYR:CD1	2.23	0.72
4:Y:40:ILE:HG23	4:Y:162:ALA:HB2	1.71	0.72
5:Z:15:PHE:HB2	6:1:23:GLN:NE2	2.04	0.72
6:1:221:HIS:HE1	6:1:223:PHE:CE1	2.06	0.72
8:H:175:VAL:HG21	8:H:191:TYR:HD1	1.53	0.72
1:V:15:PHE:H	2:W:23:GLN:HE22	1.37	0.72
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.55	0.72
11:R:4:LEU:HD12	11:R:159:ILE:HD11	1.71	0.71
7:2:233:LEU:O	7:2:236:ILE:HG13	1.91	0.71
10:Q:43:MET:SD	10:Q:101:ILE:HD11	2.30	0.71
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.71	0.71
13:T:160:ARG:HA	13:T:192:VAL:HG11	1.72	0.71
14:U:112:THR:HG22	14:U:120:HIS:HB2	1.72	0.71
8:O:112:SER:HB3	8:O:125:LEU:HD13	1.72	0.71
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.72	0.70
14:U:163:ILE:HG23	14:U:170:GLY:HA2	1.71	0.70
9:P:131:SER:OG	17:P:2011:HOH:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:198:ILE:HG23	7:G:203:THR:O	1.91	0.70
4:Y:163:LYS:HG3	4:Y:164:ALA:N	2.07	0.70
3:X:35:THR:HB	3:X:51:GLU:HG3	1.72	0.70
5:E:130:ARG:HH11	5:E:130:ARG:HG3	1.54	0.70
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.26	0.70
7:2:96:ALA:HA	7:2:107:MET:CE	2.22	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.56	0.70
6:F:42:CYS:HB2	6:F:184:LEU:O	1.91	0.70
12:L:18:THR:HG21	12:L:30:TYR:CD1	2.26	0.70
8:O:175:VAL:HG21	8:O:191:TYR:HD1	1.57	0.70
13:M:124:THR:O	13:M:125:LEU:HD23	1.92	0.69
9:P:7:THR:HG23	9:P:110:ILE:HD13	1.74	0.69
13:T:80:PHE:CE1	13:T:111:ARG:HD3	2.28	0.69
11:R:87:VAL:HG11	11:R:115:SER:HA	1.73	0.69
6:1:35:THR:HG21	6:1:51:GLU:O	1.92	0.69
6:F:36:THR:O	6:F:50:VAL:HG23	1.93	0.69
10:J:44:SER:OG	10:J:100:LEU:HB2	1.92	0.69
10:Q:105(B):LYS:HE2	2:W:143:ASP:OD2	1.93	0.69
13:T:6:MET:HG2	13:T:155:ILE:HD11	1.74	0.69
6:1:172:ALA:O	6:1:176:LEU:HD23	1.91	0.69
7:2:91:ARG:HH21	7:2:115:ARG:HH21	1.38	0.69
4:D:97:VAL:HG21	11:K:65:LEU:HD12	1.72	0.69
4:D:163:LYS:HG3	4:D:164:ALA:N	2.08	0.69
8:H:167:LEU:HD22	12:S:167:ILE:O	1.93	0.69
14:N:4:MET:CB	14:N:126:ILE:HG22	2.22	0.69
1:A:112:LEU:O	1:A:116:VAL:HG23	1.93	0.69
8:H:33:LYS:HE2	15:8:5:AKK:HA1	1.74	0.69
8:H:214:LEU:HD22	11:R:211:GLY:HA2	1.74	0.69
10:J:113:ILE:HA	10:J:118:THR:O	1.93	0.69
4:D:160:TYR:CE1	4:D:163:LYS:HD3	2.28	0.69
6:1:126:TYR:HE1	7:2:129:MET:SD	2.16	0.69
4:Y:45:GLY:HA2	4:Y:146:TYR:CE1	2.29	0.68
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.76	0.68
4:Y:46:VAL:HG11	4:Y:139:ALA:HB1	1.75	0.68
5:Z:75:GLY:HA3	5:Z:221:PHE:CE2	2.28	0.68
5:Z:194:VAL:O	5:Z:197:ILE:HG22	1.93	0.68
3:X:156:ILE:HD11	4:Y:82:THR:OG1	1.93	0.68
7:2:105:TYR:H	7:2:105:TYR:HD2	1.41	0.68
12:L:166:HIS:HD2	12:L:168:GLN:H	1.41	0.68
13:M:175:LEU:HD23	13:M:176:ALA:N	2.09	0.68
4:D:70:ILE:HB	4:D:74:ILE:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.08	0.68
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.76	0.68
5:E:66:LYS:HA	5:E:78:LEU:HD21	1.75	0.68
13:T:4:ILE:HD11	13:T:159:MET:SD	2.33	0.68
6:1:38:ILE:HG22	6:1:164:ALA:CB	2.23	0.68
2:B:126:HIS:CB	3:C:129:VAL:HG12	2.22	0.67
11:K:143:LYS:O	11:K:146:LEU:HD13	1.94	0.67
12:S:29:ARG:NH1	12:S:193:ARG:HB3	2.09	0.67
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.77	0.67
14:N:157:HIS:HD2	14:N:187(J):LEU:HD13	1.60	0.67
13:T:175:LEU:HD23	13:T:176:ALA:N	2.10	0.67
5:Z:180(C):PHE:HD1	5:Z:180(D):ILE:N	1.93	0.67
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.30	0.67
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.77	0.67
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.23	0.67
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.42	0.67
10:Q:133:TYR:OH	10:Q:166:MET:HG3	1.93	0.67
3:C:163:GLN:NE2	3:C:164:THR:H	1.91	0.67
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.25	0.67
8:O:197:ARG:NH2	9:P:139:GLU:HG3	2.10	0.67
11:R:65:LEU:HD12	4:Y:97:VAL:HG21	1.76	0.67
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.77	0.66
2:W:69:LYS:HG3	2:W:221:GLN:OE1	1.95	0.66
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.29	0.66
6:1:69:VAL:HG12	17:1:2563:HOH:O	1.94	0.66
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.59	0.66
7:G:105:TYR:H	7:G:105:TYR:HD2	1.41	0.66
12:S:163:THR:O	17:S:2012:HOH:O	2.12	0.66
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.60	0.66
7:G:12:ILE:HA	17:G:538:HOH:O	1.95	0.66
7:2:12:ILE:HG13	7:2:14:ILE:HG23	1.77	0.66
2:W:175:LEU:HB3	17:W:2109:HOH:O	1.95	0.66
3:X:38:VAL:HG22	3:X:39:GLY:N	2.11	0.66
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.31	0.66
12:S:109:ALA:HB2	12:S:121:ARG:NH2	2.11	0.66
2:W:88:LEU:HD22	2:W:116:LEU:HD22	1.77	0.66
2:B:150:THR:O	2:B:157:TYR:HA	1.95	0.65
7:G:150:LYS:O	7:G:157:TYR:HA	1.95	0.65
7:G:233:LEU:O	7:G:236:ILE:HG13	1.96	0.65
2:W:15:PHE:HB2	3:X:23:GLN:HE22	1.61	0.65
13:M:135:ASN:O	13:M:139:ARG:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:51:ASP:O	14:N:55:ILE:HG13	1.96	0.65
14:N:157:HIS:CD2	14:N:187(J):LEU:HD13	2.31	0.65
1:A:50:THR:HG21	1:A:66:LYS:HE2	1.78	0.65
13:T:78:TYR:OH	5:Z:143:LYS:HE3	1.96	0.65
9:P:64:ASN:HD22	2:W:97:GLN:HE22	1.44	0.65
10:Q:68:ILE:CD1	3:X:71:ASP:HA	2.27	0.65
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	1.79	0.65
9:I:14:ILE:HG23	9:I:34:ILE:HD13	1.78	0.65
1:A:15:PHE:H	2:B:23:GLN:HE22	1.42	0.65
14:N:4:MET:SD	14:N:159:LEU:HD21	2.37	0.65
5:Z:161:TYR:CE2	6:1:60:VAL:HA	2.31	0.65
5:Z:198:SER:HA	5:Z:201:LEU:HG	1.79	0.65
1:A:217(I):TYR:CE1	8:H:36:ARG:HD2	2.32	0.65
1:V:49:ALA:HB2	1:V:212:LEU:HG	1.78	0.64
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.79	0.64
14:N:30:VAL:HG11	13:T:199:PHE:HE2	1.62	0.64
6:F:24:VAL:O	6:F:27:ALA:HB3	1.98	0.64
11:R:105(A):ARG:HB3	11:R:105(B):LYS:HE3	1.78	0.64
12:S:4:LEU:HD13	12:S:126:ALA:HB2	1.80	0.64
5:Z:22:PHE:HD1	5:Z:26:TYR:HE1	1.46	0.64
2:W:126:HIS:HB3	3:X:129:VAL:HG12	1.79	0.64
3:X:57:LYS:HD2	3:X:58:LEU:N	2.11	0.64
6:F:126:TYR:HE1	7:G:129:MET:SD	2.20	0.64
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.27	0.64
6:1:221:HIS:HE1	6:1:223:PHE:HE1	1.46	0.64
6:F:221:HIS:HE1	6:F:223:PHE:CE1	2.16	0.64
14:U:6:VAL:HG23	14:U:155:ILE:HD11	1.80	0.64
5:Z:117:CYS:SG	6:1:86:ARG:HD3	2.38	0.64
12:S:144(W):LYS:HG2	12:S:145:TYR:N	2.13	0.63
14:N:59:VAL:HG13	14:N:82:VAL:HG11	1.79	0.63
8:O:80:LEU:HD12	8:O:113:ILE:HD11	1.80	0.63
4:Y:214:CYS:SG	4:Y:224:TYR:CE2	2.87	0.63
7:G:220:LYS:HG2	7:G:221:PHE:N	2.13	0.63
13:T:152:GLU:O	13:T:156:VAL:HG23	1.98	0.63
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.81	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.99	0.63
8:H:18:THR:HB	8:H:30:ASN:HA	1.81	0.63
12:L:24:TYR:HA	8:O:167:LEU:HD12	1.81	0.63
5:Z:48:LEU:HD13	5:Z:77:SER:HB3	1.80	0.63
8:O:113:ILE:HG12	8:O:119:THR:HG22	1.79	0.63
4:D:180(C):HIS:CD2	4:D:184:LEU:HG	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.13	0.63
12:L:133:LEU:O	12:L:136:PRO:HD2	1.99	0.63
14:N:67:THR:HA	14:N:72:GLY:O	1.99	0.63
13:T:91:ARG:HG3	13:T:92:SER:N	2.13	0.63
6:1:184:LEU:HD11	6:1:188:GLU:HB3	1.81	0.63
12:L:109:ALA:HB2	12:L:121:ARG:HH21	1.63	0.63
4:Y:46:VAL:HG11	4:Y:139:ALA:CB	2.29	0.63
3:C:163:GLN:HG3	3:C:164:THR:N	2.14	0.62
10:J:39:PRO:HD3	17:J:3265:HOH:O	1.99	0.62
6:F:186:ALA:O	6:F:190:VAL:HG23	2.00	0.62
3:X:197:LEU:O	3:X:201:VAL:HG23	1.98	0.62
2:B:6:ARG:HG3	5:E:127:TYR:OH	1.99	0.62
12:S:29:ARG:HD3	12:S:171:ASP:OD1	1.99	0.62
3:X:134:VAL:HG12	3:X:135:SER:N	2.14	0.62
4:Y:65:GLU:HA	17:Y:2028:HOH:O	1.99	0.62
6:1:160:TYR:HB3	6:1:162:GLY:O	1.99	0.62
7:2:207:LYS:HG3	7:2:208:ASN:OD1	1.99	0.62
13:M:-5:PRO:HD3	13:M:96:TRP:CD2	2.35	0.62
1:V:130:ARG:HH21	7:2:124:THR:HG22	1.65	0.62
2:W:229:ILE:O	2:W:232:ILE:HG22	1.99	0.62
6:F:12:ASN:ND2	6:F:131:PRO:HD3	2.14	0.62
11:K:5:ALA:HA	11:K:13:ILE:O	2.00	0.62
2:W:71:ASN:HD22	2:W:72:ASP:H	1.48	0.62
8:H:197:ARG:NH1	8:H:200:LYS:HD3	2.15	0.62
12:L:144(W):LYS:HG2	12:L:145:TYR:N	2.15	0.62
5:Z:226:GLY:O	5:Z:229:VAL:HG22	1.99	0.62
2:B:71:ASN:HD22	2:B:72:ASP:H	1.47	0.62
3:X:47:VAL:O	3:X:48:LEU:HD23	1.99	0.62
4:D:38:ILE:HD12	4:D:197:LEU:HG	1.80	0.62
6:1:13:SER:HB2	7:2:130:ARG:HB3	1.81	0.62
6:1:37:SER:HB3	6:1:50:VAL:CG2	2.29	0.62
2:B:163:ILE:HG13	2:B:164:SER:H	1.65	0.62
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.35	0.62
8:O:49:ALA:HB1	9:P:118:CYS:SG	2.40	0.62
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.80	0.62
12:L:190:GLU:O	12:L:191:LEU:HD23	2.00	0.62
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.81	0.62
14:N:10:ASP:O	14:N:179:THR:HG22	2.00	0.62
4:Y:78:MET:SD	4:Y:82:THR:HG22	2.40	0.62
8:O:35:HIS:HB3	8:O:56:THR:HG21	1.82	0.61
9:P:114:ASP:HB3	15:9:3:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.29	0.61
12:S:61:ASN:HD21	5:Z:97:ASN:HD21	1.47	0.61
10:Q:113:ILE:HA	10:Q:118:THR:O	2.00	0.61
9:I:113:PHE:CD2	9:I:113:PHE:N	2.68	0.61
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.81	0.61
11:K:112:TYR:O	11:K:119:ARG:HA	2.01	0.61
3:X:190:VAL:O	3:X:194:VAL:HG23	2.00	0.61
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.35	0.61
5:Z:161:TYR:OH	6:1:61:PRO:HD2	2.00	0.61
7:2:91:ARG:NH2	7:2:115:ARG:HH21	1.98	0.61
10:Q:176:LYS:HE2	10:Q:186:GLN:NE2	2.15	0.61
3:X:36:CYS:HA	3:X:166:GLY:HA3	1.83	0.61
6:F:119:TYR:O	6:F:122:ALA:HB3	2.00	0.61
12:S:134:ILE:HG22	12:S:138:LEU:HD22	1.82	0.61
14:U:134:ILE:HD12	14:U:158:SER:HB3	1.82	0.61
4:Y:214:CYS:SG	4:Y:224:TYR:HE2	2.08	0.61
6:1:176:LEU:HD22	6:1:196:ILE:HD13	1.82	0.61
3:C:38:VAL:HG22	3:C:39:GLY:N	2.16	0.61
13:M:82:TYR:O	13:M:86:VAL:HG23	2.00	0.61
2:W:124:THR:HG22	3:X:130:ARG:HH21	1.66	0.61
6:F:35:THR:HG21	6:F:51:GLU:O	2.01	0.60
6:1:122:ALA:HA	6:1:125:LEU:HD12	1.83	0.60
5:E:52:LYS:HD2	5:E:63:TYR:O	2.01	0.60
7:G:212:VAL:HG12	7:G:213:GLY:N	2.16	0.60
8:O:84:LYS:HG3	8:O:85:GLN:N	2.14	0.60
7:2:220:LYS:HG2	7:2:221:PHE:H	1.67	0.60
10:Q:180:LYS:HG3	10:Q:181:ASP:OD1	2.01	0.60
2:W:71:ASN:ND2	2:W:72:ASP:H	1.99	0.60
5:E:180(C):PHE:HD1	5:E:180(D):ILE:N	2.00	0.60
12:S:-6:PRO:HB2	13:T:91:ARG:NH1	2.15	0.60
14:U:13:ILE:HG12	14:U:177:VAL:HG13	1.83	0.60
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.83	0.60
8:H:47:GLY:O	15:8:5:AKK:ND	2.34	0.60
13:M:133:MET:O	13:M:136:PRO:HD2	2.01	0.60
12:S:177:ILE:N	12:S:177:ILE:HD12	2.16	0.60
14:U:4:MET:CB	14:U:126:ILE:HG22	2.27	0.60
14:U:55:ILE:O	14:U:59:VAL:HG23	2.01	0.60
4:Y:215:ILE:HG13	4:Y:215:ILE:O	2.00	0.60
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.14	0.60
7:G:229:ILE:O	7:G:232:ARG:HB2	2.01	0.60
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:180:LYS:HG3	10:J:181:ASP:OD1	2.01	0.60
5:E:47:VAL:HG12	5:E:48:LEU:N	2.17	0.60
5:E:73:HIS:HE1	5:E:107:LEU:O	1.83	0.60
6:F:151:LEU:HD11	6:F:155:GLY:HA2	1.83	0.60
6:F:184:LEU:HD11	6:F:188:GLU:CB	2.32	0.60
12:S:166:HIS:HD2	12:S:168:GLN:H	1.47	0.60
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.83	0.60
14:N:51:ASP:OD2	14:N:95:LEU:HA	2.01	0.60
11:R:38:ASN:O	11:R:40:PHE:N	2.34	0.60
12:S:43:MET:CB	12:S:101:ILE:HG22	2.31	0.60
5:Z:70:CYS:SG	5:Z:92:LEU:HD23	2.42	0.60
8:O:78:SER:O	8:O:82:MET:HG3	2.01	0.60
10:Q:68:ILE:HD11	3:X:71:ASP:HA	1.84	0.60
8:H:152:ILE:CG2	8:H:191:TYR:HE1	2.14	0.59
12:S:133:LEU:O	12:S:136:PRO:HD2	2.02	0.59
8:H:200:LYS:HE3	9:I:140:SER:O	2.03	0.59
11:K:102:CYS:SG	11:K:110:ILE:HG23	2.42	0.59
5:E:198:SER:HA	5:E:201:LEU:CG	2.30	0.59
10:J:43:MET:SD	10:J:101:ILE:HD11	2.43	0.59
11:K:165:ARG:NH1	9:P:171:TRP:HH2	2.00	0.59
2:B:121:GLN:O	2:B:124:THR:HB	2.03	0.59
7:G:173:THR:O	7:G:177:GLU:HG3	2.03	0.59
13:M:149:GLN:NE2	13:M:149:GLN:H	2.00	0.59
4:Y:237:LEU:HD22	4:Y:241:GLU:HG3	1.84	0.59
7:G:59:LEU:O	7:G:61:PRO:HD3	2.02	0.59
8:H:3:ILE:O	8:H:3:ILE:HG13	2.02	0.59
11:R:5:ALA:HA	11:R:13:ILE:O	2.01	0.59
5:Z:136:LEU:HD12	5:Z:151:PHE:CD2	2.37	0.59
13:M:197:TRP:CH2	14:U:171:GLY:HA2	2.37	0.59
8:H:84:LYS:HG3	8:H:85:GLN:N	2.18	0.59
11:K:196:PHE:CE2	11:K:206:PHE:CD2	2.91	0.59
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.84	0.59
12:S:-6:PRO:HB2	13:T:91:ARG:HH11	1.65	0.59
6:F:38:ILE:HG22	6:F:164:ALA:HA	1.85	0.59
13:T:-5:PRO:HD3	13:T:96:TRP:CD2	2.36	0.59
13:T:3:VAL:HG22	13:T:16:ALA:HB2	1.83	0.59
3:X:163:GLN:HE21	3:X:164:THR:N	1.99	0.59
3:X:116:VAL:O	3:X:119:VAL:HB	2.02	0.59
4:Y:197:LEU:O	4:Y:201:MET:HG3	2.02	0.59
5:Z:48:LEU:HG	5:Z:139:ILE:HD13	1.85	0.59
7:2:214:VAL:HG12	7:2:215:ALA:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:ASP:O	3:C:73:HIS:N	2.36	0.59
5:E:77:SER:OG	5:E:137:LEU:HB2	2.02	0.59
9:P:70:GLU:HB3	17:P:2524:HOH:O	2.02	0.59
4:Y:75:GLY:HA3	4:Y:221:PHE:CE2	2.38	0.59
7:2:229:ILE:O	7:2:232:ARG:HB2	2.03	0.59
12:L:19:ARG:HB2	12:L:171:ASP:HB2	1.85	0.58
8:O:69:TYR:O	8:O:69:TYR:CD1	2.56	0.58
3:X:76:LEU:HD12	3:X:138:ILE:HG12	1.84	0.58
7:2:105:TYR:CD2	7:2:105:TYR:N	2.69	0.58
1:A:79:SER:HB2	1:A:165:ILE:HD12	1.85	0.58
2:B:181:LYS:O	2:B:184:MET:HG3	2.02	0.58
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.33	0.58
3:X:115:TYR:O	3:X:119:VAL:HG23	2.04	0.58
4:Y:67:ILE:HD13	4:Y:213:SER:OG	2.03	0.58
6:1:171:SER:O	6:1:174:ALA:HB3	2.02	0.58
3:C:57:LYS:O	3:C:58:LEU:HB2	2.03	0.58
7:G:188:LYS:O	7:G:191:GLU:HB2	2.03	0.58
4:Y:160:TYR:CE1	4:Y:163:LYS:HD3	2.38	0.58
8:O:10:ASN:OD1	8:O:180:ILE:HD12	2.04	0.58
13:T:4:ILE:HD11	13:T:159:MET:HG2	1.85	0.58
1:V:27:ALA:O	1:V:31:VAL:HG23	2.02	0.58
2:W:160:TRP:CE3	2:W:163:ILE:HD13	2.39	0.58
6:1:42:CYS:HB2	6:1:184:LEU:O	2.02	0.58
7:2:67:ILE:HD12	7:2:211:GLU:HG2	1.83	0.58
1:A:78:TYR:CE2	1:A:82:GLY:HA2	2.39	0.58
1:A:79:SER:HA	17:A:252:HOH:O	2.01	0.58
8:H:52:THR:O	8:H:56:THR:HB	2.04	0.58
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.39	0.58
12:L:49:ALA:HA	17:L:531:HOH:O	2.02	0.58
11:R:65:LEU:CD1	4:Y:97:VAL:HG21	2.34	0.58
2:B:229:ILE:O	2:B:232:ILE:HG22	2.04	0.58
14:N:114:PRO:HD2	14:N:118:SER:O	2.03	0.58
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.19	0.58
12:S:109:ALA:HB2	12:S:121:ARG:HH21	1.67	0.58
13:T:124:THR:O	13:T:125:LEU:HD23	2.03	0.58
11:K:196:PHE:CE1	9:P:193:GLN:HG3	2.39	0.58
12:L:-8:PHE:HE1	13:M:115:LEU:HD12	1.68	0.58
13:M:87:MET:SD	13:M:95:LEU:HD12	2.44	0.58
8:O:172:ASN:HD22	8:O:193:THR:HA	1.69	0.58
13:T:4:ILE:CD1	13:T:159:MET:SD	2.92	0.58
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:GLU:HA	17:D:246:HOH:O	2.04	0.57
13:M:141(C):ARG:HH11	13:M:141(C):ARG:HG3	1.70	0.57
8:O:36:ARG:HD2	1:V:217(I):TYR:CE1	2.39	0.57
1:A:181:ASN:HD21	1:A:184:LEU:HD21	1.69	0.57
10:J:68:ILE:HG22	10:J:69:ARG:N	2.18	0.57
12:S:18:THR:CG2	12:S:30:TYR:HA	2.32	0.57
6:1:36:THR:O	6:1:50:VAL:HG23	2.04	0.57
7:2:105:TYR:HD2	7:2:105:TYR:N	2.01	0.57
7:G:130:ARG:HG3	7:G:131:PRO:O	2.04	0.57
7:G:151:THR:HG22	7:G:157:TYR:CB	2.31	0.57
1:V:78:TYR:CE2	1:V:82:GLY:HA2	2.39	0.57
11:K:126:CYS:SG	11:K:135:TYR:CE2	2.96	0.57
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.33	0.57
11:R:195:LEU:O	11:R:199:VAL:HG23	2.04	0.57
6:1:68:GLN:HE22	6:1:86:ARG:NH1	2.02	0.57
4:D:97:VAL:HG11	11:K:65:LEU:CD1	2.34	0.57
4:D:159:ARG:HB3	5:E:60:SER:HB3	1.85	0.57
6:1:175:GLU:O	6:1:178:LYS:HB2	2.05	0.57
2:B:20:ARG:HE	3:C:33:ARG:HH21	1.52	0.57
3:C:36:CYS:SG	3:C:37:ALA:N	2.78	0.57
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	1.86	0.57
4:Y:39:GLY:HA2	4:Y:47:VAL:O	2.03	0.57
5:Z:148:LEU:HD12	5:Z:149:LEU:N	2.19	0.57
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.52	0.57
4:D:46:VAL:HG11	4:D:139:ALA:CB	2.33	0.57
6:F:170:GLN:CD	6:F:170:GLN:H	2.08	0.57
1:V:77:VAL:HG22	1:V:78:TYR:H	1.70	0.57
1:V:86:ARG:HH21	7:2:118:ASN:HD22	1.53	0.57
3:X:57:LYS:O	3:X:58:LEU:HB2	2.03	0.57
6:1:69:VAL:HG23	6:1:74:ILE:O	2.05	0.57
4:D:177:LEU:HD22	5:E:58:LEU:HD22	1.86	0.57
7:G:46:THR:OG1	7:G:146:PRO:HB3	2.04	0.57
11:K:105(B):LYS:HD2	11:K:105(B):LYS:N	2.14	0.57
13:M:53:GLN:O	13:M:56:GLU:HB2	2.04	0.57
10:Q:35:ARG:O	10:Q:42:LEU:HD12	2.04	0.57
13:T:63:VAL:HG12	13:T:64:THR:N	2.19	0.57
13:T:76:PRO:HD2	13:T:105:GLN:OE1	2.04	0.57
14:U:163:ILE:HG21	14:U:187(G):TYR:OH	2.05	0.57
1:A:130:ARG:HG3	1:A:130:ARG:O	2.04	0.57
5:E:17:PRO:HA	6:F:26:TYR:CD2	2.40	0.57
14:N:187(D):PRO:HA	14:N:187(G):TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:78:LEU:HA	5:Z:136:LEU:HD23	1.87	0.57
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.40	0.57
11:R:142:TYR:O	11:R:143:LYS:HD2	2.05	0.57
13:T:141(C):ARG:HH11	13:T:141(C):ARG:HG3	1.70	0.57
4:Y:160:TYR:CZ	4:Y:163:LYS:HD3	2.40	0.57
8:O:197:ARG:HH21	9:P:139:GLU:HG3	1.69	0.56
11:R:1:THR:HG23	11:R:33:LYS:NZ	2.20	0.56
1:V:124:THR:CG2	2:W:130:ARG:HH21	2.15	0.56
2:W:53:LYS:HG2	2:W:54:VAL:HG23	1.87	0.56
5:Z:214:ILE:O	5:Z:221:PHE:HA	2.05	0.56
6:1:198:TYR:CE2	6:1:208:PHE:HZ	2.23	0.56
7:2:49:ILE:HD12	7:2:49:ILE:N	2.20	0.56
12:L:192:LYS:HE3	8:O:195:ASN:HB3	1.87	0.56
3:C:136:THR:O	3:C:150:GLN:HA	2.05	0.56
4:D:39:GLY:HA2	4:D:47:VAL:O	2.06	0.56
10:J:161:GLU:OE1	11:R:136:GLY:HA2	2.05	0.56
9:P:9:LYS:HD3	9:P:145:ASN:ND2	2.20	0.56
2:W:163:ILE:HG13	2:W:164:SER:H	1.70	0.56
5:Z:24:VAL:O	5:Z:27:ALA:HB3	2.05	0.56
7:2:220:LYS:HG2	7:2:221:PHE:N	2.21	0.56
12:L:166:HIS:CD2	12:L:168:GLN:HB2	2.40	0.56
