



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:58 PM UTC

PDB ID : 9U3L / pdb_00009u3l
EMDB ID : EMD-63817
Title : Substrate-engaged human 26S proteasome bound to midnolin with RPT2 at top of spiral staircase
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-03-18
Resolution : 2.91 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

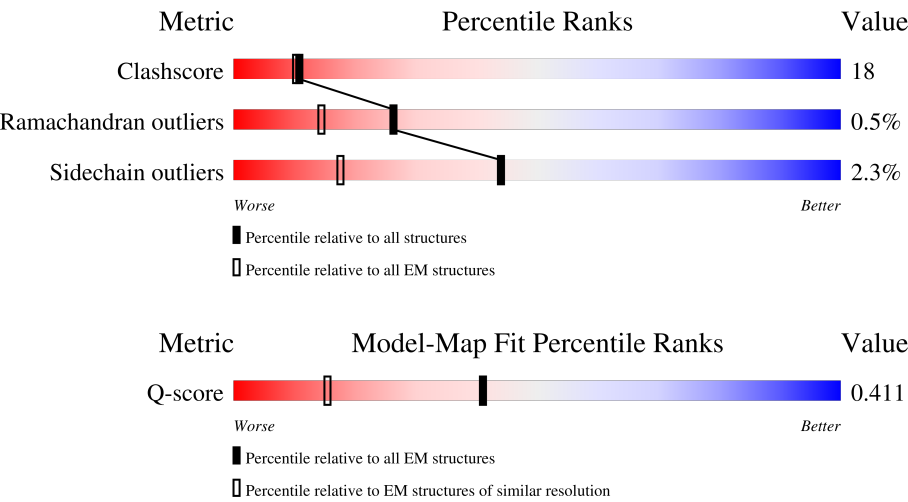
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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.



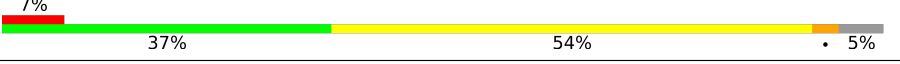

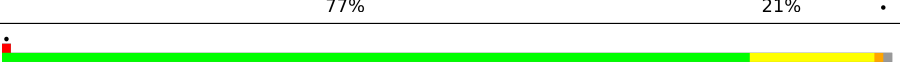
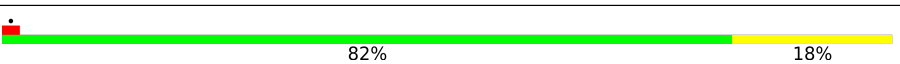


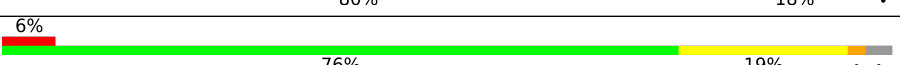

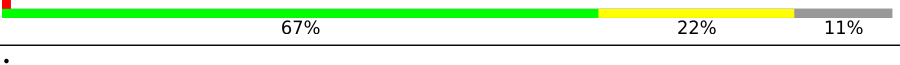




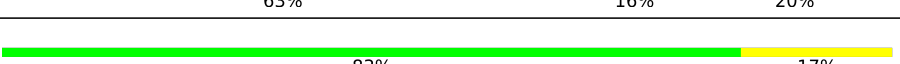

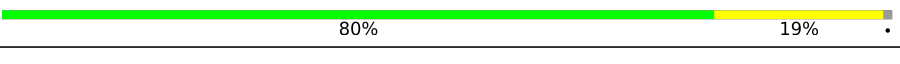

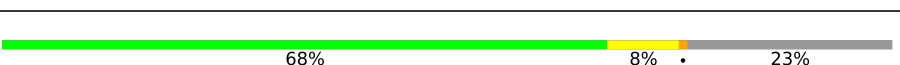





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12972 (2.41 - 3.41)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	<div><div>7%</div><div>40%</div><div>51%</div><div>5%</div></div>
2	B	440	<div><div>5%</div><div>55%</div><div>38%</div><div>7%</div></div>
3	C	398	<div><div>64%</div><div>32%</div><div>..</div></div>
4	D	418	<div><div>53%</div><div>35%</div><div>9%</div></div>











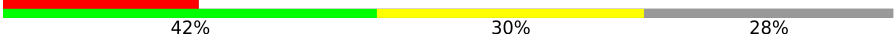


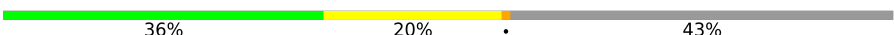




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Mol	Chain	Length	Quality of chain
5	E	403	
6	G	245	
6	g	245	
7	H	233	
7	h	233	
8	I	260	
8	i	260	
9	J	247	
9	j	247	
10	L	268	
10	l	268	
11	M	254	
11	m	254	
12	N	238	
12	n	238	
13	O	276	
13	o	276	
14	P	204	
14	p	204	
15	Q	201	
15	q	201	
16	R	262	
16	r	262	
17	S	240	
17	s	240	

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Mol	Chain	Length	Quality of chain
18	T	263	
18	t	263	
19	V	533	
20	W	456	
21	X	422	
22	Y	389	
23	Z	324	
24	a	376	
25	b	377	
26	c	309	
27	d	349	
28	u	908	
29	U	953	
30	e	70	
31	F	439	
32	K	240	
32	k	240	
33	v	15	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 104750 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3226	2033	565	610	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3201	2019	545	622	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3034	1920	521	580	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	381	Total	C	N	O	S	0	0
			3031	1903	542	569	17		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	237	Total	C	N	O	S	0	0
			1809	1151	302	343	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	240	Total	C	N	O	S	0	0
			1830	1163	306	348	13		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	231	Total	C	N	O	S	0	0
			1703	1079	289	330	5		
7	h	232	Total	C	N	O	S	0	0
			1727	1096	292	334	5		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
8	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	247	Total	C	N	O	S	0	0
			1844	1148	331	360	5		
9	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 10 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
10	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 11 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
11	m	240	Total	C	N	O	S	0	0
			1862	1181	317	353	11		

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		
12	n	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
13	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
14	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 15 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
15	q	199	Total	C	N	O	S	0	0
			1574	1009	266	290	9		

- Molecule 16 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
16	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 17 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
17	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 18 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
18	t	215	Total	C	N	O	S	0	0
			1673	1055	288	318	12		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	455	Total	C	N	O	S	0	0
			3685	2329	632	699	25		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	380	Total	C	N	O	S	0	0
			3003	1915	506	570	12		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	377	Total	C	N	O	S	0	0
			3108	1982	532	577	17		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	286	Total	C	N	O	S	0	0
			2277	1455	391	426	5		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	287	Total	C	N	O	S	0	0
			2254	1427	386	422	19		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	252	Total	C	N	O	S	0	0
			2074	1343	339	383	9		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	u	842	Total	C	N	O	S	0	0
			6514	4118	1106	1246	44		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	837	Total	C	N	O	S	0	0
			6529	4143	1109	1233	44		

- Molecule 30 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	384	Total	C	N	O	S	0	0
			3005	1896	514	577	18		

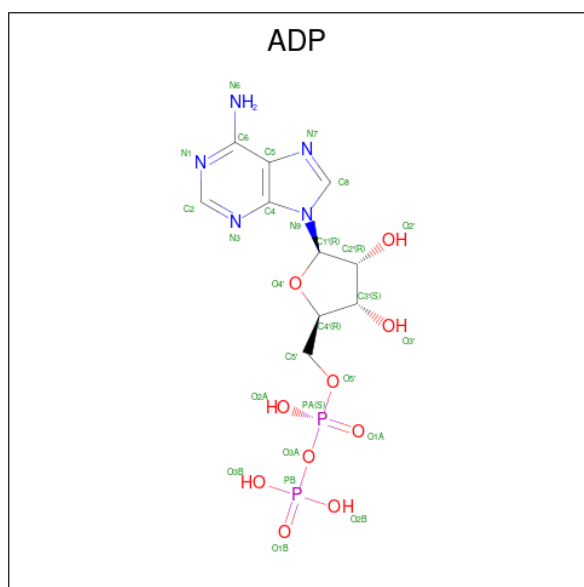
- Molecule 32 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	230	Total 1750	C 1099	N 287	O 353	S 11	0	0
32	k	228	Total 1722	C 1080	N 284	O 348	S 10	0	0

- Molecule 33 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

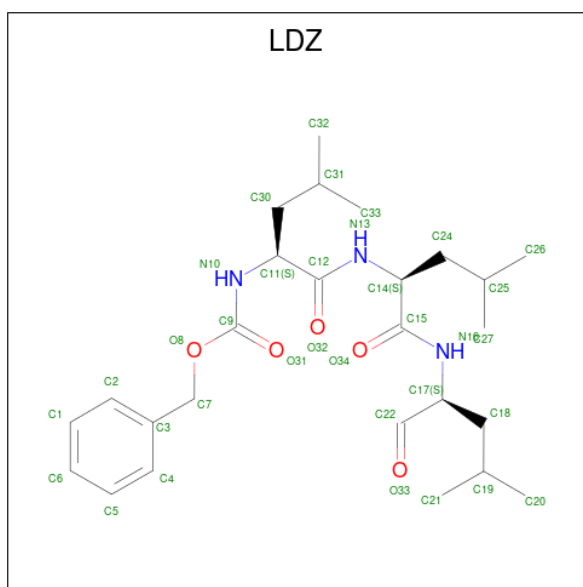


Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total 27	C 10	N 5	O 10	P 2	0
34	E	1	Total 27	C 10	N 5	O 10	P 2	0
34	F	1	Total 27	C 10	N 5	O 10	P 2	0

- # ATP

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

- Molecule 37 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
37	N	1	Total	C	N	O	0
			34	26	3	5	
37	O	1	Total	C	N	O	0
			34	26	3	5	
37	R	1	Total	C	N	O	0
			34	26	3	5	
37	n	1	Total	C	N	O	0
			34	26	3	5	
37	o	1	Total	C	N	O	0
			34	26	3	5	
37	r	1	Total	C	N	O	0
			34	26	3	5	

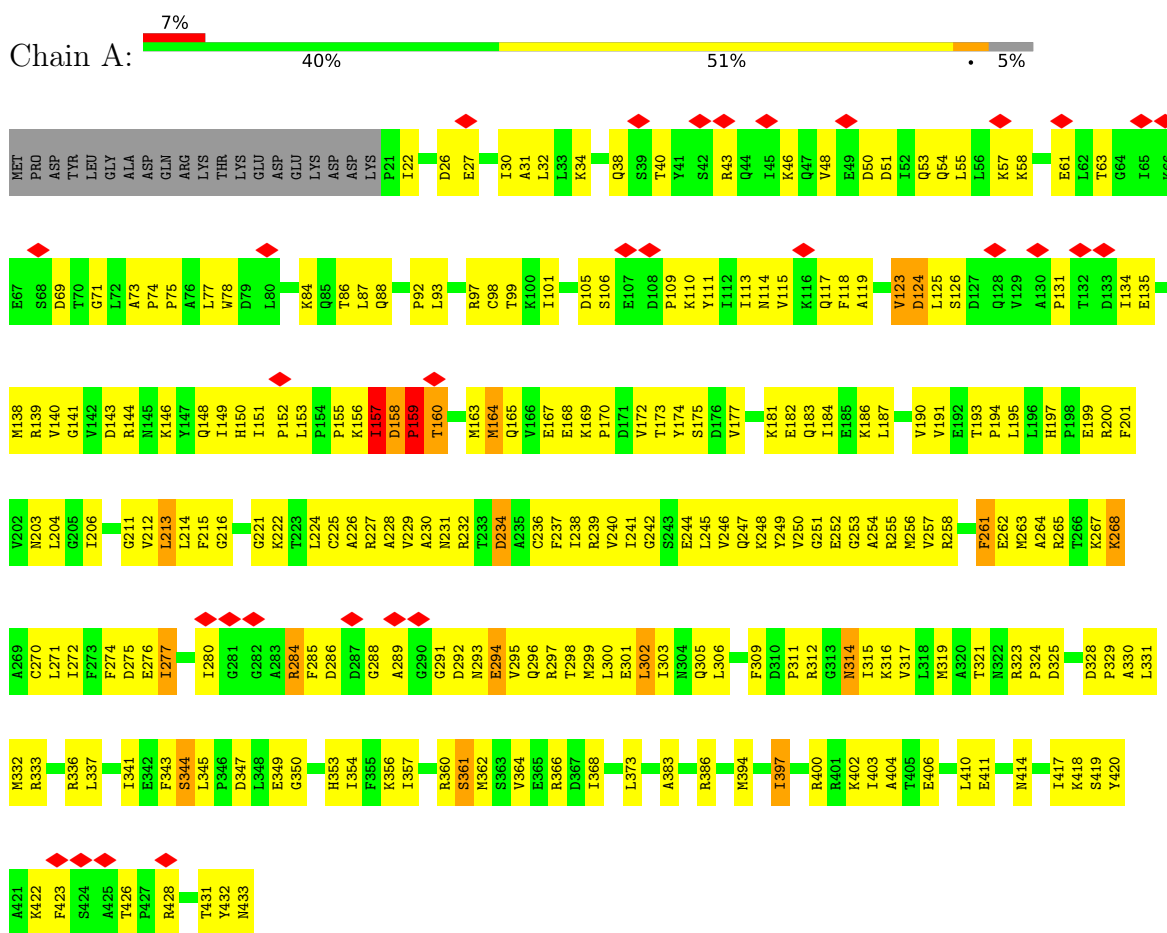
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	c	1	Total	Zn	0
			1	1	

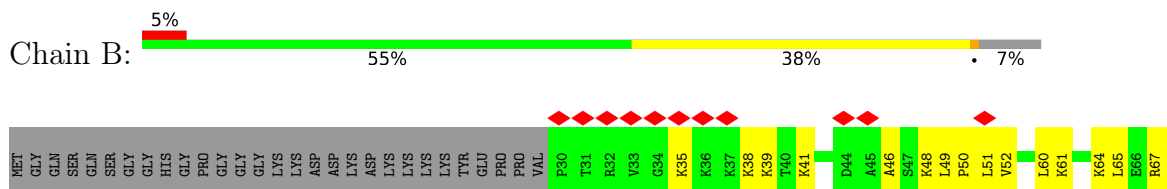
3 Residue-property plots

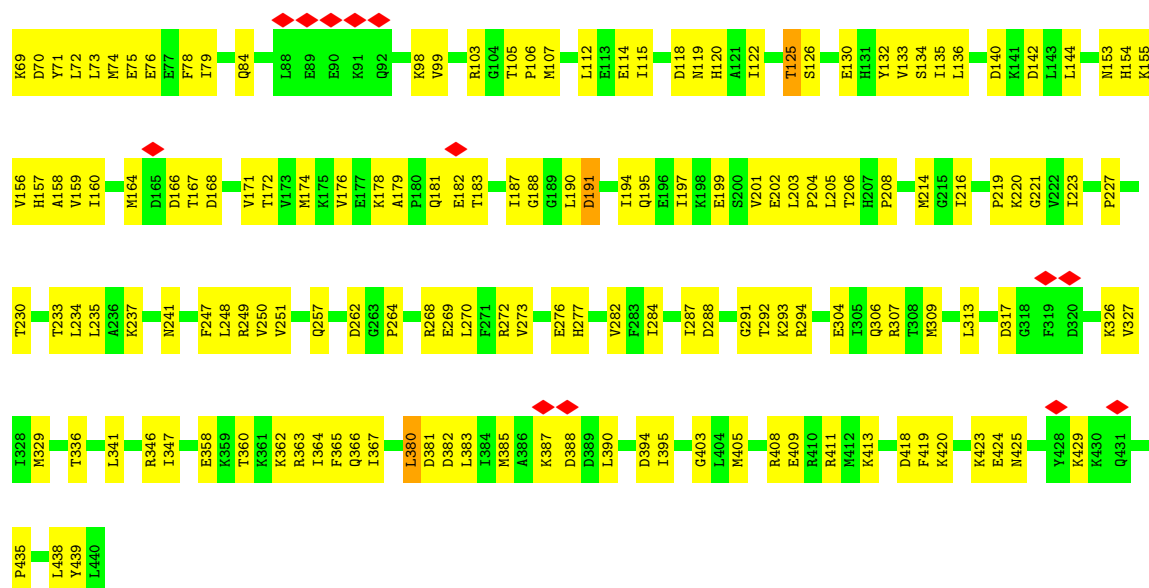
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 26S proteasome regulatory subunit 7

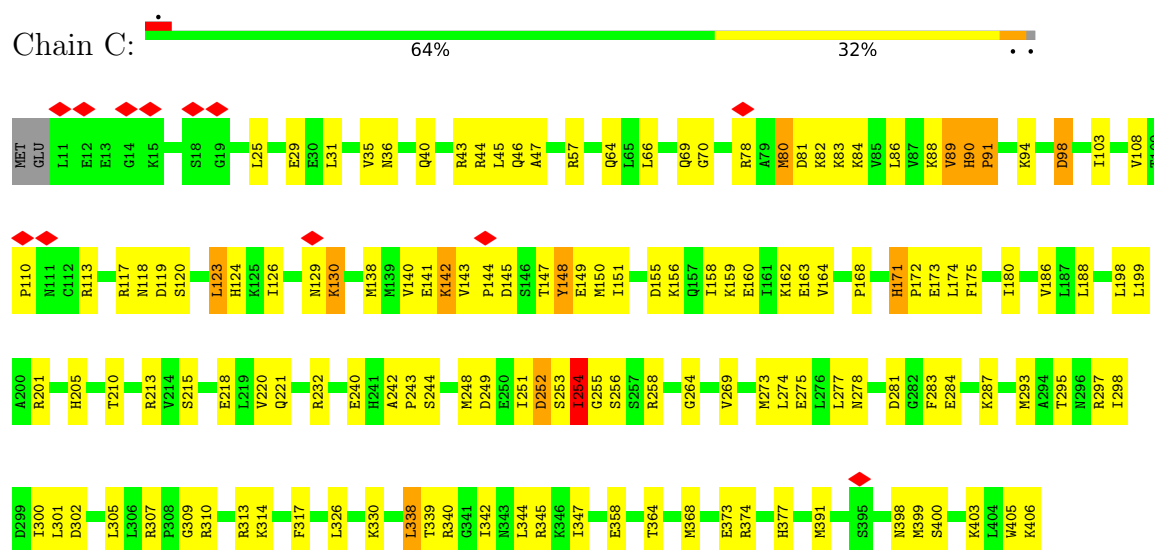


• Molecule 2: 26S proteasome regulatory subunit 4

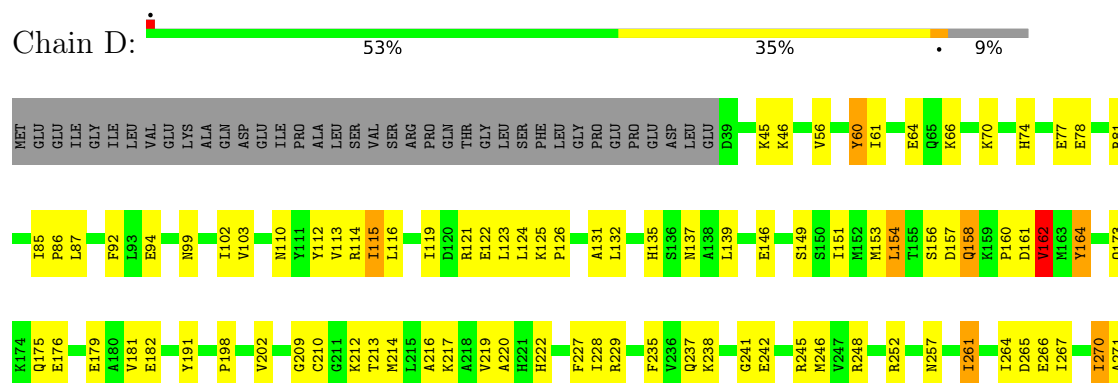


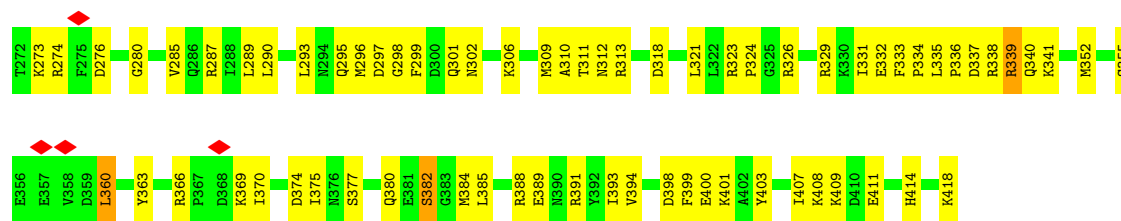


• Molecule 3: 26S proteasome regulatory subunit 8

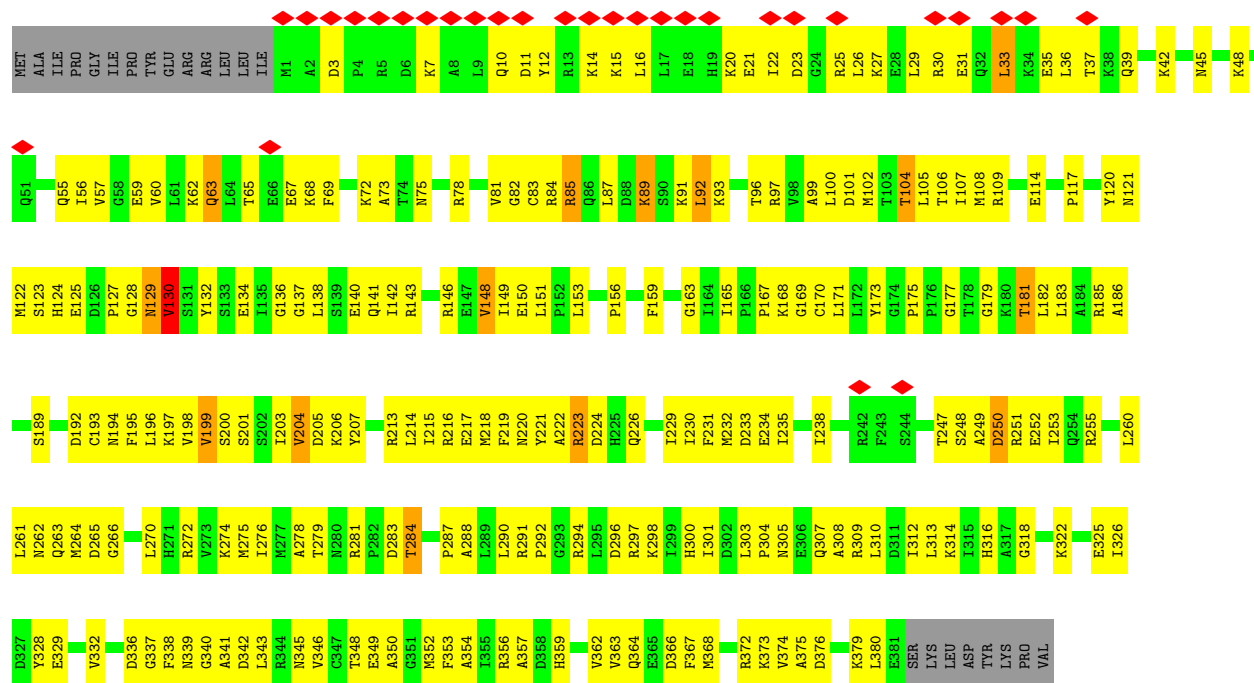


• Molecule 4: 26S proteasome regulatory subunit 6B

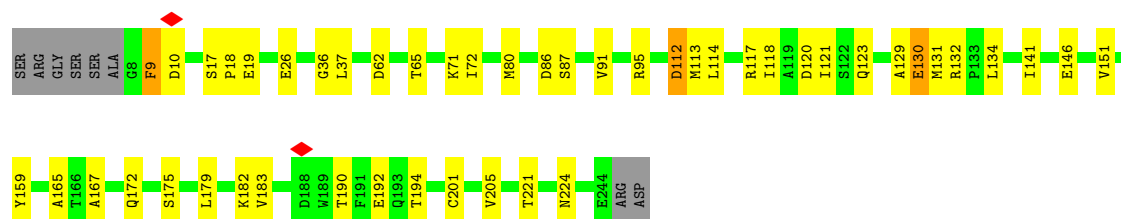
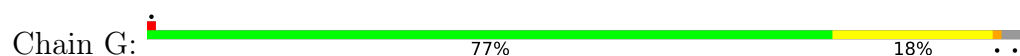




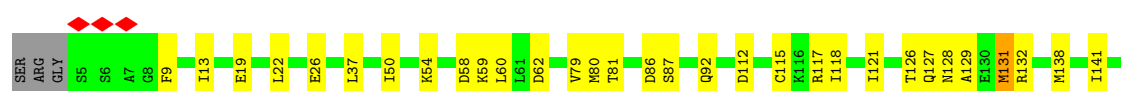
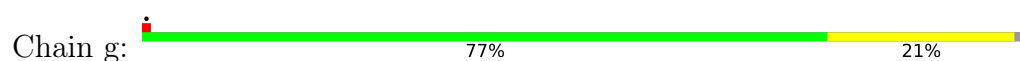
• Molecule 5: Proteasome 26S subunit, ATPase 6



• Molecule 6: Proteasome subunit alpha type-6



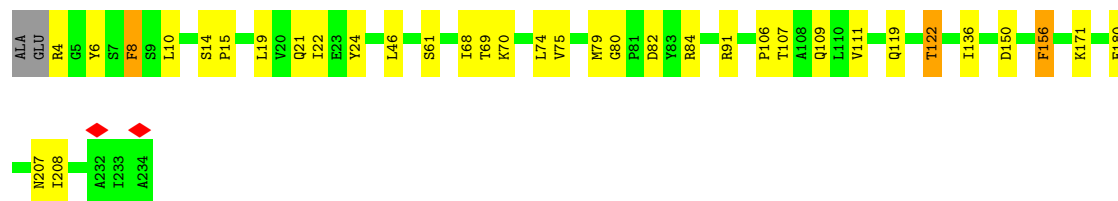
• Molecule 6: Proteasome subunit alpha type-6





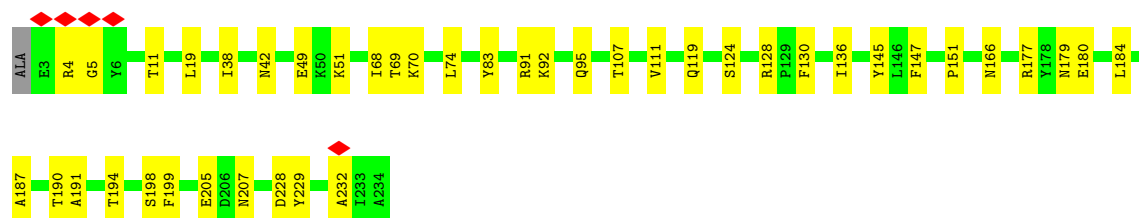
• Molecule 7: Proteasome subunit alpha type-2

Chain H: 84% 14% ..



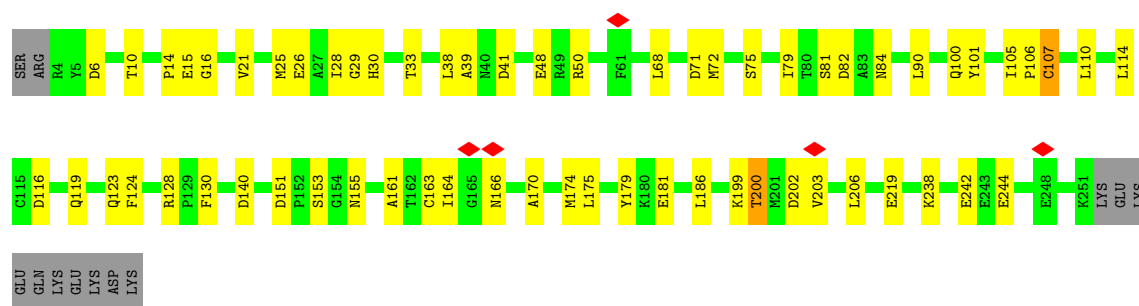
• Molecule 7: Proteasome subunit alpha type-2

Chain h: 82% 18%



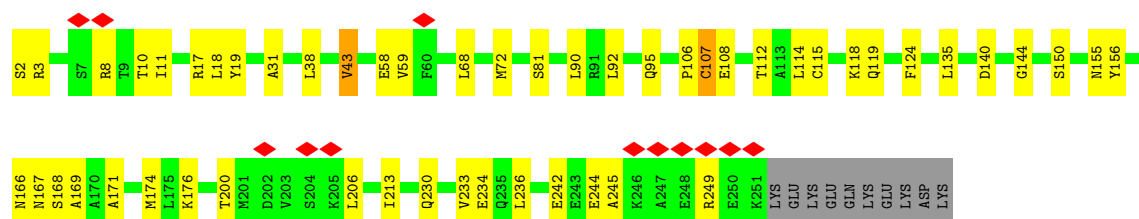
• Molecule 8: Proteasome subunit alpha type-4

Chain I: 72% 23% • 5%

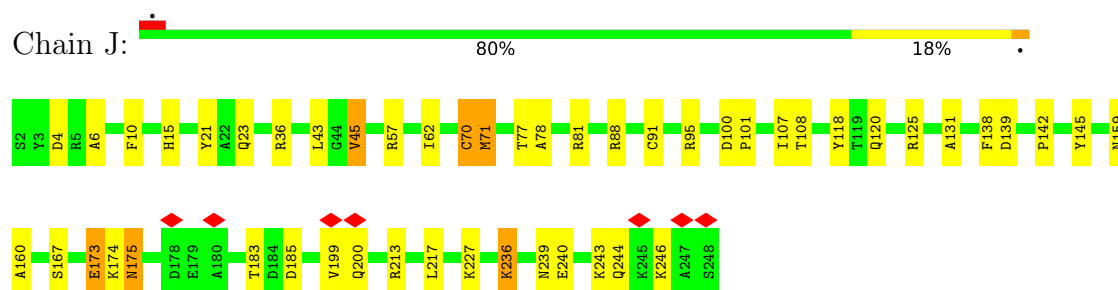


• Molecule 8: Proteasome subunit alpha type-4

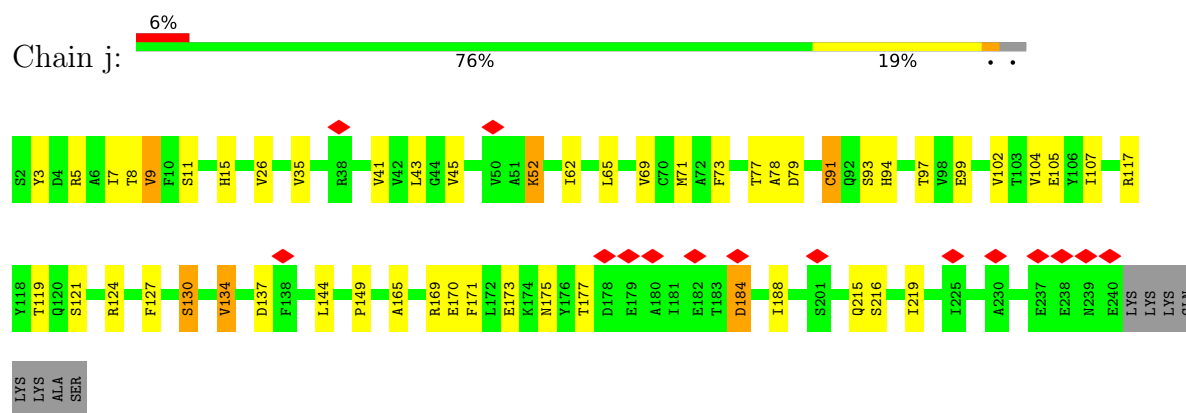
Chain i: 5% 76% 19% • •



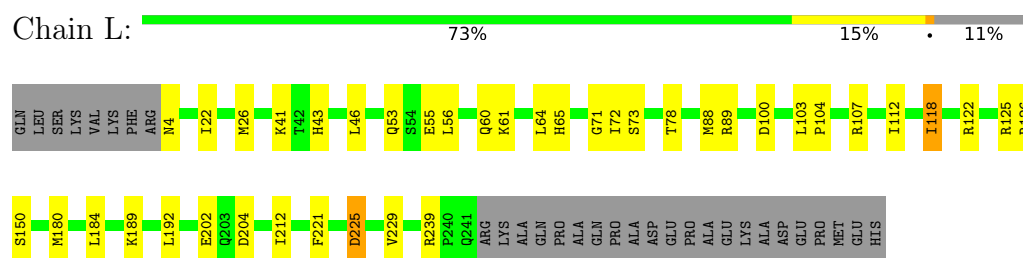
- Molecule 9: Proteasome subunit alpha type-7