5:Z:73:HIS:HE1	5:Z:107:LEU:O	1.88	0.56
5:E:48:LEU:HD13	5:E:77:SER:HB3	1.87	0.56
8:H:165:ASN:OD1	13:T:136:PRO:HA	2.05	0.56
12:S:63:VAL:HG22	12:S:74:LEU:HD23	1.86	0.56
14:U:10:ASP:O	14:U:179:THR:HG22	2.06	0.56
14:U:85:GLU:O	14:U:89:GLU:HB2	2.06	0.56
5:Z:198:SER:HA	5:Z:201:LEU:CG	2.36	0.56
4:D:215:ILE:HG13	4:D:215:ILE:O	2.05	0.56
6:F:127:ASN:HD22	6:F:127:ASN:C	2.09	0.56
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.87	0.56
9:P:101:VAL:O	9:P:110:ILE:HA	2.05	0.56
14:U:8:PHE:CZ	14:U:10:ASP:HB2	2.40	0.56
14:U:114:PRO:HD2	14:U:118:SER:O	2.06	0.56
1:V:4:MET:SD	1:V:5:THR:N	2.77	0.56
6:1:127:ASN:HD22	6:1:127:ASN:C	2.09	0.56
15:8:4:R4K:N	15:8:4:R4K:C32	2.69	0.56
1:A:4:MET:SD	1:A:5:THR:N	2.78	0.56
5:E:186:PRO:HG2	5:E:187:ASP:H	1.71	0.56
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.36	0.56
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:55:LEU:HD13	12:S:95:TYR:CD1	2.41	0.56
5:Z:114:HIS:HB3	6:1:86:ARG:NH2	2.21	0.56
12:L:43:MET:CB	12:L:101:ILE:HG22	2.36	0.56
10:Q:44:SER:OG	10:Q:100:LEU:HB2	2.05	0.56
7:2:39:ALA:HB2	7:2:48:VAL:HG12	1.86	0.56
1:A:74:ILE:HG12	1:A:140:GLY:HA3	1.88	0.56
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.05	0.56
12:L:18:THR:HG22	12:L:30:TYR:HA	1.87	0.56
2:B:46:ILE:HD11	2:B:146:TYR:HB3	1.87	0.56
12:L:-8:PHE:CE1	13:M:115:LEU:HD12	2.41	0.56
12:L:140:ASN:O	12:L:144:PHE:HA	2.05	0.56
3:X:152:GLU:CG	3:X:156:ILE:HG22	2.34	0.56
4:Y:188:GLU:O	4:Y:191:LEU:HB2	2.06	0.56
6:1:70:VAL:HB	6:1:74:ILE:HB	1.87	0.56
12:S:144(W):LYS:HG2	12:S:145:TYR:H	1.71	0.55
13:T:55:ILE:O	13:T:59:LEU:HG	2.06	0.55
5:Z:148:LEU:HD12	5:Z:149:LEU:H	1.70	0.55
7:2:48:VAL:C	7:2:49:ILE:HD12	2.26	0.55
7:G:48:VAL:C	7:G:49:ILE:HD12	2.26	0.55
5:E:78:LEU:HA	5:E:136:LEU:HD23	1.87	0.55
9:I:91:ARG:CD	9:I:116:ILE:HD12	2.36	0.55
9:I:186:LYS:HE2	9:I:188:TYR:OH	2.05	0.55
7:G:214:VAL:HG12	7:G:215:ALA:N	2.21	0.55
8:H:12:VAL:HG22	8:H:13:VAL:N	2.21	0.55
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.89	0.55
12:L:4:LEU:HD13	12:L:126:ALA:HB2	1.89	0.55
13:M:43:VAL:HG22	13:M:101:VAL:HG22	1.88	0.55
13:T:157:ASN:ND2	13:T:160:ARG:NH1	2.49	0.55
2:W:156:ASN:HD22	2:W:157:TYR:H	1.55	0.55
5:Z:40:LEU:HD23	5:Z:40:LEU:N	2.22	0.55
7:2:186:TRP:O	7:2:190:VAL:HG23	2.06	0.55
1:A:13:THR:O	2:B:130:ARG:HD3	2.07	0.55
2:B:15:PHE:HB2	3:C:23:GLN:HE22	1.72	0.55
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.89	0.55
12:L:19:ARG:HD2	12:L:168:GLN:O	2.05	0.55
13:T:165:ARG:N	13:T:165:ARG:HD2	2.20	0.55
6:1:82:ILE:HB	6:1:83:PRO:HD3	1.87	0.55
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.53	0.55
9:I:161:ASN:HD21	12:S:140:ASN:ND2	2.04	0.55
13:M:7:LYS:HD2	13:M:141(G):ILE:HD13	1.88	0.55
2:W:65:GLU:HG3	2:W:66:LYS:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:186:PRO:HG2	5:Z:187:ASP:H	1.72	0.55
6:1:150:MET:HE1	6:1:160:TYR:CE2	2.42	0.55
2:B:24:VAL:O	2:B:28:LEU:HD12	2.06	0.55
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.06	0.55
9:P:6:MET:HB3	9:P:151:LEU:HD11	1.89	0.55
14:U:112:THR:CG2	14:U:120:HIS:HB2	2.37	0.55
7:2:77:VAL:CG1	7:2:137:THR:HB	2.36	0.55
10:J:129:TYR:O	10:J:132:PHE:HB2	2.07	0.55
13:M:46:SER:OG	13:M:98:ALA:HB3	2.06	0.55
10:Q:112:GLN:HE22	10:Q:126:ALA:H	1.54	0.55
13:T:45:ILE:HG12	13:T:99:ILE:HG12	1.89	0.55
7:2:180(B):ASP:O	7:2:180(C):HIS:HB3	2.06	0.55
2:B:163:ILE:HG13	2:B:164:SER:N	2.21	0.55
4:D:160:TYR:CD2	5:E:59:SER:HB3	2.42	0.55
8:O:105:ASP:HB2	8:O:105(A):PRO:HD2	1.89	0.55
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.89	0.55
9:P:12:VAL:CG1	9:P:108:PRO:HB3	2.37	0.55
9:P:113:PHE:N	9:P:113:PHE:CD2	2.75	0.55
10:Q:85:GLN:HE21	2:W:101:LYS:HZ2	1.54	0.55
7:2:72:ARG:HB2	7:2:72:ARG:HH11	1.71	0.55
2:B:161:LYS:HE3	3:C:59:GLN:O	2.06	0.54
6:F:50:VAL:HG22	6:F:51:GLU:N	2.22	0.54
10:J:104:TYR:HD2	10:J:179:ASP:HA	1.72	0.54
14:N:38:HIS:CD2	17:N:352:HOH:O	2.59	0.54
14:U:48:SER:HB3	14:U:51:ASP:HB2	1.89	0.54
4:Y:163:LYS:HE3	4:Y:164:ALA:O	2.06	0.54
8:H:49:ALA:HB1	9:I:118:CYS:SG	2.47	0.54
5:Z:140:GLY:HA2	5:Z:215:VAL:HG11	1.88	0.54
6:F:68:GLN:OE1	6:F:89:VAL:HG21	2.07	0.54
9:I:171:TRP:HH2	11:R:165:ARG:NH1	2.04	0.54
8:O:204:TYR:CD2	8:O:204:TYR:N	2.75	0.54
13:M:100:ILE:HD13	13:M:125:LEU:HB2	1.88	0.54
8:O:49:ALA:CB	9:P:118:CYS:SG	2.96	0.54
2:W:212:PHE:O	2:W:224:PHE:HB2	2.08	0.54
4:Y:20:ARG:NH1	5:Z:33:GLN:HE22	2.05	0.54
5:Z:76:LEU:HD23	5:Z:76:LEU:O	2.07	0.54
3:C:88:LEU:HD22	3:C:116:VAL:HG13	1.90	0.54
5:E:48:LEU:O	5:E:212:ILE:HG23	2.08	0.54
11:R:37:ILE:HB	11:R:41:LEU:O	2.08	0.54
13:T:153:GLU:HG3	17:T:1470:HOH:O	2.07	0.54
3:X:40:VAL:HG12	3:X:162:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:4:LEU:O	11:R:4:LEU:HD13	2.07	0.54
13:T:133:MET:C	13:T:136:PRO:HD2	2.27	0.54
3:X:187:GLU:HA	3:X:232:TYR:OH	2.07	0.54
6:1:24:VAL:O	6:1:27:ALA:HB3	2.08	0.54
6:1:38:ILE:HG22	6:1:164:ALA:HB2	1.89	0.54
8:H:158:ALA:O	8:H:161:ALA:HB3	2.08	0.54
8:O:4:VAL:HG12	8:O:126:SER:HB2	1.90	0.54
12:S:166:HIS:CD2	12:S:168:GLN:HB2	2.43	0.54
1:V:69:LEU:HD23	1:V:70:LEU:N	2.22	0.54
2:W:126:HIS:CB	3:X:129:VAL:HG12	2.37	0.54
5:E:150:GLU:O	5:E:157:VAL:HA	2.08	0.54
6:F:212:ILE:HG22	6:F:213:SER:H	1.72	0.54
8:H:10:ASN:OD1	8:H:180:ILE:HD12	2.08	0.54
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.31	0.54
11:K:25:TRP:CH2	12:L:132:SER:HA	2.43	0.54
3:X:43:LYS:O	3:X:43:LYS:HG2	2.08	0.54
11:R:200:LYS:HE3	11:R:206:PHE:O	2.08	0.54
3:X:180(D):GLU:N	3:X:182:PRO:HD3	2.23	0.54
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.12	0.54
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.07	0.54
11:K:105(A):ARG:HB3	11:K:105(B):LYS:HE3	1.90	0.54
12:L:90:LYS:HE3	12:L:93:PHE:O	2.08	0.54
8:O:103:GLY:HA2	8:O:178:MET:SD	2.48	0.54
12:S:49:ALA:HA	17:S:2531:HOH:O	2.07	0.54
12:S:137:PHE:CE1	12:S:141:GLN:HG3	2.43	0.54
2:W:137:ILE:HD11	2:W:165:VAL:HG22	1.89	0.54
2:B:81:LEU:HD22	2:B:81:LEU:H	1.71	0.53
2:B:212:PHE:O	2:B:224:PHE:HB2	2.08	0.53
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.73	0.53
7:G:96:ALA:HA	7:G:107:MET:CE	2.29	0.53
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.53
14:U:114:PRO:O	14:U:116:GLY:N	2.41	0.53
7:2:69:CYS:O	7:2:93:LYS:HE2	2.08	0.53
4:D:59:LEU:HD13	4:D:60:GLU:N	2.22	0.53
12:L:24:TYR:O	8:O:167:LEU:HG	2.08	0.53
8:O:133:ALA:O	8:O:136:ALA:HB3	2.09	0.53
8:O:200:LYS:HE3	9:P:140:SER:O	2.08	0.53
5:Z:162:GLY:O	5:Z:163:THR:HB	2.07	0.53
4:D:52:LYS:HG3	4:D:64:ILE:HG21	1.91	0.53
4:D:188:GLU:O	4:D:191:LEU:HB2	2.08	0.53
6:F:11:SER:O	6:F:14:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:132:LEU:HD11	14:N:25:TYR:CE1	2.43	0.53
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.38	0.53
9:P:45:ILE:HG22	9:P:52:VAL:HG22	1.90	0.53
1:V:76:ALA:HB2	1:V:138:ILE:HG12	1.89	0.53
3:C:44:ASN:O	3:C:45:CYS:HB3	2.09	0.53
5:E:141:TYR:OH	5:E:217:LYS:HG3	2.09	0.53
6:F:37:SER:HB3	6:F:50:VAL:CG2	2.38	0.53
6:F:171:SER:O	6:F:174:ALA:HB3	2.08	0.53
7:G:109:CYS:HB3	17:G:754:HOH:O	2.08	0.53
12:S:61:ASN:HD21	5:Z:97:ASN:ND2	2.05	0.53
13:T:186:PHE:HE1	13:T:188:LYS:HG3	1.74	0.53
4:D:121:LEU:HB2	17:D:3156:HOH:O	2.09	0.53
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.91	0.53
10:J:52:THR:CG2	10:J:53:VAL:N	2.72	0.53
11:K:157:ARG:O	11:K:160:LEU:HB3	2.09	0.53
4:Y:221:PHE:CE1	4:Y:223:ILE:HG13	2.42	0.53
4:D:186:LEU:O	4:D:190:GLU:HG3	2.08	0.53
8:H:35:HIS:CB	8:H:56:THR:HG21	2.38	0.53
8:H:43:CYS:SG	8:H:99:LEU:HD22	2.49	0.53
8:H:195:ASN:HB3	12:S:192:LYS:HE3	1.89	0.53
14:N:55:ILE:O	14:N:59:VAL:HG23	2.09	0.53
14:N:61:TYR:CD2	14:N:62:HIS:N	2.77	0.53
6:1:65:VAL:HG12	6:1:66:LYS:N	2.23	0.53
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.72	0.53
8:H:134:ALA:HB1	8:H:158:ALA:HB1	1.89	0.53
9:I:3:VAL:HG22	9:I:16:CYS:HB3	1.89	0.53
12:L:103:GLY:HA2	12:L:178:VAL:HG11	1.89	0.53
14:N:84:LYS:HD3	17:N:920:HOH:O	2.07	0.53
8:O:3:ILE:HG13	8:O:3:ILE:O	2.07	0.53
3:X:33:ARG:HB2	3:X:33:ARG:HH11	1.73	0.53
4:Y:15:PHE:HB2	5:Z:23:GLN:OE1	2.08	0.53
2:B:120:LYS:HZ1	2:B:136:PHE:HD1	1.57	0.53
10:Q:85:GLN:NE2	2:W:101:LYS:NZ	2.56	0.53
1:V:23:GLN:OE1	7:2:15:PHE:HB2	2.09	0.53
2:B:173:GLN:HA	2:B:176:LEU:HD12	1.91	0.53
14:N:159:LEU:O	14:N:163:ILE:HG13	2.09	0.53
8:O:34:LEU:HD22	8:O:174:ASP:HB3	1.90	0.53
10:Q:166:MET:HG2	10:Q:167:PRO:HD2	1.91	0.53
12:S:114:ASP:HB2	12:S:118:SER:HB3	1.91	0.53
13:T:41:THR:HG21	13:T:79:ILE:HD12	1.91	0.53
1:A:27:ALA:O	1:A:31:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:93:ARG:O	3:X:96:ALA:HB3	2.09	0.53
7:2:77:VAL:HG12	7:2:137:THR:HB	1.90	0.53
14:N:84:LYS:HB2	14:N:119:VAL:CG2	2.39	0.52
9:P:6:MET:HE3	9:P:155:ILE:HB	1.90	0.52
5:E:130:ARG:HG3	5:E:130:ARG:NH1	2.23	0.52
5:E:214:ILE:O	5:E:221:PHE:HA	2.09	0.52
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.91	0.52
13:M:133:MET:C	13:M:136:PRO:HD2	2.29	0.52
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.52
1:V:15:PHE:N	2:W:23:GLN:HE22	2.06	0.52
3:X:38:VAL:CG2	3:X:39:GLY:N	2.73	0.52
6:1:220:LEU:N	6:1:220:LEU:HD23	2.24	0.52
6:1:224:VAL:HG13	6:1:228:LEU:HD23	1.91	0.52
5:E:22:PHE:HD1	5:E:26:TYR:HE1	1.57	0.52
5:E:24:VAL:O	5:E:27:ALA:HB3	2.08	0.52
12:L:163:THR:HB	17:L:2651:HOH:O	2.09	0.52
9:P:43:LEU:HD11	9:P:99:PRO:HB3	1.91	0.52
12:S:90:LYS:HE3	12:S:93:PHE:O	2.09	0.52
2:W:191:GLU:HG3	2:W:236:THR:HG22	1.91	0.52
5:Z:160:LEU:HD13	5:Z:163:THR:HB	1.92	0.52
4:D:215:ILE:HG22	4:D:221:PHE:CD2	2.42	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
13:M:113:VAL:HA	13:M:118:VAL:O	2.09	0.52
2:B:46:ILE:HG21	2:B:139:ALA:HB1	1.92	0.52
4:D:90:GLU:HA	17:D:509:HOH:O	2.08	0.52
11:K:4:LEU:O	11:K:4:LEU:HD13	2.09	0.52
11:K:38:ASN:O	11:K:40:PHE:N	2.42	0.52
7:G:105:TYR:CD2	7:G:105:TYR:N	2.77	0.52
10:J:176:LYS:HE2	10:J:186:GLN:HE21	1.75	0.52
13:M:112:TYR:O	13:M:119:THR:HA	2.09	0.52
9:P:2:ILE:HG21	9:P:130:ALA:HB3	1.92	0.52
11:R:105(B):LYS:HD2	11:R:105(B):LYS:N	2.14	0.52
5:E:223:ILE:HG22	5:E:223:ILE:O	2.09	0.52
12:L:140:ASN:ND2	9:P:161:ASN:HD21	2.06	0.52
8:O:134:ALA:O	8:O:137:VAL:N	2.43	0.52
12:S:79:ALA:O	12:S:83:ILE:HG13	2.10	0.52
5:Z:52:LYS:O	5:Z:63:TYR:HD2	1.92	0.52
5:E:36:VAL:HG22	5:E:37:THR:N	2.24	0.52
11:K:165:ARG:HH11	9:P:171:TRP:HH2	1.57	0.52
12:S:43:MET:HB2	12:S:101:ILE:CG2	2.33	0.52
5:Z:207:LEU:HD23	5:Z:207:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:108:PRO:HB2	7:2:111:VAL:HG23	1.91	0.52
7:2:109:CYS:HB3	17:2:2754:HOH:O	2.09	0.52
1:A:55:SER:HB2	17:G:3268:HOH:O	2.10	0.52
3:C:238:GLN:C	3:C:240:LYS:H	2.13	0.52
13:T:104:VAL:HG23	13:T:178:ILE:HG22	1.92	0.52
1:V:8:TYR:CD1	7:2:127:ALA:HB3	2.45	0.52
3:X:163:GLN:HG3	3:X:164:THR:N	2.25	0.52
5:Z:22:PHE:HD1	5:Z:26:TYR:CE1	2.27	0.52
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.73	0.52
2:B:38:ILE:HG23	2:B:164:SER:HB3	1.92	0.52
7:G:47:VAL:HG12	7:G:48:VAL:N	2.24	0.52
8:O:219:VAL:HG23	9:P:184:VAL:HG12	1.91	0.52
8:O:221:ILE:HG22	8:O:222:CYS:N	2.25	0.52
11:R:105(B):LYS:H	11:R:105(B):LYS:CD	2.13	0.52
4:Y:48:LEU:HD23	4:Y:77:ALA:HB2	1.92	0.52
5:Z:180(C):PHE:C	5:Z:180(E):LYS:H	2.14	0.52
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.45	0.51
4:D:123:PHE:CE1	4:D:131:PRO:HG3	2.44	0.51
5:E:180:LEU:HD12	5:E:180(C):PHE:HE1	1.75	0.51
9:I:79:PHE:O	9:I:82:LEU:HB3	2.10	0.51
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.90	0.51
12:L:97:VAL:O	12:L:115:PRO:HB3	2.10	0.51
8:O:172:ASN:ND2	8:O:193:THR:HA	2.23	0.51
6:1:151:LEU:HD12	6:1:156:SER:O	2.10	0.51
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.91	0.51
8:O:172:ASN:ND2	8:O:193:THR:HG22	2.25	0.51
3:X:33:ARG:HB2	3:X:33:ARG:NH1	2.25	0.51
10:J:35:ARG:O	10:J:42:LEU:HD12	2.10	0.51
10:J:147:THR:HG23	10:J:150:GLU:HG3	1.93	0.51
12:S:14:LEU:CD1	12:S:34:VAL:HG13	2.40	0.51
2:W:150:THR:O	2:W:157:TYR:HA	2.10	0.51
2:W:185:LYS:HD3	2:W:186:VAL:N	2.26	0.51
7:2:47:VAL:HG12	7:2:48:VAL:N	2.26	0.51
7:G:187:GLU:O	7:G:191:GLU:HG3	2.10	0.51
12:S:-6:PRO:O	13:T:91:ARG:NH1	2.43	0.51
6:1:121:GLN:HG2	7:2:83:PRO:HB2	1.91	0.51
6:1:130:ARG:HH11	6:1:130:ARG:HG3	1.75	0.51
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.45	0.51
8:H:221:ILE:HG22	8:H:222:CYS:N	2.25	0.51
1:V:71:THR:O	1:V:73:ASP:N	2.44	0.51
2:W:15:PHE:HB2	3:X:23:GLN:NE2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:75:GLY:HA3	4:Y:221:PHE:CD2	2.45	0.51
6:F:21:ASN:HB2	17:F:547:HOH:O	2.10	0.51
7:G:91:ARG:HH21	7:G:115:ARG:HH21	1.57	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.92	0.51
13:M:135:ASN:ND2	13:M:139:ARG:NH2	2.59	0.51
14:N:161:GLN:O	14:N:164:LYS:HB3	2.10	0.51
9:P:-2:ASN:OD1	9:P:48:LEU:HD12	2.11	0.51
11:R:45:MET:HG2	11:R:52:CYS:HB3	1.92	0.51
13:T:112:TYR:O	13:T:119:THR:HA	2.10	0.51
13:T:150:VAL:HG21	17:T:2869:HOH:O	2.10	0.51
14:U:187(D):PRO:O	14:U:187(F):GLU:N	2.44	0.51
12:L:177:ILE:HD12	12:L:177:ILE:N	2.26	0.51
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.46	0.51
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.59	0.51
11:K:8:PHE:HE2	11:K:13:ILE:HG12	1.75	0.51
11:K:126:CYS:SG	11:K:135:TYR:CD2	2.87	0.51
14:U:14:LEU:HD21	14:U:102:ALA:HB3	1.91	0.51
4:Y:112:LEU:C	4:Y:112:LEU:HD13	2.31	0.51
4:Y:186:LEU:O	4:Y:190:GLU:HG3	2.11	0.51
6:1:95:GLU:HG3	6:1:115:ARG:HH11	1.75	0.51
1:A:46:VAL:HG12	1:A:47:VAL:N	2.25	0.51
6:F:68:GLN:HE22	6:F:86:ARG:NH1	2.09	0.51
13:M:164:TYR:C	13:M:165:ARG:HD2	2.31	0.51
14:N:15:GLY:HA2	14:N:174:ARG:O	2.10	0.51
4:Y:160:TYR:CE2	5:Z:59:SER:HB3	2.46	0.51
1:A:137:LEU:HA	1:A:149:TYR:O	2.11	0.51
12:L:115:PRO:HA	17:L:613:HOH:O	2.11	0.51
14:N:30:VAL:HG11	13:T:199:PHE:CE2	2.43	0.51
12:S:14:LEU:HD12	12:S:34:VAL:HG13	1.93	0.51
7:2:14:ILE:O	7:2:21:LEU:HD23	2.11	0.51
7:2:38:LEU:HD23	7:2:197:MET:CE	2.41	0.51
7:2:222:PHE:N	7:2:222:PHE:CD2	2.79	0.51
1:A:35:VAL:HG12	1:A:36:THR:N	2.26	0.50
8:H:51:ASP:HB3	8:H:95:ILE:HG23	1.93	0.50
9:P:28:SER:HA	17:P:1086:HOH:O	2.11	0.50
14:U:14:LEU:O	14:U:175:MET:HA	2.10	0.50
6:1:109:ILE:O	6:1:110:PRO:C	2.49	0.50
4:D:180(C):HIS:NE2	4:D:184:LEU:HG	2.25	0.50
6:F:68:GLN:HG2	17:F:407:HOH:O	2.11	0.50
10:J:24:ILE:O	10:J:24:ILE:HG12	2.11	0.50
12:L:153:LYS:HG2	8:O:201:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:197:ARG:NH2	9:P:139:GLU:O	2.44	0.50
3:X:76:LEU:HD12	3:X:138:ILE:CG1	2.41	0.50
1:A:110:LYS:HG3	1:A:111:LEU:N	2.27	0.50
8:H:167:LEU:HG	12:S:24:TYR:O	2.12	0.50
10:J:143:ARG:O	10:J:146:MET:HG3	2.11	0.50
9:P:160:LEU:HD11	9:P:191:MET:HB3	1.93	0.50
5:Z:41:ARG:O	5:Z:41:ARG:HG3	2.11	0.50
5:Z:45:HIS:HB2	5:Z:189:LEU:HD12	1.92	0.50
5:E:180(C):PHE:C	5:E:180(E):LYS:H	2.15	0.50
11:K:104:TYR:CD1	11:K:180:GLU:HG3	2.45	0.50
14:N:7:THR:HA	14:N:12:VAL:HG23	1.93	0.50
5:Z:15:PHE:H	6:1:23:GLN:HE22	1.59	0.50
5:Z:207:LEU:H	5:Z:207:LEU:CD2	2.25	0.50
4:D:41:ALA:HA	4:D:46:VAL:HG22	1.92	0.50
8:H:47:GLY:H	15:8:5:AKK:HC1	1.76	0.50
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.92	0.50
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.46	0.50
13:T:32:GLU:OE1	13:T:34:LEU:HB2	2.11	0.50
7:2:179:HIS:CD2	7:2:192:PHE:HZ	2.29	0.50
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.22	0.50
4:D:14:THR:HA	17:D:3133:HOH:O	2.12	0.50
4:D:112:LEU:C	4:D:112:LEU:HD13	2.32	0.50
4:D:197:LEU:O	4:D:201:MET:HG3	2.12	0.50
9:I:171:TRP:HH2	11:R:165:ARG:HH11	1.59	0.50
6:1:18:ASP:OD1	6:1:20:ARG:HD3	2.12	0.50
6:1:68:GLN:OE1	6:1:89:VAL:HG21	2.11	0.50
4:D:100:ASN:HB3	17:D:252:HOH:O	2.11	0.50
6:F:54:ILE:HG13	6:F:208:PHE:HA	1.93	0.50
6:F:198:TYR:CE2	6:F:208:PHE:HZ	2.29	0.50
7:G:180(B):ASP:O	7:G:180(C):HIS:HB3	2.12	0.50
7:G:180(D):ILE:HG22	7:G:184:ASN:N	2.27	0.50
11:K:1:THR:HG23	11:K:33:LYS:HZ2	1.76	0.50
14:N:28:ASN:HA	17:N:319:HOH:O	2.10	0.50
8:O:128:GLY:O	8:O:131:SER:HB2	2.11	0.50
10:Q:155:LEU:O	10:Q:158:CYS:HB2	2.12	0.50
11:R:196:PHE:CE2	11:R:206:PHE:CD2	3.00	0.50
14:U:1:THR:HG23	14:U:33:LYS:NZ	2.26	0.50
5:Z:47:VAL:HG12	5:Z:48:LEU:N	2.26	0.50
3:C:134:VAL:HG12	3:C:135:SER:N	2.26	0.50
11:R:200:LYS:HG3	11:R:205:SER:O	2.12	0.50
13:T:4:ILE:HD11	13:T:159:MET:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:130:ARG:HG3	5:Z:130:ARG:NH1	2.20	0.50
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.94	0.50
5:E:5:ARG:C	5:E:7:ASN:H	2.15	0.50
10:J:38:SER:O	10:J:40:HIS:N	2.45	0.50
11:R:174:ASN:HD21	11:R:189:ASN:HB2	1.76	0.50
6:1:49:ALA:HB2	6:1:212:ILE:HG23	1.93	0.50
6:1:240:ILE:HG23	6:1:241:ASN:ND2	2.26	0.50
2:B:86:GLU:HB2	17:B:863:HOH:O	2.11	0.49
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.93	0.49
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.07	0.49
6:F:150:MET:O	6:F:157:TYR:HA	2.12	0.49
14:N:163:ILE:CG2	14:N:170:GLY:HA2	2.41	0.49
2:W:134:VAL:O	2:W:153:PRO:HD3	2.11	0.49
5:E:125:GLN:HG3	6:F:130:ARG:HG2	1.93	0.49
6:F:66:LYS:HA	17:F:670:HOH:O	2.10	0.49
7:G:49:ILE:HD12	7:G:49:ILE:N	2.27	0.49
10:J:8:VAL:HG23	10:J:9:GLN:N	2.26	0.49
14:N:175:MET:HE3	14:N:187(B):PHE:CE2	2.47	0.49
8:O:134:ALA:HB1	8:O:158:ALA:HB1	1.94	0.49
14:U:59:VAL:HG13	14:U:82:VAL:HG11	1.93	0.49
6:1:35:THR:HG22	6:1:36:THR:N	2.26	0.49
6:1:184:LEU:HD11	6:1:188:GLU:CB	2.42	0.49
2:B:39:GLY:HA2	2:B:47:VAL:O	2.12	0.49
2:B:81:LEU:HD22	2:B:81:LEU:N	2.27	0.49
8:H:55:VAL:HG23	8:H:86:HIS:HD2	1.77	0.49
8:H:213:VAL:HG12	8:H:214:LEU:N	2.27	0.49
9:I:15:ALA:CB	9:I:175:VAL:HG22	2.41	0.49
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.94	0.49
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.94	0.49
9:P:8:GLY:HA3	9:P:11:CYS:SG	2.52	0.49
12:S:19:ARG:HB2	12:S:171:ASP:HB2	1.93	0.49
1:V:11:SER:OG	2:W:129:LEU:HA	2.12	0.49
3:X:212:ILE:HG22	3:X:213:THR:N	2.27	0.49
5:Z:138:ILE:O	5:Z:148:LEU:HD12	2.11	0.49
6:1:221:HIS:CE1	6:1:223:PHE:CE1	2.95	0.49
8:H:55:VAL:HG23	8:H:86:HIS:CD2	2.45	0.49
11:K:35:ILE:CD1	11:K:45:MET:SD	3.01	0.49
13:M:35:ILE:HD13	13:M:56:GLU:HG2	1.94	0.49
2:W:86:GLU:HB2	17:W:2863:HOH:O	2.11	0.49
3:X:160:TRP:CZ2	4:Y:59:LEU:HD23	2.48	0.49
6:1:69:VAL:HG22	6:1:70:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ILE:HA	6:F:137:ILE:HD13	1.94	0.49
7:G:82:ILE:N	7:G:83:PRO:HD2	2.28	0.49
8:H:114:HIS:HE1	17:H:544:HOH:O	1.96	0.49
12:L:29:ARG:HD3	12:L:171:ASP:OD1	2.12	0.49
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.13	0.49
9:P:41:VAL:HG22	9:P:76:PRO:HG3	1.94	0.49
3:X:81:LEU:HB3	17:X:1414:HOH:O	2.12	0.49
5:Z:132:TYR:O	5:Z:153:PRO:HB3	2.13	0.49
5:Z:180(C):PHE:CD1	5:Z:180(D):ILE:N	2.79	0.49
6:F:126:TYR:CE1	7:G:129:MET:SD	3.04	0.49
7:G:105:TYR:HD2	7:G:105:TYR:N	2.09	0.49
8:H:77:VAL:HG13	17:H:952:HOH:O	2.12	0.49
12:L:134:ILE:HG22	12:L:138:LEU:CD2	2.43	0.49
10:Q:6:ILE:HD11	10:Q:142:TYR:CE1	2.47	0.49
3:X:154:SER:HB3	17:X:1000:HOH:O	2.12	0.49
15:9:4:R4K:N	15:9:4:R4K:C32	2.75	0.49
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.94	0.49
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.94	0.49
3:C:36:CYS:HA	3:C:166:GLY:HA3	1.94	0.49
6:F:148:LEU:HD12	6:F:149:TYR:N	2.27	0.49
7:G:151:THR:HA	7:G:156:TYR:O	2.13	0.49
8:O:111:PHE:HD1	8:O:121:VAL:HB	1.77	0.49
2:W:46:ILE:HG21	2:W:139:ALA:HB1	1.95	0.49
2:W:48:LEU:HD11	2:W:139:ALA:HB3	1.93	0.49
2:W:64:THR:HG23	2:W:67:LEU:O	2.13	0.49
3:X:216:LYS:HB2	3:X:220:ASP:HB3	1.95	0.49
4:Y:173:GLN:HB3	17:Y:1455:HOH:O	2.11	0.49
2:B:71:ASN:ND2	2:B:72:ASP:H	2.10	0.49
3:C:39:GLY:HA2	3:C:47:VAL:O	2.12	0.49
13:M:160:ARG:HA	13:M:192:VAL:HG11	1.95	0.49
14:N:161:GLN:HE22	14:U:139:ASP:HB3	1.77	0.49
9:P:76:PRO:O	9:P:77:GLU:C	2.51	0.49
2:W:11:ARG:O	2:W:14:ILE:HG12	2.13	0.49
4:Y:121:LEU:HB2	17:Y:1156:HOH:O	2.12	0.49
6:F:236:ALA:O	6:F:238:LYS:N	2.46	0.49
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.12	0.49
10:Q:112:GLN:NE2	10:Q:126:ALA:H	2.11	0.49
1:V:221:PHE:C	1:V:221:PHE:CD2	2.86	0.49
5:Z:77:SER:OG	5:Z:137:LEU:HB2	2.13	0.49
6:1:97:ALA:O	6:1:99:PHE:N	2.46	0.49
3:C:57:LYS:HG3	3:C:208:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:LEU:O	4:D:116:VAL:HG23	2.13	0.49
6:F:78:TYR:HB3	6:F:136:THR:HG23	1.95	0.49
8:H:90:TYR:O	8:H:93:GLY:N	2.46	0.49
14:U:41:ILE:HD13	14:U:79:ALA:HB2	1.93	0.49
1:V:112:LEU:O	1:V:116:VAL:HG23	2.13	0.49
4:Y:59:LEU:HD13	4:Y:60:GLU:N	2.27	0.49
9:I:43:LEU:HD11	9:I:99:PRO:HB3	1.94	0.48
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.80	0.48
14:N:8:PHE:CZ	14:N:10:ASP:HB2	2.48	0.48
8:O:86:HIS:CE1	8:O:90:TYR:HE2	2.30	0.48
12:S:51:ASP:OD1	12:S:95:TYR:HA	2.12	0.48
12:S:76:ILE:HG23	12:S:77:ASN:N	2.27	0.48
13:T:13:ILE:HG23	13:T:175:LEU:HD21	1.95	0.48
13:T:112:TYR:HE1	13:T:127:THR:HG22	1.78	0.48
13:T:157:ASN:O	13:T:160:ARG:N	2.46	0.48
5:Z:66:LYS:HA	5:Z:78:LEU:HD21	1.95	0.48
1:A:13:THR:HG22	1:A:21:LEU:HD22	1.95	0.48
1:A:46:VAL:CG1	1:A:47:VAL:N	2.75	0.48
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.95	0.48
6:F:31:VAL:O	6:F:34:GLY:N	2.46	0.48
6:F:221:HIS:HE1	6:F:223:PHE:HE1	1.59	0.48
12:L:49:ALA:HB1	17:M:965:HOH:O	2.13	0.48
12:L:166:HIS:HE1	17:L:233:HOH:O	1.95	0.48
13:M:40:ASN:HD22	13:M:40:ASN:N	2.11	0.48
14:N:111:TYR:HA	14:N:120:HIS:O	2.12	0.48
12:S:2:THR:HG21	12:S:130:ALA:HB3	1.94	0.48
2:W:38:ILE:HG23	2:W:164:SER:HB3	1.95	0.48
4:Y:77:ALA:HB3	4:Y:137:LEU:HB2	1.94	0.48
1:A:77:VAL:HG22	1:A:78:TYR:N	2.28	0.48
3:C:71:ASP:CA	10:J:68:ILE:HD11	2.42	0.48
11:K:208:ASN:O	9:P:30:LYS:NZ	2.46	0.48
14:U:143:ARG:O	14:U:146:MET:HG3	2.13	0.48
4:Y:170:GLU:HG2	4:Y:171:GLY:N	2.27	0.48
1:A:85:TYR:O	1:A:89:VAL:HG23	2.12	0.48
3:C:159:SER:HB2	17:C:245:HOH:O	2.13	0.48
8:H:124:TYR:N	8:H:124:TYR:CD1	2.81	0.48
10:J:132:PHE:HD1	11:R:133:PHE:CZ	2.31	0.48
10:Q:156:LYS:O	10:Q:160:GLN:HG3	2.13	0.48
13:T:19:LEU:HD11	13:T:26:LEU:HB3	1.96	0.48
2:W:121:GLN:O	2:W:124:THR:HB	2.13	0.48
1:A:130:ARG:NH1	1:A:131:PRO:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:LEU:N	5:E:40:LEU:HD23	2.28	0.48
8:H:1:THR:O	8:H:128:GLY:HA3	2.13	0.48
11:K:200:LYS:HG3	11:K:205:SER:O	2.13	0.48
14:N:1:THR:HG23	14:N:33:LYS:NZ	2.29	0.48
14:N:175:MET:HE3	14:N:187(B):PHE:HE2	1.78	0.48
8:O:18:THR:HB	8:O:30:ASN:HA	1.95	0.48
13:T:78:TYR:CE1	5:Z:105:ARG:HB2	2.48	0.48
1:V:150:GLN:O	1:V:157:TYR:HA	2.14	0.48
2:W:88:LEU:HD22	2:W:116:LEU:CD2	2.43	0.48
7:2:143(A):GLU:HG2	17:2:1127:HOH:O	2.12	0.48
3:C:95:GLU:HG3	3:C:95:GLU:O	2.13	0.48
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.48	0.48
8:H:208:ARG:NH1	9:I:149:GLU:HB2	2.28	0.48
6:1:43:ASN:HD22	6:1:43:ASN:N	2.12	0.48
2:B:117:SER:HB3	2:B:155:GLY:O	2.13	0.48
3:C:15:PHE:N	4:D:23:GLN:HE22	1.96	0.48
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.53	0.48
14:N:12:VAL:HG12	14:N:178:LEU:HB2	1.96	0.48
9:P:19:ARG:HB2	9:P:170:GLY:O	2.14	0.48
14:U:8:PHE:CE1	14:U:10:ASP:HB2	2.49	0.48
14:U:28:ASN:HA	17:U:2319:HOH:O	2.14	0.48
1:V:121:GLN:O	1:V:124:THR:HB	2.13	0.48
1:V:197:LEU:HD23	1:V:210:ILE:HD12	1.96	0.48
2:W:107:ILE:HD11	2:W:111:ILE:HG22	1.94	0.48
7:2:76:MET:SD	7:2:138:PHE:CE2	3.07	0.48
3:C:201:VAL:O	3:C:202:GLN:HB2	2.14	0.48
11:R:46:ALA:HB3	11:R:98:GLY:O	2.14	0.48
14:U:51:ASP:OD2	14:U:95:LEU:HA	2.13	0.48
7:2:179:HIS:CD2	7:2:192:PHE:CZ	3.01	0.48
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.27	0.48
5:E:180:LEU:HD12	5:E:180(C):PHE:CE1	2.49	0.48
6:F:151:LEU:HD12	6:F:156:SER:O	2.14	0.48
6:F:158:TRP:HB2	6:F:160:TYR:HE1	1.78	0.48
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.96	0.48
12:L:135:MET:CE	9:P:165:ARG:NH2	2.77	0.48
14:N:147:SER:OG	14:N:149:GLU:HG3	2.14	0.48
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.48
8:O:51:ASP:HB3	8:O:95:ILE:HG23	1.95	0.48
2:W:117:SER:HB3	2:W:155:GLY:O	2.14	0.48
3:X:134:VAL:CG1	3:X:135:SER:N	2.77	0.48
5:Z:180(C):PHE:HA	5:Z:180(F):ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:136:THR:O	6:1:150:MET:HA	2.14	0.48
7:2:151:THR:HG22	7:2:157:TYR:HB2	1.95	0.48
7:2:198:ILE:O	7:2:200:ALA:N	2.47	0.48
6:F:148:LEU:HD12	6:F:149:TYR:H	1.79	0.48
12:L:104:LEU:HD23	12:L:108:GLY:HA2	1.94	0.48
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.95	0.48
2:W:160:TRP:CD2	2:W:163:ILE:HD13	2.49	0.48
3:X:57:LYS:CG	3:X:208:LYS:NZ	2.77	0.48
7:2:170:GLN:HE21	7:2:174:THR:HG23	1.78	0.48
1:A:121:GLN:O	1:A:124:THR:HB	2.14	0.47
9:I:43:LEU:HD12	9:I:100:VAL:O	2.13	0.47
12:L:93:PHE:N	12:L:94:PRO:HD3	2.29	0.47
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.12	0.47
13:T:157:ASN:HD22	13:T:160:ARG:NH1	2.11	0.47
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.96	0.47
11:K:31:VAL:HG12	11:K:33:LYS:HG3	1.96	0.47
12:L:-6:PRO:HB2	13:M:91:ARG:NH1	2.29	0.47
8:O:152:ILE:CG2	8:O:191:TYR:HE1	2.27	0.47
10:Q:113:ILE:CG1	10:Q:119:LYS:HG3	2.37	0.47
12:S:134:ILE:HG22	12:S:138:LEU:CD2	2.43	0.47
14:U:14:LEU:HD12	14:U:14:LEU:N	2.29	0.47
14:U:51:ASP:O	14:U:55:ILE:HG13	2.15	0.47
7:2:206:SER:O	7:2:209:ASP:HB2	2.15	0.47
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.60	0.47
3:C:212:ILE:HG22	3:C:213:THR:N	2.28	0.47
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.96	0.47
5:E:117:CYS:SG	6:F:86:ARG:HD3	2.55	0.47
5:E:162:GLY:O	5:E:163:THR:HB	2.14	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.13	0.47
11:R:83:LEU:O	11:R:86:LEU:HB3	2.14	0.47
12:S:25:SER:HB3	17:S:2284:HOH:O	2.14	0.47
13:T:1:THR:OG1	13:T:2:SER:N	2.47	0.47
1:V:52:LYS:O	1:V:54:SER:N	2.47	0.47
6:1:192:GLN:O	6:1:195:LYS:HB3	2.15	0.47
1:A:41:LYS:HA	1:A:46:VAL:HG22	1.96	0.47
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.14	0.47
8:H:103:GLY:HA2	8:H:178:MET:SD	2.55	0.47
9:I:178:ILE:HG23	9:I:184:VAL:CG2	2.44	0.47
11:K:19:ARG:HA	11:K:28:SER:O	2.13	0.47
10:Q:185:ARG:HG2	10:Q:185:ARG:HH11	1.79	0.47
4:Y:160:TYR:CD2	5:Z:59:SER:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:TYR:CD1	3:C:132:PHE:HE1	2.33	0.47
4:D:97:VAL:HG11	11:K:65:LEU:HD11	1.95	0.47
5:E:28:LEU:O	5:E:31:ILE:HB	2.15	0.47
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.47
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.96	0.47
8:H:167:LEU:HD12	12:S:24:TYR:HA	1.97	0.47
8:O:124:TYR:N	8:O:124:TYR:CD1	2.82	0.47
2:B:20:ARG:NH2	3:C:33:ARG:HE	2.13	0.47
5:E:65:LYS:HG3	5:E:65:LYS:O	2.15	0.47
6:F:38:ILE:HG22	6:F:164:ALA:CA	2.44	0.47
8:H:201:GLN:CG	12:S:153:LYS:HG2	2.44	0.47
13:M:62:LEU:HA	13:M:62:LEU:HD23	1.66	0.47
8:O:55:VAL:HG23	8:O:86:HIS:HD2	1.80	0.47
10:Q:135:PHE:HZ	17:Q:2596:HOH:O	1.98	0.47
2:W:56:SER:OG	2:W:57:THR:N	2.45	0.47
3:X:135:SER:OG	3:X:152:GLU:HA	2.14	0.47
1:A:7:ARG:HH22	4:D:123(C):GLY:HA3	1.79	0.47
2:B:157:TYR:CD2	3:C:86:ARG:NH1	2.82	0.47
4:D:89:ILE:HG22	4:D:93:ARG:HD2	1.96	0.47
9:I:-2:ASN:HA	9:I:21:GLY:O	2.15	0.47
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.47
13:M:19:LEU:HD22	13:M:170:SER:HB2	1.96	0.47
8:O:3:ILE:HG22	8:O:16:ALA:HB2	1.97	0.47
9:P:75:GLU:OE1	9:P:105:ASN:HA	2.14	0.47
13:T:205:GLY:HA3	13:T:209:GLN:HB3	1.97	0.47
3:X:71:ASP:O	3:X:73:HIS:N	2.48	0.47
5:Z:38:VAL:HG12	5:Z:39:GLY:N	2.30	0.47
6:1:83:PRO:O	6:1:86:ARG:N	2.48	0.47
6:1:170:GLN:CD	6:1:170:GLN:H	2.17	0.47
7:2:67:ILE:CD1	7:2:211:GLU:HG2	2.45	0.47
7:2:136:LEU:O	7:2:150:LYS:HA	2.14	0.47
7:2:179(D):SER:O	7:2:179(E):LYS:HB2	2.15	0.47
3:C:49:GLY:C	3:C:50:CYS:SG	2.93	0.47
14:N:186:ARG:NH2	13:T:204:LYS:HB2	2.30	0.47
9:P:53:THR:HG22	10:Q:84:ARG:NH2	2.30	0.47
4:Y:29:GLU:OE2	4:Y:32:LYS:HD2	2.15	0.47
5:Z:65:LYS:HG3	5:Z:65:LYS:O	2.15	0.47
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.95	0.47
13:M:111:ARG:HG3	13:M:120:TYR:O	2.15	0.47
14:N:152:VAL:HG13	14:N:175:MET:HE1	1.96	0.47
11:R:138:LEU:HD13	11:R:158:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:161:VAL:O	13:T:164:TYR:HB2	2.14	0.47
14:U:3:ILE:HG22	14:U:16:ALA:HB2	1.96	0.47
17:1:2420:HOH:O	7:2:86:ARG:HD2	2.14	0.47
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.12	0.47
13:M:112:TYR:CD2	13:M:120:TYR:CZ	3.03	0.47
1:V:210:ILE:HG22	1:V:211:GLU:N	2.30	0.47
3:X:123:TYR:CD1	3:X:132:PHE:HE1	2.33	0.47
6:1:115:ARG:HG2	17:1:2418:HOH:O	2.14	0.47
2:B:192:LEU:HD23	2:B:192:LEU:O	2.15	0.46
6:F:53:LEU:HD23	6:F:53:LEU:HA	1.71	0.46
10:J:74:LEU:HD22	10:J:78:ALA:HB1	1.97	0.46
11:K:136:GLY:HA2	10:Q:161:GLU:OE1	2.15	0.46
9:P:3:VAL:HG22	9:P:16:CYS:HB3	1.97	0.46
9:P:71:GLU:HG2	17:P:2213:HOH:O	2.13	0.46
13:T:-6:GLN:O	13:T:-6:GLN:HG3	2.15	0.46
13:T:19:LEU:HD22	13:T:170:SER:HB2	1.95	0.46
1:V:146:GLY:HA3	17:V:2772:HOH:O	2.15	0.46
4:Y:148:LEU:HD12	4:Y:149:PHE:H	1.81	0.46
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.16	0.46
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.97	0.46
6:F:157:TYR:CE2	7:G:86:ARG:NH1	2.83	0.46
8:H:197:ARG:HH12	8:H:200:LYS:HD3	1.79	0.46
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.45	0.46
13:M:91:ARG:HG3	13:M:92:SER:N	2.30	0.46
8:O:204:TYR:O	8:O:206:PHE:CD2	2.69	0.46
8:O:219:VAL:CG2	9:P:184:VAL:HG12	2.45	0.46
9:P:67:LYS:O	9:P:71:GLU:N	2.48	0.46
11:R:155:GLY:O	11:R:156:LYS:C	2.54	0.46
17:S:1438:HOH:O	13:T:132:HIS:HE1	1.98	0.46
13:T:100:ILE:HD13	13:T:125:LEU:HB2	1.96	0.46
14:U:84:LYS:HE3	14:U:119:VAL:HG23	1.98	0.46
4:Y:139:ALA:HB2	4:Y:148:LEU:HD13	1.97	0.46
1:A:77:VAL:HG22	1:A:78:TYR:H	1.79	0.46
1:A:142:ASP:O	1:A:144:PHE:N	2.49	0.46
3:C:163:GLN:CG	3:C:164:THR:N	2.78	0.46
5:E:207:LEU:HD23	5:E:207:LEU:H	1.80	0.46
12:S:67:HIS:HD2	17:Z:2864:HOH:O	1.97	0.46
12:S:166:HIS:HE1	17:S:2233:HOH:O	1.99	0.46
13:T:198:ASP:HB3	17:T:3406:HOH:O	2.15	0.46
2:B:78:VAL:HG22	2:B:136:PHE:CE2	2.51	0.46
14:N:161:GLN:HE21	14:U:136:GLY:CA	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:187(D):PRO:O	14:N:187(F):GLU:N	2.48	0.46
10:Q:18:LYS:CD	10:Q:174:ILE:HG13	2.38	0.46
3:C:38:VAL:CG2	3:C:39:GLY:N	2.78	0.46
3:C:163:GLN:HE21	3:C:164:THR:N	2.05	0.46
4:D:89:ILE:HD13	4:D:89:ILE:HA	1.74	0.46
12:L:-6:PRO:HB2	13:M:91:ARG:HH11	1.81	0.46
9:P:97:VAL:HG23	9:P:99:PRO:HD3	1.97	0.46
12:S:60:LYS:O	12:S:63:VAL:HB	2.16	0.46
14:U:3:ILE:HG22	14:U:16:ALA:CB	2.45	0.46
1:V:66:LYS:HG2	1:V:78:TYR:HE1	1.80	0.46
6:1:109:ILE:HB	6:1:110:PRO:HD3	1.97	0.46
7:2:82:ILE:N	7:2:83:PRO:HD2	2.30	0.46
4:D:25:GLU:O	4:D:28:LEU:HB2	2.16	0.46
6:F:69:VAL:HG23	6:F:74:ILE:O	2.14	0.46
12:L:102:ALA:HB2	12:L:110:VAL:HG22	1.97	0.46
13:M:55:ILE:O	13:M:59:LEU:HG	2.15	0.46
9:P:59:PHE:CZ	9:P:83:VAL:HG22	2.50	0.46
11:R:99:THR:HA	17:R:2444:HOH:O	2.16	0.46
13:T:35:ILE:HA	13:T:36:PRO:HD3	1.82	0.46
13:T:53:GLN:O	13:T:56:GLU:HB2	2.15	0.46
1:V:175:PHE:O	1:V:175:PHE:CD1	2.68	0.46
7:2:119:LEU:HD12	7:2:119:LEU:HA	1.79	0.46
3:C:93:ARG:O	3:C:96:ALA:HB3	2.16	0.46
6:F:206(B):GLU:HG3	6:F:206(C):LYS:HG3	1.97	0.46
10:J:155:LEU:O	10:J:158:CYS:HB2	2.16	0.46
11:K:155:GLY:O	11:K:158:SER:N	2.49	0.46
9:P:6:MET:SD	9:P:142:TYR:HD1	2.38	0.46
11:R:174:ASN:ND2	11:R:189:ASN:HB2	2.30	0.46
12:S:20:ASN:O	12:S:27:ASN:HB2	2.16	0.46
13:T:42:VAL:HG23	13:T:178:ILE:HD11	1.96	0.46
13:T:164:TYR:C	13:T:165:ARG:HD2	2.36	0.46
2:W:39:GLY:HA2	2:W:47:VAL:O	2.16	0.46
3:X:35:THR:HB	3:X:51:GLU:CG	2.43	0.46
5:Z:47:VAL:O	5:Z:48:LEU:HD23	2.16	0.46
6:1:235:PHE:CD2	6:1:235:PHE:O	2.69	0.46
7:2:168:LYS:O	7:2:172:ILE:HG13	2.15	0.46
6:F:67:ILE:HG22	6:F:68:GLN:N	2.30	0.46
11:K:87:VAL:HG11	11:K:115:SER:HA	1.98	0.46
12:L:98:HIS:HE1	12:L:112:SER:HB2	1.80	0.46
9:P:7:THR:HG23	9:P:110:ILE:CD1	2.45	0.46
9:P:99:PRO:HB2	9:P:113:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:129:TYR:O	10:Q:132:PHE:HB2	2.16	0.46
12:S:19:ARG:NE	12:S:171:ASP:OD2	2.46	0.46
3:X:57:LYS:HG3	3:X:208:LYS:NZ	2.30	0.46
3:X:150:GLN:HE21	3:X:160:TRP:HE1	1.64	0.46
6:1:15:PHE:CE2	7:2:27:ALA:HB2	2.51	0.46
6:1:120:VAL:HG21	6:1:151:LEU:HD21	1.97	0.46
1:A:150:GLN:O	1:A:157:TYR:HA	2.15	0.46
2:B:120:LYS:NZ	2:B:136:PHE:HD1	2.14	0.46
3:C:154:SER:OG	3:C:156:ILE:HB	2.16	0.46
3:C:208:LYS:HE3	3:C:209:ASN:HD22	1.81	0.46
4:D:110:GLU:O	4:D:113:THR:HB	2.16	0.46
6:F:32:GLU:C	6:F:34:GLY:H	2.19	0.46
6:F:141:VAL:CG2	6:F:215:CYS:SG	2.96	0.46
11:K:200:LYS:HE3	11:K:206:PHE:O	2.16	0.46
2:W:163:ILE:HG13	2:W:164:SER:N	2.31	0.46
7:2:55:PRO:HG2	7:2:56:ASP:H	1.81	0.46
10:J:2:ILE:O	10:J:3:ILE:HD13	2.15	0.46
12:L:18:THR:HG22	12:L:31:GLU:H	1.80	0.46
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.98	0.46
10:Q:35:ARG:NH2	17:Q:2774:HOH:O	2.49	0.46
13:T:43:VAL:HG22	13:T:101:VAL:HG22	1.98	0.46
13:T:125:LEU:HA	17:T:2278:HOH:O	2.16	0.46
14:U:7:THR:HA	14:U:12:VAL:HG23	1.98	0.46
2:W:112:LEU:HD23	2:W:112:LEU:C	2.36	0.46
5:Z:37:THR:OG1	5:Z:50:ALA:HB2	2.16	0.46
4:D:40:ILE:HD11	4:D:193:VAL:HG23	1.96	0.45
6:F:180(E):GLU:HG3	6:F:180(F):GLY:O	2.16	0.45
13:M:3:VAL:O	13:M:126:ALA:HA	2.16	0.45
14:N:175:MET:CE	14:N:187(B):PHE:HE2	2.29	0.45
9:P:55:LEU:HD21	9:P:95:TYR:CD1	2.50	0.45
2:W:184:MET:HE1	2:W:189:ALA:HA	1.99	0.45
4:Y:17:PRO:HA	5:Z:26:TYR:CD2	2.51	0.45
6:1:35:THR:CG2	6:1:36:THR:N	2.78	0.45
6:1:86:ARG:HH11	6:1:86:ARG:HG2	1.81	0.45
2:B:141:TYR:CG	2:B:142:ASP:N	2.85	0.45
3:C:47:VAL:O	3:C:48:LEU:HD23	2.16	0.45
5:E:212:ILE:HG22	5:E:213:ALA:N	2.31	0.45
7:G:99:PHE:CE1	7:G:107:MET:HA	2.51	0.45
8:H:33:LYS:HE2	15:8:5:AKK:CA	2.43	0.45
8:H:126:SER:O	8:H:127:LEU:HD23	2.16	0.45
10:J:156:LYS:O	10:J:160:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:196:PHE:HE2	11:K:206:PHE:CD2	2.35	0.45
13:M:153:GLU:HG3	17:M:3470:HOH:O	2.15	0.45
14:N:113:ILE:HA	14:N:118:SER:O	2.15	0.45
8:O:4:VAL:HG22	8:O:159:ILE:HD11	1.97	0.45
11:R:88:TYR:HB2	17:R:2144:HOH:O	2.17	0.45
13:T:102:ALA:HB2	13:T:110:LEU:HD12	1.98	0.45
1:V:31:VAL:HG13	1:V:79:SER:O	2.16	0.45
3:X:198:LEU:HA	3:X:198:LEU:HD23	1.61	0.45
5:Z:17:PRO:HA	6:1:26:TYR:CD2	2.51	0.45
5:Z:47:VAL:HG11	5:Z:190:ILE:HG12	1.98	0.45
6:1:50:VAL:HG22	6:1:51:GLU:N	2.30	0.45
7:2:91:ARG:NH2	7:2:115:ARG:NH2	2.63	0.45
4:D:139:ALA:HB2	4:D:148:LEU:CD1	2.46	0.45
5:E:52:LYS:O	5:E:63:TYR:HD2	2.00	0.45
6:F:127:ASN:C	6:F:127:ASN:ND2	2.69	0.45
8:H:152:ILE:O	8:H:153:LYS:C	2.54	0.45
8:H:218:ILE:HG22	8:H:219:VAL:N	2.32	0.45
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.51	0.45
9:P:55:LEU:HD23	9:P:55:LEU:N	2.31	0.45
12:S:49:ALA:HB1	17:T:2965:HOH:O	2.17	0.45
13:T:35:ILE:HD13	13:T:56:GLU:HG2	1.98	0.45
4:Y:32:LYS:O	4:Y:167:SER:HA	2.17	0.45
4:Y:117:CYS:HB3	4:Y:155:GLY:O	2.16	0.45