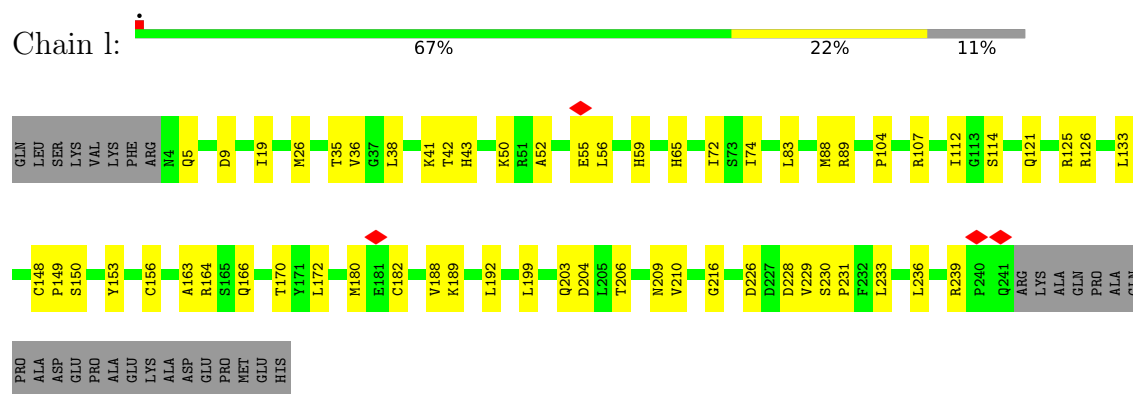
- Molecule 9: Proteasome subunit alpha type-7




- Molecule 10: Isoform Long of Proteasome subunit alpha type-1

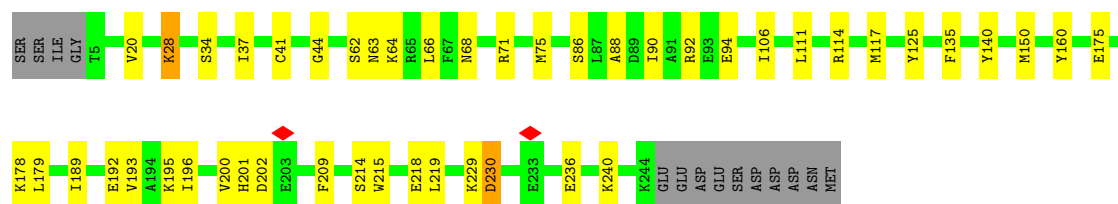


- Molecule 10: Isoform Long of Proteasome subunit alpha type-1



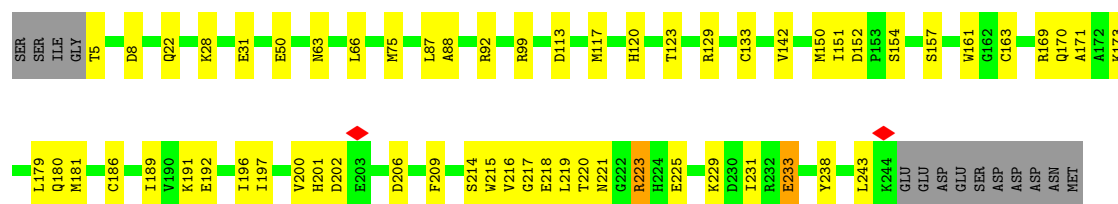
- Molecule 11: Proteasome subunit alpha type-3

Chain M:  76% 18% 6%



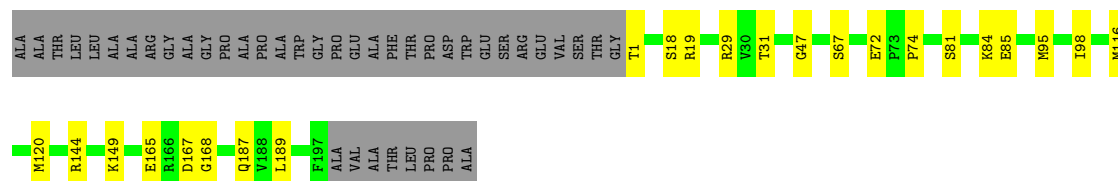
- Molecule 11: Proteasome subunit alpha type-3

Chain m:  71% 23% 6%




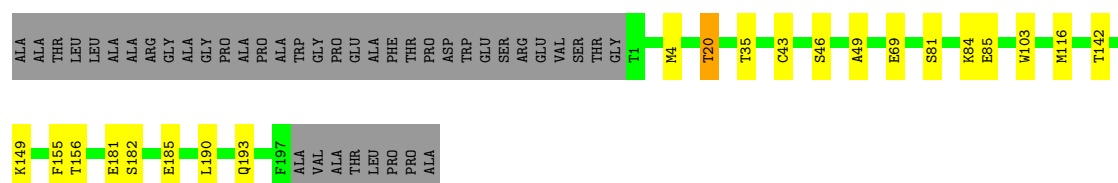
- Molecule 12: Proteasome subunit beta type-6

Chain N:  73% 10% 17%



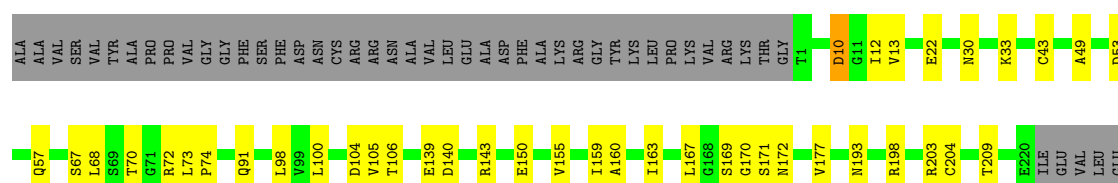
- Molecule 12: Proteasome subunit beta type-6

Chain n:  74% 8% 17%



- Molecule 13: Proteasome subunit beta type-7

Chain O:  65% 14% 20%



GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER


• Molecule 13: Proteasome subunit beta type-7

Chain o:  63% 16% 20%

ALA
ALA
VAL
SER
VAL
TYR
ALA
PRO
VAL
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ASN
ALA
VAL
LEU
GLU
ALA
PHE
ASP
ALA
LYS
ARG
GLY
TYR
LYS
LEU
PRO
LYS
VAL
ARG
LYS
THR
GLY
T1
V7
G11
I12
T18
R19
A20
C43
A46
G47
T48
A49
A50


VAL
LEU
GLU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

• Molecule 14: Proteasome subunit beta type-3

Chain P:  83% 17%


S2
M14
K15
Q31
A32
T58
Q61
T62
Q65
K77
R80
P107
D113
T116
F117
K118
P119
F120
I121
L124
D125
L126
D134
D135
C142
Q145
C150
E151
S152
H162
L163
F164
E165
N173
R177
I189
K201
D205

• Molecule 14: Proteasome subunit beta type-3

Chain p:  86% 13% .

S2
V11
M12
A13
M14
A24
R27
Q31
L73
P107
D113
F114
K115
T116
F117
C122
S123
L124
I127
D135
F136
V137
V138
C142
M146
M171
V175
D176
R177
M183
I189
I190
I195
R203
M204
D205

• Molecule 15: Proteasome subunit beta type-2

Chain Q:  80% 19% .

H1
L4
Q8
L14
V20
A21
V26
Q27
M28
K29
M35
M38
V47
M69
A81
M82
F83
T84
R85
R86
N101
L102
L103
L104
D108
E111
G112
P113
M118
L124
H132
T150
I151
S152
R155
L160
R161
K162
C163
L164

L167
T177
R181
D184
K186
S195
F196
P197
K198
Q199
GLY
SER

• Molecule 15: Proteasome subunit beta type-2

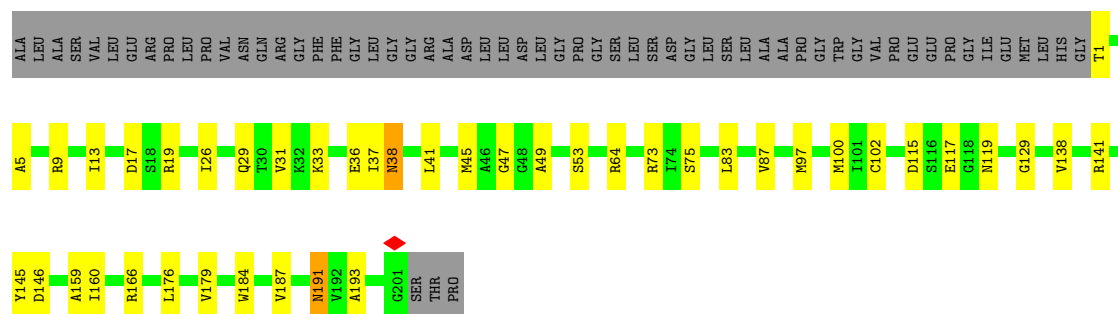
Chain q:  75% 24% .

H1
L4
Q8
G9
V13
D18
N24
M38
L43
L44
L45
C46
V47
G48
E49
A50
G51
D52
T53
V54
E58
Y59
I60
V64
L88
S94
R95
Y98
N101
L102
L103
D108
E109
H110
E111
G112
P113
M118
D119
Y120
L121
A122
H132

L138
D144
T148
R156
L164
L167
P176
T177
I183
N186
H189
D190
L191
F196
P197
K198
Q199
GLY
SER

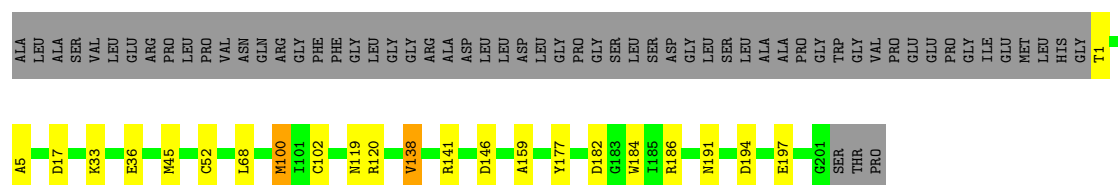
- Molecule 16: Proteasome subunit beta type-5

Chain R:  60% 16% 23%



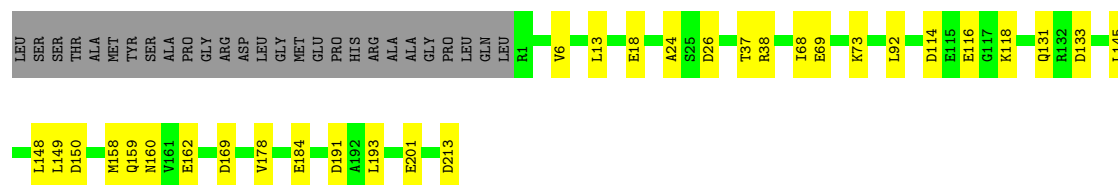
- Molecule 16: Proteasome subunit beta type-5

Chain r:  68% 8% 23%



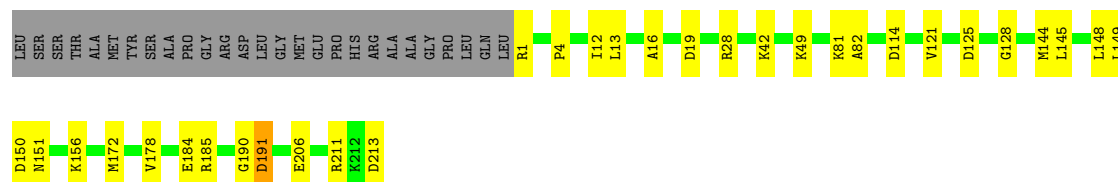
- Molecule 17: Proteasome subunit beta type-1

Chain S:  76% 13% 11%



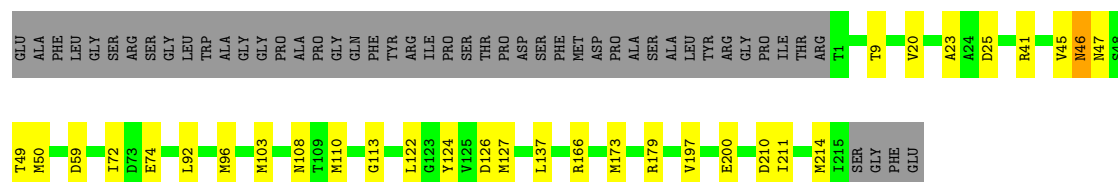
- Molecule 17: Proteasome subunit beta type-1

Chain s:  76% 12% 11%



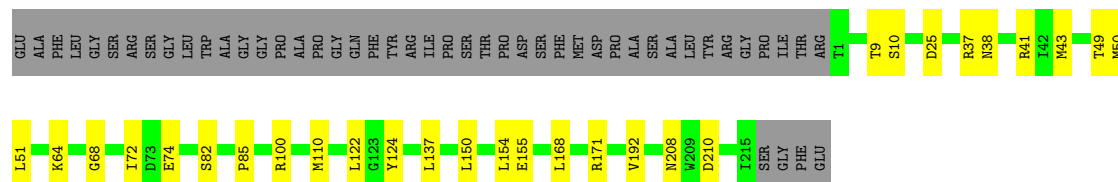
- Molecule 18: Proteasome subunit beta type-4

Chain T:  70% 12% 18%



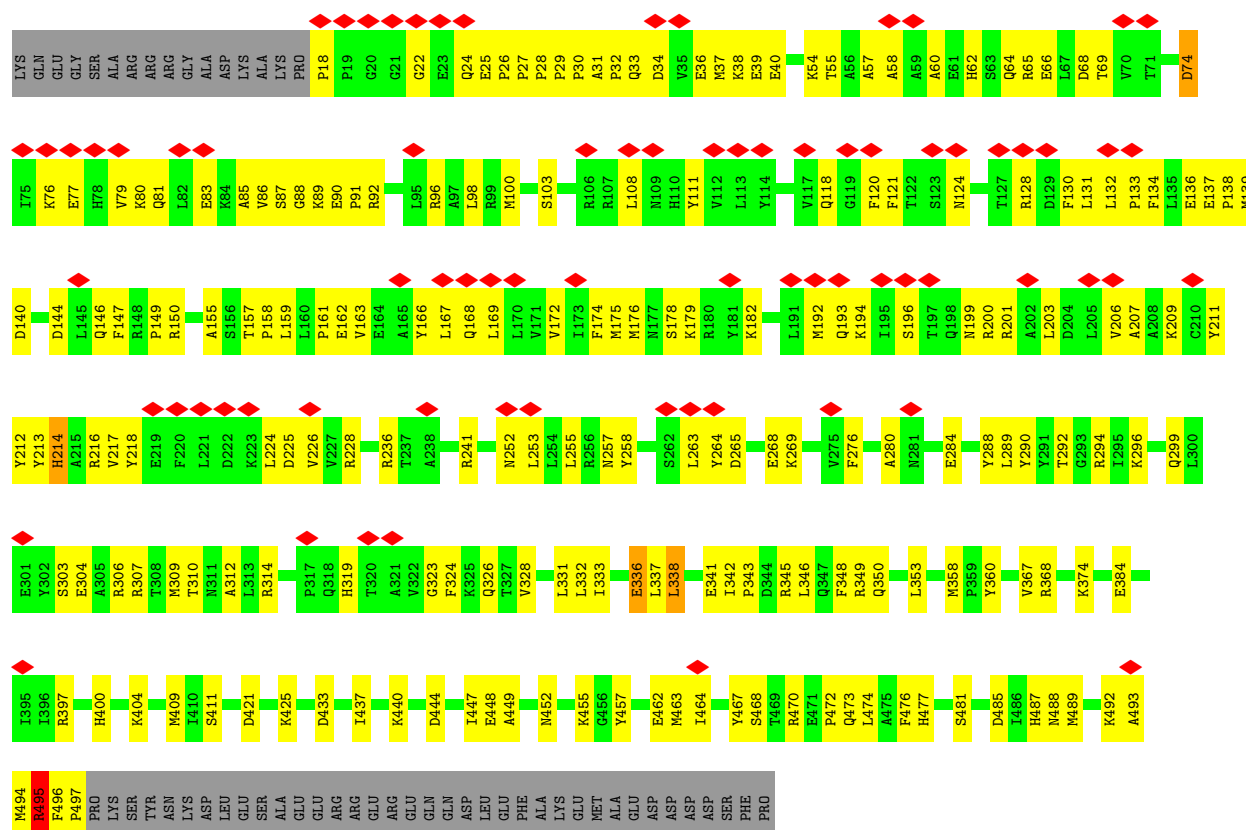
• Molecule 18: Proteasome subunit beta type-4

Chain t: 71% 11% 18%



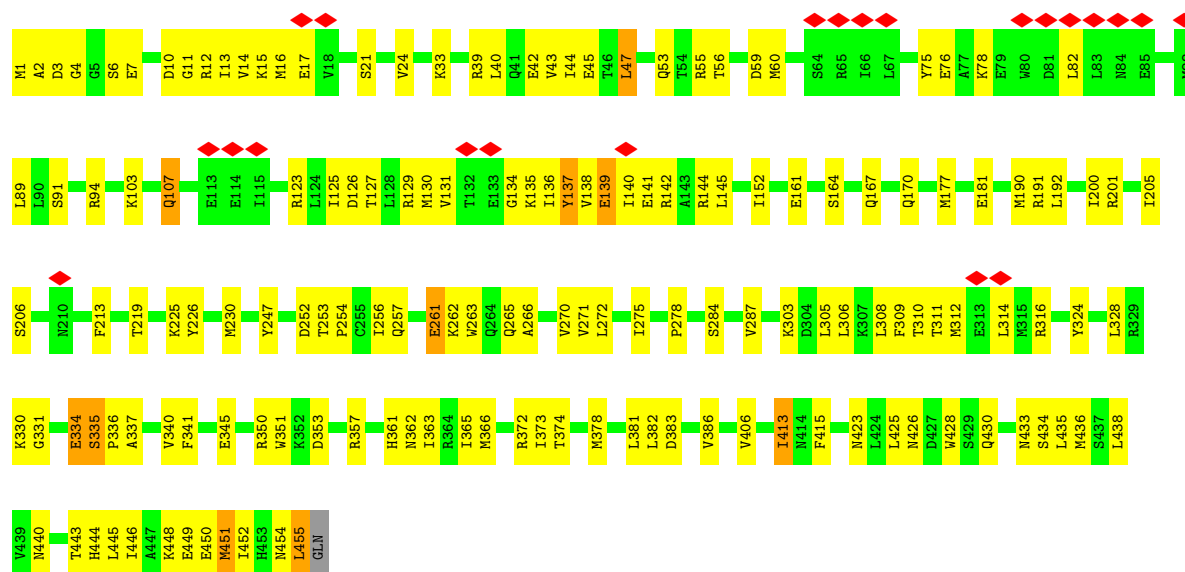
• Molecule 19: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 14% 52% 38% 10%



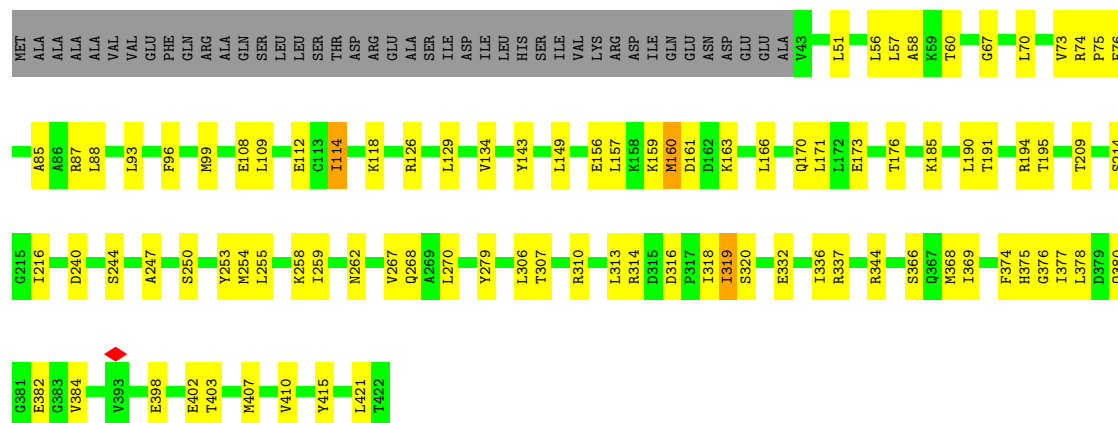
• Molecule 20: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 5% 66% 32%



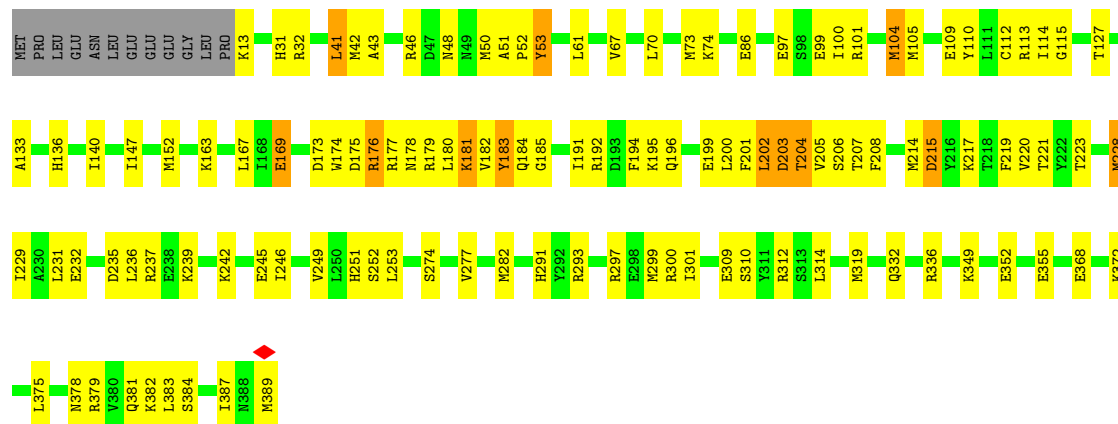
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 68% 21% 10%

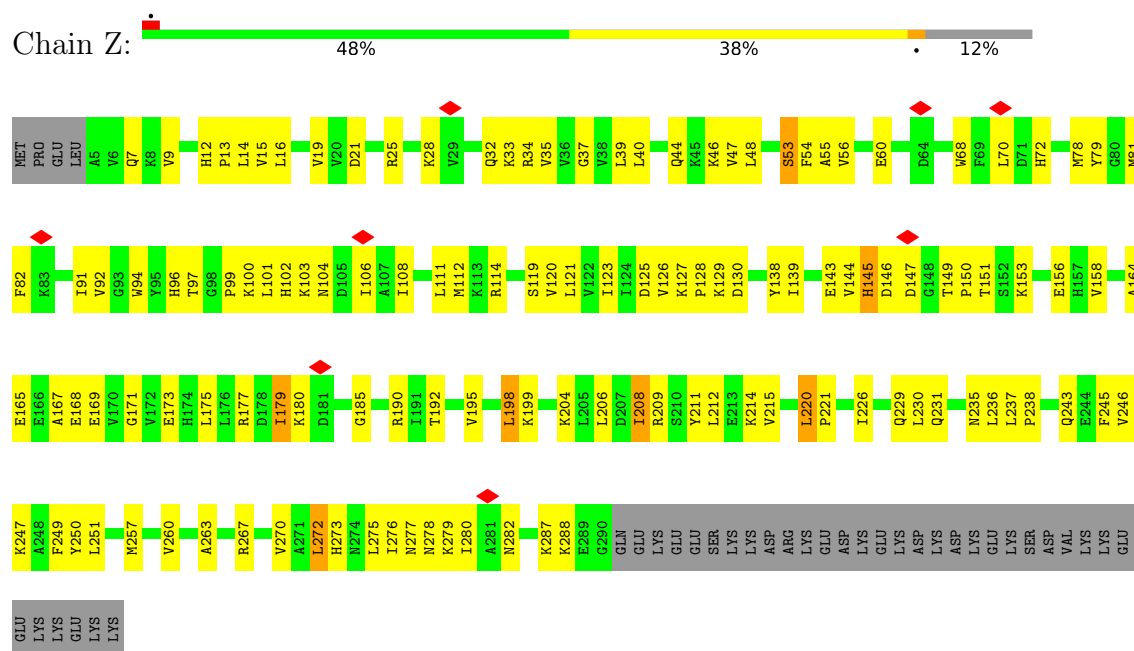


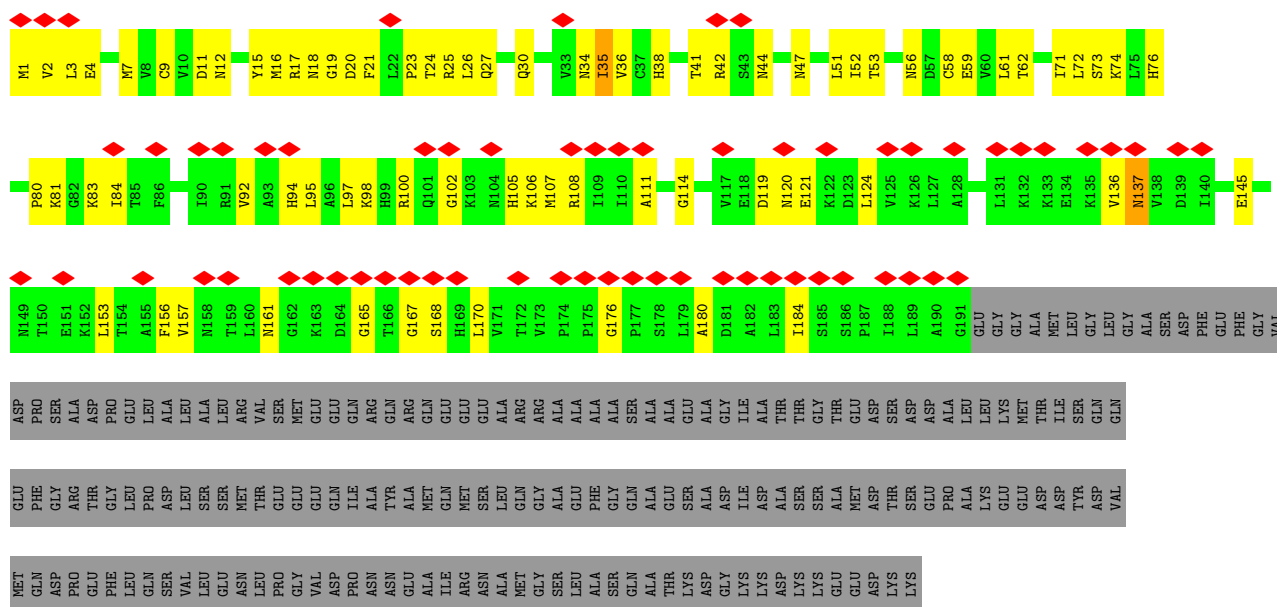
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 66% 28% 6%