5:Z:5:ARG:C	5:Z:7:ASN:H	2.20	0.45
2:B:176:LEU:C	2:B:178:MET:N	2.69	0.45
3:C:25:GLU:O	3:C:28:LEU:HB2	2.16	0.45
4:D:115:SER:O	4:D:118:ASP:HB2	2.16	0.45
4:D:224:TYR:CD2	4:D:224:TYR:N	2.84	0.45
8:O:3:ILE:HG22	8:O:16:ALA:CB	2.47	0.45
10:Q:12:VAL:HG23	10:Q:108:PRO:HB2	1.98	0.45
12:S:8:GLY:HA3	12:S:11:PHE:CZ	2.52	0.45
13:T:112:TYR:CD2	13:T:120:TYR:CZ	3.05	0.45
4:Y:123(G):GLU:HG2	4:Y:125:GLU:H	1.80	0.45
6:1:67:ILE:HG13	6:1:211:GLU:OE1	2.15	0.45
7:2:214:VAL:HG12	7:2:215:ALA:H	1.80	0.45
3:C:57:LYS:HG3	3:C:208:LYS:HZ1	1.82	0.45
7:G:221:PHE:CD1	7:G:221:PHE:C	2.90	0.45
10:Q:43:MET:HG3	10:Q:101:ILE:CG1	2.46	0.45
10:Q:129:TYR:HA	10:Q:132:PHE:HD2	1.82	0.45
14:U:84:LYS:HB2	14:U:119:VAL:CG2	2.46	0.45
4:Y:90:GLU:HA	17:Y:2509:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:194:LEU:HD12	4:Y:194:LEU:HA	1.77	0.45
6:1:107:ILE:HA	6:1:108:PRO:HD3	1.76	0.45
11:K:210:ILE:N	17:K:2742:HOH:O	2.50	0.45
12:L:184:VAL:HG12	12:L:184:VAL:O	2.16	0.45
11:R:138:LEU:HD12	11:R:138:LEU:HA	1.67	0.45
2:W:71:ASN:HD22	2:W:72:ASP:N	2.14	0.45
3:X:238:GLN:C	3:X:240:LYS:H	2.20	0.45
4:Y:156:THR:HG23	5:Z:83:PRO:HD3	1.97	0.45
6:1:54:ILE:HG13	6:1:208:PHE:HA	1.98	0.45
2:B:15:PHE:HB2	3:C:23:GLN:NE2	2.30	0.45
5:E:198:SER:HA	5:E:201:LEU:CD1	2.47	0.45
7:G:72:ARG:NH2	14:N:39:ASP:OD2	2.50	0.45
8:H:5:GLY:O	8:H:124:TYR:HA	2.16	0.45
8:H:124:TYR:HB2	8:H:138:LEU:HD13	1.99	0.45
9:I:6:MET:HE1	9:I:155:ILE:HA	1.99	0.45
10:J:171:LYS:NZ	10:Q:163:GLU:O	2.50	0.45
9:P:45:ILE:CG2	9:P:52:VAL:HG22	2.47	0.45
1:V:134:VAL:O	1:V:153:PRO:HG3	2.17	0.45
6:1:236:ALA:O	6:1:238:LYS:N	2.50	0.45
7:2:38:LEU:HD23	7:2:197:MET:HE3	1.98	0.45
1:A:23:GLN:OE1	7:G:15:PHE:HB2	2.16	0.45
3:C:57:LYS:CG	3:C:208:LYS:NZ	2.80	0.45
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.17	0.45
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.99	0.45
6:F:176:LEU:HD22	6:F:196:ILE:HD13	1.99	0.45
8:H:35:HIS:CG	8:H:56:THR:HG21	2.52	0.45
9:P:33:LYS:O	9:P:44:GLY:HA2	2.17	0.45
11:R:87:VAL:CG1	11:R:115:SER:HA	2.43	0.45
2:W:124:THR:CG2	3:X:130:ARG:HH21	2.29	0.45
6:1:52:LYS:HD2	6:1:211:GLU:OE2	2.16	0.45
6:F:208:PHE:H	6:F:208:PHE:HD2	1.64	0.45
9:I:161:ASN:ND2	12:S:140:ASN:ND2	2.64	0.45
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.35	0.45
11:K:104:TYR:CD2	11:K:179:THR:HA	2.51	0.45
13:M:136:PRO:HA	8:O:165:ASN:OD1	2.17	0.45
10:Q:54:GLN:OE1	11:R:85:ASN:ND2	2.50	0.45
13:T:8:TYR:CE2	13:T:148:VAL:HG22	2.51	0.45
14:U:51:ASP:OD2	14:U:95:LEU:HD23	2.17	0.45
14:U:65:LEU:HG	14:U:69:GLN:HE21	1.80	0.45
2:B:186:VAL:HG12	2:B:187:ASP:N	2.32	0.45
8:H:201:GLN:HG2	12:S:153:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:GLY:HA3	13:M:178:ILE:O	2.17	0.45
11:R:1:THR:HG23	11:R:33:LYS:HZ2	1.82	0.45
14:U:36:ARG:HG2	14:U:38:HIS:H	1.82	0.45
2:W:141:TYR:CG	2:W:142:ASP:N	2.85	0.45
3:X:160:TRP:CE2	4:Y:59:LEU:HD23	2.51	0.45
5:Z:28:LEU:O	5:Z:31:ILE:HB	2.17	0.45
5:Z:92:LEU:HD12	5:Z:92:LEU:HA	1.85	0.45
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.51	0.44
5:E:31:ILE:HD11	5:E:153:PRO:HD2	1.99	0.44
7:G:111:VAL:HG22	8:H:70:THR:HG22	1.98	0.44
8:H:13:VAL:HG22	8:H:14:ILE:N	2.31	0.44
12:L:42:VAL:HG22	12:L:102:ALA:O	2.17	0.44
14:N:32:ASP:OD1	13:T:204:LYS:HA	2.17	0.44
14:N:144:GLU:HG2	17:N:485:HOH:O	2.17	0.44
10:Q:136:SER:HA	17:Q:194:HOH:O	2.17	0.44
2:W:21:LEU:O	2:W:22:TYR:C	2.54	0.44
2:W:82:THR:O	2:W:85:ALA:HB3	2.17	0.44
3:X:148:LEU:HD23	3:X:160:TRP:O	2.17	0.44
4:Y:119:LEU:HD23	4:Y:119:LEU:O	2.17	0.44
6:1:32:GLU:C	6:1:34:GLY:H	2.20	0.44
4:D:134:VAL:HG22	4:D:135:ALA:N	2.32	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.44
6:F:172:ALA:O	6:F:176:LEU:HD23	2.18	0.44
7:G:55:PRO:HG2	7:G:56:ASP:H	1.82	0.44
8:H:8:PHE:CE2	8:H:12:VAL:N	2.85	0.44
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.51	0.44
10:Q:74:LEU:HD22	10:Q:78:ALA:CB	2.48	0.44
7:2:194:ILE:HD13	7:2:210:LEU:HD12	1.99	0.44
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.98	0.44
2:B:197:LEU:HA	2:B:200:THR:OG1	2.17	0.44
3:C:180(D):GLU:N	3:C:182:PRO:HD3	2.31	0.44
5:E:74:MET:HE1	5:E:109:VAL:HA	1.98	0.44
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.32	0.44
8:H:157:ASP:O	8:H:160:GLN:HB2	2.17	0.44
8:O:206:PHE:CE1	9:P:157:GLN:HG3	2.53	0.44
10:Q:10:ASP:O	10:Q:11:SER:HB3	2.18	0.44
11:R:49:ALA:HB1	12:S:118:SER:OG	2.17	0.44
11:R:85:ASN:ND2	17:R:2153:HOH:O	2.49	0.44
13:T:186:PHE:CE1	13:T:188:LYS:HG3	2.52	0.44
3:X:39:GLY:HA2	3:X:47:VAL:O	2.17	0.44
3:X:69:LYS:HA	3:X:75:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:215:VAL:O	3:X:215:VAL:HG22	2.16	0.44
3:C:89:ILE:HG22	3:C:93:ARG:HD2	1.99	0.44
4:D:216:THR:O	4:D:217:LYS:C	2.56	0.44
6:F:158:TRP:HB2	6:F:160:TYR:CE1	2.52	0.44
10:J:105:ASP:O	10:J:105(B):LYS:N	2.51	0.44
8:O:52:THR:O	8:O:56:THR:HB	2.17	0.44
10:Q:8:VAL:HG23	10:Q:9:GLN:N	2.32	0.44
10:Q:43:MET:HG3	10:Q:101:ILE:HG13	1.99	0.44
10:Q:85:GLN:HE21	2:W:101:LYS:NZ	2.16	0.44
1:V:141:HIS:CG	1:V:142:ASP:N	2.86	0.44
3:X:168:ASN:O	3:X:172:VAL:HG12	2.17	0.44
3:X:219:SER:N	17:X:2958:HOH:O	2.50	0.44
4:Y:159:ARG:HB3	5:Z:60:SER:HB3	1.99	0.44
2:B:67:LEU:HD12	2:B:77:ALA:HA	1.99	0.44
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.76	0.44
7:G:8:TYR:C	7:G:10:ARG:H	2.21	0.44
7:G:86:ARG:O	7:G:89:ALA:HB3	2.17	0.44
11:K:206:PHE:CE1	10:Q:139:ASP:HB3	2.53	0.44
8:O:48:THR:HG22	17:O:2636:HOH:O	2.18	0.44
8:O:124:TYR:HD2	8:O:138:LEU:HB3	1.82	0.44
13:T:157:ASN:O	13:T:158:ALA:C	2.56	0.44
7:2:184(G):GLU:HG2	7:2:188:LYS:CB	2.47	0.44
3:C:135:SER:OG	3:C:152:GLU:HA	2.17	0.44
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.47	0.44
7:G:194:ILE:HG23	7:G:210:LEU:HD11	2.00	0.44
10:J:74:LEU:HD22	10:J:78:ALA:CB	2.47	0.44
10:J:75:SER:HB2	17:J:835:HOH:O	2.18	0.44
10:J:112:GLN:NE2	10:J:126:ALA:H	2.15	0.44
10:J:136:SER:HA	17:J:2114:HOH:O	2.18	0.44
9:P:137:MET:HE3	9:P:141:LEU:HD11	2.00	0.44
3:X:62(A):ILE:H	3:X:62(A):ILE:HG12	1.64	0.44
3:X:110:GLU:O	3:X:113:THR:HB	2.17	0.44
5:Z:21:LEU:HD23	5:Z:21:LEU:HA	1.82	0.44
6:1:151:LEU:HD13	6:1:157:TYR:HB3	1.99	0.44
6:1:232:ALA:O	6:1:233:ILE:C	2.55	0.44
5:E:73:HIS:CE1	5:E:107:LEU:O	2.68	0.44
5:E:151:PHE:HA	5:E:157:VAL:HG22	2.00	0.44
11:K:1:THR:O	11:K:128:GLY:HA3	2.17	0.44
12:L:2:THR:HG21	12:L:130:ALA:HB3	2.00	0.44
12:L:17:ASP:HA	12:L:172:GLY:O	2.17	0.44
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:LYS:O	14:N:107:LYS:HD3	2.17	0.44
14:U:59:VAL:O	14:U:60:GLN:C	2.56	0.44
14:U:177:VAL:HG23	14:U:185:GLU:HB3	2.00	0.44
1:V:124:THR:HG22	1:V:124:THR:O	2.18	0.44
2:W:172:ALA:HB2	2:W:200:THR:HG21	1.99	0.44
1:A:71:THR:O	1:A:73:ASP:N	2.51	0.44
2:B:71:ASN:HD22	2:B:72:ASP:N	2.13	0.44
2:B:112:LEU:HD23	2:B:112:LEU:C	2.38	0.44
6:F:69:VAL:HG12	17:F:563:HOH:O	2.16	0.44
10:J:35:ARG:NH2	17:J:774:HOH:O	2.51	0.44
11:K:137:VAL:HG21	11:K:161:ALA:HB2	2.00	0.44
13:M:1:THR:OG1	13:M:2:SER:N	2.51	0.44
11:R:63:CYS:SG	11:R:74:ILE:HD13	2.58	0.44
2:B:82:THR:O	2:B:85:ALA:HB3	2.18	0.44
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.53	0.44
14:N:157:HIS:O	14:N:158:SER:C	2.55	0.44
11:R:36:GLU:HG2	11:R:184:TRP:CZ2	2.53	0.44
14:U:6:VAL:CG2	14:U:155:ILE:HD11	2.47	0.44
3:X:33:ARG:HH11	3:X:33:ARG:CB	2.30	0.44
5:Z:180(C):PHE:O	5:Z:180(E):LYS:N	2.51	0.44
7:2:109:CYS:HB2	7:2:140:SER:OG	2.17	0.44
4:D:195:LYS:O	4:D:198:LYS:HB3	2.18	0.43
13:M:35:ILE:CD1	13:M:56:GLU:HG2	2.48	0.43
13:M:141(D):GLU:O	13:M:141(G):ILE:HG13	2.18	0.43
13:T:135:ASN:HB3	13:T:139:ARG:NE	2.33	0.43
1:V:15:PHE:H	2:W:23:GLN:NE2	2.12	0.43
1:V:48:ILE:HG13	1:V:213:ALA:HB3	1.99	0.43
1:V:60:MET:HG3	7:2:159:GLY:O	2.18	0.43
1:V:124:THR:CG2	1:V:124:THR:O	2.65	0.43
5:Z:66:LYS:HA	5:Z:78:LEU:CD2	2.48	0.43
7:2:233:LEU:HD12	7:2:233:LEU:HA	1.80	0.43
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.53	0.43
2:B:10:SER:O	2:B:11:ARG:C	2.56	0.43
3:C:40:VAL:HA	3:C:162:ALA:HA	2.00	0.43
6:F:172:ALA:C	6:F:176:LEU:HD23	2.38	0.43
6:F:175:GLU:HG3	6:F:199:LEU:HD23	2.00	0.43
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.53	0.43
7:G:76:MET:HB2	7:G:138:PHE:CD2	2.53	0.43
8:H:197:ARG:NH2	9:I:139:GLU:O	2.51	0.43
12:L:1:GLY:N	17:L:866:HOH:O	2.51	0.43
12:L:167:ILE:O	8:O:167:LEU:HD22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.00	0.43
12:S:55:LEU:HD13	12:S:95:TYR:CE1	2.53	0.43
13:T:19:LEU:HD23	13:T:168:ARG:O	2.18	0.43
1:V:8:TYR:CE1	7:2:127:ALA:HB1	2.54	0.43
2:W:15:PHE:H	3:X:23:GLN:HE22	1.66	0.43
2:W:202:THR:HG22	2:W:204:SER:N	2.14	0.43
5:Z:148:LEU:HD23	5:Z:162:GLY:HA2	2.00	0.43
1:A:29:THR:O	1:A:32:LYS:HB2	2.18	0.43
6:F:108:PRO:O	6:F:111:ALA:HB3	2.19	0.43
9:I:15:ALA:HB2	9:I:175:VAL:HG22	2.01	0.43
13:M:205:GLY:HA3	13:M:209:GLN:HB3	2.00	0.43
14:N:114:PRO:O	14:N:116:GLY:N	2.50	0.43
9:P:114:ASP:CB	15:9:3:ASN:ND2	2.67	0.43
10:Q:7:ARG:HB2	10:Q:12:VAL:HG22	1.99	0.43
11:R:105(A):ARG:HB3	11:R:105(B):LYS:CE	2.46	0.43
12:S:114:ASP:HB2	12:S:118:SER:CB	2.48	0.43
14:U:173:ILE:HB	14:U:187(B):PHE:HB2	2.00	0.43
5:Z:37:THR:HG23	5:Z:137:LEU:HD12	2.00	0.43
6:1:46:VAL:HG23	6:1:48:PHE:CE1	2.53	0.43
6:1:95:GLU:HG2	6:1:115:ARG:HB3	1.99	0.43
2:B:160:TRP:CE3	2:B:163:ILE:HD13	2.54	0.43
5:E:169:SER:O	5:E:171:GLY:N	2.51	0.43
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.18	0.43
6:F:116:LEU:HA	6:F:116:LEU:HD23	1.69	0.43
6:F:148:LEU:HD23	6:F:160:TYR:O	2.18	0.43
6:F:198:TYR:CE2	6:F:208:PHE:CZ	3.06	0.43
7:G:8:TYR:O	7:G:10:ARG:N	2.51	0.43
7:G:119:LEU:HD12	7:G:119:LEU:HA	1.74	0.43
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.46	0.43
12:L:18:THR:CG2	12:L:30:TYR:HA	2.48	0.43
12:L:144(W):LYS:CG	12:L:145:TYR:N	2.81	0.43
8:O:112:SER:OG	8:O:120:ASP:HB2	2.18	0.43
9:P:99:PRO:HB2	9:P:113:PHE:CD2	2.52	0.43
12:S:184:VAL:O	12:S:184:VAL:HG12	2.18	0.43
13:T:126:ALA:N	17:T:2278:HOH:O	2.46	0.43
14:U:7:THR:HG23	14:U:123:PRO:O	2.17	0.43
4:Y:192:LEU:H	4:Y:192:LEU:HD12	1.83	0.43
6:1:102:LEU:O	6:1:102:LEU:HG	2.17	0.43
6:1:127:ASN:C	6:1:127:ASN:ND2	2.72	0.43
6:1:159:GLY:C	6:1:160:TYR:HD1	2.21	0.43
6:1:176:LEU:CD2	6:1:196:ILE:HD13	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:212:ILE:HG22	6:1:213:SER:H	1.84	0.43
7:2:72:ARG:HB2	7:2:72:ARG:NH1	2.32	0.43
7:2:110:ASP:HB3	7:2:149:TYR:CZ	2.53	0.43
2:B:40:ILE:CD1	2:B:193:ALA:HB2	2.48	0.43
4:D:28:LEU:HD12	4:D:28:LEU:HA	1.76	0.43
5:E:47:VAL:HG12	5:E:48:LEU:H	1.84	0.43
6:F:70:VAL:HB	6:F:74:ILE:HB	2.00	0.43
8:H:56:THR:HG22	8:H:57:GLN:N	2.34	0.43
13:M:51:ASP:OD1	13:M:95:LEU:HA	2.18	0.43
14:N:85:GLU:O	14:N:89:GLU:HB2	2.19	0.43
8:O:75:ARG:CZ	7:2:105:TYR:CD1	3.02	0.43
10:Q:76:PRO:O	10:Q:78:ALA:N	2.52	0.43
10:Q:133:TYR:OH	10:Q:166:MET:CG	2.63	0.43
12:S:90:LYS:HD3	12:S:95:TYR:CZ	2.53	0.43
14:U:4:MET:SD	14:U:159:LEU:HD21	2.59	0.43
14:U:20:THR:OG1	14:U:28:ASN:HB3	2.19	0.43
1:V:88:LEU:HD23	1:V:88:LEU:HA	1.68	0.43
2:W:167:ALA:O	2:W:168:ASN:HB2	2.18	0.43
5:Z:180(D):ILE:O	5:Z:180(D):ILE:HG13	2.18	0.43
7:2:78:VAL:HG11	7:2:85:ALA:HB2	2.00	0.43
5:E:176:LEU:HD22	5:E:180(C):PHE:CE2	2.40	0.43
6:F:236:ALA:C	6:F:238:LYS:H	2.22	0.43
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.34	0.43
13:M:31:VAL:HG12	13:M:33:ARG:HG2	2.00	0.43
9:P:76:PRO:O	9:P:78:THR:N	2.51	0.43
1:V:41:LYS:HA	1:V:46:VAL:HG22	2.01	0.43
1:V:111:LEU:O	1:V:114:SER:HB3	2.18	0.43
3:X:8:TYR:CE2	3:X:128:GLY:HA2	2.53	0.43
4:Y:121:LEU:HD23	4:Y:123:PHE:HE1	1.84	0.43
5:Z:17:PRO:HG3	6:1:26:TYR:CE2	2.53	0.43
5:Z:161:TYR:CZ	6:1:60:VAL:HG13	2.54	0.43
6:1:206(B):GLU:HG3	6:1:206(C):LYS:HG3	2.00	0.43
1:A:82:GLY:O	1:A:85:TYR:HB3	2.18	0.43
2:B:7:ARG:HH11	2:B:7:ARG:HG3	1.83	0.43
7:G:236:ILE:C	7:G:238:GLU:H	2.21	0.43
11:K:26:VAL:O	11:K:26:VAL:HG12	2.17	0.43
11:K:133:PHE:CB	11:K:162:ALA:HA	2.48	0.43
14:N:1:THR:O	14:N:128:GLY:HA3	2.19	0.43
14:N:4:MET:SD	14:N:159:LEU:CD2	3.07	0.43
8:O:43:CYS:SG	8:O:99:LEU:HD22	2.59	0.43
8:O:216:GLU:HG3	9:P:187:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:14:ILE:HG23	9:P:34:ILE:HD13	2.00	0.43
11:R:155:GLY:O	11:R:158:SER:N	2.52	0.43
12:S:8:GLY:HA2	12:S:145:TYR:CE1	2.53	0.43
14:U:107:LYS:HG2	14:U:108:GLY:N	2.33	0.43
1:V:130:ARG:HH21	7:2:124:THR:CG2	2.30	0.43
6:1:119:TYR:O	6:1:122:ALA:HB3	2.18	0.43
2:B:136:PHE:O	2:B:150:THR:HA	2.19	0.43
2:B:205:LEU:HD12	2:B:205:LEU:HA	1.82	0.43
17:C:3453:HOH:O	4:D:86:ARG:HB3	2.19	0.43
4:D:97:VAL:HG21	11:K:65:LEU:HD11	2.00	0.43
5:E:12:THR:HG23	5:E:23:GLN:HB2	2.01	0.43
5:E:22:PHE:HD1	5:E:26:TYR:CE1	2.35	0.43
5:E:38:VAL:HG22	5:E:164:ALA:CB	2.48	0.43
6:F:11:SER:HA	17:F:379:HOH:O	2.18	0.43
6:F:137:ILE:HD11	6:F:165:THR:HG22	2.00	0.43
7:G:15:PHE:CD1	7:G:21:LEU:HD21	2.53	0.43
7:G:45:CYS:O	7:G:146:PRO:HB3	2.19	0.43
9:I:151:LEU:O	9:I:151:LEU:HG	2.19	0.43
10:J:22:ARG:HD3	10:J:22:ARG:HA	1.85	0.43
11:K:4:LEU:HD13	11:K:15:ALA:O	2.19	0.43
11:K:172:SER:HA	11:K:192:VAL:HG23	2.00	0.43
9:P:53:THR:O	9:P:57:GLU:HG3	2.18	0.43
9:P:165:ARG:HA	9:P:165:ARG:HD3	1.85	0.43
14:U:15:GLY:HA2	14:U:174:ARG:O	2.19	0.43
1:V:52:LYS:NZ	1:V:61:SER:HB2	2.33	0.43
7:2:194:ILE:O	7:2:195:THR:C	2.57	0.43
4:D:24:VAL:O	4:D:27:SER:HB3	2.19	0.43
5:E:21:LEU:HA	5:E:21:LEU:HD23	1.81	0.43
10:J:52:THR:HG22	10:J:53:VAL:H	1.83	0.43
8:O:111:PHE:CD1	8:O:121:VAL:HB	2.54	0.43
9:P:19:ARG:HD3	9:P:168:LEU:O	2.18	0.43
10:Q:76:PRO:HD2	17:Q:2835:HOH:O	2.19	0.43
10:Q:85:GLN:NE2	2:W:101:LYS:HZ1	2.17	0.43
11:R:38:ASN:C	11:R:38:ASN:OD1	2.57	0.43
11:R:159:ILE:O	11:R:160:LEU:C	2.58	0.43
12:S:59:PHE:O	12:S:60:LYS:C	2.57	0.43
14:U:134:ILE:HD12	14:U:138:CYS:SG	2.59	0.43
1:V:66:LYS:HG2	1:V:78:TYR:CE1	2.54	0.43
2:W:141:TYR:CD1	2:W:219(E):VAL:HG21	2.54	0.43
6:1:195:LYS:O	6:1:198:TYR:N	2.51	0.43
2:B:175:LEU:O	2:B:178:MET:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:LEU:HA	5:E:162:GLY:HA2	1.99	0.43
6:F:214:TRP:N	6:F:214:TRP:CD1	2.85	0.43
7:G:222:PHE:CD2	7:G:222:PHE:N	2.86	0.43
11:K:35:ILE:HD11	11:K:45:MET:SD	2.58	0.43
11:K:197:TRP:CE2	9:P:190:LYS:HE3	2.54	0.43
8:O:1:THR:HG23	8:O:33:LYS:NZ	2.33	0.43
11:R:196:PHE:HZ	11:R:209:VAL:HG21	1.84	0.43
13:T:135:ASN:HB2	13:T:136:PRO:HD3	2.00	0.43
14:U:67:THR:O	14:U:68:SER:C	2.57	0.43
14:U:155:ILE:HG22	14:U:175:MET:HE2	2.01	0.43
3:X:163:GLN:HE21	3:X:163:GLN:HA	1.84	0.43
5:Z:15:PHE:HE1	5:Z:21:LEU:HG	1.84	0.43
5:Z:21:LEU:HA	17:Z:2539:HOH:O	2.19	0.43
1:A:17:PRO:HG3	2:B:26:TYR:CE2	2.54	0.42
5:E:44:THR:CG2	5:E:183:ASP:HB3	2.49	0.42
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.42
9:I:43:LEU:HD21	9:I:45:ILE:HD11	2.00	0.42
10:J:105:ASP:OD1	10:J:105(C):LYS:HB2	2.19	0.42
11:K:38:ASN:OD1	11:K:38:ASN:C	2.57	0.42
8:O:19:ARG:NH1	8:O:167:LEU:O	2.52	0.42
12:S:93:PHE:N	12:S:94:PRO:HD3	2.33	0.42
1:V:67:VAL:HG11	1:V:213:ALA:HB2	2.01	0.42
5:Z:68:ILE:HB	5:Z:76:LEU:CD2	2.48	0.42
6:1:77:VAL:O	6:1:136:THR:HG23	2.19	0.42
7:2:46:THR:OG1	7:2:146:PRO:HB3	2.18	0.42
7:2:87:ASN:C	7:2:87:ASN:HD22	2.22	0.42
7:2:184(G):GLU:HG2	7:2:188:LYS:HB2	2.01	0.42
4:D:97:VAL:CB	11:K:65:LEU:HD11	2.49	0.42
6:F:157:TYR:CZ	7:G:86:ARG:NH1	2.87	0.42
11:K:209:VAL:HA	17:K:2742:HOH:O	2.19	0.42
12:L:35:PHE:HZ	17:L:458:HOH:O	2.02	0.42
8:O:95:ILE:O	8:O:97:ALA:N	2.47	0.42
14:U:5:ALA:O	14:U:124:TYR:HB2	2.19	0.42
3:X:97:GLN:C	3:X:99:HIS:N	2.72	0.42
6:1:32:GLU:O	6:1:167:LYS:HG3	2.19	0.42
6:1:68:GLN:NE2	6:1:86:ARG:NH1	2.67	0.42
4:D:224:TYR:N	4:D:224:TYR:HD2	2.17	0.42
4:D:237:LEU:HD23	4:D:237:LEU:HA	1.87	0.42
6:F:69:VAL:HG22	6:F:70:VAL:N	2.35	0.42
9:I:53:THR:HG22	10:J:84:ARG:NH2	2.34	0.42
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:4:LEU:CD1	12:S:138:LEU:HD21	2.49	0.42
12:S:4:LEU:HA	12:S:126:ALA:HA	2.01	0.42
13:T:7:LYS:HD2	13:T:141(G):ILE:HD13	2.01	0.42
14:U:1:THR:O	14:U:128:GLY:HA3	2.20	0.42
1:V:21:LEU:HA	1:V:21:LEU:HD23	1.83	0.42
1:V:71:THR:C	1:V:73:ASP:H	2.22	0.42
1:V:86:ARG:HH21	7:2:118:ASN:ND2	2.16	0.42
2:W:64:THR:HG22	2:W:68:TYR:CE1	2.54	0.42
2:W:209:ARG:HG2	2:W:209:ARG:HH11	1.84	0.42
6:1:157:TYR:CD1	6:1:157:TYR:C	2.92	0.42
2:B:137:ILE:HD11	2:B:165:VAL:HG22	2.00	0.42
6:F:210:LEU:HA	6:F:210:LEU:HD12	1.84	0.42
8:H:132:LEU:CD1	14:N:25:TYR:CE1	3.02	0.42
10:J:52:THR:HG22	10:J:53:VAL:N	2.34	0.42
8:O:110:LEU:HD23	8:O:122:GLY:O	2.19	0.42
12:S:61:ASN:ND2	5:Z:101:LEU:HD21	2.35	0.42
13:T:49:ILE:O	13:T:52:MET:N	2.52	0.42
1:V:15:PHE:CE1	1:V:21:LEU:HD21	2.54	0.42
1:V:214:ILE:O	1:V:215:ILE:HD13	2.19	0.42
2:W:163:ILE:HD12	2:W:173:GLN:NE2	2.34	0.42
3:X:77:SER:OG	3:X:137:LEU:HB2	2.19	0.42
5:Z:38:VAL:HG13	5:Z:163:THR:O	2.19	0.42
5:Z:198:SER:HA	5:Z:201:LEU:CD1	2.49	0.42
6:1:7:GLY:O	6:1:9:ASP:N	2.53	0.42
6:1:12:ASN:OD1	6:1:12:ASN:C	2.58	0.42
6:1:223:PHE:N	6:1:223:PHE:CD1	2.85	0.42
2:B:172:ALA:HB2	2:B:200:THR:HG21	2.01	0.42
4:D:89:ILE:O	4:D:92:ALA:HB3	2.20	0.42
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.02	0.42
12:L:163:THR:HG23	12:L:170:GLY:HA2	2.01	0.42
13:T:13:ILE:CG2	13:T:175:LEU:HD21	2.48	0.42
13:T:62:LEU:HA	13:T:62:LEU:HD23	1.76	0.42
14:U:161:GLN:O	14:U:164:LYS:N	2.51	0.42
1:V:58:LEU:HD23	1:V:58:LEU:HA	1.77	0.42