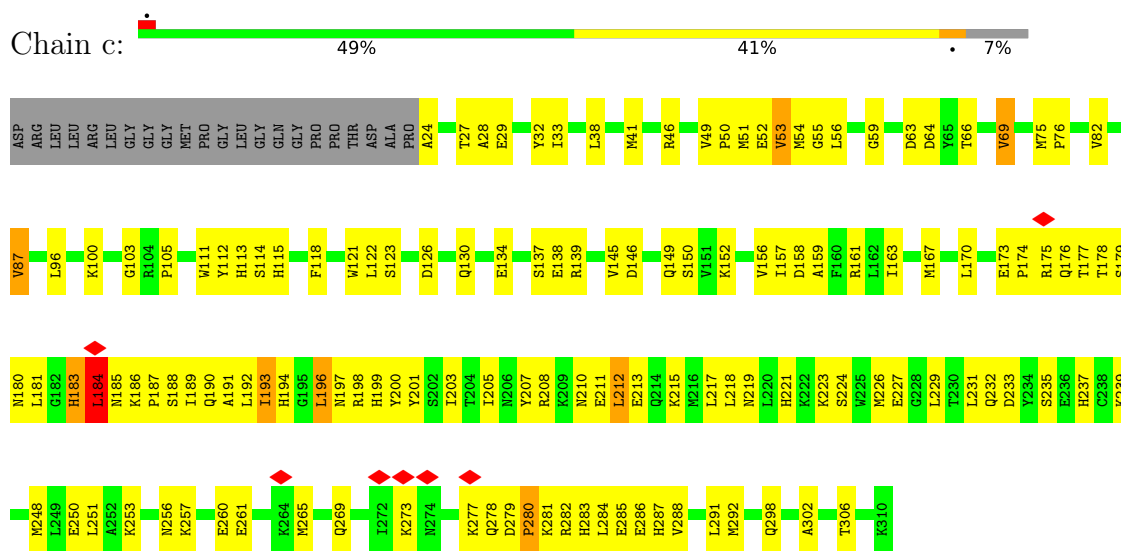


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 7

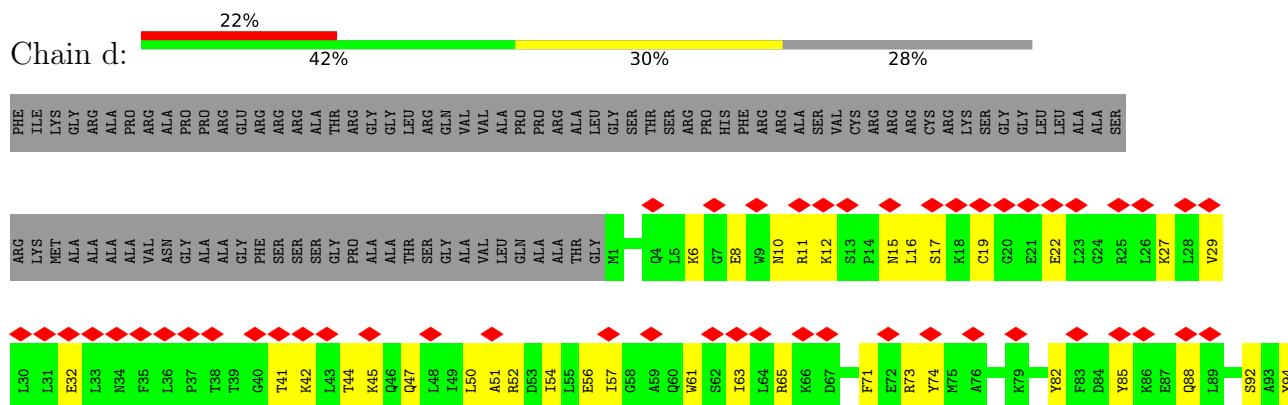


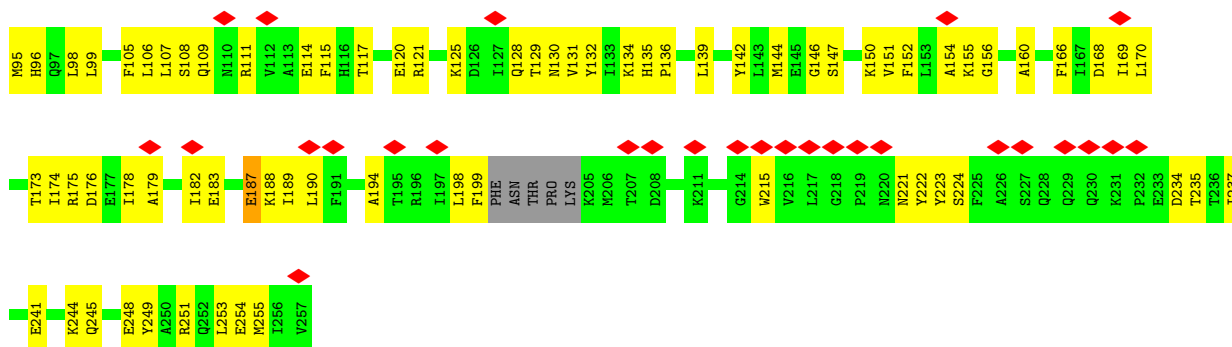


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 14

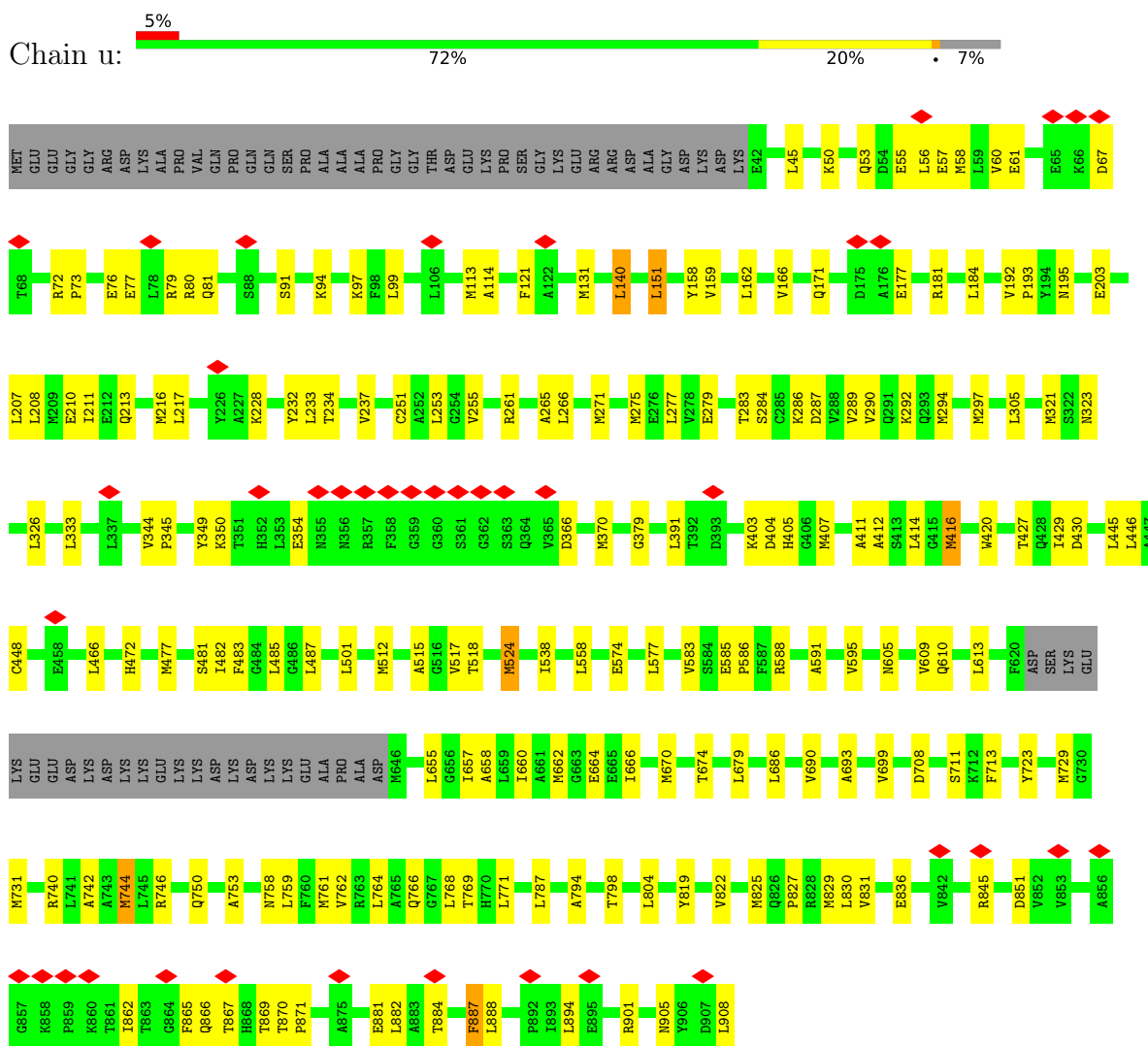


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 8

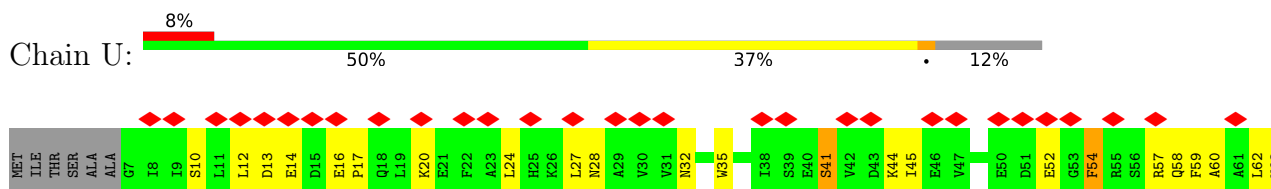


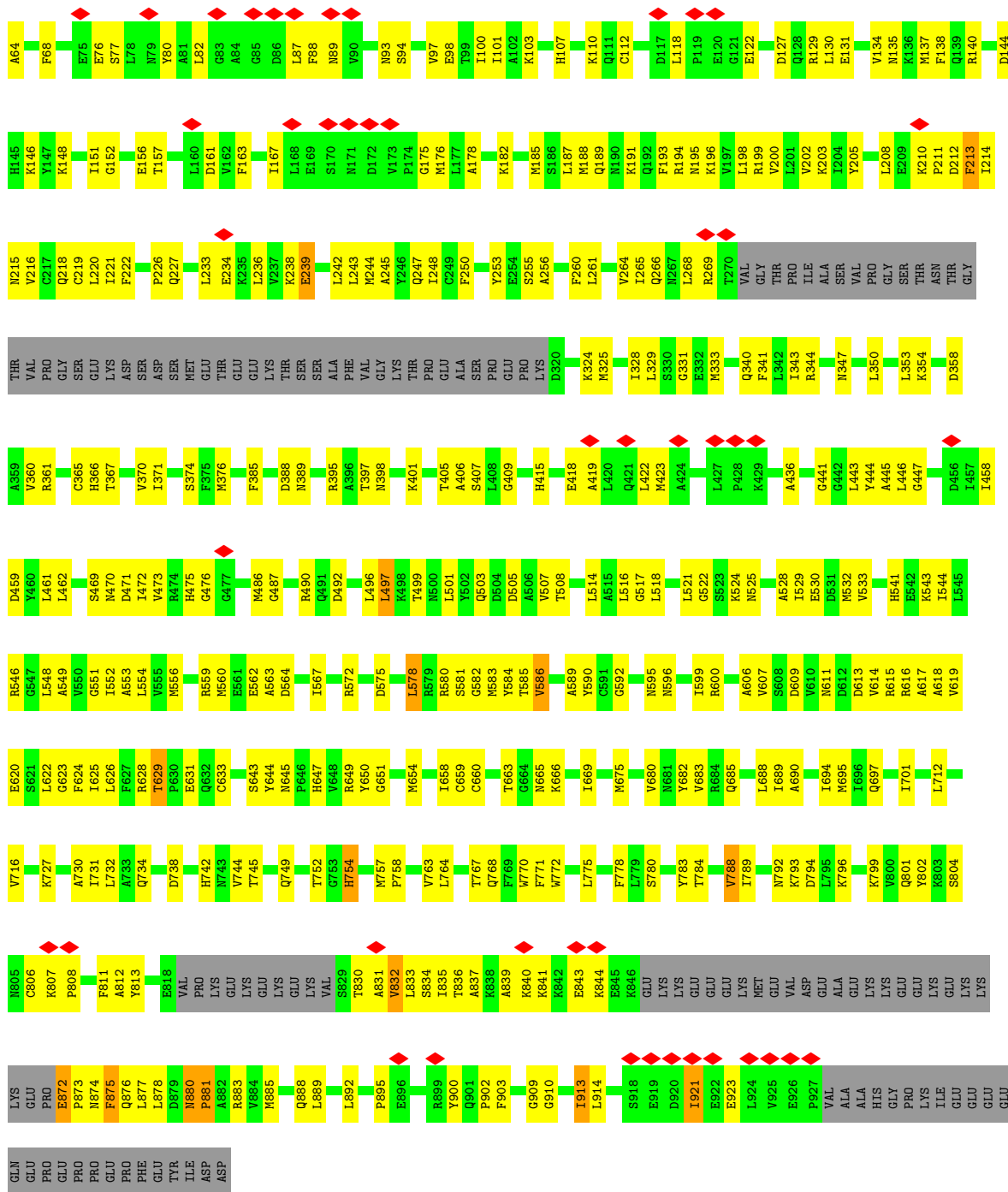


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 2



• Molecule 29: 26S proteasome non-ATPase regulatory subunit 1

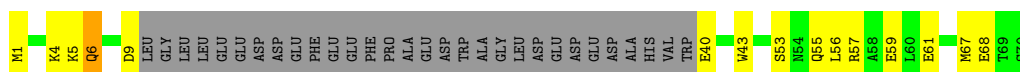




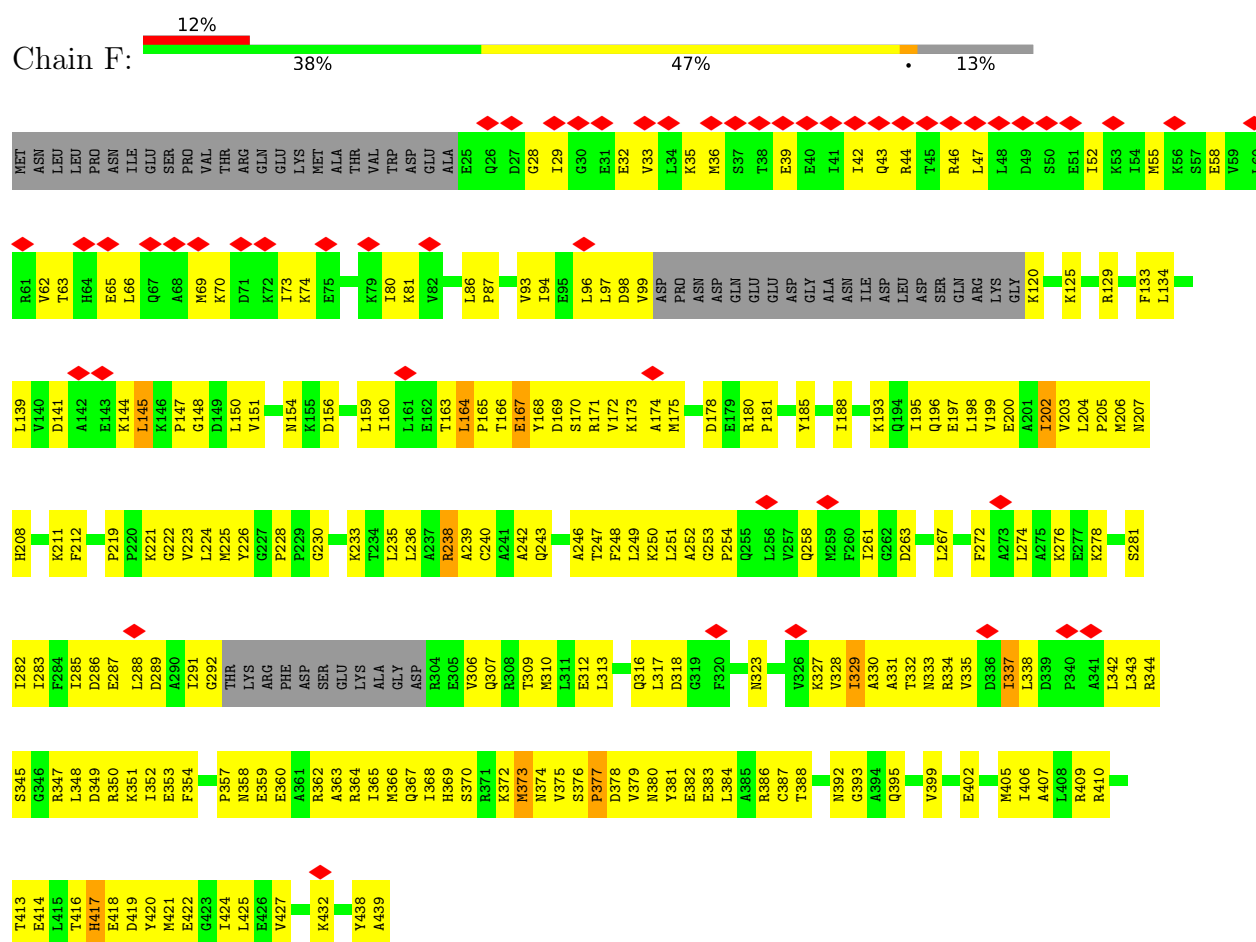
- Molecule 30: 26S proteasome complex subunit SEM1

Chain e:

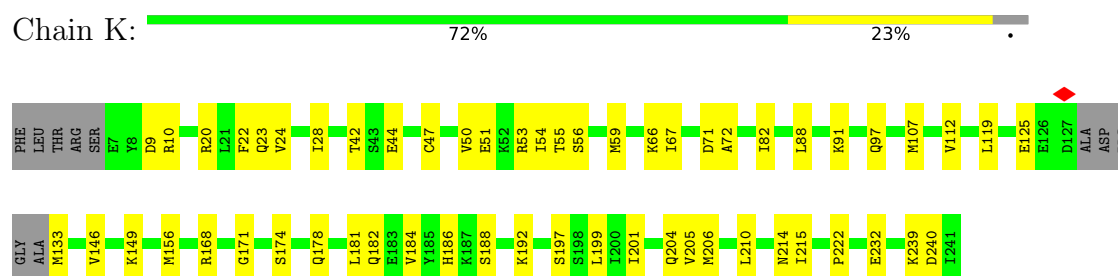
36% 20% 43%



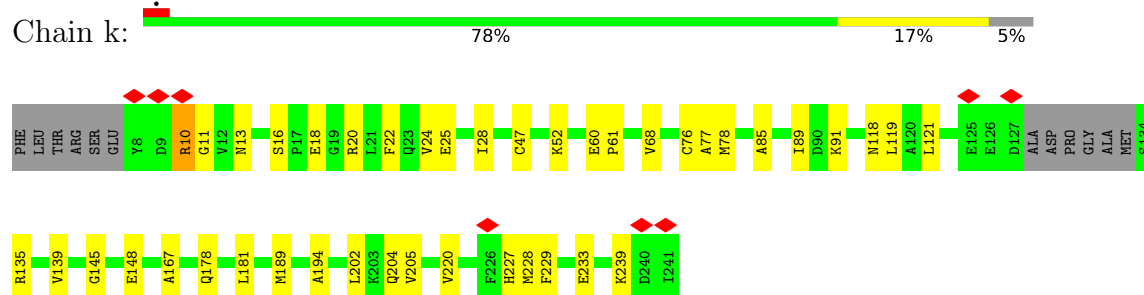
- Molecule 31: 26S proteasome regulatory subunit 6A



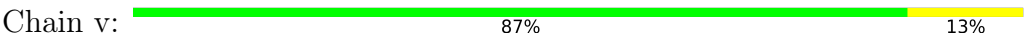
• Molecule 32: Proteasome subunit alpha type-5



• Molecule 32: Proteasome subunit alpha type-5



• Molecule 33: substrate peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.402	Depositor
Minimum map value	-1.074	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

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: ATP, LDZ, ZN, MG, ADP

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	0.40	0/3280	0.66	2/4429 (0.0%)
2	B	0.27	0/3248	0.51	0/4381
3	C	0.27	0/3146	0.50	0/4226
4	D	0.39	0/3084	0.62	2/4161 (0.0%)
5	E	0.43	0/3077	0.61	0/4141
6	G	0.18	0/1842	0.46	0/2500
6	g	0.20	0/1863	0.41	0/2527
7	H	0.16	0/1738	0.39	0/2364
7	h	0.19	0/1764	0.41	0/2399
8	I	0.25	0/1925	0.52	0/2606
8	i	0.19	0/1942	0.49	0/2628
9	J	0.19	0/1869	0.50	0/2531
9	j	0.25	0/1728	0.54	0/2358
10	L	0.14	0/1885	0.36	0/2552
10	l	0.23	0/1885	0.42	0/2552
11	M	0.24	0/1891	0.47	1/2552 (0.0%)
11	m	0.24	0/1897	0.48	0/2559
12	N	0.16	0/1508	0.42	0/2040
12	n	0.15	0/1508	0.32	0/2040
13	O	0.35	0/1670	0.55	0/2265
13	o	0.17	0/1670	0.41	0/2265
14	P	0.18	0/1620	0.42	0/2184
14	p	0.19	0/1620	0.43	0/2184
15	Q	0.13	0/1603	0.37	0/2174
15	q	0.16	0/1607	0.39	0/2178
16	R	0.18	0/1579	0.36	0/2134
16	r	0.14	0/1579	0.35	0/2134
17	S	0.16	0/1671	0.39	0/2253
17	s	0.20	0/1671	0.40	0/2253
18	T	0.16	0/1700	0.39	0/2305
18	t	0.17	0/1706	0.39	0/2312
19	V	0.31	0/3929	0.58	1/5309 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
20	W	0.29	0/3733	0.52	0/5021
21	X	0.34	0/3047	0.51	0/4108
22	Y	0.39	0/3165	0.62	0/4262
23	Z	0.35	0/2320	0.62	0/3145
24	a	0.28	0/3053	0.52	0/4133
25	b	0.17	0/1478	0.41	0/2001
26	c	0.43	0/2296	0.68	0/3103
27	d	0.25	0/2117	0.49	0/2856
28	u	0.25	0/6625	0.43	0/8968
29	U	0.32	0/6642	0.54	0/8983
30	e	0.37	0/338	0.72	0/450
31	F	0.35	0/3042	0.61	0/4097
32	K	0.16	0/1776	0.39	0/2401
32	k	0.18	0/1747	0.45	0/2364
All	All	0.27	0/106084	0.50	6/143388 (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
8	I	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	123	LEU	N-CA-C	-6.93	105.38	114.31
1	A	159	PRO	N-CA-CB	-6.08	96.87	103.25
1	A	314	ASN	N-CA-C	-5.82	105.45	112.54
4	D	158	GLN	N-CA-C	-5.53	104.78	113.02
19	V	214	HIS	N-CA-C	-5.11	105.79	111.36
11	M	44	GLY	CA-C-O	-5.03	118.25	122.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	128	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3226	0	3259	321	0
2	B	3201	0	3267	167	0
3	C	3105	0	3219	176	0
4	D	3034	0	3065	162	0
5	E	3031	0	3103	277	0
6	G	1809	0	1781	40	0
6	g	1830	0	1807	37	0
7	H	1703	0	1599	31	0
7	h	1727	0	1619	36	0
8	I	1895	0	1833	55	0
8	i	1912	0	1851	44	0
9	J	1844	0	1747	38	0
9	j	1704	0	1517	53	0
10	L	1850	0	1822	31	0
10	l	1850	0	1822	41	0
11	M	1856	0	1816	32	0
11	m	1862	0	1827	45	0
12	N	1482	0	1450	14	0
12	n	1482	0	1450	12	0
13	O	1643	0	1644	34	0
13	o	1643	0	1644	37	0
14	P	1591	0	1609	32	0
14	p	1591	0	1609	20	0
15	Q	1570	0	1547	26	0
15	q	1574	0	1558	31	0
16	R	1548	0	1499	30	0
16	r	1548	0	1499	15	0
17	S	1641	0	1618	21	0
17	s	1641	0	1618	25	0
18	T	1667	0	1628	25	0
18	t	1673	0	1639	23	0
19	V	3852	0	3893	227	0
20	W	3685	0	3799	192	0
21	X	3003	0	3102	88	0
22	Y	3108	0	3112	173	0
23	Z	2277	0	2306	169	0
24	a	2995	0	3012	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	b	1458	0	1505	74	0
26	c	2254	0	2265	160	0
27	d	2074	0	2103	125	0
28	u	6514	0	6527	178	0
29	U	6529	0	6572	362	0
30	e	334	0	294	24	0
31	F	3005	0	3093	246	0
32	K	1750	0	1706	50	0
32	k	1722	0	1673	39	0
33	v	75	0	20	1	0
34	A	27	0	12	2	0
34	E	27	0	12	3	0
34	F	27	0	12	2	0
35	B	31	0	12	1	0
35	C	31	0	12	0	0
35	D	31	0	12	3	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
37	N	34	0	41	2	0
37	O	34	0	41	5	0
37	R	34	0	41	4	0
37	n	34	0	41	2	0
37	o	34	0	41	4	0
37	r	34	0	41	1	0
38	c	1	0	0	0	0
All	All	104750	0	104266	3856	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 18.

All (3856) 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)
29:U:623:GLY:HA2	29:U:659:CYS:SG	1.78	1.24
19:V:62:HIS:CE1	22:Y:389:MET:HE1	1.81	1.15
21:X:159:LYS:HA	21:X:159:LYS:HE3	1.19	1.15
22:Y:282:MET:HE3	22:Y:291:HIS:HB3	1.26	1.14
1:A:156:LYS:HE2	2:B:114:GLU:HB3	1.15	1.14
3:C:66:LEU:HD12	4:D:114:ARG:HD3	1.26	1.13
3:C:147:THR:HG22	3:C:150:MET:HE3	1.29	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:65:ARG:HH21	19:V:66:GLU:HG3	1.04	1.11
29:U:812:ALA:HA	29:U:885:MET:HE1	1.16	1.11
4:D:45:LYS:HG2	29:U:187:LEU:HD11	1.30	1.11
28:u:56:LEU:HD23	28:u:99:LEU:HD21	1.33	1.10
29:U:623:GLY:CA	29:U:659:CYS:SG	2.40	1.09
27:d:120:GLU:OE2	27:d:121:ARG:NH1	1.86	1.09
20:W:425:LEU:HD11	23:Z:247:LYS:HD3	1.33	1.08
1:A:268:LYS:HE3	1:A:314:ASN:H	1.13	1.08
29:U:529:ILE:O	29:U:533:VAL:HG12	1.52	1.07
1:A:418:LYS:HA	1:A:422:LYS:HB2	1.34	1.07
20:W:275:ILE:HG13	20:W:308:LEU:HD22	1.36	1.06
29:U:836:THR:HB	29:U:840:LYS:HE2	1.37	1.05
1:A:22:ILE:HG12	3:C:159:LYS:HD3	1.04	1.04
19:V:62:HIS:HE1	22:Y:389:MET:HE1	0.94	1.04
5:E:310:LEU:HG	5:E:332:VAL:HG21	1.38	1.03
4:D:408:LYS:HE2	4:D:408:LYS:HA	1.39	1.02
31:F:93:VAL:HG23	31:F:147:PRO:HA	1.40	1.02
31:F:309:THR:HG23	31:F:312:GLU:OE1	1.57	1.02
7:H:68:ILE:HD11	7:H:74:LEU:HG	1.41	1.01
5:E:81:VAL:HG21	5:E:107:ILE:HD11	1.42	1.00
29:U:560:MET:HE1	29:U:590:TYR:HA	1.43	1.00
5:E:127:PRO:HA	5:E:185:ARG:HH22	1.28	0.99
2:B:176:VAL:HG12	2:B:247:PHE:O	1.64	0.98
1:A:135:GLU:H	1:A:138:MET:HE2	1.22	0.98
22:Y:113:ARG:HG2	22:Y:114:ILE:HD12	1.44	0.98
1:A:157:ILE:HG12	1:A:158:ASP:H	1.28	0.98
2:B:382:ASP:HA	2:B:385:MET:SD	2.02	0.98
1:A:173:THR:HA	1:A:231:ASN:HD21	1.28	0.96
20:W:1:MET:HE3	20:W:43:VAL:HG13	1.47	0.96
21:X:369:ILE:HG21	22:Y:310:SER:HB2	1.44	0.96
2:B:75:GLU:OE1	28:u:674:THR:HG22	1.64	0.96
20:W:316:ARG:HH22	20:W:381:LEU:HA	1.27	0.96
1:A:268:LYS:CE	1:A:314:ASN:H	1.79	0.95
20:W:372:ARG:NH1	24:a:327:VAL:HG23	1.80	0.95
1:A:258:ARG:HA	1:A:305:GLN:HE22	1.31	0.95
28:u:711:SER:HB2	28:u:729:MET:HE1	1.46	0.95
5:E:303:LEU:HG	5:E:338:PHE:HB3	1.47	0.95
19:V:255:LEU:HD13	19:V:269:LYS:HZ3	1.31	0.95
1:A:329:PRO:HA	1:A:332:MET:HE1	1.47	0.95
28:u:731:MET:O	28:u:731:MET:HE3	1.66	0.95
29:U:694:ILE:HG23	29:U:695:MET:HE3	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:334:GLU:HG2	20:W:337:ALA:HB3	1.49	0.94
1:A:156:LYS:CE	2:B:114:GLU:HB3	1.97	0.94
1:A:250:VAL:HA	1:A:294:GLU:HB2	1.48	0.94
3:C:213:ARG:NH1	4:D:299:PHE:HB2	1.83	0.94
24:a:80:ILE:O	24:a:84:VAL:HG23	1.67	0.94
24:a:308:GLU:HG3	24:a:312:MET:CE	1.98	0.94
31:F:225:MET:HE1	31:F:329:ILE:HG22	1.48	0.94
14:p:190:ILE:HG22	14:p:195:ILE:HG12	1.50	0.93
23:Z:167:ALA:HB2	26:c:46:ARG:HH11	1.33	0.93
19:V:130:PHE:HB3	19:V:133:PRO:HG2	1.45	0.93
28:u:609:VAL:O	28:u:613:LEU:HD12	1.69	0.93
22:Y:229:ILE:HD12	22:Y:299:MET:HE2	1.48	0.92
19:V:65:ARG:NH2	19:V:66:GLU:HG3	1.82	0.92
22:Y:43:ALA:HA	22:Y:46:ARG:CZ	1.99	0.92
23:Z:129:LYS:HZ1	26:c:215:LYS:HG3	1.30	0.92
32:K:107:MET:HE3	32:K:112:VAL:HG22	1.52	0.92
1:A:394:MET:HE2	1:A:394:MET:HA	1.51	0.92
23:Z:220:LEU:HB2	23:Z:221:PRO:HD2	1.51	0.92
24:a:308:GLU:HG3	24:a:312:MET:HE1	1.52	0.91
2:B:221:GLY:HA3	2:B:347:ILE:HD12	1.49	0.91
29:U:58:GLN:OE1	29:U:58:GLN:N	2.02	0.91
31:F:309:THR:HA	31:F:312:GLU:HG2	1.52	0.91
10:L:60:GLN:NE2	31:F:439:ALA:HB3	1.83	0.91
1:A:268:LYS:HE3	1:A:314:ASN:N	1.85	0.91
1:A:317:VAL:HG12	1:A:319:MET:HE1	1.49	0.91
22:Y:70:LEU:HB3	22:Y:73:MET:HE3	1.53	0.91
3:C:338:LEU:HD21	3:C:342:ILE:HG21	1.52	0.91
1:A:296:GLN:HG2	31:F:174:ALA:HB1	1.50	0.90
24:a:12:GLN:HG2	24:a:18:GLN:HG2	1.51	0.90
20:W:372:ARG:HH12	24:a:327:VAL:H	1.15	0.90
20:W:430:GLN:HA	20:W:433:ASN:ND2	1.86	0.90
4:D:121:ARG:HA	4:D:124:LEU:HD13	1.50	0.90
5:E:121:ASN:OD1	5:E:122:MET:N	2.04	0.90
27:d:22:GLU:HG2	27:d:61:TRP:HZ3	1.36	0.90
31:F:381:TYR:HA	31:F:384:LEU:HG	1.52	0.90
5:E:101:ASP:HA	5:E:108:MET:HE2	1.54	0.89
29:U:836:THR:HB	29:U:840:LYS:CE	2.02	0.89
1:A:292:ASP:C	31:F:171:ARG:HH22	1.79	0.89
1:A:200:ARG:HA	1:A:203:ASN:OD1	1.73	0.89
1:A:332:MET:HA	1:A:337:LEU:HB2	1.55	0.89
28:u:275:MET:HA	28:u:275:MET:HE3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:65:ARG:HH21	19:V:66:GLU:CG	1.85	0.88
23:Z:263:ALA:HB1	26:c:292:MET:HE2	1.53	0.88
31:F:378:ASP:HA	31:F:417:HIS:HA	1.56	0.88
26:c:279:ASP:HA	26:c:283:HIS:HB2	1.55	0.88
29:U:532:MET:HE1	29:U:551:GLY:HA3	1.55	0.88
5:E:179:GLY:HA2	5:E:182:LEU:HD23	1.53	0.88
5:E:26:LEU:HD21	31:F:55:MET:HE3	1.55	0.88
24:a:12:GLN:HA	24:a:22:TRP:CZ3	2.09	0.87
28:u:266:LEU:HD23	28:u:297:MET:HE3	1.56	0.87
29:U:52:GLU:HA	29:U:57:ARG:HH21	1.40	0.87
1:A:169:LYS:HG2	1:A:234:ASP:OD1	1.74	0.87
20:W:142:ARG:HD2	20:W:145:LEU:HD11	1.55	0.87
23:Z:257:MET:HA	23:Z:257:MET:HE2	1.54	0.87
29:U:532:MET:SD	29:U:552:ILE:HG23	2.14	0.87
3:C:405:TRP:HE1	8:I:30:HIS:HB2	1.37	0.87
28:u:213:GLN:HB3	28:u:216:MET:CE	2.04	0.87
10:L:88:MET:HG2	10:L:112:ILE:HD11	1.54	0.87
23:Z:167:ALA:HB2	26:c:46:ARG:NH1	1.88	0.87
19:V:358:MET:HA	19:V:358:MET:HE3	1.55	0.87
4:D:45:LYS:CG	29:U:187:LEU:HD11	2.04	0.86
18:T:126:ASP:OD2	18:T:127:MET:N	2.07	0.86
29:U:836:THR:CB	29:U:840:LYS:HE2	2.06	0.86
22:Y:192:ARG:HH21	22:Y:194:PHE:HB3	1.41	0.86
1:A:191:VAL:HG21	1:A:232:ARG:NH2	1.89	0.86
29:U:701:ILE:HD11	29:U:811:PHE:HB3	1.56	0.86
21:X:368:MET:HG2	21:X:374:PHE:HB3	1.57	0.86
21:X:159:LYS:HE3	21:X:159:LYS:CA	2.03	0.85
24:a:12:GLN:HA	24:a:22:TRP:CE3	2.11	0.85
24:a:308:GLU:O	24:a:312:MET:HE3	1.76	0.85
28:u:869:THR:HG23	28:u:871:PRO:HD2	1.57	0.85
29:U:250:PHE:CE2	29:U:328:ILE:HG13	2.10	0.85
21:X:368:MET:HE2	21:X:374:PHE:HB2	1.57	0.85
1:A:22:ILE:HG12	3:C:159:LYS:CD	2.00	0.85
29:U:675:MET:HA	29:U:675:MET:HE3	1.59	0.85
4:D:338:ARG:C	4:D:340:GLN:H	1.85	0.84
29:U:844:LYS:HA	29:U:844:LYS:HE3	1.59	0.84
32:K:51:GLU:HB2	32:K:206:MET:HE2	1.58	0.84
1:A:285:PHE:HA	1:A:296:GLN:HE22	1.41	0.84
4:D:374:ASP:OD1	5:E:292:PRO:HG2	1.76	0.84
22:Y:110:TYR:HA	22:Y:113:ARG:NH1	1.93	0.84
23:Z:236:LEU:HD23	23:Z:236:LEU:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:224:SER:HB2	26:c:227:GLU:HG3	1.60	0.84
28:u:213:GLN:O	28:u:216:MET:HE3	1.77	0.84
20:W:275:ILE:CG1	20:W:308:LEU:HD22	2.07	0.84
28:u:723:TYR:HB3	28:u:761:MET:HE2	1.57	0.84
10:l:83:LEU:HD11	32:k:121:LEU:HD11	1.60	0.84
1:A:305:GLN:HA	1:A:309:PHE:HB2	1.60	0.84
19:V:489:MET:N	19:V:489:MET:HE3	1.93	0.84
2:B:191:ASP:HA	2:B:194:ILE:HD12	1.59	0.83
27:d:144:MET:HA	27:d:144:MET:HE3	1.59	0.83
3:C:338:LEU:HD21	3:C:342:ILE:HD13	1.60	0.83
33:v:23:UNK:O	33:v:24:UNK:CB	2.24	0.83
20:W:425:LEU:CD1	23:Z:247:LYS:HD3	2.08	0.83
27:d:10:ASN:HB2	27:d:11:ARG:NH1	1.94	0.83
26:c:152:LYS:HA	26:c:152:LYS:CE	2.09	0.82
1:A:22:ILE:HG21	3:C:159:LYS:NZ	1.93	0.82
3:C:129:ASN:HB2	4:D:94:GLU:OE2	1.80	0.82
9:J:239:ASN:HA	9:J:243:LYS:HB2	1.61	0.82
11:M:66:LEU:HD13	11:M:214:SER:OG	1.79	0.82
23:Z:179:ILE:HD12	23:Z:180:LYS:H	1.45	0.82
5:E:121:ASN:OD1	5:E:122:MET:SD	2.37	0.82
10:l:26:MET:HE3	10:l:150:SER:HB3	1.61	0.82
29:U:244:MET:HG3	29:U:903:PHE:CZ	2.15	0.82
22:Y:205:VAL:HG23	22:Y:219:PHE:CE2	2.14	0.82
11:m:243:LEU:O	11:m:243:LEU:HD13	1.80	0.82
29:U:185:MET:HE1	29:U:222:PHE:CE2	2.14	0.82
31:F:366:MET:HA	31:F:366:MET:HE3	1.62	0.82
5:E:336:ASP:HB3	5:E:338:PHE:CZ	2.14	0.82
29:U:446:LEU:HD12	29:U:447:GLY:N	1.94	0.82
6:g:212:PRO:HG3	6:g:236:ASP:OD2	1.78	0.81
28:u:487:LEU:HD23	28:u:524:MET:HE1	1.62	0.81
29:U:205:TYR:HB3	29:U:215:ASN:HD22	1.43	0.81
1:A:22:ILE:CG1	3:C:159:LYS:HD3	2.00	0.81
5:E:214:LEU:O	5:E:218:MET:HG3	1.80	0.81
26:c:100:LYS:HG2	26:c:105:PRO:HB3	1.61	0.81
26:c:212:LEU:H	26:c:215:LYS:HG2	1.42	0.81
4:D:394:VAL:HG11	4:D:399:PHE:CE2	2.15	0.81
2:B:362:LYS:HD2	2:B:362:LYS:O	1.81	0.81
19:V:176:MET:N	19:V:176:MET:SD	2.54	0.81
21:X:407:MET:HE2	21:X:407:MET:HA	1.62	0.81
26:c:152:LYS:HA	26:c:152:LYS:HE3	1.62	0.81
1:A:51:ASP:HA	1:A:54:GLN:HG2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HA	1:A:258:ARG:HD2	1.63	0.81
4:D:235:PHE:HB3	4:D:246:MET:SD	2.20	0.81
2:B:362:LYS:HD2	2:B:362:LYS:C	2.04	0.81
3:C:255:GLY:HA2	3:C:273:MET:HG3	1.63	0.81
5:E:87:LEU:HD11	5:E:92:LEU:HD23	1.62	0.81
24:a:308:GLU:C	24:a:312:MET:HE3	2.05	0.81
27:d:254:GLU:HB2	27:d:255:MET:CE	2.10	0.81
4:D:266:GLU:N	4:D:266:GLU:OE2	2.15	0.80
2:B:176:VAL:HG11	2:B:247:PHE:HB3	1.64	0.80
23:Z:129:LYS:NZ	26:c:215:LYS:HG3	1.95	0.80
21:X:159:LYS:HA	21:X:159:LYS:CE	2.04	0.80
24:a:247:ARG:NH1	24:a:251:LEU:HD21	1.97	0.80
1:A:263:MET:HE3	1:A:267:LYS:NZ	1.96	0.80
2:B:84:GLN:OE1	2:B:84:GLN:HA	1.82	0.80
27:d:251:ARG:HA	27:d:255:MET:HE3	1.62	0.79
2:B:174:MET:HG2	2:B:249:ARG:O	1.82	0.79
21:X:114:ILE:HD13	21:X:129:LEU:HD13	1.64	0.79
20:W:316:ARG:NH2	20:W:381:LEU:HA	1.97	0.79
8:i:8:ARG:HB3	8:i:11:ILE:HB	1.64	0.79
31:F:307:GLN:O	31:F:310:MET:HB2	1.83	0.79
20:W:177:MET:HG2	20:W:181:GLU:HB2	1.65	0.79
24:a:141:MET:N	24:a:141:MET:HE2	1.98	0.79
1:A:329:PRO:HA	1:A:332:MET:CE	2.12	0.78
5:E:231:PHE:CD1	5:E:276:ILE:HD11	2.18	0.78
2:B:174:MET:SD	2:B:250:VAL:HG22	2.23	0.78
1:A:84:LYS:HA	1:A:87:LEU:HD23	1.65	0.78
3:C:147:THR:CG2	3:C:150:MET:HE3	2.13	0.78
3:C:171:HIS:O	3:C:174:LEU:HD23	1.83	0.78
7:h:228:ASP:OD2	7:h:229:TYR:N	2.16	0.78
29:U:694:ILE:CG2	29:U:695:MET:HE3	2.13	0.78
29:U:222:PHE:CE1	29:U:754:HIS:CE1	2.71	0.78
31:F:377:PRO:HA	31:F:380:ASN:HB2	1.65	0.78
4:D:369:LYS:H	4:D:369:LYS:HD3	1.47	0.78
25:b:108:ARG:HH11	25:b:137:ASN:HD22	1.31	0.78
2:B:358:GLU:OE1	2:B:358:GLU:N	2.15	0.78
29:U:518:LEU:HD23	29:U:554:LEU:CD2	2.14	0.78
5:E:310:LEU:HG	5:E:332:VAL:CG2	2.12	0.78
5:E:322:LYS:HA	5:E:362:VAL:H	1.49	0.78
1:A:317:VAL:HG12	1:A:319:MET:CE	2.12	0.78
24:a:267:GLN:HB3	24:a:270:ARG:HH12	1.49	0.78
12:N:95:MET:HG3	12:N:116:MET:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:38:LYS:HA	19:V:38:LYS:HE3	1.64	0.77
24:a:83:VAL:O	24:a:87:MET:HE2	1.83	0.77
21:X:262:ASN:O	21:X:262:ASN:OD1	2.02	0.77
15:q:38:MET:HE1	15:q:60:ILE:HG22	1.67	0.77
31:F:282:ILE:HG22	31:F:327:LYS:HB2	1.65	0.77
28:u:515:ALA:O	28:u:518:THR:HG22	1.84	0.77
23:Z:139:ILE:HB	23:Z:156:GLU:OE2	1.84	0.77
2:B:429:LYS:O	2:B:429:LYS:NZ	2.15	0.77
4:D:408:LYS:HA	4:D:408:LYS:CE	2.15	0.77
22:Y:199:GLU:O	22:Y:203:ASP:HB3	1.85	0.77
22:Y:229:ILE:CD1	22:Y:299:MET:HE2	2.16	0.77
9:j:45:VAL:HG23	9:j:62:ILE:HD11	1.67	0.77
28:u:113:MET:HE2	28:u:113:MET:HA	1.64	0.77
21:X:369:ILE:CG2	22:Y:310:SER:HB2	2.15	0.76
29:U:236:LEU:HA	29:U:239:GLU:OE1	1.85	0.76
5:E:87:LEU:O	5:E:87:LEU:HD13	1.86	0.76
29:U:844:LYS:HA	29:U:844:LYS:CE	2.14	0.76
8:i:17:ARG:HH12	8:i:19:TYR:HD1	1.34	0.76
31:F:224:LEU:HB3	31:F:351:LYS:HA	1.66	0.76
3:C:138:MET:SD	3:C:138:MET:N	2.58	0.76
19:V:131:LEU:HB3	19:V:174:PHE:CE2	2.20	0.76
18:t:9:THR:HG22	18:t:10:SER:H	1.50	0.76
29:U:58:GLN:HG2	29:U:87:LEU:HD12	1.68	0.76
1:A:153:LEU:HD22	2:B:132:TYR:OH	1.85	0.76
1:A:270:CYS:HB2	1:A:315:ILE:HG22	1.68	0.76
2:B:71:TYR:HB2	28:u:670:MET:HE3	1.68	0.76
9:j:170:GLU:HA	9:j:173:GLU:OE1	1.86	0.76
20:W:444:HIS:HE1	23:Z:204:LYS:HB3	1.51	0.76
21:X:369:ILE:HG21	22:Y:310:SER:CB	2.16	0.76
23:Z:78:MET:HA	23:Z:78:MET:HE3	1.68	0.76
1:A:254:ALA:HB2	1:A:298:THR:HA	1.68	0.76
4:D:45:LYS:HG2	29:U:187:LEU:CD1	2.14	0.76
20:W:75:TYR:HB3	20:W:123:ARG:HH22	1.51	0.76
26:c:146:ASP:HB3	26:c:156:VAL:CG2	2.16	0.76
31:F:252:ALA:HA	31:F:286:ASP:HB2	1.68	0.76
1:A:272:ILE:HD11	1:A:315:ILE:HB	1.67	0.75
13:O:33:LYS:HE2	37:O:301:LDZ:H19	1.68	0.75
31:F:93:VAL:CG2	31:F:147:PRO:HA	2.15	0.75
27:d:22:GLU:CG	27:d:61:TRP:HZ3	1.98	0.75
27:d:108:SER:HA	27:d:170:LEU:HD13	1.68	0.75
11:M:215:TRP:CZ2	11:M:219:LEU:HD11	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:205:VAL:HG23	22:Y:219:PHE:HE2	1.51	0.75
27:d:251:ARG:HA	27:d:255:MET:CE	2.17	0.75
1:A:53:GLN:OE1	1:A:53:GLN:N	2.19	0.75
5:E:231:PHE:HA	5:E:276:ILE:HG12	1.68	0.75
26:c:239:LYS:N	26:c:239:LYS:HE2	2.02	0.75
2:B:223:ILE:HG12	2:B:347:ILE:HG21	1.68	0.74
19:V:306:ARG:O	19:V:310:THR:HG23	1.87	0.74
22:Y:173:ASP:HA	22:Y:177:ARG:HG3	1.68	0.74
24:a:123:LEU:HD12	24:a:161:LYS:HB2	1.69	0.74
29:U:789:ILE:HG23	29:U:880:ASN:HD21	1.51	0.74
31:F:272:PHE:CE1	31:F:276:LYS:HE3	2.21	0.74
5:E:229:ILE:HD11	5:E:276:ILE:HG23	1.69	0.74
5:E:375:ALA:O	5:E:379:LYS:HE3	1.87	0.74
29:U:836:THR:CA	29:U:840:LYS:HE2	2.17	0.74
22:Y:110:TYR:HA	22:Y:113:ARG:HH12	1.53	0.74
2:B:52:VAL:HG12	2:B:61:LYS:HE3	1.69	0.74
22:Y:42:MET:O	22:Y:46:ARG:HG3	1.87	0.74
26:c:41:MET:HE1	26:c:112:TYR:CG	2.22	0.74
1:A:293:ASN:HB2	31:F:171:ARG:NH1	2.02	0.74
27:d:10:ASN:ND2	27:d:11:ARG:NH2	2.35	0.74
3:C:147:THR:HG23	3:C:149:GLU:H	1.51	0.74
19:V:280:ALA:HB1	19:V:284:GLU:HB3	1.68	0.74
20:W:56:THR:O	20:W:60:MET:HG3	1.87	0.74
13:o:7:VAL:HG22	13:o:12:ILE:HD12	1.69	0.74
1:A:22:ILE:HG21	3:C:159:LYS:HZ2	1.52	0.74
1:A:156:LYS:HE2	2:B:114:GLU:CB	2.08	0.74
12:N:95:MET:HG3	12:N:116:MET:HE3	1.70	0.74
20:W:425:LEU:HD11	23:Z:247:LYS:CD	2.15	0.74
27:d:150:LYS:HZ2	27:d:154:ALA:HB2	1.53	0.74
28:u:213:GLN:HB3	28:u:216:MET:HE1	1.69	0.74
32:k:91:LYS:HG3	32:k:119:LEU:HD13	1.70	0.74
1:A:240:VAL:HB	1:A:274:PHE:HA	1.70	0.73
19:V:199:ASN:O	19:V:203:LEU:HG	1.88	0.73
21:X:368:MET:CG	21:X:374:PHE:HB3	2.16	0.73
5:E:213:ARG:O	5:E:217:GLU:HG2	1.88	0.73
13:O:160:ALA:HA	13:O:163:ILE:HG12	1.70	0.73
10:l:83:LEU:HD11	32:k:121:LEU:CD1	2.18	0.73
10:l:210:VAL:HG13	10:l:229:VAL:HG11	1.70	0.73
32:k:189:MET:HE2	32:k:194:ALA:HA	1.69	0.73
1:A:265:ARG:NH1	1:A:309:PHE:O	2.21	0.73
2:B:122:ILE:HD11	2:B:130:GLU:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:170:VAL:HG13	6:g:171:LYS:HG2	1.70	0.73
4:D:270:ILE:HG22	4:D:285:VAL:HG13	1.69	0.73
22:Y:175:ASP:O	22:Y:179:ARG:HG2	1.88	0.73
28:u:266:LEU:HD23	28:u:297:MET:CE	2.19	0.73
20:W:60:MET:HE1	20:W:107:GLN:HB3	1.70	0.73
23:Z:112:MET:HE1	23:Z:119:SER:HB3	1.70	0.73
25:b:161:ASN:HB2	25:b:165:GLY:HA3	1.70	0.73
29:U:436:ALA:HB3	29:U:472:ILE:HD11	1.70	0.73
1:A:157:ILE:HB	1:A:255:ARG:CZ	2.19	0.73
20:W:137:TYR:CE1	20:W:139:GLU:HG2	2.23	0.73
29:U:62:LEU:HD13	29:U:88:PHE:HE2	1.54	0.73
4:D:385:LEU:HD21	4:D:401:LYS:HE3	1.70	0.73
5:E:303:LEU:HD12	5:E:338:PHE:HB2	1.71	0.73
5:E:205:ASP:OD2	5:E:206:LYS:N	2.21	0.73
24:a:284:ARG:NH1	24:a:284:ARG:O	2.22	0.73
1:A:54:GLN:HG3	1:A:58:LYS:NZ	2.04	0.73
1:A:204:LEU:HD13	1:A:206:ILE:HD12	1.70	0.73
2:B:383:LEU:HD11	2:B:419:PHE:HB3	1.70	0.73
22:Y:113:ARG:NH1	22:Y:113:ARG:HB3	2.04	0.73
27:d:109:GLN:HB2	27:d:111:ARG:HH21	1.53	0.73
10:L:72:ILE:HG21	10:L:88:MET:HE1	1.71	0.72
27:d:150:LYS:NZ	27:d:154:ALA:HB2	2.04	0.72
27:d:188:LYS:HD2	27:d:221:ASN:HD21	1.54	0.72
29:U:843:GLU:OE1	29:U:844:LYS:HD2	1.88	0.72
10:L:53:GLN:HE21	32:K:168:ARG:HH12	1.34	0.72
20:W:137:TYR:CD1	20:W:139:GLU:HG2	2.24	0.72
20:W:21:SER:HA	20:W:24:VAL:HG22	1.70	0.72
24:a:291:LEU:HB3	24:a:295:GLU:HG2	1.71	0.72
18:t:50:MET:HE2	18:t:192:VAL:HG23	1.71	0.72
1:A:258:ARG:HE	1:A:301:GLU:HG3	1.52	0.72
20:W:152:ILE:HG22	20:W:161:GLU:HB3	1.70	0.72
21:X:319:ILE:HD12	21:X:320:SER:H	1.54	0.72
24:a:21:VAL:HG23	24:a:22:TRP:CD1	2.25	0.72
28:u:605:ASN:H	28:u:660:ILE:HD11	1.53	0.72
1:A:193:THR:OG1	1:A:200:ARG:NH1	2.22	0.72
12:n:4:MET:HG2	12:n:156:THR:HG23	1.70	0.72
20:W:426:ASN:ND2	26:c:233:ASP:OD2	2.23	0.72
26:c:279:ASP:O	26:c:280:PRO:C	2.33	0.72
27:d:198:LEU:O	27:d:199:PHE:CD2	2.43	0.72
28:u:195:ASN:ND2	28:u:203:GLU:OE1	2.23	0.72
3:C:368:MET:HE1	4:D:191:TYR:HE1	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:114:ILE:HD11	21:X:129:LEU:HB3	1.72	0.72
26:c:251:LEU:HD11	26:c:283:HIS:HB3	1.70	0.72
29:U:486:MET:SD	29:U:518:LEU:HB3	2.29	0.72
1:A:256:MET:N	1:A:256:MET:SD	2.63	0.71
2:B:249:ARG:HD3	3:C:283:PHE:HD2	1.54	0.71
21:X:85:ALA:O	21:X:88:LEU:HD12	1.89	0.71
28:u:131:MET:HE1	28:u:158:TYR:HA	1.70	0.71
31:F:310:MET:HE1	31:F:338:LEU:HA	1.72	0.71
1:A:250:VAL:HG13	1:A:293:ASN:O	1.90	0.71
5:E:27:LYS:HA	5:E:30:ARG:HD2	1.72	0.71
2:B:405:MET:HE2	2:B:408:ARG:HD3	1.73	0.71
29:U:82:LEU:HD23	29:U:129:ARG:HE	1.56	0.71
31:F:348:LEU:C	31:F:350:ARG:H	1.98	0.71
21:X:421:LEU:O	23:Z:279:LYS:NZ	2.23	0.71
28:u:56:LEU:O	28:u:60:VAL:HG23	1.91	0.71
29:U:24:LEU:HD21	29:U:59:PHE:O	1.90	0.71
29:U:518:LEU:HD23	29:U:554:LEU:HD21	1.71	0.71
1:A:422:LYS:HZ2	1:A:422:LYS:HB3	1.55	0.71
3:C:164:VAL:HG21	3:C:313:ARG:HG3	1.73	0.71
7:H:69:THR:HG22	7:H:70:LYS:H	1.55	0.71
10:L:202:GLU:OE2	10:L:202:GLU:N	2.23	0.71
22:Y:206:SER:HA	22:Y:245:GLU:OE1	1.90	0.71
23:Z:106:ILE:HD12	23:Z:153:LYS:HG2	1.72	0.71
23:Z:214:LYS:HG3	23:Z:220:LEU:HD21	1.72	0.71
1:A:214:LEU:HD23	1:A:341:ILE:HB	1.73	0.71
1:A:364:VAL:HA	1:A:404:ALA:H	1.56	0.71
19:V:477:HIS:CE1	27:d:245:GLN:HG2	2.26	0.71
20:W:335:SER:HB3	20:W:336:PRO:HD3	1.72	0.71
26:c:212:LEU:N	26:c:215:LYS:HG2	2.06	0.71
29:U:62:LEU:HD13	29:U:88:PHE:CE2	2.25	0.71
29:U:807:LYS:HB2	29:U:808:PRO:HD3	1.71	0.71
31:F:175:MET:O	31:F:250:LYS:NZ	2.24	0.71
1:A:394:MET:HA	1:A:394:MET:CE	2.18	0.71
15:q:111:GLU:N	15:q:111:GLU:OE2	2.23	0.71
28:u:445:LEU:HD11	28:u:466:LEU:HA	1.72	0.71
31:F:309:THR:HA	31:F:312:GLU:CG	2.21	0.71
5:E:26:LEU:HD21	31:F:55:MET:CE	2.20	0.71
29:U:812:ALA:HA	29:U:885:MET:CE	2.10	0.71
22:Y:309:GLU:O	22:Y:310:SER:HB3	1.89	0.70
5:E:231:PHE:HA	5:E:276:ILE:CG1	2.21	0.70
27:d:234:ASP:OD2	27:d:237:ILE:HD11	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:187:LEU:O	29:U:187:LEU:HD23	1.91	0.70
5:E:310:LEU:HD21	5:E:328:TYR:C	2.17	0.70
6:G:18:PRO:O	6:G:19:GLU:HG2	1.91	0.70
22:Y:180:LEU:O	22:Y:183:TYR:HD2	1.74	0.70
25:b:108:ARG:HG3	25:b:137:ASN:ND2	2.06	0.70
1:A:158:ASP:N	1:A:159:PRO:HD3	2.06	0.70
4:D:298:GLY:O	4:D:301:GLN:NE2	2.24	0.70
26:c:146:ASP:HB3	26:c:156:VAL:HG21	1.72	0.70
6:g:127:GLN:HA	7:h:128:ARG:NH1	2.07	0.70
29:U:185:MET:HE1	29:U:222:PHE:HE2	1.56	0.70
29:U:880:ASN:HB3	29:U:881:PRO:HD3	1.73	0.70
8:I:29:GLY:HA3	8:I:166:ASN:HB3	1.73	0.70
27:d:234:ASP:HB3	27:d:237:ILE:HG12	1.74	0.70
4:D:394:VAL:HG11	4:D:399:PHE:CD2	2.26	0.70
5:E:33:LEU:HA	5:E:36:LEU:HD21	1.72	0.70
19:V:172:VAL:O	19:V:176:MET:HE2	1.91	0.70
20:W:452:ILE:HG12	23:Z:101:LEU:HD21	1.74	0.70
4:D:64:GLU:HA	4:D:64:GLU:OE2	1.90	0.70
20:W:1:MET:HG2	20:W:42:GLU:HB3	1.72	0.70
20:W:130:MET:HE2	20:W:130:MET:O	1.91	0.70
23:Z:226:ILE:HA	23:Z:229:GLN:HG2	1.72	0.70
24:a:278:MET:HE3	24:a:319:LEU:HD23	1.74	0.70
27:d:194:ALA:HA	27:d:198:LEU:HD13	1.72	0.70
29:U:532:MET:HE1	29:U:551:GLY:CA	2.22	0.70
31:F:364:ARG:HE	31:F:367:GLN:HE21	1.37	0.70
32:K:201:ILE:O	32:K:205:VAL:HG22	1.91	0.70
3:C:213:ARG:NH2	4:D:299:PHE:CD1	2.60	0.70
5:E:33:LEU:HA	5:E:36:LEU:CD2	2.21	0.70
20:W:436:MET:HE3	23:Z:236:LEU:HD22	1.74	0.69
9:j:43:LEU:HD11	9:j:62:ILE:HG13	1.74	0.69
3:C:86:LEU:HD11	3:C:94:LYS:HD2	1.72	0.69
5:E:23:ASP:HA	5:E:26:LEU:HD12	1.74	0.69
18:T:96:MET:HE2	18:T:110:MET:CE	2.23	0.69
20:W:253:THR:O	20:W:257:GLN:HG2	1.91	0.69
6:g:132:ARG:NH1	11:m:123:THR:O	2.25	0.69
28:u:349:TYR:O	28:u:350:LYS:HG2	1.92	0.69
8:I:219:GLU:HA	8:I:219:GLU:OE2	1.90	0.69
20:W:47:LEU:HD23	20:W:47:LEU:H	1.56	0.69
20:W:451:MET:HE3	20:W:455:LEU:HD21	1.73	0.69
2:B:70:ASP:O	2:B:74:MET:HG3	1.91	0.69
26:c:235:SER:O	26:c:239:LYS:HE3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:6:LYS:HG2	27:d:10:ASN:ND2	2.07	0.69
27:d:50:LEU:O	27:d:54:ILE:HG12	1.93	0.69
9:j:41:VAL:HG11	9:j:134:VAL:HG13	1.74	0.69
1:A:26:ASP:OD2	1:A:27:GLU:N	2.25	0.69
4:D:64:GLU:OE1	29:U:607:VAL:HG22	1.93	0.69
28:u:326:LEU:HD21	28:u:420:TRP:HB3	1.74	0.69
29:U:486:MET:HE1	29:U:521:LEU:HD23	1.72	0.69
25:b:11:ASP:HB3	25:b:16:MET:HE3	1.75	0.69
1:A:262:GLU:HA	1:A:265:ARG:HD2	1.75	0.69
3:C:168:PRO:HA	3:C:175:PHE:HE1	1.57	0.69