2:W:7:ARG:HH11	2:W:7:ARG:HG3	1.85	0.42
5:Z:66:LYS:O	5:Z:77:SER:HA	2.20	0.42
5:Z:76:LEU:HD23	5:Z:76:LEU:C	2.40	0.42
6:1:194:ALA:O	6:1:198:TYR:HD1	2.03	0.42
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.02	0.42
14:N:29:ARG:HD2	13:T:197:TRP:CH2	2.54	0.42
8:O:12:VAL:HG22	8:O:13:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:105(B):LYS:N	11:R:105(B):LYS:CD	2.80	0.42
14:U:42:TRP:N	14:U:42:TRP:CD1	2.85	0.42
3:X:25:GLU:O	3:X:28:LEU:HB2	2.20	0.42
4:Y:70:ILE:HB	4:Y:74:ILE:CG2	2.44	0.42
7:2:9:ASP:HA	7:2:14:ILE:HD11	2.00	0.42
7:2:41:ARG:NH2	7:2:180(B):ASP:O	2.51	0.42
1:A:197:LEU:O	1:A:202:VAL:HG23	2.20	0.42
4:D:211:GLN:HA	17:D:916:HOH:O	2.19	0.42
5:E:107:LEU:HD12	17:E:389:HOH:O	2.19	0.42
6:F:82:ILE:O	6:F:83:PRO:C	2.58	0.42
7:G:179(D):SER:O	7:G:179(E):LYS:HB2	2.19	0.42
8:H:160:GLN:O	8:H:164:TRP:CD1	2.73	0.42
10:J:53:VAL:O	10:J:54:GLN:C	2.58	0.42
12:L:58:ARG:NH2	17:L:3067:HOH:O	2.53	0.42
8:O:55:VAL:HG23	8:O:86:HIS:CD2	2.53	0.42
8:O:84:LYS:HE2	8:O:119:THR:HG23	2.02	0.42
11:R:4:LEU:HD11	11:R:15:ALA:HB3	2.02	0.42
1:V:15:PHE:HB2	2:W:23:GLN:NE2	2.35	0.42
3:X:63:THR:HG23	3:X:64:PRO:HD2	2.02	0.42
3:X:182:PRO:HA	3:X:183:PRO:HD3	1.97	0.42
7:2:25:GLU:O	7:2:28:PHE:HB2	2.20	0.42
1:A:221:PHE:CD2	1:A:221:PHE:C	2.93	0.42
3:C:15:PHE:CE2	4:D:27:SER:HB2	2.55	0.42
3:C:70:ILE:HG21	3:C:112:LEU:HD21	2.00	0.42
4:D:180(C):HIS:O	4:D:184:LEU:HD12	2.20	0.42
4:D:243:ALA:O	4:D:244:GLU:HG2	2.20	0.42
6:F:135:SER:HA	17:F:408:HOH:O	2.20	0.42
12:L:43:MET:HB2	12:L:101:ILE:CG2	2.44	0.42
8:O:47:GLY:O	15:9:5:AKK:ND	2.52	0.42
9:P:12:VAL:HG13	9:P:108:PRO:HB3	2.01	0.42
13:T:128:GLY:HA3	17:T:2312:HOH:O	2.18	0.42
13:T:171:ARG:CG	13:T:192:VAL:HG23	2.38	0.42
14:U:78:THR:O	14:U:79:ALA:C	2.58	0.42
1:V:46:VAL:HG12	1:V:47:VAL:N	2.34	0.42
2:W:20:ARG:HE	3:X:33:ARG:HH21	1.67	0.42
2:W:107:ILE:HG13	2:W:108:PRO:HD2	2.02	0.42
3:X:81:LEU:HD23	3:X:81:LEU:HA	1.86	0.42
3:X:97:GLN:O	3:X:99:HIS:N	2.53	0.42
3:X:212:ILE:CG2	3:X:213:THR:N	2.83	0.42
5:Z:92:LEU:HD11	5:Z:112:ALA:HB1	2.01	0.42
6:1:67:ILE:HG22	6:1:68:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:108:PRO:O	6:1:111:ALA:HB3	2.19	0.42
3:C:197:LEU:O	3:C:201:VAL:HG23	2.20	0.42
6:F:113:ALA:O	6:F:116:LEU:N	2.52	0.42
8:O:90:TYR:O	8:O:93:GLY:N	2.53	0.42
12:S:144(W):LYS:CG	12:S:145:TYR:N	2.83	0.42
14:U:63:LEU:O	14:U:66:TYR:HB3	2.20	0.42
14:U:111:TYR:HA	14:U:120:HIS:O	2.20	0.42
2:W:66:LYS:HB2	2:W:211:GLU:OE1	2.20	0.42
4:Y:138:ILE:O	4:Y:148:LEU:HD12	2.20	0.42
7:2:16:SER:O	7:2:18:GLU:N	2.53	0.42
7:G:74:ILE:HG21	7:G:112:LEU:HD23	2.02	0.42
7:G:212:VAL:CG1	7:G:213:GLY:N	2.82	0.42
8:H:152:ILE:HG21	8:H:191:TYR:HE1	1.84	0.42
8:H:167:LEU:HB3	12:S:167:ILE:HB	2.02	0.42
11:K:151:ALA:O	11:K:152:LEU:C	2.58	0.42
14:N:187(C):TYR:CE1	13:T:198:ASP:HA	2.55	0.42
8:O:19:ARG:HG2	8:O:21:THR:HG23	2.02	0.42
8:O:34:LEU:HD12	8:O:34:LEU:HA	1.78	0.42
1:V:35:VAL:HG12	1:V:36:THR:N	2.35	0.42
5:Z:180(C):PHE:C	5:Z:180(E):LYS:N	2.72	0.42
6:1:7:GLY:C	6:1:9:ASP:H	2.22	0.42
1:A:69:LEU:O	1:A:93:ARG:NH2	2.51	0.41
3:C:62(A):ILE:H	3:C:62(A):ILE:HG12	1.71	0.41
7:G:27:ALA:O	7:G:30:ALA:N	2.51	0.41
10:J:119:LYS:HG2	10:J:120:VAL:N	2.35	0.41
13:M:-4:ILE:HG22	13:M:-3:VAL:N	2.34	0.41
13:M:135:ASN:HB2	13:M:136:PRO:HD3	2.02	0.41
14:N:52:THR:O	14:N:53:GLN:C	2.58	0.41
10:Q:166:MET:HA	10:Q:167:PRO:HD3	1.88	0.41
11:R:41:LEU:HD23	11:R:41:LEU:HA	1.75	0.41
1:V:72:PRO:HB3	17:V:1013:HOH:O	2.20	0.41
1:V:221:PHE:O	1:V:221:PHE:HD2	2.01	0.41
3:X:33:ARG:O	3:X:33:ARG:HG2	2.19	0.41
3:X:49:GLY:C	3:X:50:CYS:SG	2.98	0.41
3:X:52:ARG:HD2	3:X:208:LYS:O	2.20	0.41
3:X:163:GLN:CG	3:X:164:THR:N	2.82	0.41
5:Z:139:ILE:HG22	5:Z:148:LEU:HD13	2.02	0.41
6:1:53:LEU:HD23	6:1:53:LEU:HA	1.77	0.41
1:A:176:LEU:O	1:A:178:LYS:N	2.53	0.41
1:A:210:ILE:HG22	1:A:211:GLU:N	2.35	0.41
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13:ALA:CB	9:I:151:LEU:HD21	2.51	0.41
9:I:152:PHE:O	9:I:155:ILE:HG22	2.20	0.41
12:L:107:LYS:HA	12:L:107:LYS:HD3	1.86	0.41
13:M:157:ASN:O	13:M:160:ARG:N	2.53	0.41
8:O:91:GLN:HA	8:O:91:GLN:NE2	2.35	0.41
10:Q:143:ARG:O	10:Q:146:MET:HG3	2.20	0.41
11:R:52:CYS:SG	11:R:97:MET:CB	3.08	0.41
12:S:156:ARG:HD2	12:S:189:TYR:CE1	2.55	0.41
1:V:26:TYR:O	1:V:29:THR:HB	2.20	0.41
1:V:65:SER:HA	1:V:211:GLU:OE1	2.19	0.41
1:V:118:LYS:O	1:V:122:GLU:HG3	2.20	0.41
3:X:201:VAL:O	3:X:202:GLN:HB2	2.19	0.41
6:1:51:GLU:OE1	6:1:53:LEU:HD21	2.20	0.41
6:1:208:PHE:H	6:1:208:PHE:HD2	1.67	0.41
7:G:120:SER:O	7:G:121:GLN:C	2.57	0.41
10:J:38:SER:OG	10:J:41:THR:HB	2.20	0.41
10:J:43:MET:HG3	10:J:101:ILE:HG13	2.02	0.41
10:J:133:TYR:C	17:J:441:HOH:O	2.58	0.41
11:K:133:PHE:HB2	11:K:162:ALA:HA	2.02	0.41
11:K:142:TYR:C	11:K:143:LYS:HD2	2.39	0.41
8:O:35:HIS:CB	8:O:56:THR:HG21	2.50	0.41
1:V:86:ARG:HE	7:2:118:ASN:HD21	1.69	0.41
4:Y:15:PHE:CE1	4:Y:21:LEU:HG	2.54	0.41
5:Z:215:VAL:HG23	5:Z:221:PHE:N	2.35	0.41
6:1:116:LEU:HD23	6:1:116:LEU:HA	1.81	0.41
7:2:225:SER:O	7:2:226:ALA:C	2.58	0.41
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.02	0.41
1:A:171:ALA:O	1:A:174:THR:HB	2.21	0.41
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.01	0.41
5:E:76:LEU:HD23	5:E:76:LEU:C	2.40	0.41
6:F:113:ALA:O	6:F:114:ASP:C	2.55	0.41
9:I:12:VAL:HG23	9:I:178:ILE:HD12	2.02	0.41
9:I:55:LEU:HD21	9:I:95:TYR:CE1	2.56	0.41
10:J:44:SER:HG	10:J:100:LEU:HB2	1.84	0.41
10:J:73:GLU:HG2	17:J:870:HOH:O	2.19	0.41
13:T:134:ALA:O	13:T:135:ASN:C	2.58	0.41
1:V:85:TYR:O	1:V:89:VAL:HG23	2.21	0.41
3:X:172:VAL:O	3:X:175:PHE:HB3	2.20	0.41
7:2:49:ILE:HG22	7:2:50:SER:N	2.35	0.41
7:2:160:TYR:HB3	7:2:162:ALA:O	2.20	0.41
7:2:179:HIS:ND1	7:2:179:HIS:C	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:ASN:O	5:E:93:ARG:N	2.53	0.41
9:I:13:ALA:HB2	9:I:151:LEU:HD21	2.02	0.41
9:I:131:SER:HB2	17:I:3153:HOH:O	2.20	0.41
9:I:133:GLN:HB3	9:I:162:ALA:HB1	2.02	0.41
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.49	0.41
10:Q:112:GLN:NE2	10:Q:126:ALA:N	2.68	0.41
12:S:177:ILE:N	12:S:177:ILE:CD1	2.84	0.41
13:T:149:GLN:NE2	13:T:149:GLN:H	2.18	0.41
14:U:38:HIS:NE2	14:U:74:PRO:HD2	2.35	0.41
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.74	0.41
7:G:194:ILE:O	7:G:198:ILE:HG13	2.20	0.41
9:I:29:ASN:HB3	9:I:171:TRP:CE3	2.56	0.41
11:K:138:LEU:HA	11:K:138:LEU:HD12	1.89	0.41
12:L:113:PHE:CD1	12:L:113:PHE:N	2.89	0.41
13:M:49:ILE:O	13:M:50:SER:C	2.57	0.41
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.86	0.41
8:O:175:VAL:HG21	8:O:191:TYR:CD1	2.46	0.41
12:S:59:PHE:O	12:S:62:SER:N	2.53	0.41
5:Z:176:LEU:C	5:Z:178:ARG:N	2.73	0.41
7:G:9:ASP:HA	7:G:14:ILE:HD11	2.02	0.41
11:K:85:ASN:HD22	11:K:85:ASN:HA	1.74	0.41
12:L:63:VAL:HG22	12:L:74:LEU:HD23	2.02	0.41
12:L:100:ILE:HG22	12:L:101:ILE:N	2.36	0.41
12:S:20:ASN:OD1	12:S:27:ASN:HB2	2.21	0.41
14:U:133:PHE:HE2	14:U:166:ASP:HB2	1.83	0.41
14:U:163:ILE:CG2	14:U:170:GLY:HA2	2.44	0.41
1:V:15:PHE:O	2:W:26:TYR:HD2	2.04	0.41
2:W:176:LEU:C	2:W:178:MET:H	2.24	0.41
3:X:183:PRO:HB3	3:X:189:CYS:HA	2.03	0.41
5:Z:48:LEU:O	5:Z:212:ILE:HG23	2.20	0.41
7:2:132:LEU:O	7:2:153:PRO:HG3	2.20	0.41
7:2:165:THR:HG22	7:2:166:GLY:N	2.36	0.41
1:A:124:THR:CG2	1:A:124:THR:O	2.69	0.41
3:C:185:THR:CB	3:C:188:GLU:HG2	2.34	0.41
6:F:26:TYR:N	6:F:26:TYR:CD1	2.87	0.41
7:G:35:ILE:HG23	7:G:51:GLN:HB2	2.03	0.41
13:M:149:GLN:H	13:M:149:GLN:CD	2.23	0.41
8:O:6:VAL:O	8:O:13:VAL:HG12	2.21	0.41
8:O:105:ASP:O	8:O:106:THR:N	2.53	0.41
8:O:132:LEU:N	8:O:132:LEU:CD1	2.84	0.41
8:O:197:ARG:NH1	8:O:200:LYS:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:68:TYR:OH	6:1:71:ASP:N	2.50	0.41
13:T:169:SER:HB2	17:T:2472:HOH:O	2.20	0.41
1:V:161:LYS:HD3	1:V:180:TRP:CH2	2.55	0.41
3:X:58:LEU:HG	3:X:58:LEU:O	2.20	0.41
5:Z:121:GLN:NE2	6:1:87:HIS:ND1	2.69	0.41
5:Z:138:ILE:O	5:Z:148:LEU:HA	2.21	0.41
7:2:59:LEU:O	7:2:61:PRO:CD	2.64	0.41
7:2:120:SER:HA	7:2:123:TYR:CD2	2.56	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
1:A:147(A):SER:HB2	1:A:149:TYR:CE2	2.56	0.41
2:B:15:PHE:N	3:C:23:GLN:HE22	2.18	0.41
2:B:64:THR:HG23	2:B:67:LEU:O	2.20	0.41
2:B:175:LEU:HD23	2:B:175:LEU:HA	1.88	0.41
2:B:176:LEU:C	2:B:178:MET:H	2.23	0.41
2:B:207:TYR:CG	2:B:208:ASP:N	2.89	0.41
5:E:220:PRO:O	5:E:221:PHE:C	2.59	0.41
6:F:35:THR:HG22	6:F:36:THR:N	2.34	0.41
6:F:147:HIS:HB3	6:F:149:TYR:HE2	1.86	0.41
6:F:160:TYR:HB3	6:F:162:GLY:O	2.21	0.41
8:H:49:ALA:CB	9:I:118:CYS:SG	3.09	0.41
8:H:133:ALA:O	8:H:136:ALA:HB3	2.21	0.41
10:J:43:MET:HG3	10:J:101:ILE:CG1	2.50	0.41
10:J:137:LEU:HA	10:J:137:LEU:HD23	1.84	0.41
10:J:157:LEU:HD12	10:J:157:LEU:HA	1.80	0.41
11:K:58:TRP:O	11:K:59:LEU:C	2.59	0.41
11:K:165:ARG:NH1	9:P:26:GLY:O	2.53	0.41
12:L:148:VAL:HG13	12:L:149:GLU:N	2.36	0.41
13:M:150:VAL:HG21	17:M:869:HOH:O	2.21	0.41
14:N:6:VAL:CG2	14:N:155:ILE:HD11	2.46	0.41
14:N:174:ARG:HD2	17:N:564:HOH:O	2.21	0.41
8:O:21:THR:HG22	8:O:26:VAL:HA	2.03	0.41
8:O:221:ILE:N	8:O:221:ILE:CD1	2.84	0.41
9:P:5:ALA:HB2	9:P:14:ILE:HG13	2.03	0.41
10:Q:3:ILE:HD13	10:Q:3:ILE:HA	1.85	0.41
11:R:40:PHE:HB2	17:R:2501:HOH:O	2.20	0.41
11:R:52:CYS:SG	11:R:97:MET:HB2	2.60	0.41
12:S:29:ARG:HB2	17:S:2276:HOH:O	2.21	0.41
12:S:113:PHE:CD2	12:S:119:TYR:HB3	2.56	0.41
14:U:107:LYS:HG2	14:U:108:GLY:H	1.86	0.41
1:V:50:THR:HG21	1:V:66:LYS:HE2	2.03	0.41
1:V:100:TYR:CE1	1:V:107:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:15:PHE:CB	3:X:23:GLN:HE22	2.31	0.41
3:X:96:ALA:O	3:X:100:ARG:HG3	2.21	0.41
4:Y:45:GLY:HA2	4:Y:146:TYR:CD1	2.56	0.41
4:Y:47:VAL:HG12	4:Y:48:LEU:N	2.36	0.41
4:Y:147:GLN:HA	17:Y:1042:HOH:O	2.21	0.41
4:Y:215:ILE:HG22	4:Y:221:PHE:HD2	1.84	0.41
5:Z:35:SER:OG	5:Z:36:VAL:N	2.54	0.41
5:Z:44:THR:O	5:Z:45:HIS:ND1	2.53	0.41
5:Z:73:HIS:CE1	5:Z:107:LEU:O	2.72	0.41
5:Z:176:LEU:HD22	5:Z:180(C):PHE:HE2	1.86	0.41
7:2:12:ILE:HA	17:2:2538:HOH:O	2.20	0.41
1:A:109:THR:O	1:A:113:VAL:HG23	2.21	0.41
2:B:70:LEU:CD2	2:B:89:ILE:HG23	2.50	0.41
3:C:183:PRO:HB3	3:C:189:CYS:HA	2.02	0.41
4:D:121:LEU:HD23	4:D:123:PHE:HE1	1.85	0.41
11:K:139:ASP:OD2	10:Q:164:LYS:HD3	2.21	0.41
13:M:165:ARG:HD2	13:M:165:ARG:N	2.36	0.41
8:O:163:ILE:HG22	8:O:164:TRP:CE3	2.55	0.41
11:R:41:LEU:HD21	11:R:76:VAL:HG22	2.02	0.41
12:S:4:LEU:CD1	12:S:126:ALA:HB2	2.48	0.41
5:Z:160:LEU:CD2	6:1:59:LEU:HD12	2.51	0.41
5:Z:161:TYR:CE2	6:1:61:PRO:HD3	2.56	0.41
7:2:158:VAL:HG22	7:2:159:GLY:N	2.36	0.41
1:A:60:MET:HG3	7:G:159:GLY:O	2.21	0.40
1:A:149:TYR:CE1	1:A:159:PRO:HB3	2.57	0.40
3:C:212:ILE:CG2	3:C:213:THR:N	2.84	0.40
5:E:28:LEU:HA	5:E:31:ILE:HD12	2.03	0.40
5:E:180(C):PHE:C	5:E:180(E):LYS:N	2.74	0.40
6:F:50:VAL:CG2	6:F:51:GLU:N	2.84	0.40
6:F:192:GLN:O	6:F:195:LYS:HB3	2.21	0.40
10:J:63:ILE:HD13	10:J:63:ILE:HA	1.91	0.40
11:K:99:THR:HA	17:K:444:HOH:O	2.21	0.40
13:M:83:LEU:HA	13:M:83:LEU:HD23	1.87	0.40
10:Q:52:THR:CG2	10:Q:53:VAL:N	2.84	0.40
10:Q:105:ASP:O	10:Q:105(B):LYS:N	2.53	0.40
1:V:55:SER:HB2	17:2:1268:HOH:O	2.21	0.40
3:X:57:LYS:HG3	3:X:208:LYS:HZ1	1.86	0.40
4:Y:243:ALA:O	4:Y:244:GLU:HG2	2.20	0.40
5:Z:4:PHE:O	5:Z:7:ASN:HB2	2.21	0.40
2:B:116:LEU:HA	2:B:116:LEU:HD23	1.84	0.40
3:C:77:SER:OG	3:C:137:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:GLN:HG2	3:C:151:THR:N	2.36	0.40
17:E:864:HOH:O	12:L:67:HIS:HD2	2.03	0.40
6:F:17:PRO:HA	7:G:26:TYR:CD2	2.57	0.40
7:G:130:ARG:HG3	7:G:130:ARG:HH11	1.86	0.40
7:G:214:VAL:HG12	7:G:215:ALA:H	1.87	0.40
8:H:13:VAL:CG2	8:H:14:ILE:N	2.85	0.40
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.04	0.40
12:L:18:THR:HG22	12:L:31:GLU:N	2.36	0.40
13:M:12:VAL:HG21	13:M:102:ALA:HB1	2.03	0.40
13:M:82:TYR:O	13:M:85:THR:HB	2.21	0.40
8:O:3:ILE:O	8:O:126:SER:HA	2.22	0.40
8:O:114:HIS:HD2	17:O:2814:HOH:O	2.03	0.40
9:P:53:THR:CG2	10:Q:84:ARG:CZ	2.99	0.40
10:Q:120:VAL:HG13	10:Q:122:LEU:HG	2.02	0.40
10:Q:157:LEU:HD12	10:Q:157:LEU:HA	1.87	0.40
13:T:78:TYR:CD1	5:Z:105:ARG:HB2	2.55	0.40
1:V:79:SER:HB2	1:V:165:ILE:HD12	2.02	0.40
5:Z:15:PHE:HD1	5:Z:15:PHE:HA	1.75	0.40
5:Z:82:ALA:O	5:Z:83:PRO:C	2.60	0.40
5:Z:194:VAL:O	5:Z:195:GLU:C	2.60	0.40
6:1:198:TYR:CE2	6:1:208:PHE:CZ	3.06	0.40
2:B:225:LYS:O	2:B:228:GLU:HB2	2.20	0.40
17:C:2999:HOH:O	4:D:86:ARG:HG3	2.21	0.40
4:D:91:HIS:CD2	4:D:91:HIS:O	2.74	0.40
7:G:225:SER:O	7:G:226:ALA:C	2.59	0.40
9:I:19:ARG:NH1	17:I:211:HOH:O	2.55	0.40
12:L:167:ILE:HA	17:L:2973:HOH:O	2.21	0.40
13:M:70(A):ALA:O	13:M:71(D):ALA:HB2	2.21	0.40
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.22	0.40
10:Q:38:SER:O	10:Q:40:HIS:N	2.54	0.40
10:Q:59:ILE:HG23	10:Q:59:ILE:HD12	1.86	0.40
12:S:18:THR:HG22	12:S:18:THR:O	2.21	0.40
13:T:55:ILE:O	13:T:55:ILE:HG22	2.22	0.40
13:T:122:SER:N	13:T:125:LEU:HD21	2.36	0.40
14:U:175:MET:CE	14:U:187(B):PHE:HE2	2.34	0.40
1:V:62:GLU:CD	1:V:62:GLU:H	2.24	0.40
1:V:77:VAL:HG22	1:V:78:TYR:N	2.35	0.40
2:W:176:LEU:C	2:W:178:MET:N	2.74	0.40
3:X:232:TYR:O	3:X:236:ILE:HG13	2.21	0.40
4:Y:160:TYR:HA	5:Z:59:SER:HA	2.03	0.40
5:Z:207:LEU:HD23	5:Z:207:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:63:LYS:O	6:1:65:VAL:N	2.53	0.40
6:1:236:ALA:C	6:1:238:LYS:H	2.25	0.40
2:B:189:ALA:O	2:B:190:ILE:C	2.59	0.40
3:C:208:LYS:HE3	3:C:209:ASN:ND2	2.37	0.40
4:D:49:GLY:HA2	4:D:211:GLN:O	2.22	0.40
4:D:139:ALA:HB2	4:D:148:LEU:HD13	2.04	0.40
7:G:59:LEU:O	7:G:61:PRO:CD	2.70	0.40
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.04	0.40
8:H:13:VAL:HG23	8:H:176:CYS:O	2.20	0.40
8:H:204:TYR:CD2	8:H:204:TYR:N	2.89	0.40
9:I:3:VAL:HA	9:I:15:ALA:O	2.21	0.40
9:I:76:PRO:O	9:I:77:GLU:C	2.60	0.40
11:K:85:ASN:ND2	17:K:227:HOH:O	2.53	0.40
11:K:196:PHE:CE2	11:K:206:PHE:CG	3.09	0.40
13:M:63:VAL:HG12	13:M:64:THR:N	2.35	0.40
14:N:112:THR:O	14:N:112:THR:HG23	2.21	0.40
14:N:187:LEU:HA	14:N:187:LEU:HD23	1.90	0.40
11:R:175:LEU:O	11:R:186:TYR:HD1	2.05	0.40
12:S:17:ASP:HA	12:S:172:GLY:O	2.22	0.40
12:S:99:THR:HG23	12:S:113:PHE:HB2	2.03	0.40
13:T:-6:GLN:HA	13:T:-5:PRO:HD2	1.93	0.40
13:T:42:VAL:CG2	13:T:178:ILE:HD11	2.51	0.40
13:T:82:TYR:O	13:T:86:VAL:HG23	2.21	0.40
14:U:52:THR:HG22	14:U:97:ALA:HB1	2.03	0.40
14:U:187(D):PRO:C	14:U:187(F):GLU:N	2.75	0.40
1:V:130:ARG:O	1:V:130:ARG:HG3	2.20	0.40
3:X:19:GLY:O	4:Y:30:ALA:HB2	2.22	0.40
3:X:241:GLN:C	3:X:243:GLN:H	2.25	0.40
5:Z:161:TYR:OH	6:1:61:PRO:CD	2.66	0.40
5:Z:179:THR:O	5:Z:179:THR:HG22	2.21	0.40
7:2:82:ILE:O	7:2:83:PRO:C	2.59	0.40
7:2:87:ASN:N	17:2:2404:HOH:O	2.54	0.40
1:A:50:THR:OG1	1:A:51:GLU:N	2.55	0.40
5:E:167:ALA:HB3	17:E:982:HOH:O	2.22	0.40
6:F:38:ILE:HG22	6:F:164:ALA:HB2	2.03	0.40
6:F:198:TYR:CD2	6:F:208:PHE:HZ	2.40	0.40
8:H:95:ILE:O	8:H:97:ALA:N	2.52	0.40
10:J:138:LEU:O	10:J:139:ASP:C	2.57	0.40
13:M:114:ASN:O	13:M:116:LEU:N	2.55	0.40
14:N:13:ILE:HG12	14:N:177:VAL:HG13	2.04	0.40
14:N:171:GLY:HA2	13:T:197:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:27:VAL:HG13	17:Q:2596:HOH:O	2.20	0.40
10:Q:2:ILE:HD12	10:Q:170:PHE:CG	2.55	0.40
10:Q:78:ALA:O	10:Q:79:VAL:C	2.60	0.40
12:S:21:ILE:C	12:S:21:ILE:HD12	2.41	0.40
1:V:197:LEU:HD12	1:V:197:LEU:HA	1.79	0.40
2:W:71:ASN:ND2	2:W:72:ASP:N	2.68	0.40
2:W:120:LYS:NZ	2:W:151:SER:OG	2.53	0.40
3:X:122:ARG:NH2	17:X:2046:HOH:O	2.55	0.40
5:Z:216:GLY:O	5:Z:219:THR:N	2.50	0.40
7:2:99:PHE:CE1	7:2:107:MET:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/250 (99%)	207 (84%)	38 (15%)	3 (1%)	13 48
1	V	248/250 (99%)	212 (86%)	32 (13%)	4 (2%)	9 40
2	B	242/244 (99%)	210 (87%)	26 (11%)	6 (2%)	5 28
2	W	242/244 (99%)	209 (86%)	24 (10%)	9 (4%)	3 19
3	C	239/241 (99%)	207 (87%)	25 (10%)	7 (3%)	4 24
3	X	239/241 (99%)	203 (85%)	29 (12%)	7 (3%)	4 24
4	D	240/242 (99%)	205 (85%)	30 (12%)	5 (2%)	7 33
4	Y	240/242 (99%)	210 (88%)	24 (10%)	6 (2%)	5 28
5	E	231/233 (99%)	196 (85%)	30 (13%)	5 (2%)	6 31
5	Z	231/233 (99%)	196 (85%)	28 (12%)	7 (3%)	4 24
6	1	242/244 (99%)	203 (84%)	33 (14%)	6 (2%)	5 28
6	F	242/244 (99%)	206 (85%)	34 (14%)	2 (1%)	19 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2	241/243 (99%)	211 (88%)	24 (10%)	6 (2%)	5	28
7	G	241/243 (99%)	209 (87%)	27 (11%)	5 (2%)	7	33
8	H	220/222 (99%)	192 (87%)	25 (11%)	3 (1%)	11	43
8	O	220/222 (99%)	198 (90%)	17 (8%)	5 (2%)	6	30
9	I	202/204 (99%)	181 (90%)	20 (10%)	1 (0%)	29	68
9	P	202/204 (99%)	185 (92%)	16 (8%)	1 (0%)	29	68
10	J	196/198 (99%)	175 (89%)	17 (9%)	4 (2%)	7	34
10	Q	196/198 (99%)	175 (89%)	16 (8%)	5 (3%)	5	27
11	K	210/212 (99%)	190 (90%)	17 (8%)	3 (1%)	11	43
11	R	210/212 (99%)	187 (89%)	21 (10%)	2 (1%)	15	53
12	L	220/222 (99%)	191 (87%)	27 (12%)	2 (1%)	17	55
12	S	220/222 (99%)	196 (89%)	23 (10%)	1 (0%)	29	68
13	M	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	9	39
13	T	231/233 (99%)	200 (87%)	29 (13%)	2 (1%)	17	55
14	N	194/196 (99%)	175 (90%)	16 (8%)	3 (2%)	10	42
14	U	194/196 (99%)	171 (88%)	20 (10%)	3 (2%)	10	42
15	8	1/5 (20%)	1 (100%)	0	0	100	100
15	9	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6314/6378 (99%)	5504 (87%)	693 (11%)	117 (2%)	8	36