22:Y:282:MET:CE	22:Y:291:HIS:HB3	2.15	0.69
29:U:567:ILE:HD12	29:U:586:VAL:HG12	1.74	0.69
3:C:251:ILE:HG13	3:C:293:MET:HE2	1.72	0.69
3:C:338:LEU:HD13	3:C:339:THR:O	1.92	0.69
5:E:33:LEU:HD21	31:F:62:VAL:HB	1.75	0.69
10:L:125:ARG:NH1	10:L:126:ARG:O	2.26	0.69
20:W:2:ALA:HB3	20:W:47:LEU:HD12	1.75	0.69
26:c:180:ASN:HA	26:c:183:HIS:CD2	2.27	0.69
15:q:176:PRO:HB2	15:q:177:THR:HG23	1.74	0.69
29:U:623:GLY:HA3	29:U:659:CYS:SG	2.33	0.69
19:V:309:MET:SD	19:V:328:VAL:HG23	2.32	0.69
26:c:224:SER:HB2	26:c:227:GLU:CG	2.23	0.69
29:U:532:MET:CE	29:U:551:GLY:HA3	2.22	0.69
5:E:303:LEU:CG	5:E:338:PHE:HB3	2.22	0.69
5:E:328:TYR:HE1	5:E:367:PHE:HE2	1.37	0.69
28:u:213:GLN:HB3	28:u:216:MET:HE3	1.73	0.69
31:F:188:ILE:HG21	31:F:236:LEU:HD23	1.75	0.69
5:E:222:ALA:C	5:E:224:ASP:H	2.00	0.68
5:E:375:ALA:C	5:E:379:LYS:HE3	2.19	0.68
10:L:60:GLN:HE22	31:F:439:ALA:HB3	1.58	0.68
22:Y:43:ALA:HB2	22:Y:46:ARG:HH22	1.56	0.68
22:Y:282:MET:HE3	22:Y:291:HIS:CB	2.16	0.68
1:A:299:MET:HE3	1:A:330:ALA:HB3	1.73	0.68
4:D:338:ARG:O	4:D:340:GLN:N	2.26	0.68
9:j:171:PHE:HE2	9:j:175:ASN:HD22	1.39	0.68
2:B:201:VAL:O	2:B:205:LEU:HD23	1.92	0.68
5:E:45:ASN:HA	5:E:48:LYS:HD3	1.74	0.68
23:Z:111:LEU:HG	23:Z:114:ARG:HH21	1.58	0.68
24:a:267:GLN:HB3	24:a:270:ARG:NH1	2.07	0.68
29:U:233:LEU:HD11	29:U:268:LEU:HD11	1.75	0.68
29:U:503:GLN:OE1	29:U:503:GLN:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:682:TYR:O	29:U:685:GLN:HG2	1.93	0.68
17:s:184:GLU:OE1	17:s:211:ARG:NH1	2.26	0.68
3:C:83:LYS:HE3	3:C:84:LYS:HG3	1.76	0.68
5:E:215:ILE:HD13	5:E:260:LEU:HB2	1.76	0.68
22:Y:274:SER:HA	22:Y:277:VAL:HG12	1.75	0.68
24:a:141:MET:HE2	24:a:141:MET:H	1.56	0.68
27:d:22:GLU:HG2	27:d:61:TRP:CZ3	2.26	0.68
31:F:172:VAL:HG21	31:F:274:LEU:HG	1.76	0.68
32:k:68:VAL:HG21	32:k:89:ILE:HD13	1.75	0.68
1:A:155:PRO:HD2	1:A:255:ARG:HH22	1.57	0.68
1:A:268:LYS:HE3	1:A:314:ASN:CB	2.24	0.68
2:B:250:VAL:HG12	2:B:284:ILE:HG23	1.76	0.68
4:D:182:GLU:HA	4:D:182:GLU:OE1	1.93	0.68
6:g:80:MET:HE2	6:g:87:SER:HA	1.75	0.68
9:j:5:ARG:HD2	32:k:10:ARG:O	1.94	0.68
4:D:173:GLN:HE22	4:D:334:PRO:HD2	1.59	0.68
19:V:485:ASP:O	19:V:489:MET:SD	2.52	0.68
23:Z:171:GLY:O	23:Z:175:LEU:HD23	1.94	0.68
4:D:352:MET:HE3	4:D:352:MET:HA	1.75	0.68
5:E:25:ARG:O	5:E:29:LEU:HG	1.94	0.68
5:E:122:MET:HE2	5:E:198:VAL:HG22	1.75	0.68
20:W:2:ALA:HB3	20:W:47:LEU:CD1	2.23	0.68
20:W:44:ILE:H	20:W:47:LEU:HD21	1.59	0.68
22:Y:43:ALA:HB2	22:Y:46:ARG:NH2	2.08	0.68
2:B:187:ILE:HD12	2:B:187:ILE:O	1.94	0.68
5:E:221:TYR:O	5:E:224:ASP:HB3	1.92	0.68
24:a:180:LEU:HD21	24:a:221:VAL:HG11	1.74	0.68
24:a:281:THR:O	24:a:284:ARG:NH1	2.27	0.68
26:c:211:GLU:O	26:c:212:LEU:HB3	1.92	0.68
1:A:432:TYR:O	1:A:433:ASN:C	2.36	0.68
5:E:83:CYS:SG	5:E:87:LEU:HD12	2.32	0.68
22:Y:181:LYS:HZ2	22:Y:181:LYS:HB3	1.57	0.68
15:q:38:MET:HE3	15:q:64:VAL:HG21	1.76	0.68
29:U:609:ASP:OD2	29:U:614:VAL:HG13	1.93	0.68
20:W:444:HIS:NE2	23:Z:208:ILE:HG12	2.09	0.67
25:b:62:THR:HG21	25:b:71:ILE:HG22	1.76	0.67
1:A:238:ILE:HD12	1:A:272:ILE:HG13	1.75	0.67
3:C:174:LEU:HD22	3:C:174:LEU:N	2.09	0.67
3:C:258:ARG:HD3	3:C:273:MET:HE1	1.77	0.67
9:J:10:PHE:H	32:K:23:GLN:HE22	1.42	0.67
26:c:158:ASP:OD1	26:c:159:ALA:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:139:ILE:O	23:Z:156:GLU:HG3	1.94	0.67
19:V:228:ARG:HH12	27:d:85:TYR:HE1	1.39	0.67
24:a:270:ARG:HH11	24:a:271:LYS:HG3	1.57	0.67
26:c:269:GLN:OE1	26:c:269:GLN:O	2.12	0.67
1:A:87:LEU:HD22	1:A:87:LEU:H	1.60	0.67
3:C:307:ARG:HD2	3:C:309:GLY:H	1.58	0.67
20:W:60:MET:CE	20:W:107:GLN:HB3	2.25	0.67
27:d:107:LEU:CD2	27:d:170:LEU:HD11	2.24	0.67
29:U:213:PHE:CD1	29:U:214:ILE:HG13	2.29	0.67
1:A:285:PHE:HA	1:A:296:GLN:NE2	2.08	0.67
29:U:738:ASP:HB3	29:U:742:HIS:CE1	2.30	0.67
10:l:126:ARG:HB3	32:k:13:ASN:HB3	1.77	0.67
14:P:177:ARG:NH2	17:s:150:ASP:OD2	2.26	0.67
15:Q:26:VAL:HG12	15:q:138:LEU:HD21	1.76	0.67
20:W:435:LEU:O	20:W:435:LEU:HD12	1.95	0.67
8:i:17:ARG:NH1	8:i:19:TYR:HA	2.09	0.67
32:K:186:HIS:CE1	32:K:188:SER:OG	2.47	0.67
4:D:60:TYR:O	4:D:64:GLU:N	2.27	0.67
19:V:476:PHE:CZ	23:Z:257:MET:HE1	2.29	0.67
26:c:174:PRO:O	26:c:176:GLN:NE2	2.28	0.67
27:d:117:THR:O	27:d:121:ARG:NH2	2.28	0.67
12:n:149:LYS:NZ	12:n:185:GLU:OE2	2.28	0.67
31:F:420:TYR:CE2	31:F:424:ILE:HD11	2.30	0.67
26:c:191:ALA:HB1	26:c:196:LEU:HG	1.76	0.67
32:k:227:HIS:CE1	32:k:233:GLU:OE1	2.48	0.67
1:A:194:PRO:HB3	1:A:316:LYS:HE3	1.77	0.66
2:B:35:LYS:HZ2	2:B:38:LYS:HG3	1.60	0.66
2:B:48:LYS:HD3	2:B:49:LEU:H	1.60	0.66
4:D:384:MET:HE3	4:D:384:MET:C	2.19	0.66
20:W:406:VAL:HG23	20:W:413:ILE:HG22	1.75	0.66
27:d:183:GLU:OE2	27:d:215:TRP:NE1	2.28	0.66
29:U:12:LEU:O	29:U:20:LYS:NZ	2.24	0.66
1:A:293:ASN:HB2	31:F:171:ARG:CZ	2.25	0.66
3:C:163:GLU:OE2	3:C:164:VAL:HG23	1.95	0.66
3:C:174:LEU:HD22	3:C:174:LEU:H	1.61	0.66
5:E:288:ALA:O	5:E:291:ARG:HG2	1.96	0.66
5:E:328:TYR:HE1	5:E:367:PHE:CE2	2.12	0.66
23:Z:179:ILE:HD12	23:Z:180:LYS:N	2.09	0.66
28:u:53:GLN:NE2	28:u:57:GLU:OE2	2.27	0.66
28:u:56:LEU:HD23	28:u:99:LEU:CD2	2.20	0.66
3:C:251:ILE:O	3:C:252:ASP:C	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:267:ILE:HG12	4:D:309:MET:HG2	1.76	0.66
6:g:127:GLN:HA	7:h:128:ARG:HH11	1.59	0.66
29:U:521:LEU:HD22	29:U:554:LEU:HD11	1.77	0.66
29:U:583:MET:HE1	29:U:614:VAL:HG22	1.77	0.66
1:A:146:LYS:HE2	1:A:148:GLN:HG3	1.77	0.66
1:A:157:ILE:HG12	1:A:158:ASP:N	2.06	0.66
5:E:179:GLY:HA2	5:E:182:LEU:CD2	2.24	0.66
19:V:167:LEU:HD12	19:V:169:LEU:H	1.60	0.66
31:F:208:HIS:CE1	31:F:211:LYS:HE3	2.31	0.66
20:W:314:LEU:HD22	24:a:309:LEU:HG	1.77	0.66
27:d:120:GLU:CD	27:d:121:ARG:HH12	1.97	0.66
28:u:192:VAL:HG23	28:u:193:PRO:HD3	1.77	0.66
29:U:843:GLU:CD	29:U:844:LYS:HD2	2.21	0.66
31:F:58:GLU:O	31:F:62:VAL:HG22	1.95	0.66
31:F:223:VAL:HB	31:F:329:ILE:HA	1.78	0.66
1:A:229:VAL:O	1:A:232:ARG:NE	2.29	0.66
2:B:174:MET:CG	2:B:249:ARG:O	2.43	0.66
2:B:385:MET:HB3	9:J:200:GLN:HA	1.76	0.66
4:D:124:LEU:O	4:D:125:LYS:C	2.39	0.66
5:E:22:ILE:HD12	5:E:25:ARG:HG3	1.78	0.66
19:V:79:VAL:HG13	19:V:81:GLN:H	1.59	0.66
32:k:189:MET:CE	32:k:194:ALA:HA	2.26	0.66
2:B:118:ASP:O	2:B:119:ASN:OD1	2.14	0.66
5:E:26:LEU:CD2	31:F:55:MET:HE3	2.26	0.66
9:J:120:GLN:HG2	32:K:133:MET:HE3	1.77	0.66
27:d:198:LEU:O	27:d:199:PHE:CG	2.49	0.66
28:u:412:ALA:HB1	28:u:446:LEU:HD22	1.78	0.66
1:A:225:CYS:SG	1:A:229:VAL:HG13	2.35	0.66
4:D:115:ILE:HD12	4:D:116:LEU:O	1.95	0.66
8:I:181:GLU:CD	8:I:181:GLU:H	2.04	0.66
20:W:448:LYS:NZ	23:Z:99:PRO:O	2.27	0.66
21:X:114:ILE:HG12	21:X:129:LEU:HD22	1.78	0.66
22:Y:113:ARG:CB	22:Y:113:ARG:HH11	2.08	0.66
31:F:386:ARG:HB2	31:F:386:ARG:NH1	2.11	0.66
32:k:118:ASN:HA	32:k:121:LEU:HD23	1.77	0.66
3:C:215:SER:HA	3:C:249:ASP:HB2	1.78	0.65
19:V:96:ARG:HB2	19:V:150:ARG:HH22	1.61	0.65
27:d:10:ASN:HD22	27:d:11:ARG:NH2	1.95	0.65
31:F:362:ARG:HD2	31:F:388:THR:HB	1.77	0.65
3:C:117:ARG:NH1	3:C:124:HIS:CD2	2.64	0.65
22:Y:70:LEU:CB	22:Y:73:MET:HE3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:t:68:GLY:O	18:t:72:ILE:HG13	1.96	0.65
1:A:31:ALA:HA	1:A:34:LYS:HB2	1.78	0.65
2:B:171:VAL:HG21	2:B:269:GLU:OE2	1.97	0.65
11:M:68:ASN:O	11:M:92:ARG:NH1	2.29	0.65
20:W:1:MET:CE	20:W:43:VAL:HG13	2.24	0.65
20:W:435:LEU:HG	20:W:436:MET:HE2	1.78	0.65
21:X:255:LEU:HD22	21:X:267:VAL:HG13	1.77	0.65
10:l:192:LEU:HD13	10:l:236:LEU:HD11	1.77	0.65
1:A:139:ARG:HG2	1:A:155:PRO:HA	1.76	0.65
3:C:155:ASP:HA	3:C:158:ILE:HD12	1.78	0.65
20:W:253:THR:O	20:W:256:ILE:HG22	1.95	0.65
23:Z:112:MET:HE1	23:Z:119:SER:CB	2.27	0.65
26:c:156:VAL:HG23	26:c:156:VAL:O	1.95	0.65
29:U:250:PHE:CD2	29:U:328:ILE:HG13	2.32	0.65
5:E:117:PRO:HA	5:E:120:TYR:HB3	1.78	0.65
24:a:28:LEU:HG	24:a:33:LEU:HD11	1.77	0.65
28:u:213:GLN:O	28:u:216:MET:HG2	1.96	0.65
29:U:529:ILE:HD12	29:U:530:GLU:N	2.12	0.65
31:F:357:PRO:O	31:F:362:ARG:NH1	2.29	0.65
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.77	0.65
3:C:253:SER:HB3	4:D:290:LEU:HD12	1.78	0.65
4:D:102:ILE:HG13	4:D:112:TYR:HD1	1.61	0.65
5:E:97:ARG:HH21	5:E:114:GLU:H	1.44	0.65
5:E:203:ILE:HD11	5:E:218:MET:HE1	1.79	0.65
10:l:41:LYS:HB3	10:l:180:MET:HE2	1.79	0.65
28:u:253:LEU:CD2	28:u:277:LEU:HD21	2.26	0.65
19:V:130:PHE:CB	19:V:133:PRO:HG2	2.23	0.65
22:Y:232:GLU:OE2	22:Y:232:GLU:N	2.26	0.65
6:g:126:THR:O	7:h:128:ARG:NH1	2.29	0.65
5:E:310:LEU:HA	5:E:313:LEU:HD12	1.77	0.65
7:h:177:ARG:HH11	7:h:177:ARG:HB2	1.62	0.65
28:u:766:GLN:O	28:u:769:THR:HG22	1.97	0.65
5:E:75:ASN:ND2	31:F:129:ARG:O	2.30	0.65
5:E:127:PRO:HA	5:E:185:ARG:NH2	2.07	0.65
20:W:11:GLY:O	20:W:15:LYS:NZ	2.28	0.65
26:c:167:MET:HG2	26:c:170:LEU:HB3	1.77	0.65
15:q:88:LEU:HB3	15:q:122:ALA:HB2	1.78	0.65
5:E:310:LEU:HD12	5:E:329:GLU:OE1	1.97	0.65
19:V:64:GLN:NE2	19:V:68:ASP:OD2	2.28	0.65
19:V:468:SER:OG	23:Z:250:TYR:CE1	2.50	0.65
20:W:303:LYS:HA	20:W:306:LEU:CD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:7:MET:HE3	25:b:52:ILE:HB	1.78	0.65
6:g:92:GLN:NE2	12:n:69:GLU:OE1	2.29	0.65
7:h:95:GLN:HG3	13:o:65:LEU:HD13	1.78	0.65
29:U:835:ILE:HG13	29:U:836:THR:H	1.62	0.65
1:A:265:ARG:NH2	1:A:305:GLN:HG2	2.12	0.64
5:E:30:ARG:HA	5:E:33:LEU:HD22	1.79	0.64
19:V:211:TYR:HD1	19:V:253:LEU:HD13	1.61	0.64
29:U:486:MET:HE3	29:U:487:GLY:N	2.11	0.64
29:U:628:ARG:NH1	29:U:749:GLN:OE1	2.30	0.64
3:C:45:LEU:HB3	4:D:61:ILE:HD13	1.79	0.64
22:Y:381:GLN:HG2	22:Y:382:LYS:HD2	1.78	0.64
1:A:400:ARG:HH21	28:u:866:GLN:HB3	1.62	0.64
12:N:67:SER:HB2	12:N:74:PRO:HG3	1.79	0.64
22:Y:43:ALA:CA	22:Y:46:ARG:CZ	2.75	0.64
3:C:298:ILE:HD12	3:C:301:LEU:HD21	1.79	0.64
4:D:418:LYS:HE3	7:H:80:GLY:HA3	1.79	0.64
19:V:62:HIS:HE1	22:Y:389:MET:CE	1.89	0.64
26:c:232:GLN:NE2	26:c:233:ASP:O	2.30	0.64
1:A:284:ARG:HB3	1:A:288:GLY:HA3	1.78	0.64
12:N:18:SER:HB3	12:N:31:THR:H	1.62	0.64
25:b:7:MET:HE3	25:b:52:ILE:CG2	2.27	0.64
29:U:553:ALA:HA	29:U:585:THR:HG22	1.78	0.64
1:A:34:LYS:NZ	3:C:174:LEU:HD22	2.12	0.64
1:A:170:PRO:HG3	1:A:237:PHE:HB2	1.79	0.64
3:C:201:ARG:HG3	4:D:299:PHE:CD1	2.32	0.64
4:D:156:SER:O	4:D:157:ASP:HB3	1.96	0.64
5:E:181:THR:O	5:E:185:ARG:HG2	1.98	0.64
5:E:303:LEU:HD23	5:E:304:PRO:HD3	1.80	0.64
20:W:2:ALA:O	20:W:6:SER:N	2.29	0.64
22:Y:70:LEU:HB3	22:Y:73:MET:CE	2.28	0.64
26:c:279:ASP:O	26:c:281:LYS:N	2.31	0.64
10:l:125:ARG:HD3	10:l:126:ARG:H	1.63	0.64
6:G:192:GLU:CD	6:G:192:GLU:H	2.04	0.64
22:Y:110:TYR:HA	22:Y:113:ARG:CZ	2.28	0.64
24:a:145:LEU:HD22	24:a:147:GLY:H	1.62	0.64
24:a:312:MET:HA	24:a:315:LEU:HD21	1.79	0.64
29:U:889:LEU:HD13	29:U:909:GLY:H	1.63	0.64
19:V:120:PHE:HB3	19:V:121:PHE:CE2	2.33	0.64
19:V:131:LEU:HA	19:V:134:PHE:HB2	1.80	0.64
19:V:200:ARG:H	19:V:200:ARG:HE	1.45	0.64
25:b:16:MET:HE2	25:b:114:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:119:GLN:HB2	8:i:81:SER:OG	1.98	0.64
4:D:103:VAL:HG11	4:D:132:LEU:HD11	1.78	0.64
20:W:142:ARG:HD2	20:W:145:LEU:CD1	2.26	0.64
17:s:190:GLY:O	17:s:191:ASP:HB2	1.98	0.64
6:G:120:ASP:OD1	7:H:84:ARG:NH1	2.31	0.63
16:r:17:ASP:OD2	16:r:33:LYS:NZ	2.31	0.63
29:U:806:CYS:O	29:U:874:ASN:HB3	1.98	0.63
1:A:134:ILE:HG23	1:A:138:MET:HE3	1.79	0.63
5:E:26:LEU:HD11	31:F:55:MET:HE3	1.79	0.63
19:V:324:PHE:HB2	30:e:5:LYS:HE3	1.78	0.63
25:b:24:THR:HG22	25:b:26:LEU:H	1.64	0.63
11:m:151:ILE:HG13	11:m:157:SER:HB3	1.80	0.63
2:B:171:VAL:HG21	2:B:269:GLU:CD	2.23	0.63
2:B:171:VAL:HG11	2:B:269:GLU:OE1	1.97	0.63
5:E:33:LEU:HA	5:E:36:LEU:CG	2.27	0.63
20:W:444:HIS:CE1	23:Z:204:LYS:HB3	2.33	0.63
22:Y:382:LYS:HD2	22:Y:382:LYS:N	2.14	0.63
27:d:254:GLU:HB2	27:d:255:MET:HE1	1.80	0.63
1:A:194:PRO:HG3	1:A:201:PHE:HE2	1.63	0.63
1:A:236:CYS:HB3	1:A:270:CYS:HA	1.80	0.63
5:E:87:LEU:HD11	5:E:92:LEU:CD2	2.28	0.63
10:L:88:MET:CG	10:L:112:ILE:HD11	2.28	0.63
13:O:105:VAL:HG23	13:O:106:THR:HG23	1.79	0.63
21:X:316:ASP:O	21:X:319:ILE:HD11	1.98	0.63
22:Y:192:ARG:HA	22:Y:192:ARG:CZ	2.29	0.63
23:Z:129:LYS:HZ2	26:c:215:LYS:HE2	1.62	0.63
18:t:50:MET:CE	18:t:192:VAL:HG23	2.28	0.63
29:U:669:ILE:HG21	29:U:695:MET:HE1	1.80	0.63
3:C:147:THR:HG23	3:C:148:TYR:N	2.13	0.63
8:I:119:GLN:HG3	9:J:78:ALA:HB1	1.81	0.63
31:F:383:GLU:HG3	31:F:421:MET:SD	2.38	0.63
31:F:432:LYS:H	31:F:432:LYS:HD2	1.64	0.63
3:C:213:ARG:CZ	4:D:299:PHE:CG	2.81	0.63
3:C:338:LEU:CD2	3:C:342:ILE:HD13	2.27	0.63
19:V:194:LYS:H	19:V:194:LYS:HD2	1.64	0.63
23:Z:212:LEU:HD23	23:Z:212:LEU:O	1.99	0.63
26:c:279:ASP:CA	26:c:283:HIS:HB2	2.28	0.63
29:U:572:ARG:NE	29:U:572:ARG:O	2.32	0.63
1:A:263:MET:HE3	1:A:267:LYS:HZ1	1.62	0.63
5:E:33:LEU:O	5:E:36:LEU:HG	1.99	0.63
24:a:11:SER:O	24:a:22:TRP:CZ3	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:56:LEU:HD21	32:k:178:GLN:HE22	1.64	0.63
1:A:323:ARG:HH21	1:A:325:ASP:HB3	1.64	0.63
22:Y:101:ARG:O	22:Y:104:MET:HG2	1.99	0.63
26:c:152:LYS:HE3	26:c:152:LYS:CA	2.24	0.63
27:d:178:ILE:O	27:d:182:ILE:HG22	1.98	0.63
29:U:836:THR:O	29:U:839:ALA:N	2.31	0.63
3:C:140:VAL:O	3:C:141:GLU:HG3	1.99	0.62
5:E:325:GLU:OE2	5:E:325:GLU:N	2.31	0.62
6:G:175:SER:OG	6:G:201:CYS:SG	2.58	0.62
19:V:323:GLY:HA3	30:e:9:ASP:O	1.99	0.62
21:X:114:ILE:CG1	21:X:129:LEU:HD22	2.29	0.62
7:h:179:ASN:OD1	7:h:180:GLU:N	2.32	0.62
18:t:9:THR:O	18:t:41:ARG:NH2	2.31	0.62
22:Y:152:MET:HE3	22:Y:152:MET:C	2.24	0.62
23:Z:54:PHE:HD1	23:Z:82:PHE:CE2	2.16	0.62
24:a:350:LYS:HA	24:a:353:LEU:HD12	1.81	0.62
26:c:188:SER:HB2	26:c:190:GLN:OE1	1.98	0.62
9:j:45:VAL:CG2	9:j:62:ILE:HD11	2.27	0.62
29:U:244:MET:SD	29:U:244:MET:N	2.73	0.62
31:F:381:TYR:HA	31:F:384:LEU:CG	2.26	0.62
1:A:86:THR:HG22	2:B:136:LEU:HD12	1.80	0.62
22:Y:387:ILE:HG21	23:Z:275:LEU:HD21	1.81	0.62
28:u:287:ASP:OD2	28:u:901:ARG:NH2	2.32	0.62
31:F:251:LEU:HB3	31:F:285:ILE:HG23	1.81	0.62
2:B:73:LEU:HA	2:B:76:GLU:HG3	1.81	0.62
3:C:147:THR:HG22	3:C:150:MET:CE	2.18	0.62
4:D:114:ARG:CZ	4:D:114:ARG:HB2	2.29	0.62
5:E:310:LEU:HD11	5:E:329:GLU:HA	1.80	0.62
19:V:80:LYS:HZ2	19:V:128:ARG:HA	1.64	0.62
28:u:794:ALA:O	28:u:798:THR:HG23	2.00	0.62
31:F:207:ASN:OD1	31:F:207:ASN:O	2.18	0.62
31:F:286:ASP:HB3	31:F:287:GLU:OE2	1.99	0.62
31:F:410:ARG:NH2	31:F:416:THR:H	1.98	0.62
4:D:64:GLU:CD	29:U:607:VAL:HG13	2.24	0.62
19:V:488:ASN:C	19:V:489:MET:HE3	2.23	0.62
20:W:137:TYR:O	20:W:144:ARG:NH2	2.33	0.62
24:a:308:GLU:CG	24:a:312:MET:HE1	2.27	0.62
28:u:404:ASP:N	28:u:407:MET:HE1	2.14	0.62
28:u:711:SER:HB2	28:u:729:MET:CE	2.27	0.62
29:U:242:LEU:CD1	29:U:325:MET:HE3	2.29	0.62
28:u:764:LEU:O	28:u:768:LEU:HG	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HA	1:A:46:LYS:HG2	1.81	0.62
4:D:119:ILE:H	4:D:119:ILE:HD12	1.64	0.62
5:E:33:LEU:HD12	5:E:36:LEU:HD21	1.82	0.62
17:s:172:MET:HE1	17:s:206:GLU:OE2	2.00	0.62
30:e:67:MET:C	30:e:67:MET:HE2	2.24	0.62
31:F:405:MET:HE3	31:F:405:MET:HA	1.80	0.62
32:K:178:GLN:O	32:K:182:GLN:HG3	2.00	0.62
32:k:220:VAL:HG12	32:k:228:MET:HG3	1.82	0.62
2:B:294:ARG:HA	2:B:306:GLN:HE22	1.63	0.62
29:U:804:SER:HA	29:U:892:LEU:HA	1.82	0.62
1:A:258:ARG:HA	1:A:305:GLN:NE2	2.11	0.62
3:C:264:GLY:O	4:D:280:GLY:N	2.32	0.62
22:Y:180:LEU:HD22	22:Y:183:TYR:HE2	1.65	0.62
22:Y:382:LYS:N	22:Y:382:LYS:CD	2.63	0.62
24:a:308:GLU:HG3	24:a:312:MET:HE3	1.79	0.62
26:c:186:LYS:H	26:c:186:LYS:HD2	1.65	0.62
29:U:789:ILE:HG23	29:U:880:ASN:ND2	2.15	0.62
2:B:106:PRO:O	2:B:154:HIS:NE2	2.33	0.62
2:B:405:MET:HE2	2:B:405:MET:HA	1.82	0.62
5:E:231:PHE:HD1	5:E:276:ILE:CD1	2.13	0.62
19:V:309:MET:CG	19:V:332:LEU:HD13	2.30	0.62
26:c:53:VAL:HG22	26:c:114:SER:OG	1.99	0.62
1:A:174:TYR:HA	1:A:228:ALA:HB1	1.80	0.61
14:P:113:ASP:HB3	14:P:116:THR:O	2.00	0.61
29:U:443:LEU:O	29:U:446:LEU:CD1	2.48	0.61
5:E:12:TYR:HA	5:E:16:LEU:HB2	1.81	0.61
17:S:158:MET:HG2	13:o:208:THR:CG2	2.30	0.61
28:u:845:ARG:HB3	28:u:865:PHE:HB2	1.80	0.61
2:B:197:ILE:HG21	2:B:235:LEU:HD21	1.81	0.61
16:R:87:VAL:HG11	16:R:97:MET:HE1	1.82	0.61
20:W:247:TYR:HB3	20:W:270:VAL:HG22	1.81	0.61
22:Y:50:MET:N	22:Y:50:MET:SD	2.73	0.61
24:a:291:LEU:HD13	24:a:295:GLU:OE1	1.99	0.61
28:u:430:ASP:OD2	28:u:430:ASP:N	2.28	0.61
29:U:469:SER:H	29:U:473:VAL:HG21	1.65	0.61
30:e:6:GLN:HB2	30:e:9:ASP:O	1.99	0.61
1:A:250:VAL:HA	1:A:294:GLU:CB	2.27	0.61
2:B:52:VAL:CG1	2:B:61:LYS:HE3	2.29	0.61
4:D:216:ALA:O	4:D:219:VAL:HG12	2.00	0.61
5:E:92:LEU:C	5:E:93:LYS:HE2	2.25	0.61
5:E:136:GLY:HA3	5:E:312:ILE:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:76:GLU:OE2	20:W:129:ARG:NH2	2.33	0.61
11:m:117:MET:HE2	11:m:117:MET:HA	1.83	0.61
4:D:389:GLU:HB2	4:D:391:ARG:NE	2.15	0.61
20:W:362:ASN:O	20:W:366:MET:HG3	2.00	0.61
17:s:4:PRO:O	18:t:100:ARG:NH1	2.33	0.61
29:U:532:MET:SD	29:U:552:ILE:CG2	2.86	0.61
31:F:62:VAL:HG23	31:F:63:THR:N	2.15	0.61
32:k:60:GLU:N	32:k:60:GLU:OE1	2.34	0.61
3:C:273:MET:SD	3:C:277:LEU:HD11	2.41	0.61
4:D:210:CYS:N	35:D:501:ATP:O2B	2.32	0.61
8:I:123:GLN:HG3	9:J:125:ARG:HE	1.65	0.61
20:W:1:MET:HE3	20:W:43:VAL:CG1	2.27	0.61
27:d:73:ARG:HD2	29:U:10:SER:HB2	1.81	0.61
29:U:366:HIS:HE1	29:U:395:ARG:HD2	1.65	0.61
29:U:446:LEU:HD12	29:U:447:GLY:H	1.65	0.61
32:k:204:GLN:C	32:k:204:GLN:OE1	2.44	0.61
1:A:134:ILE:HG13	1:A:152:PRO:HB3	1.81	0.61
2:B:133:VAL:HB	2:B:158:ALA:HA	1.83	0.61
5:E:303:LEU:HD23	5:E:304:PRO:CD	2.30	0.61
24:a:311:VAL:O	24:a:315:LEU:HD22	2.01	0.61
9:j:137:ASP:O	9:j:137:ASP:OD2	2.18	0.61
29:U:885:MET:H	29:U:888:GLN:HE21	1.48	0.61
31:F:223:VAL:N	31:F:328:VAL:O	2.31	0.61
19:V:37:MET:HE3	19:V:92:ARG:HH22	1.65	0.61
19:V:212:TYR:CG	30:e:4:LYS:HE2	2.36	0.61
9:j:134:VAL:CG2	9:j:144:LEU:HD12	2.31	0.61
1:A:165:GLN:HE21	1:A:238:ILE:HG12	1.66	0.61
2:B:120:HIS:HA	2:B:134:SER:HA	1.82	0.61
5:E:33:LEU:HA	5:E:36:LEU:HG	1.82	0.61
5:E:89:LYS:O	5:E:89:LYS:NZ	2.24	0.61
19:V:345:ARG:NH1	19:V:360:TYR:HB2	2.16	0.61
24:a:148:VAL:HG12	24:a:150:SER:H	1.66	0.61
24:a:267:GLN:HG2	24:a:270:ARG:NH2	2.16	0.61
29:U:208:LEU:HD23	29:U:210:LYS:H	1.64	0.61
31:F:272:PHE:CZ	31:F:276:LYS:HE3	2.36	0.61
1:A:187:LEU:CD1	1:A:229:VAL:HG11	2.31	0.61
1:A:268:LYS:NZ	1:A:314:ASN:H	1.98	0.61
5:E:21:GLU:OE1	5:E:21:GLU:N	2.33	0.61
5:E:132:TYR:HE1	5:E:146:ARG:HD3	1.66	0.61
22:Y:41:LEU:HD12	22:Y:61:LEU:HD12	1.83	0.61
22:Y:105:MET:SD	22:Y:140:ILE:HD11	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:7:MET:CE	25:b:52:ILE:HB	2.31	0.61
25:b:35:ILE:HD13	25:b:184:ILE:HD11	1.83	0.61
29:U:214:ILE:HD13	29:U:218:GLN:HG3	1.83	0.61
32:K:51:GLU:CB	32:K:206:MET:HE2	2.30	0.61
1:A:215:PHE:HB2	1:A:324:PRO:HB3	1.83	0.60
5:E:109:ARG:NH1	31:F:99:VAL:O	2.33	0.60
15:Q:81:ALA:HB2	15:Q:104:LEU:HD22	1.83	0.60
16:R:31:VAL:HG11	37:R:301:LDZ:H17	1.82	0.60
23:Z:173:GLU:O	23:Z:180:LYS:NZ	2.34	0.60
24:a:83:VAL:C	24:a:87:MET:HE2	2.24	0.60
29:U:24:LEU:HD11	29:U:60:ALA:HA	1.83	0.60
29:U:560:MET:HE2	29:U:560:MET:HA	1.83	0.60
31:F:224:LEU:HB2	31:F:348:LEU:HD23	1.81	0.60
1:A:299:MET:O	1:A:302:LEU:HD23	2.01	0.60
5:E:140:GLU:HA	5:E:143:ARG:HE	1.67	0.60
19:V:65:ARG:NH2	19:V:66:GLU:CG	2.54	0.60
19:V:130:PHE:HB3	19:V:133:PRO:CG	2.26	0.60
29:U:559:ARG:HB3	29:U:562:GLU:HB2	1.83	0.60
31:F:225:MET:HE1	31:F:329:ILE:O	2.01	0.60
32:K:42:THR:HG22	32:K:44:GLU:H	1.65	0.60
5:E:198:VAL:HB	5:E:232:MET:SD	2.42	0.60
9:J:91:CYS:SG	9:J:107:ILE:HD13	2.41	0.60
24:a:227:ASN:O	24:a:231:GLN:NE2	2.34	0.60
24:a:370:GLN:HE21	27:d:244:LYS:HE2	1.66	0.60
28:u:609:VAL:HG13	28:u:657:ILE:HG13	1.82	0.60
2:B:287:ILE:HG21	2:B:329:MET:HG2	1.83	0.60
8:I:33:THR:HG21	8:I:200:THR:HG21	1.82	0.60
19:V:65:ARG:NH2	19:V:66:GLU:CD	2.59	0.60
21:X:118:LYS:HD2	21:X:126:ARG:HD2	1.84	0.60
24:a:57:ILE:HG13	24:a:61:GLU:OE2	2.02	0.60
13:o:7:VAL:HG22	13:o:12:ILE:CD1	2.31	0.60
28:u:445:LEU:HD12	28:u:481:SER:HA	1.83	0.60
31:F:80:ILE:HD11	31:F:139:LEU:HD11	1.84	0.60
31:F:226:TYR:HB2	31:F:335:VAL:HG22	1.83	0.60
3:C:198:LEU:HD12	3:C:199:LEU:H	1.66	0.60
13:O:67:SER:HB3	13:O:74:PRO:HG3	1.84	0.60
22:Y:70:LEU:HA	22:Y:73:MET:HG3	1.84	0.60
24:a:309:LEU:HA	24:a:312:MET:SD	2.40	0.60
25:b:58:CYS:HB3	25:b:92:VAL:HG11	1.83	0.60
16:r:36:GLU:HG2	16:r:184:TRP:CZ2	2.37	0.60
28:u:77:GLU:HA	28:u:80:ARG:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:TYR:CB	28:u:670:MET:HE3	2.32	0.60
19:V:384:GLU:HA	19:V:384:GLU:OE2	2.02	0.60
9:j:8:THR:HG22	32:k:135:ARG:HD3	1.83	0.60
28:u:94:LYS:O	28:u:97:LYS:HG2	2.01	0.60
28:u:766:GLN:HA	28:u:769:THR:HG22	1.82	0.60
29:U:486:MET:CE	29:U:521:LEU:HD23	2.31	0.60
1:A:414:ASN:HA	1:A:418:LYS:HB3	1.82	0.60
3:C:89:VAL:HG23	3:C:90:HIS:H	1.66	0.60
18:T:96:MET:HE2	18:T:110:MET:HE1	1.83	0.60
19:V:120:PHE:HB3	19:V:121:PHE:CD2	2.36	0.60
6:g:192:GLU:HA	6:g:192:GLU:OE2	2.01	0.60
18:t:208:ASN:OD1	18:t:210:ASP:OD1	2.20	0.60
28:u:829:MET:C	28:u:829:MET:HE2	2.26	0.60
29:U:529:ILE:HD12	29:U:530:GLU:H	1.65	0.60
31:F:287:GLU:HA	31:F:332:THR:HA	1.84	0.60
1:A:106:SER:O	1:A:110:LYS:NZ	2.35	0.60
1:A:251:GLY:H	1:A:294:GLU:CB	2.15	0.60
3:C:110:PRO:HG2	3:C:130:LYS:NZ	2.16	0.60
5:E:101:ASP:HB3	5:E:105:LEU:N	2.17	0.60
19:V:324:PHE:HB2	30:e:5:LYS:HG3	1.82	0.60
20:W:265:GLN:NE2	20:W:335:SER:HB3	2.16	0.60
22:Y:101:ARG:HH21	22:Y:136:HIS:HB3	1.67	0.60
23:Z:72:HIS:CE1	23:Z:114:ARG:HH22	2.19	0.60
27:d:187:GLU:OE1	27:d:188:LYS:HB3	2.02	0.60
29:U:161:ASP:OD1	29:U:161:ASP:N	2.34	0.60
3:C:66:LEU:HD12	4:D:114:ARG:CD	2.18	0.60
5:E:281:ARG:HH22	5:E:283:ASP:HB2	1.66	0.60
5:E:345:ASN:CG	31:F:345:SER:HB2	2.27	0.60
6:G:165:ALA:HB1	6:G:179:LEU:HD13	1.83	0.60
19:V:338:LEU:HD21	19:V:397:ARG:HG3	1.83	0.60
20:W:435:LEU:HD23	23:Z:236:LEU:CD1	2.31	0.60
22:Y:231:LEU:HG	22:Y:236:LEU:HD23	1.84	0.60
29:U:643:SER:O	29:U:649:ARG:NH1	2.34	0.60
29:U:873:PRO:HA	29:U:875:PHE:CZ	2.37	0.60
31:F:288:LEU:HD21	31:F:330:ALA:HB1	1.84	0.60
1:A:164:MET:HA	1:A:241:ILE:HD13	1.83	0.60
1:A:257:VAL:O	1:A:261:PHE:HB2	2.02	0.60
5:E:336:ASP:HA	5:E:338:PHE:CE1	2.37	0.60
21:X:366:SER:O	21:X:369:ILE:HG22	2.02	0.60
23:Z:138:TYR:C	23:Z:139:ILE:HD13	2.26	0.60
23:Z:139:ILE:HB	23:Z:156:GLU:CD	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:236:LEU:HD23	23:Z:236:LEU:C	2.26	0.60
26:c:46:ARG:HH11	26:c:46:ARG:HG2	1.67	0.60
29:U:243:LEU:HB3	29:U:244:MET:SD	2.42	0.60
1:A:187:LEU:HD13	1:A:229:VAL:HG11	1.84	0.59
3:C:98:ASP:N	3:C:98:ASP:OD2	2.35	0.59
11:M:196:ILE:O	11:M:200:VAL:HG23	2.02	0.59
19:V:179:LYS:HA	19:V:182:LYS:HZ2	1.66	0.59
20:W:39:ARG:H	20:W:39:ARG:HD3	1.66	0.59
25:b:124:LEU:HD13	25:b:156:PHE:HB2	1.84	0.59
26:c:161:ARG:HG2	26:c:201:TYR:OH	2.01	0.59
10:l:125:ARG:HD3	10:l:126:ARG:N	2.16	0.59
29:U:422:LEU:HD13	29:U:423:MET:HE2	1.83	0.59
29:U:581:SER:O	29:U:585:THR:HG23	2.01	0.59
31:F:382:GLU:OE1	31:F:382:GLU:N	2.34	0.59
29:U:68:PHE:CD2	29:U:76:GLU:HG2	2.37	0.59
5:E:231:PHE:CD1	5:E:276:ILE:CD1	2.85	0.59
6:G:71:LYS:O	6:G:95:ARG:NH1	2.35	0.59
26:c:212:LEU:CA	26:c:215:LYS:HG2	2.32	0.59
26:c:217:LEU:O	26:c:218:LEU:C	2.45	0.59
29:U:360:VAL:HG13	29:U:365:CYS:HB3	1.84	0.59
31:F:73:ILE:HG23	31:F:74:LYS:HE2	1.84	0.59
31:F:333:ASN:C	31:F:334:ARG:HE	2.11	0.59
1:A:411:GLU:HA	1:A:414:ASN:HD22	1.67	0.59
2:B:68:ILE:HA	28:u:670:MET:HE1	1.85	0.59
2:B:292:THR:HG22	2:B:293:LYS:HG2	1.84	0.59
3:C:83:LYS:O	3:C:83:LYS:NZ	2.34	0.59
18:T:59:ASP:HB2	18:T:108:ASN:HD21	1.66	0.59
22:Y:113:ARG:HG2	22:Y:114:ILE:CD1	2.28	0.59
23:Z:54:PHE:C	23:Z:54:PHE:CD2	2.81	0.59
9:j:105:GLU:OE2	9:j:105:GLU:C	2.44	0.59
29:U:325:MET:HA	29:U:328:ILE:HG22	1.83	0.59
23:Z:44:GLN:OE1	23:Z:44:GLN:N	2.36	0.59
29:U:666:LYS:HD2	29:U:666:LYS:O	2.02	0.59
1:A:115:VAL:HG12	1:A:117:GLN:H	1.66	0.59
2:B:291:GLY:HA2	2:B:309:MET:HE2	1.84	0.59
5:E:181:THR:HG23	34:E:401:ADP:O3B	2.02	0.59
19:V:463:MET:HE3	19:V:464:ILE:N	2.18	0.59
10:l:35:THR:OG1	10:l:133:LEU:HD12	2.03	0.59
29:U:189:GLN:NE2	29:U:595:ASN:OD1	2.35	0.59
29:U:212:ASP:O	29:U:213:PHE:C	2.45	0.59
4:D:293:LEU:HD21	4:D:321:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:95:MET:HG3	12:N:116:MET:HE1	1.83	0.59
17:S:148:LEU:HD23	17:S:178:VAL:HG12	1.83	0.59
26:c:49:VAL:N	26:c:50:PRO:HD2	2.17	0.59
8:i:176:LYS:HZ2	9:j:52:LYS:HG2	1.67	0.59
32:K:186:HIS:CE1	32:K:188:SER:HG	2.19	0.59
1:A:115:VAL:HG12	1:A:118:PHE:H	1.67	0.59
2:B:221:GLY:HA3	2:B:347:ILE:CD1	2.29	0.59
4:D:274:ARG:NH1	4:D:276:ASP:O	2.35	0.59
8:I:21:VAL:O	8:I:25:MET:HG3	2.03	0.59
13:O:143:ARG:HB2	13:O:143:ARG:CZ	2.32	0.59
31:F:382:GLU:CD	31:F:383:GLU:H	2.11	0.59
4:D:122:GLU:OE1	4:D:122:GLU:N	2.36	0.59
20:W:436:MET:HE1	23:Z:236:LEU:HD13	1.85	0.59
22:Y:191:ILE:HD11	22:Y:293:ARG:NH2	2.18	0.59
22:Y:217:LYS:HD2	22:Y:253:LEU:HD21	1.84	0.59
23:Z:40:LEU:HD23	23:Z:91:ILE:HD13	1.85	0.59
8:i:3:ARG:NE	8:i:3:ARG:O	2.35	0.59
28:u:233:LEU:O	28:u:237:VAL:HG13	2.03	0.59
5:E:342:ASP:O	5:E:346:VAL:HG23	2.02	0.59
19:V:33:GLN:NE2	19:V:83:GLU:O	2.36	0.59
21:X:268:GLN:OE1	21:X:268:GLN:O	2.20	0.59
23:Z:28:LYS:O	23:Z:28:LYS:HD3	2.03	0.59
29:U:446:LEU:HD11	29:U:461:LEU:HD21	1.85	0.59
1:A:249:TYR:HB2	1:A:252:GLU:HB2	1.83	0.58
18:T:179:ARG:HD3	13:o:139:GLU:OE1	2.02	0.58
19:V:494:MET:HE2	19:V:494:MET:HA	1.85	0.58
20:W:372:ARG:HH12	24:a:327:VAL:HG23	1.64	0.58
22:Y:201:PHE:CD1	22:Y:219:PHE:HE1	2.21	0.58
22:Y:220:VAL:O	22:Y:223:THR:HG22	2.02	0.58
11:m:223:ARG:HG2	11:m:223:ARG:O	2.02	0.58
29:U:744:VAL:HG21	29:U:783:TYR:HB3	1.85	0.58
32:K:240:ASP:OD1	32:K:240:ASP:O	2.21	0.58
3:C:368:MET:HG3	4:D:329:ARG:HH22	1.67	0.58
22:Y:314:LEU:HD22	22:Y:319:MET:HE3	1.84	0.58
26:c:175:ARG:HG3	26:c:181:LEU:HD22	1.85	0.58
27:d:61:TRP:HB3	27:d:65:ARG:HH22	1.69	0.58
1:A:333:ARG:HH22	1:A:336:ARG:HE	1.51	0.58
3:C:198:LEU:HD12	3:C:199:LEU:N	2.19	0.58
4:D:64:GLU:OE2	29:U:607:VAL:HG13	2.03	0.58
13:O:203:ARG:NH1	14:P:162:HIS:CE1	2.71	0.58
19:V:36:GLU:N	19:V:36:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:130:MET:HE2	20:W:130:MET:C	2.28	0.58
25:b:84:ILE:H	25:b:84:ILE:HD12	1.66	0.58
10:l:121:GLN:HG3	11:m:129:ARG:HG3	1.84	0.58
28:u:699:VAL:HA	28:u:731:MET:HE2	1.85	0.58
3:C:358:GLU:HA	4:D:324:PRO:HG2	1.84	0.58
5:E:122:MET:HB2	5:E:196:LEU:HA	1.84	0.58
5:E:200:SER:HB3	5:E:233:ASP:O	2.02	0.58
16:R:166:ARG:NH1	15:q:144:ASP:OD2	2.36	0.58
19:V:209:LYS:HA	19:V:212:TYR:CD2	2.39	0.58
22:Y:300:ARG:NH1	30:e:59:GLU:OE1	2.32	0.58
23:Z:230:LEU:HD12	23:Z:231:GLN:N	2.18	0.58
24:a:309:LEU:HA	24:a:312:MET:CG	2.34	0.58
11:m:50:GLU:HG2	11:m:50:GLU:O	2.03	0.58
16:r:197:GLU:HA	16:r:197:GLU:OE2	2.02	0.58
28:u:427:THR:O	28:u:430:ASP:OD2	2.20	0.58
29:U:247:GLN:OE1	29:U:913:ILE:HG23	2.03	0.58
31:F:309:THR:O	31:F:312:GLU:HG3	2.03	0.58
1:A:54:GLN:O	1:A:58:LYS:HG3	2.03	0.58
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.83	0.58
14:P:173:ASN:HD21	17:s:151:ASN:ND2	2.01	0.58
19:V:55:THR:HG21	19:V:196:SER:HB3	1.85	0.58
20:W:47:LEU:H	20:W:47:LEU:CD2	2.16	0.58
22:Y:181:LYS:HB3	22:Y:181:LYS:NZ	2.17	0.58
26:c:29:GLU:HB3	26:c:203:ILE:HD11	1.85	0.58
27:d:10:ASN:ND2	27:d:11:ARG:CZ	2.67	0.58
29:U:213:PHE:HD1	29:U:214:ILE:HG13	1.68	0.58
31:F:376:SER:O	31:F:378:ASP:N	2.36	0.58
32:K:206:MET:CE	32:K:215:ILE:HG22	2.33	0.58
1:A:197:HIS:CD2	1:A:199:GLU:HB2	2.39	0.58
4:D:271:ALA:HA	4:D:289:LEU:HD21	1.85	0.58
8:I:116:ASP:OD2	9:J:81:ARG:NH1	2.36	0.58
19:V:137:GLU:OE2	19:V:137:GLU:N	2.30	0.58
19:V:178:SER:O	19:V:182:LYS:HG3	2.04	0.58
28:u:208:LEU:HD12	28:u:217:LEU:HD13	1.85	0.58
30:e:61:GLU:OE1	30:e:61:GLU:N	2.36	0.58
31:F:249:LEU:HD23	31:F:283:ILE:HG13	1.85	0.58
1:A:418:LYS:CA	1:A:422:LYS:HB2	2.22	0.58
2:B:362:LYS:NZ	2:B:366:GLN:HB2	2.19	0.58
4:D:408:LYS:HE2	4:D:408:LYS:CA	2.20	0.58
14:P:151:GLU:OE1	17:s:185:ARG:CG	2.51	0.58
19:V:62:HIS:O	19:V:66:GLU:OE1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:175:LEU:HD21	26:c:38:LEU:HD22	1.85	0.58
27:d:139:LEU:HD11	27:d:151:VAL:HG13	1.86	0.58
31:F:180:ARG:HD3	31:F:181:PRO:HD2	1.85	0.58
31:F:272:PHE:CD1	31:F:272:PHE:O	2.57	0.58
1:A:270:CYS:H	1:A:315:ILE:HA	1.68	0.58
14:P:118:LYS:HG2	14:P:119:PRO:HD2	1.86	0.58
19:V:304:GLU:OE1	19:V:307:ARG:NH2	2.32	0.58
20:W:4:GLY:HA2	20:W:7:GLU:HG2	1.84	0.58
27:d:106:LEU:HD11	27:d:114:GLU:HG3	1.85	0.58
13:o:190:THR:HG22	13:o:192:PRO:HD3	1.86	0.58
1:A:164:MET:HE3	1:A:240:VAL:HA	1.86	0.58
1:A:272:ILE:HD13	1:A:317:VAL:HG22	1.86	0.58
2:B:41:LYS:HE2	28:u:708:ASP:OD2	2.02	0.58
24:a:168:ASN:OD1	24:a:171:SER:OG	2.20	0.58
31:F:292:GLY:CA	31:F:310:MET:HG2	2.34	0.58
1:A:105:ASP:HB2	1:A:110:LYS:HB2	1.85	0.58
2:B:429:LYS:HG2	3:C:314:LYS:HD3	1.85	0.58
25:b:108:ARG:HH11	25:b:137:ASN:ND2	1.98	0.58
13:o:46:ALA:HA	37:o:301:LDZ:H22	1.86	0.58
29:U:443:LEU:O	29:U:446:LEU:HD12	2.04	0.58
1:A:251:GLY:H	1:A:294:GLU:CA	2.17	0.57
19:V:58:ALA:O	22:Y:389:MET:SD	2.62	0.57
21:X:332:GLU:O	21:X:336:ILE:HG13	2.04	0.57
22:Y:104:MET:HG3	22:Y:127:THR:HB	1.86	0.57
23:Z:263:ALA:CB	26:c:292:MET:HE2	2.29	0.57
1:A:135:GLU:H	1:A:138:MET:CE	2.07	0.57
4:D:369:LYS:HD3	4:D:369:LYS:N	2.18	0.57
5:E:59:GLU:HG2	5:E:72:LYS:HB3	1.87	0.57
5:E:78:ARG:H	5:E:78:ARG:HD2	1.67	0.57
19:V:211:TYR:O	19:V:212:TYR:C	2.45	0.57
20:W:33:LYS:O	20:W:33:LYS:NZ	2.33	0.57
21:X:407:MET:HE2	21:X:407:MET:CA	2.34	0.57
22:Y:67:VAL:HA	22:Y:70:LEU:HD12	1.86	0.57
22:Y:112:CYS:SG	22:Y:147:ILE:HD11	2.44	0.57
24:a:6:GLY:HA2	24:a:9:GLN:HB2	1.85	0.57
27:d:41:THR:HG22	27:d:44:THR:H	1.69	0.57
27:d:114:GLU:HA	27:d:117:THR:HG22	1.85	0.57
27:d:150:LYS:O	27:d:150:LYS:HD3	2.04	0.57
1:A:140:VAL:HB	1:A:149:ILE:HG23	1.85	0.57
4:D:153:MET:O	4:D:154:LEU:C	2.47	0.57
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:235:ILE:HG22	5:E:279:THR:HB	1.86	0.57
13:O:70:THR:HG22	13:O:72:ARG:HE	1.69	0.57
19:V:492:LYS:C	19:V:494:MET:H	2.11	0.57
21:X:114:ILE:CD1	21:X:129:LEU:HD13	2.33	0.57
1:A:330:ALA:O	1:A:336:ARG:HD2	2.02	0.57
2:B:191:ASP:CA	2:B:194:ILE:HD12	2.31	0.57
16:R:115:ASP:OD2	16:R:117:GLU:OE2	2.21	0.57
24:a:201:GLY:HA3	24:a:233:LEU:HD21	1.85	0.57
7:h:68:ILE:HD11	7:h:74:LEU:HD22	1.86	0.57
5:E:303:LEU:CD2	5:E:304:PRO:HD3	2.33	0.57
8:I:174:MET:CE	8:I:199:LYS:HD3	2.35	0.57
20:W:191:ARG:HD3	20:W:192:LEU:N	2.19	0.57
21:X:380:GLN:HB2	22:Y:314:LEU:HA	1.85	0.57
16:r:45:MET:HG2	16:r:52:CYS:HB3	1.85	0.57
29:U:613:ASP:HA	29:U:616:ARG:HE	1.68	0.57
31:F:188:ILE:O	31:F:188:ILE:HG22	2.04	0.57
1:A:190:VAL:HG13	1:A:212:VAL:HG21	1.87	0.57
2:B:35:LYS:NZ	2:B:38:LYS:HG3	2.19	0.57
5:E:60:VAL:HG23	5:E:96:THR:O	2.05	0.57
10:L:103:LEU:HD12	10:L:104:PRO:HD2	1.86	0.57
20:W:436:MET:O	20:W:440:ASN:OD1	2.23	0.57
7:h:228:ASP:OD2	7:h:229:TYR:CD1	2.58	0.57
9:j:165:ALA:O	9:j:169:ARG:N	2.35	0.57
28:u:829:MET:HE2	28:u:830:LEU:N	2.20	0.57
31:F:199:VAL:HG13	31:F:203:VAL:HB	1.87	0.57
31:F:348:LEU:C	31:F:350:ARG:N	2.62	0.57
31:F:378:ASP:CA	31:F:417:HIS:HA	2.31	0.57
2:B:78:PHE:HD2	28:u:613:LEU:HB3	1.68	0.57
16:R:38:ASN:N	16:R:38:ASN:HD22	2.02	0.57
25:b:24:THR:HB	25:b:27:GLN:HG2	1.87	0.57
25:b:108:ARG:HG3	25:b:137:ASN:HD22	1.67	0.57
29:U:415:HIS:HB3	29:U:419:ALA:HB2	1.87	0.57
1:A:291:GLY:O	31:F:171:ARG:NH2	2.37	0.57
5:E:326:ILE:HG23	5:E:364:GLN:HG2	1.86	0.57
19:V:36:GLU:HA	19:V:39:GLU:OE2	2.04	0.57
24:a:370:GLN:HG2	27:d:244:LYS:HD2	1.85	0.57
26:c:232:GLN:HE22	26:c:237:HIS:HB2	1.69	0.57
11:m:221:ASN:HB2	11:m:223:ARG:HH21	1.70	0.57
29:U:462:LEU:HD11	29:U:492:ASP:OD2	2.04	0.57
5:E:55:GLN:HB2	31:F:133:PHE:HD2	1.69	0.57
5:E:151:LEU:H	5:E:151:LEU:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:53:ASP:O	13:O:57:GLN:HG3	2.04	0.57
26:c:186:LYS:HD2	26:c:186:LYS:N	2.20	0.57
13:o:80:ASN:HD21	13:o:119:THR:HG21	1.69	0.57
31:F:39:GLU:HA	31:F:42:ILE:HB	1.86	0.57
31:F:225:MET:CE	31:F:329:ILE:HG22	2.29	0.57
1:A:75:PRO:HA	1:A:78:TRP:CE2	2.39	0.57
1:A:111:TYR:HE2	1:A:134:ILE:HB	1.69	0.57
1:A:159:PRO:O	1:A:160:THR:HB	2.05	0.57
1:A:246:VAL:HG22	1:A:280:ILE:HD12	1.87	0.57
1:A:293:ASN:N	31:F:171:ARG:HH22	2.02	0.57
2:B:190:LEU:HB3	2:B:194:ILE:HD11	1.87	0.57
2:B:425:ASN:HD21	3:C:313:ARG:HH12	1.53	0.57
9:J:88:ARG:NH1	15:Q:69:MET:O	2.38	0.57
11:M:236:GLU:O	11:M:240:LYS:HG2	2.05	0.57
19:V:437:ILE:HD13	27:d:146:GLY:HA3	1.85	0.57
23:Z:146:ASP:HB3	23:Z:149:THR:OG1	2.05	0.57
6:g:153:LYS:HD3	6:g:166:THR:HG21	1.87	0.57
29:U:24:LEU:HD21	29:U:60:ALA:HA	1.87	0.57
5:E:120:TYR:HA	5:E:123:SER:HB3	1.86	0.56
8:I:238:LYS:O	8:I:238:LYS:NZ	2.33	0.56
14:P:164:PHE:HB2	14:P:189:ILE:HD11	1.87	0.56
20:W:328:LEU:HD22	20:W:351:TRP:CZ2	2.40	0.56
7:h:228:ASP:OD2	7:h:228:ASP:C	2.48	0.56
10:l:153:TYR:O	11:m:63:ASN:ND2	2.38	0.56
14:p:190:ILE:CG2	14:p:195:ILE:HG12	2.30	0.56
31:F:178:ASP:HA	31:F:248:PHE:HB3	1.86	0.56
1:A:57:LYS:O	1:A:61:GLU:HG2	2.05	0.56
2:B:182:GLU:HG2	2:B:183:THR:H	1.69	0.56
3:C:82:LYS:HG3	3:C:82:LYS:O	2.04	0.56
5:E:177:GLY:O	5:E:339:ASN:ND2	2.38	0.56
8:I:84:ASN:HD22	8:I:84:ASN:N	2.01	0.56
16:R:49:ALA:O	16:R:53:SER:OG	2.22	0.56
18:T:211:ILE:HA	18:T:214:MET:HE3	1.87	0.56
19:V:66:GLU:HA	19:V:69:THR:HG22	1.85	0.56
21:X:415:TYR:HE1	22:Y:383:LEU:HB2	1.70	0.56
24:a:138:VAL:HG11	24:a:155:PHE:HB2	1.86	0.56
25:b:157:VAL:HG21	25:b:170:LEU:HB2	1.86	0.56
27:d:57:ILE:HB	27:d:61:TRP:CE2	2.40	0.56
8:i:118:LYS:NZ	8:i:150:SER:OG	2.36	0.56
13:o:1:THR:OG1	37:o:301:LDZ:O33	2.23	0.56
1:A:197:HIS:HB3	1:A:200:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:PRO:HG3	28:u:740:ARG:HE	1.70	0.56
4:D:87:LEU:HD13	4:D:131:ALA:HB1	1.88	0.56
22:Y:174:TRP:O	22:Y:175:ASP:C	2.48	0.56
23:Z:34:ARG:NH1	23:Z:60:GLU:OE1	2.39	0.56
26:c:219:ASN:O	26:c:223:LYS:HG3	2.05	0.56
31:F:151:VAL:HG22	31:F:163:THR:HG23	1.86	0.56
31:F:240:CYS:O	31:F:243:GLN:NE2	2.38	0.56
31:F:312:GLU:O	31:F:316:GLN:HB2	2.04	0.56
31:F:418:GLU:O	31:F:422:GLU:HG3	2.05	0.56
1:A:265:ARG:HH21	1:A:305:GLN:HG2	1.69	0.56
2:B:195:GLN:O	2:B:199:GLU:HG3	2.06	0.56
4:D:181:VAL:HG13	4:D:261:ILE:HD11	1.88	0.56
19:V:60:ALA:HB3	19:V:62:HIS:HD2	1.71	0.56
19:V:211:TYR:O	19:V:214:HIS:N	2.38	0.56
19:V:225:ASP:OD1	19:V:228:ARG:HD3	2.05	0.56
26:c:189:ILE:O	26:c:192:LEU:HG	2.06	0.56
28:u:512:MET:HE3	28:u:515:ALA:HB3	1.88	0.56
31:F:406:ILE:HA	31:F:409:ARG:HG2	1.87	0.56
1:A:22:ILE:HG21	3:C:159:LYS:HZ3	1.69	0.56
1:A:265:ARG:HH22	1:A:309:PHE:HB3	1.70	0.56
2:B:411:ARG:NH1	2:B:413:LYS:O	2.38	0.56
3:C:251:ILE:HG13	3:C:293:MET:CE	2.35	0.56
19:V:85:ALA:O	19:V:89:LYS:NZ	2.38	0.56
19:V:296:LYS:HA	19:V:299:GLN:OE1	2.05	0.56
29:U:443:LEU:HA	29:U:446:LEU:HG	1.87	0.56
29:U:583:MET:SD	29:U:618:ALA:HA	2.45	0.56
32:K:204:GLN:HA	32:K:204:GLN:HE21	1.71	0.56
23:Z:35:VAL:O	23:Z:96:HIS:HA	2.05	0.56
25:b:7:MET:HE3	25:b:52:ILE:CB	2.35	0.56
25:b:7:MET:HE3	25:b:52:ILE:HG22	1.87	0.56
25:b:18:ASN:HD22	25:b:25:ARG:NH2	2.04	0.56
7:h:111:VAL:HG22	7:h:136:ILE:HG13	1.87	0.56
8:i:95:GLN:HG2	14:p:73:LEU:HG	1.87	0.56
8:i:242:GLU:O	8:i:242:GLU:CD	2.49	0.56
29:U:406:ALA:HA	29:U:445:ALA:HB2	1.87	0.56
1:A:183:GLN:HG2	1:A:343:PHE:CD1	2.41	0.56
4:D:389:GLU:HB2	4:D:391:ARG:HE	1.71	0.56
18:T:96:MET:HE2	18:T:110:MET:HE2	1.88	0.56
19:V:81:GLN:HB3	19:V:85:ALA:HB3	1.86	0.56
20:W:423:ASN:HA	20:W:426:ASN:OD1	2.05	0.56
24:a:312:MET:HA	24:a:315:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:278:GLN:CG	26:c:282:ARG:HH21	2.18	0.56
28:u:228:LYS:HE2	28:u:228:LYS:H	1.71	0.56
29:U:94:SER:HB3	29:U:97:VAL:HG12	1.87	0.56
1:A:73:ALA:HB2	2:B:140:ASP:H	1.71	0.56
2:B:61:LYS:O	2:B:65:LEU:HG	2.06	0.56
2:B:304:GLU:HG3	2:B:307:ARG:HH21	1.71	0.56
2:B:425:ASN:ND2	3:C:313:ARG:HH12	2.03	0.56
3:C:158:ILE:HG22	3:C:162:LYS:HE2	1.86	0.56
10:L:118:ILE:HG23	10:L:122:ARG:HE	1.69	0.56
14:P:65:GLN:OE1	15:Q:86:ARG:NH2	2.38	0.56
22:Y:105:MET:O	22:Y:105:MET:HG3	2.04	0.56
14:p:12:MET:HG3	14:p:138:VAL:HG12	1.87	0.56
29:U:188:MET:HE1	29:U:193:PHE:CZ	2.41	0.56
29:U:764:LEU:O	29:U:767:THR:OG1	2.21	0.56
4:D:332:GLU:C	4:D:332:GLU:OE1	2.49	0.56
14:P:58:THR:O	14:P:62:THR:HG23	2.06	0.56
14:P:151:GLU:OE1	17:s:185:ARG:HG2	2.07	0.56
19:V:487:HIS:CE1	23:Z:267:ARG:HH21	2.24	0.56
20:W:334:GLU:O	20:W:335:SER:C	2.49	0.56
26:c:269:GLN:OE1	26:c:273:LYS:HB3	2.06	0.56
27:d:125:LYS:HE3	27:d:130:ASN:HB2	1.88	0.56
1:A:229:VAL:O	1:A:232:ARG:HG3	2.05	0.55
4:D:261:ILE:HD13	4:D:306:LYS:HB2	1.88	0.55
10:L:53:GLN:NE2	32:K:168:ARG:HH12	2.02	0.55
10:L:107:ARG:NH1	18:T:74:GLU:OE1	2.36	0.55
19:V:258:TYR:HB2	19:V:269:LYS:NZ	2.21	0.55
19:V:397:ARG:HA	19:V:400:HIS:HE1	1.71	0.55
22:Y:50:MET:SD	22:Y:73:MET:HE1	2.46	0.55
23:Z:167:ALA:CB	26:c:46:ARG:NH1	2.67	0.55
25:b:161:ASN:HD21	25:b:168:SER:H	1.53	0.55
8:i:17:ARG:NH1	8:i:19:TYR:HD1	2.02	0.55
28:u:766:GLN:C	28:u:769:THR:HG22	2.32	0.55
29:U:68:PHE:HE2	29:U:80:TYR:CD2	2.24	0.55
29:U:205:TYR:O	29:U:211:PRO:HB3	2.06	0.55
31:F:141:ASP:H	31:F:144:LYS:HE3	1.70	0.55
21:X:114:ILE:O	21:X:118:LYS:HG2	2.05	0.55
21:X:240:ASP:OD1	21:X:279:TYR:OH	2.25	0.55
27:d:128:GLN:HG3	27:d:129:THR:HG22	1.86	0.55
27:d:152:PHE:CE1	27:d:199:PHE:HE1	2.25	0.55
28:u:290:VAL:O	28:u:294:MET:HG3	2.06	0.55
1:A:99:THR:HG21	1:A:115:VAL:HG22	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LYS:HD2	1:A:422:LYS:HD3	1.87	0.55
3:C:43:ARG:HA	3:C:46:GLN:HG2	1.88	0.55
7:H:4:ARG:NH1	7:H:4:ARG:HA	2.22	0.55
11:M:94:GLU:OE2	11:M:114:ARG:NE	2.21	0.55
19:V:211:TYR:CD1	19:V:253:LEU:HD13	2.39	0.55
22:Y:13:LYS:HE3	22:Y:112:CYS:O	2.05	0.55
15:q:38:MET:HE1	15:q:60:ILE:CG2	2.36	0.55
15:q:94:SER:OG	15:q:95:ARG:N	2.39	0.55
29:U:556:MET:HE1	29:U:589:ALA:HA	1.88	0.55
1:A:306:LEU:HB3	1:A:336:ARG:NH1	2.22	0.55
3:C:213:ARG:CZ	4:D:299:PHE:HB2	2.37	0.55
5:E:305:ASN:HB2	5:E:309:ARG:N	2.21	0.55
19:V:258:TYR:HD1	19:V:269:LYS:HE2	1.70	0.55
26:c:121:TRP:CE2	26:c:194:HIS:CE1	2.94	0.55
9:j:170:GLU:HA	9:j:173:GLU:HB2	1.87	0.55
31:F:359:GLU:HG2	31:F:360:GLU:OE2	2.05	0.55
1:A:51:ASP:CA	1:A:54:GLN:HG2	2.35	0.55
4:D:135:HIS:CG	26:c:149:GLN:HE22	2.24	0.55
4:D:374:ASP:OD1	5:E:292:PRO:CG	2.53	0.55
5:E:216:ARG:HG2	5:E:263:GLN:HE21	1.72	0.55
6:G:112:ASP:OD2	13:O:72:ARG:NH2	2.38	0.55
7:H:10:LEU:HD13	7:H:21:GLN:HB2	1.88	0.55
7:H:22:ILE:HD11	7:H:122:THR:OG1	2.07	0.55
13:O:91:GLN:HA	13:O:91:GLN:OE1	2.07	0.55
19:V:463:MET:HE3	19:V:464:ILE:C	2.31	0.55
25:b:18:ASN:ND2	25:b:25:ARG:NH2	2.54	0.55
6:g:207:SER:C	6:g:208:ILE:HD13	2.32	0.55
31:F:365:ILE:HD13	31:F:393:GLY:HA2	1.89	0.55
1:A:155:PRO:HG2	1:A:255:ARG:HH12	1.70	0.55
2:B:105:THR:HG23	2:B:106:PRO:HD3	1.88	0.55
2:B:125:THR:OG1	2:B:126:SER:N	2.37	0.55
2:B:382:ASP:CA	2:B:385:MET:SD	2.88	0.55
5:E:185:ARG:HH11	5:E:185:ARG:HA	1.72	0.55
18:T:47:ASN:O	18:T:47:ASN:ND2	2.40	0.55
19:V:349:ARG:HA	19:V:353:LEU:HD23	1.89	0.55
21:X:56:LEU:O	21:X:60:THR:HG23	2.06	0.55
29:U:873:PRO:HB2	29:U:876:GLN:NE2	2.22	0.55
1:A:428:ARG:HA	9:J:23:GLN:HE22	1.71	0.55
4:D:154:LEU:HD21	4:D:229:ARG:HD3	1.89	0.55
6:G:117:ARG:O	6:G:121:ILE:HG12	2.06	0.55
6:G:141:ILE:HG22	6:G:151:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:220:LEU:HB2	23:Z:221:PRO:CD	2.30	0.55
7:h:5:GLY:C	9:j:3:TYR:OH	2.50	0.55
29:U:575:ASP:OD2	29:U:578:LEU:HD13	2.06	0.55
29:U:624:PHE:HE2	29:U:764:LEU:HD23	1.72	0.55
31:F:196:GLN:O	31:F:200:GLU:HG2	2.06	0.55
31:F:370:SER:HB2	31:F:375:VAL:HG11	1.89	0.55
1:A:242:GLY:HA3	1:A:276:GLU:O	2.07	0.55
1:A:295:VAL:O	1:A:296:GLN:C	2.50	0.55
2:B:71:TYR:O	2:B:75:GLU:HG2	2.07	0.55
2:B:155:LYS:H	2:B:155:LYS:HE2	1.72	0.55
3:C:253:SER:O	3:C:254:ILE:HG13	2.07	0.55
15:Q:197:PRO:HA	15:q:199:GLN:H	1.72	0.55
19:V:37:MET:HE3	19:V:92:ARG:HH12	1.70	0.55
26:c:256:ASN:O	26:c:260:GLU:HG3	2.07	0.55
28:u:286:LYS:HA	28:u:286:LYS:HE3	1.88	0.55
29:U:625:ILE:HG13	29:U:626:LEU:HG	1.88	0.55