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	167	LYS
2	B	54	VAL
2	B	204(A)	SER
3	C	58	LEU
3	C	72	SER
3	C	183	PRO
3	C	203	THR
5	E	217	LYS
8	H	91	GLN
10	J	39	PRO
13	M	71(B)	GLU
8	O	91	GLN

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Mol	Chain	Res	Type
11	R	39	PRO
1	V	167	LYS
2	W	54	VAL
2	W	204(A)	SER
2	W	218(C)	ASP
3	X	58	LEU
3	X	183	PRO
3	X	203	THR
5	Z	217	LYS
2	B	219(C)	ASP
3	C	184	ALA
4	D	120	ALA
4	D	121	LEU
4	D	180(E)	SER
5	E	202	ARG
5	E	231	LYS
7	G	9	ASP
7	G	180(C)	HIS
10	J	49	ALA
14	N	115	LEU
10	Q	105(A)	LYS
13	T	71(B)	GLU
14	U	115	LEU
1	V	53	LYS
1	V	143	GLU
2	W	182	ASP
3	X	72	SER
4	Y	120	ALA
4	Y	180(E)	SER
5	Z	163	THR
5	Z	202	ARG
5	Z	231	LYS
7	2	9	ASP
7	2	55	PRO
7	2	180(C)	HIS
2	B	11	ARG
4	D	22	PHE
5	E	170	GLN
6	F	206	LYS
6	F	237	GLN
8	H	30	ASN
10	J	105(A)	LYS