1:A:157:ILE:HB	1:A:255:ARG:NH2	2.22	0.55
10:L:65:HIS:O	10:L:89:ARG:NH1	2.39	0.55
20:W:170:GLN:OE1	20:W:170:GLN:N	2.40	0.55
21:X:403:THR:O	21:X:407:MET:HG2	2.06	0.55
24:a:21:VAL:HG23	24:a:22:TRP:HD1	1.68	0.55
24:a:236:THR:HA	24:a:249:GLN:NE2	2.21	0.55
26:c:198:ARG:HG3	26:c:199:HIS:ND1	2.22	0.55
27:d:10:ASN:CG	27:d:11:ARG:CZ	2.80	0.55
1:A:274:PHE:HB2	1:A:277:ILE:HG23	1.89	0.55
2:B:106:PRO:HG2	2:B:154:HIS:CD2	2.41	0.55
5:E:222:ALA:C	5:E:224:ASP:N	2.65	0.55
5:E:233:ASP:HA	5:E:278:ALA:HB3	1.88	0.55
5:E:337:GLY:O	5:E:339:ASN:N	2.40	0.55
20:W:254:PRO:HA	20:W:257:GLN:HG2	1.88	0.55
22:Y:192:ARG:HH21	22:Y:194:PHE:CB	2.18	0.55
27:d:19:CYS:SG	27:d:65:ARG:NH2	2.80	0.55
28:u:208:LEU:HD22	28:u:216:MET:HG3	1.87	0.55
29:U:844:LYS:HE3	29:U:844:LYS:CA	2.32	0.55
8:I:68:LEU:HD22	8:I:90:LEU:HB3	1.89	0.54
15:Q:118:MET:HE2	15:Q:124:LEU:HD13	1.89	0.54
18:T:9:THR:O	18:T:41:ARG:NH2	2.33	0.54
19:V:96:ARG:CB	19:V:150:ARG:HH22	2.20	0.54
19:V:176:MET:HE1	19:V:217:VAL:HG21	1.88	0.54
21:X:368:MET:SD	21:X:374:PHE:CD2	3.00	0.54
6:g:145:GLU:C	6:g:145:GLU:OE1	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:605:ASN:O	28:u:609:VAL:HG23	2.06	0.54
29:U:458:ILE:HD13	29:U:490:ARG:HH12	1.71	0.54
29:U:633:CYS:SG	29:U:659:CYS:HB3	2.47	0.54
1:A:173:THR:HG22	1:A:175:SER:H	1.72	0.54
1:A:197:HIS:CE1	1:A:200:ARG:HG3	2.43	0.54
2:B:181:GLN:O	2:B:241:ASN:ND2	2.41	0.54
19:V:192:MET:SD	19:V:193:GLN:HB2	2.47	0.54
19:V:358:MET:HA	19:V:358:MET:CE	2.33	0.54
22:Y:381:GLN:HB3	22:Y:382:LYS:HZ2	1.71	0.54
13:o:159:ILE:O	13:o:163:ILE:HG13	2.07	0.54
29:U:609:ASP:OD2	29:U:614:VAL:CG1	2.55	0.54
1:A:238:ILE:HB	1:A:271:LEU:O	2.07	0.54
4:D:296:MET:HE3	4:D:326:ARG:HG3	1.88	0.54
5:E:11:ASP:OD1	5:E:15:LYS:HB2	2.08	0.54
5:E:199:VAL:HA	5:E:233:ASP:HB3	1.89	0.54
5:E:219:PHE:CD2	5:E:263:GLN:HB3	2.42	0.54
20:W:43:VAL:HG23	20:W:43:VAL:O	2.05	0.54
20:W:135:LYS:NZ	20:W:137:TYR:HB3	2.22	0.54
20:W:438:LEU:HD12	20:W:438:LEU:H	1.71	0.54
8:i:17:ARG:HD2	8:i:18:LEU:O	2.07	0.54
29:U:492:ASP:OD2	29:U:492:ASP:C	2.50	0.54
29:U:532:MET:HG3	29:U:548:LEU:HG	1.90	0.54
2:B:234:LEU:HD11	35:B:501:ATP:H2'	1.89	0.54
4:D:382:SER:HG	4:D:399:PHE:HD2	1.55	0.54
5:E:310:LEU:CD1	5:E:329:GLU:OE1	2.56	0.54
11:M:75:MET:HE2	11:M:135:PHE:CG	2.43	0.54
19:V:90:GLU:HG2	19:V:134:PHE:HB3	1.87	0.54
19:V:400:HIS:O	19:V:404:LYS:HG2	2.07	0.54
26:c:145:VAL:HG22	26:c:157:ILE:HD12	1.89	0.54
26:c:280:PRO:O	26:c:284:LEU:HD12	2.07	0.54
8:i:59:VAL:O	8:i:59:VAL:HG22	2.06	0.54
15:q:101:ASN:HD21	15:q:120:TYR:HB3	1.73	0.54
28:u:686:LEU:O	28:u:690:VAL:HG23	2.07	0.54
29:U:799:LYS:HB2	29:U:923:GLU:HG3	1.90	0.54
29:U:833:LEU:HD23	29:U:833:LEU:H	1.72	0.54
31:F:383:GLU:HG3	31:F:421:MET:HE1	1.89	0.54
1:A:347:ASP:C	1:A:347:ASP:OD1	2.50	0.54
3:C:338:LEU:HD13	3:C:338:LEU:C	2.32	0.54
5:E:159:PHE:O	5:E:163:GLY:N	2.40	0.54
5:E:313:LEU:HD23	5:E:343:LEU:HB3	1.88	0.54
20:W:303:LYS:O	20:W:306:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:119:GLN:HG3	9:j:78:ALA:HB1	1.90	0.54
8:i:155:ASN:ND2	9:j:77:THR:OG1	2.41	0.54
31:F:366:MET:HA	31:F:366:MET:CE	2.34	0.54
31:F:421:MET:O	31:F:425:LEU:HD12	2.07	0.54
1:A:250:VAL:CA	1:A:294:GLU:HB2	2.30	0.54
1:A:428:ARG:HA	9:J:23:GLN:NE2	2.22	0.54
2:B:105:THR:CG2	2:B:106:PRO:HD3	2.38	0.54
2:B:181:GLN:OE1	2:B:182:GLU:N	2.38	0.54
2:B:237:LYS:HG2	3:C:283:PHE:CE1	2.43	0.54
5:E:219:PHE:O	5:E:223:ARG:HG3	2.07	0.54
7:H:19:LEU:H	7:H:19:LEU:HD12	1.71	0.54
24:a:140:GLU:O	24:a:143:ASN:ND2	2.40	0.54
24:a:256:GLY:O	24:a:258:GLN:NE2	2.40	0.54
29:U:514:LEU:O	29:U:518:LEU:HG	2.08	0.54
1:A:88:GLN:O	1:A:92:PRO:HD2	2.08	0.54
1:A:303:ILE:HB	1:A:336:ARG:CZ	2.38	0.54
19:V:397:ARG:HA	19:V:400:HIS:CE1	2.43	0.54
22:Y:163:LYS:HG3	22:Y:167:LEU:HD12	1.90	0.54
27:d:147:SER:OG	27:d:150:LYS:HB3	2.08	0.54
10:l:230:SER:HB2	10:l:231:PRO:HD3	1.90	0.54
14:p:122:CYS:SG	14:p:123:SER:N	2.81	0.54
29:U:221:ILE:CG2	29:U:754:HIS:NE2	2.71	0.54
32:k:189:MET:HE2	32:k:194:ALA:CA	2.36	0.54
3:C:248:MET:HB3	3:C:251:ILE:HD11	1.88	0.54
4:D:154:LEU:HD12	4:D:227:PHE:HD2	1.72	0.54
10:L:56:LEU:HD23	10:L:56:LEU:H	1.72	0.54
22:Y:180:LEU:HD13	22:Y:183:TYR:CE2	2.43	0.54
24:a:308:GLU:O	24:a:312:MET:HG2	2.07	0.54
26:c:192:LEU:HA	26:c:196:LEU:HB2	1.90	0.54
8:i:245:ALA:O	8:i:249:ARG:HG2	2.08	0.54
28:u:253:LEU:HD12	28:u:265:ALA:HA	1.90	0.54
5:E:148:VAL:HG11	5:E:170:CYS:SG	2.48	0.54
20:W:430:GLN:HA	20:W:433:ASN:HD21	1.71	0.54
26:c:239:LYS:HE2	26:c:239:LYS:H	1.73	0.54
9:j:175:ASN:OD1	9:j:175:ASN:O	2.26	0.54
28:u:472:HIS:ND1	28:u:477:MET:HG3	2.22	0.54
31:F:253:GLY:H	31:F:287:GLU:HG2	1.73	0.54
1:A:51:ASP:HA	1:A:54:GLN:CG	2.37	0.54
1:A:246:VAL:HG22	1:A:280:ILE:HB	1.88	0.54
1:A:299:MET:HA	1:A:302:LEU:CD2	2.38	0.54
19:V:496:PHE:CD2	19:V:497:PRO:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:319:ILE:HD12	21:X:320:SER:N	2.21	0.54
7:h:51:LYS:HG3	7:h:51:LYS:O	2.05	0.54
29:U:68:PHE:HE2	29:U:80:TYR:HD2	1.54	0.54
31:F:272:PHE:CD1	31:F:272:PHE:C	2.85	0.54
1:A:182:GLU:H	1:A:182:GLU:CD	2.16	0.53
4:D:77:GLU:O	4:D:81:ARG:HG2	2.08	0.53
4:D:297:ASP:OD2	4:D:323:ARG:NH2	2.41	0.53
5:E:120:TYR:CE1	5:E:124:HIS:HB3	2.43	0.53
5:E:146:ARG:C	5:E:151:LEU:HD23	2.33	0.53
6:G:9:PHE:CE2	7:H:8:PHE:CE1	2.96	0.53
7:H:150:ASP:N	7:H:150:ASP:OD1	2.41	0.53
17:S:13:LEU:HD11	17:S:149:LEU:HD11	1.90	0.53
18:T:92:LEU:O	18:T:96:MET:HG2	2.08	0.53
19:V:57:ALA:C	19:V:201:ARG:HH22	2.15	0.53
21:X:73:VAL:HA	21:X:76:PHE:HE1	1.72	0.53
23:Z:35:VAL:H	23:Z:97:THR:HG22	1.74	0.53
23:Z:145:HIS:HD2	23:Z:149:THR:HB	1.73	0.53
23:Z:177:ARG:HA	23:Z:180:LYS:HE2	1.90	0.53
24:a:50:PHE:HE1	24:a:52:GLN:HE21	1.52	0.53
25:b:107:MET:HA	25:b:107:MET:HE3	1.90	0.53
9:j:171:PHE:C	9:j:171:PHE:CD2	2.86	0.53
31:F:285:ILE:H	31:F:285:ILE:HD12	1.73	0.53
1:A:242:GLY:HA2	1:A:245:LEU:HG	1.89	0.53
5:E:33:LEU:CA	5:E:36:LEU:HG	2.38	0.53
14:P:201:LYS:NZ	16:r:197:GLU:OE1	2.41	0.53
17:S:158:MET:HG2	13:o:208:THR:HG22	1.91	0.53
22:Y:113:ARG:HB3	22:Y:113:ARG:HH11	1.71	0.53
23:Z:257:MET:HE2	23:Z:257:MET:CA	2.31	0.53
31:F:202:ILE:O	31:F:206:MET:HG2	2.07	0.53
1:A:159:PRO:HD2	1:A:256:MET:HE2	1.90	0.53
1:A:191:VAL:HG21	1:A:232:ARG:HH22	1.69	0.53
1:A:236:CYS:CB	1:A:270:CYS:HA	2.38	0.53
4:D:161:ASP:O	4:D:162:VAL:C	2.52	0.53
5:E:336:ASP:CA	5:E:338:PHE:CE1	2.91	0.53
6:G:9:PHE:CD2	7:H:8:PHE:CE1	2.96	0.53
9:J:36:ARG:HG3	9:J:142:PRO:HB2	1.91	0.53
10:L:189:LYS:HA	10:L:192:LEU:HG	1.91	0.53
13:O:43:CYS:HB2	13:O:100:LEU:HD12	1.89	0.53
14:P:205:ASP:C	14:P:205:ASP:OD1	2.51	0.53
19:V:159:LEU:HD11	19:V:182:LYS:HE2	1.91	0.53
19:V:319:HIS:HE1	30:e:1:MET:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:316:ARG:HH22	20:W:381:LEU:CA	2.13	0.53
22:Y:99:GLU:H	22:Y:99:GLU:CD	2.16	0.53
9:j:5:ARG:C	9:j:7:ILE:H	2.15	0.53
28:u:679:LEU:HD13	28:u:713:PHE:CD1	2.44	0.53
29:U:100:ILE:HA	29:U:103:LYS:HE3	1.89	0.53
29:U:525:ASN:OD1	29:U:528:ALA:N	2.40	0.53
4:D:355:SER:HB3	4:D:393:ILE:HD11	1.90	0.53
5:E:196:LEU:HB2	5:E:230:ILE:HD13	1.91	0.53
5:E:281:ARG:HH12	5:E:283:ASP:HB2	1.73	0.53
6:G:221:THR:HG23	6:G:224:ASN:H	1.72	0.53
11:M:41:CYS:SG	11:M:189:ILE:HG13	2.48	0.53
20:W:334:GLU:CG	20:W:337:ALA:HB3	2.33	0.53
26:c:63:ASP:OD1	26:c:66:THR:OG1	2.22	0.53
26:c:122:LEU:HB2	26:c:200:TYR:CE1	2.44	0.53
27:d:107:LEU:HD22	27:d:170:LEU:HD11	1.88	0.53
27:d:117:THR:HA	27:d:120:GLU:OE1	2.09	0.53
28:u:354:GLU:OE1	28:u:750:GLN:NE2	2.41	0.53
31:F:386:ARG:HB2	31:F:386:ARG:HH11	1.72	0.53
1:A:139:ARG:HB3	1:A:139:ARG:NH1	2.24	0.53
2:B:50:PRO:HG2	2:B:51:LEU:HD22	1.89	0.53
19:V:467:TYR:HD2	23:Z:250:TYR:CD1	2.26	0.53
22:Y:220:VAL:HG21	22:Y:249:VAL:HG11	1.90	0.53
22:Y:381:GLN:CD	22:Y:382:LYS:HZ1	2.15	0.53
23:Z:263:ALA:HB2	26:c:291:LEU:HD11	1.91	0.53
24:a:278:MET:HA	24:a:281:THR:HG22	1.90	0.53
25:b:17:ARG:HD3	25:b:81:LYS:HZ3	1.73	0.53
11:m:152:ASP:C	11:m:152:ASP:OD1	2.51	0.53
28:u:427:THR:O	28:u:430:ASP:CG	2.52	0.53
1:A:241:ILE:HG22	1:A:244:GLU:H	1.74	0.53
1:A:274:PHE:CE2	1:A:319:MET:HE2	2.43	0.53
2:B:251:VAL:HG11	3:C:278:ASN:CG	2.33	0.53
5:E:36:LEU:HD12	5:E:37:THR:N	2.23	0.53
7:H:106:PRO:HG3	14:P:80:ARG:HH22	1.73	0.53
21:X:191:THR:O	21:X:195:THR:HG23	2.08	0.53
23:Z:276:ILE:O	23:Z:280:ILE:HG12	2.08	0.53
18:t:50:MET:HE2	18:t:192:VAL:CG2	2.38	0.53
29:U:361:ARG:N	29:U:361:ARG:HD2	2.24	0.53
31:F:97:LEU:O	31:F:120:LYS:N	2.42	0.53
4:D:408:LYS:HD3	4:D:411:GLU:OE2	2.07	0.53
6:G:201:CYS:O	6:G:205:VAL:HG23	2.08	0.53
25:b:4:GLU:HA	25:b:106:LYS:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:257:LYS:NZ	26:c:261:GLU:HB2	2.24	0.53
6:g:141:ILE:HG22	6:g:151:VAL:HG22	1.91	0.53
28:u:822:VAL:HA	28:u:825:MET:HG3	1.90	0.53
1:A:98:CYS:HA	1:A:140:VAL:O	2.08	0.53
1:A:299:MET:HA	1:A:302:LEU:HD22	1.91	0.53
1:A:397:ILE:CD1	2:B:214:MET:SD	2.96	0.53
5:E:232:MET:O	5:E:278:ALA:N	2.41	0.53
19:V:57:ALA:O	19:V:62:HIS:NE2	2.41	0.53
19:V:203:LEU:N	19:V:203:LEU:HD23	2.24	0.53
24:a:156:TYR:O	24:a:160:SER:N	2.39	0.53
26:c:279:ASP:N	26:c:280:PRO:HD2	2.24	0.53
31:F:399:VAL:HG22	31:F:427:VAL:HG12	1.91	0.53
31:F:438:TYR:OH	32:K:20:ARG:HA	2.09	0.53
1:A:397:ILE:HD13	2:B:214:MET:SD	2.49	0.53
5:E:125:GLU:OE1	5:E:197:LYS:HB3	2.09	0.53
8:I:202:ASP:OD2	8:I:203:VAL:N	2.42	0.53
15:Q:162:LYS:HD2	16:r:141:ARG:HD2	1.90	0.53
19:V:225:ASP:O	19:V:228:ARG:HG2	2.08	0.53
19:V:263:LEU:HG	19:V:264:TYR:H	1.74	0.53
20:W:138:VAL:O	20:W:139:GLU:C	2.52	0.53
26:c:27:THR:OG1	26:c:28:ALA:N	2.41	0.53
10:l:228:ASP:O	10:l:231:PRO:HD2	2.09	0.53
11:m:113:ASP:C	11:m:113:ASP:OD1	2.51	0.53
28:u:658:ALA:O	28:u:662:MET:HG2	2.09	0.53
29:U:28:ASN:HB2	29:U:63:VAL:HG22	1.90	0.53
32:k:220:VAL:HG23	32:k:220:VAL:O	2.09	0.53
1:A:111:TYR:HB3	1:A:113:ILE:HD11	1.91	0.53
1:A:181:LYS:HA	1:A:184:ILE:HB	1.91	0.53
5:E:272:ARG:HG2	5:E:272:ARG:HH11	1.73	0.53
5:E:303:LEU:CD1	5:E:338:PHE:HB2	2.38	0.53
5:E:353:PHE:HA	5:E:356:ARG:HG2	1.90	0.53
20:W:265:GLN:CD	20:W:335:SER:HB3	2.33	0.53
22:Y:169:GLU:HG2	22:Y:180:LEU:HD11	1.90	0.53
24:a:68:GLU:CG	24:a:69:HIS:H	2.22	0.53
25:b:71:ILE:HD12	25:b:72:LEU:N	2.24	0.53
26:c:278:GLN:O	26:c:283:HIS:N	2.41	0.53
9:j:171:PHE:C	9:j:171:PHE:HD2	2.16	0.53
9:j:184:ASP:O	9:j:188:ILE:HD12	2.09	0.53
14:p:27:ARG:HB2	14:p:183:MET:HB2	1.91	0.53
29:U:367:THR:HA	29:U:370:VAL:HG12	1.91	0.53
31:F:246:ALA:O	31:F:281:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:HA	1:A:134:ILE:CD1	2.40	0.52
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.74	0.52
3:C:44:ARG:HA	19:V:495:ARG:HG3	1.90	0.52
4:D:202:VAL:HA	4:D:329:ARG:HB2	1.92	0.52
16:R:117:GLU:HG2	16:R:119:ASN:OD1	2.09	0.52
22:Y:177:ARG:O	22:Y:180:LEU:HB2	2.08	0.52
23:Z:32:GLN:HG2	23:Z:34:ARG:H	1.74	0.52
23:Z:139:ILE:HG12	23:Z:158:VAL:HG23	1.91	0.52
24:a:247:ARG:O	24:a:251:LEU:HG	2.09	0.52
26:c:265:MET:SD	26:c:273:LYS:NZ	2.81	0.52
26:c:288:VAL:O	26:c:292:MET:HG2	2.09	0.52
28:u:723:TYR:CB	28:u:761:MET:HE2	2.33	0.52
2:B:75:GLU:O	2:B:79:ILE:HG22	2.09	0.52
4:D:264:ILE:HG23	4:D:309:MET:HG3	1.92	0.52
4:D:360:LEU:CD2	4:D:399:PHE:HE1	2.22	0.52
5:E:101:ASP:OD2	5:E:104:THR:N	2.39	0.52
37:O:301:LDZ:H3	14:P:126:LEU:HD21	1.90	0.52
21:X:332:GLU:OE1	21:X:368:MET:HE3	2.09	0.52
22:Y:70:LEU:CA	22:Y:73:MET:HE3	2.39	0.52
24:a:32:LYS:O	24:a:32:LYS:HD2	2.09	0.52
25:b:2:VAL:O	25:b:44:ASN:ND2	2.40	0.52
25:b:18:ASN:HD22	25:b:25:ARG:CZ	2.21	0.52
25:b:83:LYS:HD2	25:b:84:ILE:N	2.24	0.52
27:d:106:LEU:HD21	27:d:114:GLU:HG3	1.90	0.52
29:U:244:MET:HE3	29:U:903:PHE:CE1	2.43	0.52
31:F:235:LEU:HD22	34:F:501:ADP:C4	2.44	0.52
31:F:251:LEU:HB3	31:F:285:ILE:HA	1.91	0.52
31:F:383:GLU:HG3	31:F:421:MET:CE	2.39	0.52
9:J:95:ARG:HH12	9:J:101:PRO:HB3	1.74	0.52
10:L:125:ARG:NH2	32:K:125:GLU:OE2	2.41	0.52
19:V:467:TYR:HD2	23:Z:250:TYR:CE1	2.28	0.52
20:W:12:ARG:NE	20:W:24:VAL:HG12	2.24	0.52
29:U:409:GLY:HA3	29:U:445:ALA:HB1	1.91	0.52
31:F:384:LEU:HD22	31:F:420:TYR:CE2	2.43	0.52
1:A:242:GLY:N	1:A:275:ASP:O	2.43	0.52
1:A:328:ASP:O	1:A:332:MET:SD	2.67	0.52
3:C:174:LEU:H	3:C:174:LEU:CD2	2.23	0.52
20:W:55:ARG:NH1	20:W:59:ASP:OD2	2.42	0.52
23:Z:46:LYS:O	23:Z:46:LYS:HD2	2.08	0.52
24:a:164:GLN:OE1	24:a:164:GLN:N	2.43	0.52
8:i:244:GLU:OE2	8:i:244:GLU:N	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:69:VAL:HG12	9:j:104:VAL:HG23	1.90	0.52
13:o:163:ILE:HG21	13:o:171:SER:OG	2.09	0.52
31:F:175:MET:O	31:F:175:MET:SD	2.68	0.52
31:F:338:LEU:HG	31:F:343:LEU:HD11	1.91	0.52
31:F:376:SER:HB2	31:F:377:PRO:HD2	1.91	0.52
32:k:189:MET:HE2	32:k:194:ALA:CB	2.40	0.52
1:A:126:SER:HB3	1:A:150:HIS:HA	1.91	0.52
1:A:293:ASN:CB	31:F:171:ARG:NH1	2.71	0.52
5:E:101:ASP:HB3	5:E:105:LEU:H	1.75	0.52
5:E:376:ASP:O	5:E:379:LYS:HG2	2.09	0.52
8:I:29:GLY:CA	8:I:166:ASN:HB3	2.39	0.52
19:V:207:ALA:O	19:V:211:TYR:CG	2.62	0.52
22:Y:379:ARG:NH1	22:Y:379:ARG:HA	2.24	0.52
23:Z:143:GLU:HG2	23:Z:145:HIS:N	2.24	0.52
23:Z:273:HIS:CE1	23:Z:277:ASN:HD21	2.26	0.52
24:a:83:VAL:HG12	24:a:87:MET:CE	2.39	0.52
27:d:152:PHE:CZ	27:d:199:PHE:HE1	2.28	0.52
10:l:166:GLN:O	10:l:170:THR:HG23	2.10	0.52
28:u:80:ARG:HG3	28:u:81:GLN:N	2.25	0.52
29:U:107:HIS:HA	29:U:110:LYS:HE3	1.90	0.52
31:F:238:ARG:HG2	31:F:239:ALA:N	2.25	0.52
15:Q:4:LEU:HD11	15:Q:47:VAL:HG13	1.92	0.52
19:V:288:TYR:CD1	19:V:288:TYR:C	2.86	0.52
20:W:126:ASP:O	20:W:130:MET:HG3	2.10	0.52
27:d:144:MET:HA	27:d:144:MET:CE	2.37	0.52
28:u:275:MET:HA	28:u:275:MET:CE	2.35	0.52
28:u:407:MET:N	28:u:407:MET:SD	2.82	0.52
28:u:829:MET:HE2	28:u:830:LEU:CA	2.39	0.52
29:U:216:VAL:HA	29:U:220:LEU:HD13	1.91	0.52
31:F:254:PRO:HD3	31:F:287:GLU:HG3	1.91	0.52
3:C:373:GLU:O	3:C:374:ARG:C	2.51	0.52
5:E:137:GLY:HA3	5:E:308:ALA:HB1	1.91	0.52
5:E:376:ASP:HA	5:E:379:LYS:CE	2.40	0.52
9:J:138:PHE:O	9:J:139:ASP:OD1	2.27	0.52
26:c:189:ILE:HA	26:c:192:LEU:HD21	1.92	0.52
9:j:91:CYS:SG	9:j:107:ILE:HD13	2.50	0.52
1:A:34:LYS:HZ3	3:C:174:LEU:HD22	1.74	0.52
4:D:398:ASP:N	4:D:398:ASP:OD1	2.43	0.52
5:E:345:ASN:HD22	5:E:374:VAL:HG22	1.75	0.52
8:I:106:PRO:O	8:I:140:ASP:HB3	2.10	0.52
13:O:105:VAL:CG2	13:O:106:THR:HG23	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:21:ALA:HB3	15:Q:29:LYS:HB2	1.91	0.52
19:V:132:LEU:N	19:V:174:PHE:HE2	2.08	0.52
24:a:12:GLN:O	24:a:22:TRP:CZ2	2.63	0.52
24:a:331:VAL:HG13	24:a:333:MET:CE	2.40	0.52
29:U:243:LEU:HD12	29:U:244:MET:CE	2.39	0.52
30:e:57:ARG:HG3	30:e:57:ARG:O	2.09	0.52
31:F:212:PHE:CD2	31:F:219:PRO:HB3	2.45	0.52
31:F:285:ILE:HD13	31:F:330:ALA:HB2	1.90	0.52
1:A:126:SER:N	1:A:149:ILE:O	2.41	0.52
1:A:134:ILE:CG2	1:A:138:MET:HE3	2.40	0.52
2:B:381:ASP:O	2:B:385:MET:HG3	2.10	0.52
8:I:174:MET:HE3	8:I:199:LYS:NZ	2.25	0.52
9:J:240:GLU:O	9:J:244:GLN:HB2	2.10	0.52
11:M:140:TYR:CE2	11:M:218:GLU:HG2	2.45	0.52
19:V:130:PHE:CD2	19:V:133:PRO:HG3	2.45	0.52
24:a:20:ALA:HA	24:a:24:ARG:CZ	2.40	0.52
2:B:103:ARG:HB2	2:B:160:ILE:HD13	1.91	0.52
3:C:220:VAL:HG23	4:D:241:GLY:HA3	1.92	0.52
4:D:153:MET:HE1	4:D:257:ASN:ND2	2.25	0.52
20:W:436:MET:CE	23:Z:236:LEU:HD13	2.39	0.52
22:Y:176:ARG:HA	22:Y:176:ARG:HE	1.75	0.52
10:l:55:GLU:OE2	10:l:55:GLU:N	2.40	0.52
28:u:753:ALA:HA	28:u:759:LEU:HD21	1.92	0.52
28:u:908:LEU:HD12	28:u:908:LEU:H	1.75	0.52
29:U:583:MET:SD	29:U:618:ALA:CA	2.98	0.52
31:F:170:SER:HA	31:F:173:LYS:HD2	1.90	0.52
1:A:169:LYS:HG2	1:A:234:ASP:CG	2.36	0.51
2:B:64:LYS:O	2:B:68:ILE:HG13	2.09	0.51
3:C:338:LEU:CD1	3:C:339:THR:O	2.58	0.51
5:E:65:THR:H	5:E:68:LYS:HB2	1.74	0.51
5:E:87:LEU:CD1	5:E:92:LEU:HD23	2.36	0.51
16:R:37:ILE:HG22	16:R:38:ASN:ND2	2.25	0.51
19:V:91:PRO:HB3	19:V:124:ASN:HB2	1.91	0.51
20:W:451:MET:N	20:W:451:MET:SD	2.83	0.51
21:X:157:LEU:HA	21:X:160:MET:CE	2.39	0.51
24:a:137:ASP:O	24:a:141:MET:CE	2.58	0.51
24:a:210:VAL:HG13	24:a:213:PHE:CG	2.45	0.51
24:a:270:ARG:NH1	24:a:271:LYS:HE3	2.26	0.51
18:t:49:THR:HG22	18:t:85:PRO:HG3	1.92	0.51
29:U:324:LYS:NZ	29:U:794:ASP:HB3	2.25	0.51
31:F:43:GLN:HG2	31:F:44:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:O	1:A:38:GLN:NE2	2.44	0.51
1:A:331:LEU:O	1:A:336:ARG:HB2	2.09	0.51
1:A:414:ASN:O	1:A:419:SER:HB2	2.11	0.51
2:B:68:ILE:HA	28:u:670:MET:CE	2.39	0.51
2:B:237:LYS:HG2	3:C:283:PHE:HE1	1.75	0.51
3:C:89:VAL:HG23	3:C:90:HIS:N	2.25	0.51
4:D:242:GLU:CD	4:D:245:ARG:HH12	2.18	0.51
19:V:324:PHE:N	30:e:6:GLN:HB3	2.25	0.51
22:Y:180:LEU:HB3	22:Y:183:TYR:CE2	2.44	0.51
22:Y:192:ARG:NH2	22:Y:194:PHE:HB3	2.18	0.51
23:Z:287:LYS:HG3	23:Z:288:LYS:HD3	1.92	0.51
26:c:49:VAL:HG23	26:c:50:PRO:HD3	1.92	0.51
16:r:1:THR:HG23	37:r:301:LDZ:H23	1.91	0.51
28:u:881:GLU:N	28:u:881:GLU:OE2	2.40	0.51
29:U:422:LEU:HD13	29:U:423:MET:CE	2.39	0.51
29:U:796:LYS:HE3	29:U:921:ILE:HD12	1.93	0.51
32:k:239:LYS:O	32:k:239:LYS:HG2	2.10	0.51
1:A:155:PRO:HG2	1:A:255:ARG:NH1	2.25	0.51
4:D:377:SER:HA	4:D:380:GLN:HB2	1.91	0.51
5:E:30:ARG:HA	5:E:33:LEU:CD2	2.40	0.51
6:G:167:ALA:O	6:G:172:GLN:NE2	2.44	0.51
8:I:174:MET:HE1	8:I:199:LYS:HD3	1.91	0.51
10:L:148:CYS:SG	10:L:150:SER:OG	2.67	0.51
17:S:184:GLU:OE1	13:o:195:LYS:HD2	2.11	0.51
20:W:3:ASP:OD1	20:W:3:ASP:N	2.43	0.51
24:a:184:ASP:OD1	24:a:185:ILE:N	2.44	0.51
25:b:56:ASN:OD1	25:b:83:LYS:N	2.43	0.51
27:d:108:SER:HA	27:d:170:LEU:CD1	2.39	0.51
29:U:521:LEU:HD21	29:U:757:MET:SD	2.50	0.51
1:A:300:LEU:HA	1:A:303:ILE:HG12	1.92	0.51
1:A:333:ARG:NH2	1:A:336:ARG:HE	2.08	0.51
2:B:176:VAL:CG1	2:B:247:PHE:HB3	2.38	0.51
13:O:155:VAL:O	13:O:159:ILE:HG12	2.10	0.51
17:S:159:GLN:HG3	17:S:160:ASN:ND2	2.26	0.51
19:V:218:TYR:HD2	19:V:224:LEU:HA	1.76	0.51
19:V:476:PHE:HB3	23:Z:260:VAL:HG21	1.92	0.51
23:Z:145:HIS:HB3	23:Z:150:PRO:O	2.10	0.51
25:b:17:ARG:HD3	25:b:81:LYS:NZ	2.25	0.51
25:b:108:ARG:NH1	25:b:137:ASN:HD22	2.05	0.51
27:d:107:LEU:HD23	27:d:170:LEU:HD11	1.93	0.51
6:g:62:ASP:OD2	11:m:161:TRP:NE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:174:GLU:OE1	6:g:174:GLU:N	2.40	0.51
31:F:98:ASP:OD1	31:F:120:LYS:N	2.43	0.51
2:B:429:LYS:HE2	3:C:298:ILE:HG13	1.93	0.51
3:C:339:THR:HA	22:Y:174:TRP:NE1	2.25	0.51
5:E:107:ILE:HD13	5:E:107:ILE:N	2.25	0.51
5:E:252:GLU:HA	5:E:255:ARG:HE	1.76	0.51
16:R:5:ALA:HB3	16:R:100:MET:HE1	1.92	0.51
22:Y:97:GLU:HA	22:Y:101:ARG:HB2	1.92	0.51
24:a:77:VAL:HG11	24:a:110:ALA:HB1	1.92	0.51
24:a:140:GLU:HB2	24:a:141:MET:HE1	1.93	0.51
28:u:379:GLY:C	28:u:416:MET:SD	2.93	0.51
2:B:75:GLU:CD	28:u:674:THR:HG22	2.31	0.51
19:V:163:VAL:HG11	19:V:213:TYR:CG	2.45	0.51
21:X:344:ARG:HG3	21:X:384:VAL:HG21	1.92	0.51
24:a:83:VAL:O	24:a:87:MET:CE	2.55	0.51
24:a:140:GLU:HB2	24:a:141:MET:CE	2.41	0.51
24:a:284:ARG:HE	24:a:289:ARG:HA	1.76	0.51
26:c:183:HIS:O	26:c:184:LEU:C	2.53	0.51
27:d:248:GLU:N	27:d:248:GLU:OE1	2.44	0.51
11:m:191:LYS:HB3	11:m:238:TYR:HD2	1.75	0.51
14:p:142:CYS:O	14:p:146:MET:HE2	2.10	0.51
28:u:279:GLU:O	28:u:283:THR:OG1	2.24	0.51
29:U:900:TYR:HB3	29:U:914:LEU:HD21	1.92	0.51
31:F:235:LEU:HD21	34:F:501:ADP:H2'	1.91	0.51
32:k:24:VAL:O	32:k:28:ILE:HG12	2.10	0.51
1:A:211:GLY:HA3	1:A:336:ARG:O	2.11	0.51
1:A:292:ASP:CA	31:F:171:ARG:HH22	2.22	0.51
2:B:363:ARG:HH11	2:B:363:ARG:HA	1.75	0.51
5:E:182:LEU:HD22	34:E:401:ADP:O2A	2.10	0.51
19:V:309:MET:HG2	19:V:332:LEU:HD13	1.93	0.51
21:X:407:MET:HA	21:X:410:VAL:HG22	1.93	0.51
24:a:363:MET:HE3	24:a:363:MET:C	2.36	0.51
6:g:128:ASN:OD1	6:g:131:MET:HE3	2.11	0.51
31:F:198:LEU:HD23	31:F:223:VAL:HG11	1.93	0.51
31:F:225:MET:HA	31:F:352:ILE:O	2.10	0.51
1:A:357:ILE:HG12	1:A:360:ARG:NH2	2.25	0.51
5:E:33:LEU:C	5:E:36:LEU:HG	2.35	0.51
5:E:78:ARG:H	5:E:78:ARG:CD	2.24	0.51
5:E:262:ASN:O	5:E:266:GLY:HA3	2.10	0.51
9:J:45:VAL:HB	9:J:62:ILE:HD11	1.93	0.51
9:J:159:ASN:OD1	9:J:160:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:18:GLU:OE1	17:S:118:LYS:NZ	2.32	0.51