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Mol	Chain	Res	Type
11	K	9	GLN
11	K	39	PRO
12	L	71	ASP
13	M	2	SER
14	N	187(E)	ASP
8	O	205	LYS
10	Q	8	VAL
10	Q	49	ALA
11	R	9	GLN
14	U	187(E)	ASP
2	W	35	GLY
3	X	184	ALA
4	Y	22	PHE
4	Y	121	LEU
5	Z	227	GLU
6	1	8	TYR
6	1	143	LYS
6	1	237	GLN
5	E	186	PRO
7	G	55	PRO
7	G	237	ALA
13	M	72	ALA
8	O	9	ASN
10	Q	39	PRO
10	Q	115	TYR
3	X	64	PRO
5	Z	170	GLN
5	Z	186	PRO
6	1	12	ASN
6	1	206	LYS
7	2	199	ASP
2	B	219(D)	GLY
3	C	239	GLU
9	I	93	GLY
11	K	138	LEU
13	M	115	LEU
14	U	67	THR
2	W	22	TYR
3	X	242	GLU
6	1	98	SER
1	A	72	PRO
14	N	67	THR

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Mol	Chain	Res	Type
8	O	105(A)	PRO
9	P	76	PRO
13	T	72	ALA
2	W	226	PRO
7	2	60	ASP
7	2	208	ASN
7	G	60	ASP
8	H	105(A)	PRO
10	J	8	VAL
8	O	96	GLY
2	W	153	PRO
3	C	64	PRO
1	V	159	PRO
2	W	218(D)	GLY
4	Y	123(F)	GLY
2	B	186	VAL
4	D	123(F)	GLY
12	L	94	PRO
12	S	-6	PRO
4	Y	11	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	198 (95%)	11 (5%)	22	58
1	V	209/209 (100%)	200 (96%)	9 (4%)	29	66
2	B	203/203 (100%)	188 (93%)	15 (7%)	13	44
2	W	203/203 (100%)	186 (92%)	17 (8%)	11	38
3	C	213/213 (100%)	194 (91%)	19 (9%)	9	35
3	X	213/213 (100%)	196 (92%)	17 (8%)	12	40
4	D	198/198 (100%)	185 (93%)	13 (7%)	16	49
4	Y	198/198 (100%)	185 (93%)	13 (7%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	25
5	Z	192/192 (100%)	173 (90%)	19 (10%)	8	30
6	1	201/201 (100%)	181 (90%)	20 (10%)	7	29
6	F	201/201 (100%)	183 (91%)	18 (9%)	9	35
7	2	207/207 (100%)	188 (91%)	19 (9%)	9	34
7	G	207/207 (100%)	191 (92%)	16 (8%)	13	42
8	H	181/181 (100%)	169 (93%)	12 (7%)	16	49
8	O	181/181 (100%)	167 (92%)	14 (8%)	13	42
9	I	172/172 (100%)	160 (93%)	12 (7%)	15	47
9	P	172/172 (100%)	163 (95%)	9 (5%)	23	59
10	J	175/175 (100%)	164 (94%)	11 (6%)	18	51
10	Q	175/175 (100%)	165 (94%)	10 (6%)	20	56
11	K	169/169 (100%)	156 (92%)	13 (8%)	13	42
11	R	169/169 (100%)	158 (94%)	11 (6%)	17	50
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	50
12	S	185/185 (100%)	173 (94%)	12 (6%)	17	50
13	M	199/199 (100%)	186 (94%)	13 (6%)	17	50
13	T	199/199 (100%)	188 (94%)	11 (6%)	21	57
14	N	162/162 (100%)	152 (94%)	10 (6%)	18	52
14	U	162/162 (100%)	147 (91%)	15 (9%)	9	33
15	8	2/2 (100%)	2 (100%)	0	100	100
15	9	2/2 (100%)	2 (100%)	0	100	100
All	All	5336/5336 (100%)	4944 (93%)	392 (7%)	14	44

All (392) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	64	LEU
1	A	78	TYR
1	A	124	THR
1	A	135	SER
1	A	136	LEU
1	A	158	PHE

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Mol	Chain	Res	Type
1	A	170	VAL
1	A	200	SER
1	A	212	LEU
1	A	236	LEU
2	B	58	LEU
2	B	61	GLN
2	B	63	THR
2	B	65	GLU
2	B	67	LEU
2	B	71	ASN
2	B	150	THR
2	B	156	ASN
2	B	169	THR
2	B	185	LYS
2	B	198	SER
2	B	203	ASP
2	B	206	THR
2	B	226	PRO
2	B	236	THR
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	61	THR
3	C	62(A)	ILE
3	C	66	LYS
3	C	75	VAL
3	C	124	THR
3	C	135	SER
3	C	144(B)	ASP
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	178	LYS
3	C	196	SER
3	C	209	ASN
3	C	215	VAL
3	C	224	LEU
4	D	13	SER
4	D	27	SER
4	D	28	LEU
4	D	76	CYS

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Mol	Chain	Res	Type
4	D	119	LEU
4	D	126	ARG
4	D	156	THR
4	D	170	GLU
4	D	177	LEU
4	D	184	LEU
4	D	191	LEU
4	D	215	ILE
4	D	237	LEU
5	E	11	ASP
5	E	12	THR
5	E	15	PHE
5	E	18	THR
5	E	32	LYS
5	E	33	GLN
5	E	58	LEU
5	E	76	LEU
5	E	97	ASN
5	E	121	GLN
5	E	153	PRO
5	E	178	ARG
5	E	180(C)	PHE
5	E	185	ASN
5	E	189	LEU
5	E	198	SER
5	E	199	GLN
5	E	203	ASP
5	E	207(C)	VAL
5	E	222	THR
5	E	231	LYS
6	F	36	THR
6	F	43	ASN
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	153	PRO
6	F	169	ARG
6	F	170	GLN
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU
6	F	204	ASP

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Mol	Chain	Res	Type
6	F	205	ASN
6	F	208	PHE
6	F	214	TRP
6	F	218(C)	ASN
6	F	227	ASP
6	F	233	ILE
7	G	40	VAL
7	G	72	ARG
7	G	87	ASN
7	G	105	TYR
7	G	119	LEU
7	G	121	GLN
7	G	157	TYR
7	G	169	GLN
7	G	171	GLU
7	G	184	ASN
7	G	201	LEU
7	G	204	GLU
7	G	217	LYS
7	G	221	PHE
7	G	232	ARG
7	G	233	LEU
8	H	22	GLN
8	H	30	ASN
8	H	31	CYS
8	H	34	LEU
8	H	56	THR
8	H	105(A)	PRO
8	H	124	TYR
8	H	135	MET
8	H	185	GLU
8	H	191	TYR
8	H	196	VAL
8	H	197	ARG
9	I	-5	SER
9	I	29	ASN
9	I	55	LEU
9	I	61	TYR
9	I	70	GLU
9	I	113	PHE
9	I	131	SER
9	I	148	PRO

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Mol	Chain	Res	Type
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
9	I	185	VAL
10	J	7	ARG
10	J	17	SER
10	J	34	THR
10	J	52	THR
10	J	68	ILE
10	J	77	GLN
10	J	91	SER
10	J	104	TYR
10	J	133	TYR
10	J	147	THR
10	J	166	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	39	PRO
11	K	69	ARG
11	K	70	GLU
11	K	97	MET
11	K	100	MET
11	K	104	TYR
11	K	105(B)	LYS
11	K	138	LEU
11	K	139	ASP
11	K	145	ASP
12	L	14	LEU
12	L	33	LYS
12	L	40	ASN
12	L	48	PHE
12	L	62	SER
12	L	98	HIS
12	L	99	THR
12	L	138	LEU
12	L	144(J)	ASN
12	L	145	TYR
12	L	150	GLU
12	L	184	VAL
13	M	21	SER
13	M	40	ASN

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Mol	Chain	Res	Type
13	M	61	ASP
13	M	62	LEU
13	M	112	TYR
13	M	115	LEU
13	M	122	SER
13	M	141(C)	ARG
13	M	181(A)	THR
13	M	184	LEU
13	M	190	LEU
13	M	192	VAL
13	M	204	LYS
14	N	12	VAL
14	N	20	THR
14	N	36	ARG
14	N	61	TYR
14	N	81	SER
14	N	105	ASP
14	N	105(A)	ASP
14	N	123	PRO
14	N	132	THR
14	N	149	GLU
8	O	22	GLN
8	O	30	ASN
8	O	34	LEU
8	O	56	THR
8	O	68	LEU
8	O	105(A)	PRO
8	O	121	VAL
8	O	124	TYR
8	O	156	SER
8	O	189	ARG
8	O	191	TYR
8	O	193	THR
8	O	197	ARG
8	O	221	ILE
9	P	-5	SER
9	P	29	ASN
9	P	55	LEU
9	P	113	PHE
9	P	131	SER
9	P	159	LEU
9	P	160	LEU

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Mol	Chain	Res	Type
9	P	171	TRP
9	P	185	VAL
10	Q	7	ARG
10	Q	17	SER
10	Q	34	THR
10	Q	52	THR
10	Q	68	ILE
10	Q	77	GLN
10	Q	91	SER
10	Q	104	TYR
10	Q	133	TYR
10	Q	147	THR
11	R	4	LEU
11	R	9	GLN
11	R	39	PRO
11	R	70	GLU
11	R	100	MET
11	R	102	CYS
11	R	104	TYR
11	R	105(B)	LYS
11	R	135	TYR
11	R	138	LEU
11	R	145	ASP
12	S	14	LEU
12	S	40	ASN
12	S	43	MET
12	S	62	SER
12	S	82	ASN
12	S	98	HIS
12	S	99	THR
12	S	138	LEU
12	S	144(I)	ASN
12	S	145	TYR
12	S	150	GLU
12	S	179	THR
13	T	21	SER
13	T	40	ASN
13	T	61	ASP
13	T	62	LEU
13	T	63	VAL
13	T	123	PRO
13	T	141(C)	ARG

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Mol	Chain	Res	Type
13	T	165	ARG
13	T	181(A)	THR
13	T	192	VAL
13	T	204	LYS
14	U	6	VAL
14	U	8	PHE
14	U	20	THR
14	U	36	ARG
14	U	70	TYR
14	U	81	SER
14	U	105(A)	ASP
14	U	115	LEU
14	U	122	LEU
14	U	124	TYR
14	U	132	THR
14	U	144	GLU
14	U	169	SER
14	U	177	VAL
14	U	178	LEU
1	V	64	LEU
1	V	78	TYR
1	V	135	SER
1	V	136	LEU
1	V	158	PHE
1	V	170	VAL
1	V	212	LEU
1	V	221	PHE
1	V	236	LEU
2	W	38	ILE
2	W	58	LEU
2	W	61	GLN
2	W	63	THR
2	W	67	LEU
2	W	71	ASN
2	W	121	GLN
2	W	150	THR
2	W	153	PRO
2	W	156	ASN
2	W	169	THR
2	W	185	LYS
2	W	198	SER
2	W	203	ASP

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Mol	Chain	Res	Type
2	W	218(C)	ASP
2	W	226	PRO
2	W	236	THR
3	X	10	ARG
3	X	17	PRO
3	X	25	GLU
3	X	57	LYS
3	X	61	THR
3	X	62(A)	ILE
3	X	66	LYS
3	X	75	VAL
3	X	121	GLN
3	X	135	SER
3	X	163	GLN
3	X	174	GLU
3	X	178	LYS
3	X	196	SER
3	X	209	ASN
3	X	215	VAL
3	X	224	LEU
4	Y	28	LEU
4	Y	56	SER
4	Y	76	CYS
4	Y	119	LEU
4	Y	126	ARG
4	Y	154	SER
4	Y	156	THR
4	Y	177	LEU
4	Y	184	LEU
4	Y	191	LEU
4	Y	208	ASP
4	Y	215	ILE
4	Y	237	LEU
5	Z	11	ASP
5	Z	12	THR
5	Z	15	PHE
5	Z	18	THR
5	Z	32	LYS
5	Z	58	LEU
5	Z	76	LEU
5	Z	97	ASN
5	Z	117	CYS

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Mol	Chain	Res	Type
5	Z	153	PRO
5	Z	178	ARG
5	Z	180(C)	PHE
5	Z	185	ASN
5	Z	198	SER
5	Z	199	GLN
5	Z	207	LEU
5	Z	207(C)	VAL
5	Z	222	THR
5	Z	231	LYS
6	1	36	THR
6	1	43	ASN
6	1	73	HIS
6	1	83	PRO
6	1	121	GLN
6	1	127	ASN
6	1	135	SER
6	1	153	PRO
6	1	169	ARG
6	1	170	GLN
6	1	187	ARG
6	1	192	GLN
6	1	203	GLU
6	1	204	ASP
6	1	205	ASN
6	1	208	PHE
6	1	214	TRP
6	1	218(C)	ASN
6	1	227	ASP
6	1	233	ILE
7	2	29	LYS
7	2	56	ASP
7	2	62	THR
7	2	72	ARG
7	2	87	ASN
7	2	105	TYR
7	2	119	LEU
7	2	121	GLN
7	2	152	ASP
7	2	157	TYR
7	2	169	GLN
7	2	171	GLU

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Mol	Chain	Res	Type
7	2	184	ASN
7	2	201	LEU
7	2	204	GLU
7	2	217	LYS
7	2	222	PHE
7	2	232	ARG
7	2	233	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	145	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	177	GLN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	120	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	235	GLN
4	D	23	GLN
4	D	99	HIS
4	D	108	ASN
4	D	150	HIS
4	D	211	GLN
4	D	226	ASN
5	E	6	ASN
5	E	7	ASN
5	E	33	GLN
5	E	73	HIS
5	E	97	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN

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Mol	Chain	Res	Type
5	E	152	GLN
5	E	185	ASN
5	E	199	GLN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	123	HIS
6	F	221	HIS
6	F	241	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	170	GLN
7	G	184	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	109	HIS
8	H	114	HIS
8	H	144	GLN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
9	I	145	ASN
10	J	54	GLN
10	J	64	GLN
10	J	77	GLN
10	J	85	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
12	L	-7	ASN
12	L	40	ASN
12	L	67	HIS

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Mol	Chain	Res	Type
12	L	70(A)	ASN
12	L	123	GLN
12	L	140	ASN
12	L	141	GLN
12	L	144(B)	ASN
12	L	144(J)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	135	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	38	HIS
14	N	62	HIS
14	N	157	HIS
14	N	161	GLN
8	O	22	GLN
8	O	30	ASN
8	O	66	HIS
8	O	91	GLN
8	O	114	HIS
8	O	144	GLN
8	O	172	ASN
8	O	190	ASN
9	P	29	ASN
9	P	81	GLN
9	P	145	ASN
10	Q	54	GLN
10	Q	64	GLN
10	Q	77	GLN
10	Q	85	GLN
10	Q	112	GLN
10	Q	141	HIS
10	Q	186	GLN
11	R	9	GLN
11	R	85	ASN
11	R	174	ASN
12	S	40	ASN

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Mol	Chain	Res	Type
12	S	61	ASN
12	S	70(A)	ASN
12	S	140	ASN
12	S	141	GLN
12	S	144(B)	ASN
12	S	144(I)	ASN
12	S	166	HIS
13	T	10	ASN
13	T	40	ASN
13	T	89	GLN
13	T	93	ASN
13	T	132	HIS
13	T	135	ASN
13	T	149	GLN
13	T	157	ASN
13	T	172	ASN
13	T	191	GLN
14	U	69	GLN
14	U	161	GLN
1	V	97	HIS
1	V	145	ASN
1	V	181	ASN
1	V	217(B)	ASN
2	W	23	GLN
2	W	71	ASN
2	W	97	GLN
2	W	121	GLN
2	W	125	GLN
2	W	156	ASN
2	W	177	GLN
2	W	227	GLN
3	X	23	GLN
3	X	82	ASN
3	X	97	GLN
3	X	150	GLN
3	X	163	GLN
3	X	209	ASN
4	Y	23	GLN
4	Y	108	ASN
4	Y	150	HIS
4	Y	211	GLN
4	Y	226	ASN

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Mol	Chain	Res	Type
5	Z	6	ASN
5	Z	7	ASN
5	Z	33	GLN
5	Z	54	ASN
5	Z	73	HIS
5	Z	121	GLN
5	Z	123	ASN
5	Z	125	GLN
5	Z	152	GLN
5	Z	185	ASN
5	Z	199	GLN
6	1	23	GLN
6	1	43	ASN
6	1	90	ASN
6	1	121	GLN
6	1	123	HIS
6	1	147	HIS
6	1	192	GLN
6	1	241	ASN
7	2	33	GLN
7	2	34(A)	ASN
7	2	87	ASN
7	2	118	ASN
7	2	121	GLN
7	2	125	GLN
7	2	170	GLN
7	2	184	ASN
7	2	239	GLN
15	8	3	ASN
15	9	3	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	R4K	8	4	15	16,18,19	3.01	5 (31%)	18,27,29	2.51	8 (44%)
15	R4K	9	4	15	16,18,19	3.83	8 (50%)	18,27,29	3.62	10 (55%)

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	R4K	8	4	15	-	4/11/28/30	0/2/2/2
15	R4K	9	4	15	-	4/11/28/30	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	9	4	R4K	C32-N31	-9.11	1.24	1.35
15	9	4	R4K	C55-C50	-8.49	1.30	1.39
15	8	4	R4K	C29-C50	-6.85	1.41	1.51
15	8	4	R4K	C55-C50	-6.49	1.32	1.39
15	8	4	R4K	C32-N31	-5.46	1.28	1.35
15	9	4	R4K	C29-CB	-4.29	1.53	1.55
15	9	4	R4K	C55-N31	-4.07	1.31	1.38
15	8	4	R4K	C51-C50	3.54	1.44	1.39
15	9	4	R4K	C29-C50	-3.48	1.46	1.51
15	9	4	R4K	CB-CA	3.25	1.61	1.53
15	9	4	R4K	C51-C50	2.91	1.43	1.39
15	9	4	R4K	O33-C32	2.37	1.27	1.22
15	8	4	R4K	O34-CB	2.12	1.47	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	9	4	R4K	C51-C50-C55	10.34	128.82	119.81
15	9	4	R4K	C54-C55-C50	-6.68	115.56	121.91
15	8	4	R4K	C51-C50-C55	4.63	123.84	119.81
15	9	4	R4K	C50-C55-N31	4.43	112.56	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	8	4	R4K	C54-C55-C50	-4.04	118.06	121.91
15	9	4	R4K	C51-C50-C29	-4.00	124.91	130.76
15	8	4	R4K	O-C-CA	-3.89	114.58	124.78
15	8	4	R4K	C29-CB-CA	-3.70	109.84	112.78
15	8	4	R4K	O33-C32-N31	3.25	129.51	126.31
15	8	4	R4K	C55-N31-C32	-3.02	110.05	111.86
15	9	4	R4K	C29-CB-CA	-2.91	110.47	112.78
15	8	4	R4K	CB-CA-C	-2.81	107.29	111.77
15	9	4	R4K	O-C-CA	-2.75	117.58	124.78
15	9	4	R4K	C52-C51-C50	-2.74	114.98	119.96
15	9	4	R4K	C55-N31-C32	-2.72	110.23	111.86
15	8	4	R4K	C51-C50-C29	-2.64	126.90	130.76
15	9	4	R4K	C52-C53-C54	2.60	124.15	120.19
15	9	4	R4K	CB-CA-C	-2.47	107.83	111.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	8	4	R4K	O-C-CA-CB
15	8	4	R4K	C-CA-CB-C29
15	9	4	R4K	C-CA-CB-C29
15	8	4	R4K	N-CA-CB-C29
15	9	4	R4K	N-CA-CB-C29
15	8	4	R4K	N-CA-CB-O34
15	9	4	R4K	N-CA-CB-O34
15	9	4	R4K	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	8	4	R4K	2	0
15	9	4	R4K	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.