19:V:31:ALA:HB3	19:V:32:PRO:HD3	1.92	0.51
20:W:137:TYR:O	20:W:144:ARG:NE	2.44	0.51
22:Y:300:ARG:HH22	30:e:59:GLU:HB3	1.75	0.51
25:b:25:ARG:NH1	25:b:145:GLU:OE1	2.20	0.51
7:h:42:ASN:HD21	7:h:184:LEU:H	1.58	0.51
7:h:69:THR:HG22	7:h:70:LYS:H	1.75	0.51
13:o:167:LEU:O	13:o:167:LEU:HD13	2.11	0.51
29:U:242:LEU:HD13	29:U:325:MET:HE3	1.92	0.51
31:F:62:VAL:HG23	31:F:63:THR:H	1.74	0.51
31:F:221:LYS:HD2	31:F:323:ASN:HB2	1.93	0.51
31:F:226:TYR:HE1	31:F:351:LYS:O	1.93	0.51
5:E:33:LEU:HD13	5:E:33:LEU:N	2.26	0.51
5:E:250:ASP:OD1	5:E:250:ASP:N	2.44	0.51
13:O:143:ARG:NH2	13:O:150:GLU:OE2	2.44	0.51
19:V:136:GLU:O	19:V:139:MET:HG3	2.10	0.51
19:V:258:TYR:HB2	19:V:269:LYS:HZ1	1.75	0.51
23:Z:212:LEU:HD23	23:Z:212:LEU:C	2.36	0.51
12:n:35:THR:OG1	12:n:43:CYS:SG	2.69	0.51
15:q:52:ASP:HB3	15:q:98:TYR:HD1	1.75	0.51
16:r:5:ALA:HB3	16:r:100:MET:HE3	1.93	0.51
28:u:67:ASP:C	28:u:67:ASP:OD2	2.54	0.51
28:u:207:LEU:O	28:u:211:ILE:HG13	2.11	0.51
29:U:191:LYS:HD2	29:U:194:ARG:HD2	1.91	0.51
1:A:48:VAL:HG13	2:B:69:LYS:HZ3	1.76	0.51
1:A:97:ARG:HH12	1:A:144:ARG:HA	1.75	0.51
2:B:164:MET:SD	2:B:166:ASP:HB2	2.51	0.51
3:C:269:VAL:HG11	4:D:287:ARG:HH12	1.76	0.51
5:E:87:LEU:HD13	5:E:87:LEU:C	2.36	0.51
25:b:52:ILE:HD11	25:b:58:CYS:HB3	1.93	0.51
26:c:46:ARG:HD3	26:c:49:VAL:HG11	1.93	0.51
27:d:187:GLU:OE1	27:d:223:TYR:CD2	2.64	0.51
7:h:5:GLY:O	9:j:3:TYR:CE1	2.64	0.51
29:U:17:PRO:HB3	29:U:54:PHE:CZ	2.46	0.51
29:U:831:ALA:HB1	29:U:833:LEU:HD22	1.92	0.51
31:F:224:LEU:HA	31:F:330:ALA:O	2.11	0.51
1:A:109:PRO:HB3	1:A:111:TYR:CE1	2.46	0.50
1:A:213:LEU:HD22	1:A:337:LEU:HD13	1.93	0.50
3:C:258:ARG:CD	3:C:273:MET:HE1	2.40	0.50
5:E:308:ALA:O	5:E:312:ILE:HG13	2.12	0.50
6:G:80:MET:HE2	6:G:87:SER:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:100:GLN:HE21	15:Q:83:PHE:HD1	1.59	0.50
19:V:88:GLY:O	19:V:118:GLN:NE2	2.44	0.50
19:V:303:SER:O	19:V:306:ARG:NE	2.45	0.50
20:W:430:GLN:HA	20:W:433:ASN:HD22	1.75	0.50
22:Y:201:PHE:HD1	22:Y:219:PHE:HE1	1.57	0.50
24:a:186:LYS:HB3	24:a:193:GLN:HE22	1.76	0.50
26:c:41:MET:HE1	26:c:112:TYR:CB	2.40	0.50
26:c:161:ARG:HG2	26:c:201:TYR:CZ	2.46	0.50
17:s:28:ARG:O	17:s:42:LYS:NZ	2.40	0.50
29:U:68:PHE:CE2	29:U:80:TYR:CD2	2.99	0.50
29:U:211:PRO:O	29:U:212:ASP:C	2.55	0.50
29:U:789:ILE:HG12	29:U:881:PRO:HB3	1.92	0.50
31:F:383:GLU:CG	31:F:421:MET:HE1	2.41	0.50
1:A:99:THR:HB	1:A:115:VAL:HA	1.93	0.50
1:A:135:GLU:N	1:A:138:MET:HE2	2.07	0.50
1:A:157:ILE:CG1	1:A:158:ASP:H	2.13	0.50
3:C:305:LEU:HA	3:C:310:ARG:HD2	1.94	0.50
5:E:63:GLN:O	5:E:63:GLN:NE2	2.44	0.50
5:E:127:PRO:CA	5:E:185:ARG:HH22	2.12	0.50
5:E:310:LEU:CG	5:E:332:VAL:HG21	2.27	0.50
5:E:376:ASP:HA	5:E:379:LYS:CD	2.42	0.50
19:V:30:PRO:HA	19:V:33:GLN:HB2	1.93	0.50
19:V:421:ASP:O	19:V:425:LYS:HG2	2.12	0.50
20:W:125:ILE:O	20:W:129:ARG:HG3	2.12	0.50
21:X:377:ILE:HD12	22:Y:310:SER:O	2.10	0.50
22:Y:152:MET:HE3	22:Y:152:MET:O	2.12	0.50
22:Y:182:VAL:O	22:Y:183:TYR:C	2.54	0.50
23:Z:15:VAL:O	23:Z:19:VAL:HG23	2.11	0.50
18:t:124:TYR:HB2	18:t:137:LEU:HD13	1.94	0.50
31:F:202:ILE:HD13	31:F:327:LYS:HG2	1.93	0.50
31:F:247:THR:HG21	31:F:278:LYS:HG2	1.94	0.50
2:B:364:ILE:HG22	2:B:395:ILE:HG21	1.93	0.50
3:C:297:ARG:HE	3:C:300:ILE:HD13	1.77	0.50
19:V:411:SER:OG	19:V:447:ILE:HG21	2.12	0.50
20:W:372:ARG:HH11	20:W:372:ARG:HG3	1.76	0.50
21:X:255:LEU:O	21:X:259:ILE:HG12	2.12	0.50
22:Y:202:LEU:HG	22:Y:203:ASP:N	2.25	0.50
8:i:242:GLU:O	8:i:242:GLU:OE1	2.29	0.50
28:u:213:GLN:CB	28:u:216:MET:CE	2.86	0.50
1:A:336:ARG:NH1	1:A:336:ARG:HG2	2.27	0.50
4:D:113:VAL:HG11	4:D:137:ASN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:THR:HG23	5:E:68:LYS:HD2	1.93	0.50
15:Q:101:ASN:HB3	15:Q:132:HIS:CE1	2.46	0.50
17:S:150:ASP:OD1	14:p:177:ARG:NH2	2.44	0.50
21:X:316:ASP:O	21:X:319:ILE:CD1	2.59	0.50
27:d:56:GLU:HG2	27:d:98:LEU:HD21	1.92	0.50
10:l:50:LYS:HB3	10:l:59:HIS:HB3	1.93	0.50
28:u:658:ALA:HB2	28:u:693:ALA:HB1	1.92	0.50
29:U:175:GLY:O	29:U:178:ALA:N	2.45	0.50
29:U:583:MET:SD	29:U:618:ALA:HB2	2.51	0.50
31:F:272:PHE:O	31:F:272:PHE:HD1	1.94	0.50
1:A:187:LEU:HA	1:A:190:VAL:HB	1.93	0.50
2:B:269:GLU:CD	2:B:269:GLU:C	2.80	0.50
5:E:368:MET:HE2	5:E:368:MET:HA	1.91	0.50
18:T:166:ARG:NH2	18:T:200:GLU:OE2	2.39	0.50
19:V:25:GLU:O	19:V:28:PRO:HD2	2.11	0.50
19:V:38:LYS:HE3	19:V:38:LYS:CA	2.37	0.50
19:V:58:ALA:HA	19:V:201:ARG:NH2	2.27	0.50
19:V:192:MET:SD	19:V:193:GLN:OE1	2.69	0.50
20:W:135:LYS:HD2	20:W:144:ARG:HH22	1.76	0.50
21:X:143:TYR:OH	22:Y:251:HIS:HB3	2.11	0.50
22:Y:217:LYS:HD2	22:Y:253:LEU:HD11	1.92	0.50
24:a:26:GLU:HA	24:a:29:TYR:CE1	2.46	0.50
25:b:53:THR:HG22	25:b:59:GLU:H	1.77	0.50
27:d:182:ILE:HG13	27:d:215:TRP:CH2	2.47	0.50
28:u:213:GLN:CB	28:u:216:MET:HE3	2.41	0.50
28:u:305:LEU:HB2	28:u:321:MET:HE1	1.94	0.50
29:U:205:TYR:HB3	29:U:215:ASN:ND2	2.21	0.50
29:U:837:ALA:O	29:U:841:LYS:HB2	2.11	0.50
31:F:188:ILE:N	31:F:188:ILE:HD12	2.25	0.50
1:A:51:ASP:O	1:A:54:GLN:HG2	2.12	0.50
1:A:272:ILE:HG22	1:A:274:PHE:HE1	1.76	0.50
2:B:257:GLN:HB2	2:B:262:ASP:HB3	1.92	0.50
2:B:385:MET:HB3	9:J:200:GLN:CA	2.42	0.50
3:C:284:GLU:OE1	3:C:284:GLU:N	2.44	0.50
5:E:260:LEU:O	5:E:264:MET:HG2	2.12	0.50
5:E:310:LEU:CD2	5:E:328:TYR:HB3	2.42	0.50
13:O:203:ARG:NH1	14:P:162:HIS:HE1	2.08	0.50
14:P:173:ASN:ND2	17:s:151:ASN:ND2	2.60	0.50
19:V:289:LEU:HA	19:V:292:THR:HG22	1.92	0.50
20:W:47:LEU:HD23	20:W:47:LEU:N	2.25	0.50
22:Y:113:ARG:NH1	22:Y:113:ARG:CB	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:144:VAL:O	23:Z:151:THR:HA	2.11	0.50
23:Z:247:LYS:HD2	23:Z:247:LYS:C	2.36	0.50
23:Z:263:ALA:HB1	26:c:292:MET:CE	2.33	0.50
26:c:173:GLU:HG3	26:c:175:ARG:HD2	1.94	0.50
27:d:88:GLN:OE1	27:d:88:GLN:N	2.45	0.50
9:j:65:LEU:HB2	9:j:69:VAL:HG23	1.94	0.50
18:t:74:GLU:OE1	18:t:82:SER:HA	2.11	0.50
28:u:379:GLY:O	28:u:416:MET:SD	2.70	0.50
29:U:486:MET:HE3	29:U:486:MET:C	2.36	0.50
32:K:22:PHE:O	32:K:23:GLN:HB2	2.11	0.50
1:A:265:ARG:NH2	1:A:309:PHE:HB3	2.26	0.50
1:A:268:LYS:HE3	1:A:314:ASN:CA	2.41	0.50
1:A:286:ASP:HB2	31:F:171:ARG:CD	2.42	0.50
1:A:423:PHE:CD2	1:A:426:THR:HG23	2.47	0.50
2:B:140:ASP:O	2:B:142:ASP:N	2.40	0.50
3:C:213:ARG:NH2	4:D:299:PHE:CG	2.80	0.50
4:D:164:TYR:N	4:D:222:HIS:CE1	2.79	0.50
16:R:26:ILE:HG22	16:R:26:ILE:O	2.11	0.50
24:a:112:ILE:HA	24:a:115:LYS:HZ2	1.76	0.50
24:a:257:GLN:HB3	24:a:261:LEU:HD22	1.93	0.50
25:b:52:ILE:HD12	25:b:59:GLU:O	2.12	0.50
11:m:191:LYS:HB3	11:m:238:TYR:CD2	2.47	0.50
28:u:271:MET:HE2	28:u:787:LEU:HG	1.94	0.50
28:u:292:LYS:NZ	28:u:836:GLU:OE2	2.45	0.50
29:U:560:MET:HE2	29:U:560:MET:CA	2.42	0.50
31:F:204:LEU:O	31:F:208:HIS:HB2	2.12	0.50
1:A:286:ASP:HB2	31:F:171:ARG:HD3	1.93	0.50
1:A:402:LYS:HD2	1:A:402:LYS:N	2.27	0.50
1:A:431:THR:O	32:K:82:ILE:HG13	2.11	0.50
5:E:97:ARG:NH2	5:E:114:GLU:H	2.10	0.50
5:E:140:GLU:HG3	5:E:141:GLN:OE1	2.11	0.50
8:I:14:PRO:O	8:I:15:GLU:HG3	2.11	0.50
10:L:43:HIS:CD2	10:L:184:LEU:HD12	2.47	0.50
16:R:83:LEU:O	16:R:87:VAL:HG22	2.11	0.50
20:W:426:ASN:HD22	26:c:233:ASP:CG	2.17	0.50
21:X:382:GLU:HB2	21:X:384:VAL:HG12	1.94	0.50
26:c:52:GLU:HG3	26:c:82:VAL:HG22	1.93	0.50
27:d:8:GLU:HG2	27:d:12:LYS:O	2.12	0.50
27:d:237:ILE:HD13	27:d:237:ILE:N	2.27	0.50
29:U:250:PHE:CD2	29:U:328:ILE:CG1	2.94	0.50
29:U:376:MET:HE1	29:U:738:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:K:146:VAL:HG11	32:K:222:PRO:HA	1.94	0.50
1:A:329:PRO:HA	1:A:332:MET:SD	2.52	0.50
3:C:160:GLU:OE1	3:C:313:ARG:NH2	2.45	0.50
5:E:81:VAL:CG2	5:E:107:ILE:HD11	2.30	0.50
19:V:472:PRO:HB3	19:V:476:PHE:CE2	2.47	0.50
20:W:275:ILE:HD11	20:W:308:LEU:HD13	1.94	0.50
23:Z:94:TRP:CE2	23:Z:121:LEU:HD23	2.47	0.50
24:a:27:GLU:O	24:a:31:LYS:HD2	2.11	0.50
24:a:282:PHE:CD1	24:a:335:TRP:HH2	2.30	0.50
26:c:184:LEU:HD13	26:c:184:LEU:N	2.27	0.50
9:j:7:ILE:O	9:j:9:VAL:HG12	2.12	0.50
17:s:13:LEU:HD11	17:s:149:LEU:HD11	1.94	0.50
28:u:512:MET:HE3	28:u:512:MET:HA	1.94	0.50
28:u:829:MET:HE3	28:u:831:VAL:HG23	1.93	0.50
29:U:151:ILE:HD11	29:U:163:PHE:CD2	2.47	0.50
29:U:196:LYS:O	29:U:200:VAL:HG13	2.12	0.50
29:U:840:LYS:O	29:U:844:LYS:N	2.34	0.50
29:U:902:PRO:HA	29:U:914:LEU:HA	1.93	0.50
31:F:226:TYR:CZ	31:F:353:GLU:HB3	2.46	0.50
31:F:282:ILE:C	31:F:283:ILE:HD12	2.37	0.50
1:A:167:GLU:O	1:A:168:GLU:HG2	2.11	0.49
1:A:344:SER:OG	1:A:345:LEU:N	2.45	0.49
13:O:104:ASP:OD1	13:O:104:ASP:N	2.45	0.49
19:V:289:LEU:HB3	19:V:312:ALA:HB2	1.94	0.49
20:W:1:MET:HG3	20:W:43:VAL:CG1	2.42	0.49
20:W:428:TRP:HZ3	23:Z:238:PRO:HG2	1.75	0.49
23:Z:130:ASP:OD1	23:Z:130:ASP:N	2.38	0.49
24:a:232:TRP:CH2	24:a:257:GLN:HB2	2.47	0.49
26:c:163:ILE:HG22	26:c:199:HIS:O	2.12	0.49
6:g:80:MET:HE2	6:g:87:SER:CA	2.41	0.49
6:g:86:ASP:OD1	11:m:120:HIS:NE2	2.42	0.49
17:s:19:ASP:N	17:s:19:ASP:OD1	2.43	0.49
28:u:323:ASN:O	28:u:326:LEU:HD22	2.12	0.49
29:U:82:LEU:HA	29:U:129:ARG:NE	2.26	0.49
31:F:93:VAL:HG22	31:F:148:GLY:H	1.77	0.49
1:A:247:GLN:HB3	1:A:252:GLU:HG3	1.94	0.49
5:E:314:LYS:O	5:E:318:GLY:N	2.45	0.49
5:E:340:GLY:HA3	34:E:401:ADP:C8	2.48	0.49
12:N:81:SER:O	12:N:85:GLU:HG2	2.12	0.49
19:V:147:PHE:O	19:V:150:ARG:HG2	2.12	0.49
19:V:350:GLN:HB2	19:V:353:LEU:H	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:368:ARG:HE	19:V:368:ARG:C	2.19	0.49
20:W:324:TYR:O	20:W:328:LEU:HD12	2.12	0.49
20:W:444:HIS:CD2	23:Z:208:ILE:HG12	2.47	0.49
26:c:250:GLU:HA	26:c:253:LYS:HG3	1.95	0.49
27:d:187:GLU:CD	27:d:223:TYR:CE2	2.91	0.49
6:g:54:LYS:HD3	6:g:216:GLU:OE2	2.11	0.49
9:j:137:ASP:O	9:j:137:ASP:CG	2.55	0.49
28:u:766:GLN:O	28:u:769:THR:CG2	2.60	0.49
29:U:58:GLN:CD	29:U:59:PHE:H	2.20	0.49
32:K:54:ILE:H	32:K:54:ILE:HD12	1.77	0.49
32:K:197:SER:O	32:K:201:ILE:HG12	2.12	0.49
3:C:155:ASP:OD2	3:C:156:LYS:N	2.45	0.49
5:E:33:LEU:HD21	31:F:62:VAL:CB	2.41	0.49
5:E:192:ASP:N	5:E:192:ASP:OD1	2.43	0.49
7:H:46:LEU:HB3	7:H:75:VAL:HG21	1.95	0.49
11:M:230:ASP:C	11:M:230:ASP:OD1	2.55	0.49
14:P:134:ASP:OD2	14:P:134:ASP:N	2.39	0.49
14:P:135:ASP:OD1	14:P:135:ASP:N	2.45	0.49
16:R:36:GLU:HG2	16:R:184:TRP:CZ2	2.47	0.49
19:V:194:LYS:HE2	19:V:241:ARG:HH12	1.77	0.49
22:Y:110:TYR:HA	22:Y:113:ARG:NH2	2.27	0.49
22:Y:110:TYR:CA	22:Y:113:ARG:HH12	2.24	0.49
27:d:47:GLN:HA	27:d:50:LEU:HG	1.94	0.49
28:u:113:MET:SD	28:u:114:ALA:N	2.85	0.49
28:u:162:LEU:O	28:u:166:VAL:HG23	2.12	0.49
29:U:615:ARG:O	29:U:619:VAL:HG22	2.12	0.49
29:U:689:ILE:HD12	29:U:690:ALA:N	2.27	0.49
30:e:53:SER:N	30:e:55:GLN:HE22	2.09	0.49
1:A:131:PRO:HA	1:A:134:ILE:HD12	1.95	0.49
1:A:383:ALA:HA	1:A:386:ARG:HG2	1.93	0.49
2:B:98:LYS:HD2	2:B:99:VAL:N	2.27	0.49
3:C:277:LEU:O	3:C:310:ARG:NH1	2.46	0.49
19:V:467:TYR:CD2	23:Z:250:TYR:CD1	3.01	0.49
27:d:29:VAL:HA	27:d:32:GLU:OE1	2.12	0.49
28:u:766:GLN:HA	28:u:769:THR:CG2	2.41	0.49
29:U:10:SER:HA	29:U:13:ASP:OD2	2.12	0.49
29:U:611:ASN:HB3	29:U:614:VAL:HG12	1.95	0.49
5:E:148:VAL:HG22	5:E:167:PRO:HB2	1.93	0.49
5:E:310:LEU:HD21	5:E:329:GLU:N	2.26	0.49
5:E:310:LEU:HD11	5:E:329:GLU:CA	2.42	0.49
8:I:14:PRO:C	8:I:16:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:131:GLN:NE2	17:S:133:ASP:OD2	2.45	0.49
19:V:474:LEU:H	19:V:474:LEU:HD22	1.76	0.49
20:W:127:THR:HA	20:W:130:MET:SD	2.52	0.49
20:W:425:LEU:CG	23:Z:247:LYS:HD3	2.42	0.49
20:W:443:THR:HG22	23:Z:229:GLN:NE2	2.26	0.49
22:Y:46:ARG:C	22:Y:48:ASN:H	2.20	0.49
24:a:34:TRP:CZ3	24:a:64:ILE:HG23	2.47	0.49
24:a:135:ILE:HG12	24:a:158:LEU:HD13	1.95	0.49
11:m:202:ASP:HB2	11:m:209:PHE:CE1	2.46	0.49
18:t:43:MET:SD	18:t:64:LYS:HG3	2.52	0.49
29:U:836:THR:C	29:U:840:LYS:HE2	2.37	0.49
4:D:85:ILE:HG13	4:D:86:PRO:HD2	1.94	0.49
5:E:42:LYS:HA	5:E:45:ASN:HD22	1.77	0.49
5:E:231:PHE:HB2	5:E:276:ILE:HD11	1.95	0.49
20:W:75:TYR:HB3	20:W:123:ARG:NH2	2.24	0.49
20:W:256:ILE:HG22	20:W:257:GLN:OE1	2.12	0.49
22:Y:43:ALA:CA	22:Y:46:ARG:NH2	2.76	0.49
22:Y:113:ARG:HH11	22:Y:113:ARG:HB2	1.75	0.49
22:Y:274:SER:O	22:Y:277:VAL:HG12	2.12	0.49
24:a:190:VAL:HG12	24:a:225:LEU:HD22	1.95	0.49
25:b:119:ASP:OD2	25:b:120:ASN:N	2.45	0.49
7:h:166:ASN:OD1	7:h:198:SER:OG	2.30	0.49
8:i:168:SER:HA	8:i:171:ALA:HB3	1.95	0.49
9:j:93:SER:O	9:j:97:THR:HG23	2.13	0.49
11:m:169:ARG:O	11:m:173:LYS:HG3	2.12	0.49
29:U:185:MET:CE	29:U:222:PHE:HE2	2.24	0.49
1:A:138:MET:CB	1:A:155:PRO:HD3	2.43	0.49
4:D:296:MET:CE	4:D:326:ARG:HG3	2.42	0.49
5:E:357:ALA:HB3	5:E:359:HIS:CE1	2.48	0.49
19:V:200:ARG:H	19:V:200:ARG:NE	2.11	0.49
19:V:306:ARG:CZ	19:V:307:ARG:HB3	2.43	0.49
20:W:361:HIS:CE1	20:W:365:ILE:HD13	2.46	0.49
23:Z:245:PHE:O	23:Z:249:PHE:HD1	1.96	0.49
9:j:215:GLN:CD	9:j:216:SER:H	2.21	0.49
14:p:107:PRO:HG2	14:p:124:LEU:HD13	1.95	0.49
28:u:655:LEU:HD21	28:u:804:LEU:HD21	1.94	0.49
29:U:195:ASN:O	29:U:199:ARG:HG2	2.12	0.49
29:U:793:LYS:HB3	29:U:796:LYS:HB2	1.93	0.49
31:F:208:HIS:NE2	31:F:211:LYS:HE3	2.27	0.49
31:F:366:MET:HE3	31:F:366:MET:CA	2.37	0.49
3:C:253:SER:HB3	4:D:290:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:GLN:HB3	5:E:14:LYS:HZ3	1.78	0.49
5:E:226:GLN:HG3	5:E:272:ARG:HB3	1.95	0.49
5:E:336:ASP:CB	5:E:338:PHE:CZ	2.93	0.49
19:V:26:PRO:O	19:V:29:PRO:HD2	2.13	0.49
19:V:155:ALA:C	19:V:158:PRO:HD2	2.38	0.49
20:W:265:GLN:NE2	20:W:335:SER:CB	2.75	0.49
20:W:435:LEU:HG	20:W:436:MET:CE	2.41	0.49
21:X:75:PRO:HD2	21:X:76:PHE:H	1.77	0.49
22:Y:113:ARG:CG	22:Y:114:ILE:HD12	2.29	0.49
24:a:87:MET:N	24:a:87:MET:SD	2.85	0.49
26:c:286:GLU:OE2	26:c:286:GLU:N	2.33	0.49
28:u:485:LEU:HD13	28:u:501:LEU:HD21	1.94	0.49
28:u:882:LEU:HG	28:u:884:THR:H	1.78	0.49
31:F:195:ILE:HG12	31:F:236:LEU:HD21	1.94	0.49
31:F:424:ILE:HA	31:F:427:VAL:HG13	1.94	0.49
1:A:101:ILE:HG12	1:A:113:ILE:HD12	1.95	0.49
1:A:325:ASP:O	1:A:325:ASP:OD2	2.31	0.49
2:B:423:LYS:HE2	2:B:424:GLU:HG3	1.94	0.49
3:C:163:GLU:OE2	3:C:164:VAL:CG2	2.61	0.49
4:D:154:LEU:HD12	4:D:227:PHE:CD2	2.48	0.49
5:E:270:LEU:HD23	5:E:270:LEU:H	1.78	0.49
5:E:310:LEU:O	5:E:314:LYS:HG3	2.13	0.49
20:W:200:ILE:C	20:W:200:ILE:HD12	2.37	0.49
20:W:266:ALA:O	20:W:270:VAL:HG23	2.12	0.49
22:Y:202:LEU:HD11	22:Y:239:LYS:HG2	1.95	0.49
22:Y:274:SER:O	22:Y:277:VAL:CG1	2.61	0.49
22:Y:378:ASN:O	22:Y:382:LYS:HD3	2.13	0.49
23:Z:167:ALA:HB2	26:c:46:ARG:HG2	1.95	0.49
24:a:115:LYS:HZ3	24:a:138:VAL:HG22	1.76	0.49
32:K:206:MET:HE3	32:K:215:ILE:HG22	1.95	0.49
1:A:177:VAL:HG21	34:A:501:ADP:HN62	1.78	0.49
1:A:186:LYS:HG3	1:A:341:ILE:HG12	1.93	0.49
3:C:66:LEU:HD21	4:D:116:LEU:HD21	1.94	0.49
4:D:61:ILE:HA	4:D:64:GLU:HB2	1.94	0.49
4:D:66:LYS:HD2	4:D:70:LYS:HZ3	1.78	0.49
4:D:160:PRO:HG3	4:D:220:ALA:HB3	1.95	0.49
4:D:191:TYR:CD1	4:D:198:PRO:HB3	2.48	0.49
5:E:350:ALA:CB	5:E:367:PHE:CD1	2.96	0.49
7:H:111:VAL:HG22	7:H:136:ILE:HD12	1.95	0.49
20:W:303:LYS:HA	20:W:306:LEU:HD23	1.94	0.49
20:W:450:GLU:OE2	23:Z:211:TYR:OH	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:73:VAL:CA	21:X:76:PHE:HE1	2.25	0.49
24:a:57:ILE:O	24:a:61:GLU:OE2	2.30	0.49
25:b:3:LEU:HB3	25:b:105:HIS:CD2	2.48	0.49
26:c:27:THR:HB	26:c:176:GLN:OE1	2.13	0.49
26:c:161:ARG:HB3	26:c:201:TYR:CE2	2.48	0.49
27:d:106:LEU:HA	27:d:111:ARG:NH2	2.28	0.49
12:n:142:THR:HB	12:n:155:PHE:HE1	1.76	0.49
28:u:429:ILE:HD13	28:u:448:CYS:SG	2.53	0.49
28:u:766:GLN:CA	28:u:769:THR:HG22	2.42	0.49
29:U:347:ASN:HB2	29:U:813:TYR:OH	2.13	0.49
1:A:99:THR:O	1:A:139:ARG:HA	2.13	0.48
2:B:172:THR:HG21	3:C:78:ARG:HH21	1.78	0.48
19:V:98:LEU:O	19:V:146:GLN:NE2	2.46	0.48
22:Y:195:LYS:HZ3	22:Y:200:LEU:HD21	1.77	0.48
22:Y:381:GLN:O	22:Y:384:SER:OG	2.27	0.48
23:Z:32:GLN:O	23:Z:33:LYS:HG3	2.13	0.48
23:Z:127:LYS:HB3	23:Z:128:PRO:HD3	1.95	0.48
23:Z:212:LEU:HD22	24:a:353:LEU:HD13	1.95	0.48
24:a:74:LEU:HD23	24:a:110:ALA:HB2	1.94	0.48
26:c:46:ARG:HD3	26:c:49:VAL:CG1	2.43	0.48
8:i:17:ARG:HH12	8:i:19:TYR:HA	1.76	0.48
15:q:8:GLN:HG3	15:q:9:GLY:N	2.27	0.48
29:U:532:MET:HE1	29:U:551:GLY:C	2.38	0.48
29:U:727:LYS:O	29:U:731:ILE:HG22	2.13	0.48
31:F:134:LEU:HD12	31:F:134:LEU:O	2.12	0.48
32:k:227:HIS:CE1	32:k:233:GLU:CD	2.91	0.48
1:A:197:HIS:ND1	1:A:200:ARG:HG3	2.28	0.48
4:D:414:HIS:CE1	6:G:26:GLU:HB2	2.48	0.48
5:E:26:LEU:CD1	31:F:55:MET:HE3	2.42	0.48
20:W:44:ILE:O	20:W:47:LEU:HD23	2.12	0.48
20:W:275:ILE:CG1	20:W:308:LEU:CD2	2.86	0.48
20:W:312:MET:HB2	20:W:365:ILE:HD12	1.94	0.48
20:W:314:LEU:HD11	24:a:313:LYS:HD3	1.95	0.48
23:Z:143:GLU:HG2	23:Z:145:HIS:H	1.78	0.48
27:d:131:VAL:HA	27:d:134:LYS:HB3	1.94	0.48
27:d:251:ARG:O	27:d:255:MET:HE2	2.13	0.48
13:o:19:ARG:HB3	13:o:169:SER:HA	1.95	0.48
31:F:36:MET:HE2	31:F:36:MET:HA	1.95	0.48
31:F:204:LEU:HB3	31:F:205:PRO:HD3	1.95	0.48
2:B:76:GLU:C	2:B:76:GLU:OE1	2.56	0.48
8:I:100:GLN:NE2	15:Q:83:PHE:CE1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:124:PHE:HE1	9:J:118:TYR:CE2	2.31	0.48
10:L:46:LEU:HD13	10:L:73:SER:HB2	1.94	0.48
11:M:86:SER:O	11:M:90:ILE:HG12	2.14	0.48
19:V:467:TYR:CD2	23:Z:250:TYR:HD1	2.31	0.48
20:W:16:MET:SD	20:W:17:GLU:N	2.86	0.48
24:a:145:LEU:HD11	24:a:148:VAL:HG23	1.95	0.48
24:a:291:LEU:HB2	24:a:333:MET:HE1	1.96	0.48
24:a:293:PHE:HE2	24:a:331:VAL:HB	1.77	0.48
11:m:209:PHE:H	11:m:209:PHE:HD1	1.62	0.48
29:U:245:ALA:HA	29:U:248:ILE:HG22	1.94	0.48
29:U:388:ASP:OD1	29:U:389:ASN:N	2.44	0.48
29:U:629:THR:O	29:U:629:THR:OG1	2.28	0.48
31:F:94:ILE:HD11	31:F:125:LYS:HB2	1.95	0.48
31:F:222:GLY:O	31:F:350:ARG:HB2	2.13	0.48
3:C:213:ARG:CZ	4:D:299:PHE:CD2	2.96	0.48
12:N:84:LYS:NZ	12:N:85:GLU:OE1	2.47	0.48
17:S:114:ASP:C	17:S:114:ASP:OD1	2.56	0.48
19:V:440:LYS:O	19:V:444:ASP:OD2	2.32	0.48
21:X:57:LEU:O	21:X:99:MET:HE3	2.13	0.48
26:c:211:GLU:HG3	26:c:212:LEU:H	1.78	0.48
7:h:95:GLN:CG	13:o:65:LEU:HD13	2.41	0.48
29:U:546:ARG:HD2	29:U:771:PHE:CD2	2.48	0.48
2:B:153:ASN:O	2:B:157:HIS:ND1	2.47	0.48
2:B:233:THR:O	2:B:237:LYS:HG3	2.14	0.48
2:B:250:VAL:CG1	2:B:284:ILE:HG23	2.42	0.48
3:C:117:ARG:NH1	3:C:124:HIS:CG	2.81	0.48
18:T:50:MET:HE3	18:T:197:VAL:HG13	1.94	0.48
19:V:34:ASP:O	19:V:38:LYS:HG2	2.14	0.48
19:V:255:LEU:HD13	19:V:269:LYS:NZ	2.17	0.48
20:W:164:SER:O	20:W:167:GLN:NE2	2.46	0.48
20:W:190:MET:HE1	20:W:206:SER:HA	1.94	0.48
20:W:449:GLU:HG2	20:W:452:ILE:HD12	1.95	0.48
24:a:119:GLY:O	24:a:123:LEU:HG	2.13	0.48
25:b:9:CYS:HB3	25:b:111:ALA:HA	1.94	0.48
25:b:106:LYS:HE3	25:b:107:MET:H	1.78	0.48
15:q:46:CYS:SG	15:q:53:THR:HG23	2.54	0.48
17:s:148:LEU:O	17:s:148:LEU:HD22	2.13	0.48
28:u:171:GLN:NE2	28:u:210:GLU:OE1	2.44	0.48
29:U:580:ARG:HG3	29:U:617:ALA:HB2	1.95	0.48
31:F:52:ILE:HA	31:F:55:MET:HB2	1.95	0.48
32:K:50:VAL:HB	32:K:67:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:K:71:ASP:OD2	32:K:72:ALA:N	2.46	0.48
1:A:309:PHE:C	1:A:311:PRO:HD3	2.38	0.48
3:C:171:HIS:HB2	3:C:174:LEU:HD21	1.96	0.48
3:C:213:ARG:NE	4:D:299:PHE:CD2	2.81	0.48
5:E:63:GLN:HB2	5:E:69:PHE:CE1	2.48	0.48
20:W:201:ARG:O	20:W:205:ILE:HG12	2.14	0.48
23:Z:70:LEU:HD11	23:Z:108:ILE:HG23	1.96	0.48
23:Z:212:LEU:HA	23:Z:215:VAL:HG12	1.93	0.48
24:a:94:LEU:HA	24:a:97:LEU:HG	1.95	0.48
24:a:342:ASP:O	24:a:344:GLN:N	2.46	0.48
10:l:19:ILE:H	10:l:19:ILE:HD12	1.78	0.48
28:u:679:LEU:HD23	28:u:679:LEU:HA	1.57	0.48
28:u:758:ASN:O	28:u:762:VAL:HG13	2.13	0.48
29:U:127:ASP:HB3	29:U:130:LEU:HG	1.95	0.48
29:U:167:ILE:HG12	29:U:176:MET:SD	2.54	0.48
29:U:772:TRP:HB3	29:U:775:LEU:HG	1.95	0.48
5:E:22:ILE:O	5:E:26:LEU:HG	2.14	0.48
5:E:33:LEU:HD21	31:F:62:VAL:CG1	2.44	0.48
8:I:6:ASP:C	8:I:6:ASP:OD1	2.56	0.48
11:M:37:ILE:HD11	11:M:193:VAL:HG13	1.96	0.48
15:Q:14:LEU:HD21	15:Q:160:LEU:HD22	1.95	0.48
19:V:236:ARG:HH22	29:U:35:TRP:HE1	1.61	0.48
19:V:290:TYR:C	19:V:290:TYR:CD2	2.92	0.48
19:V:342:ILE:HD12	19:V:343:PRO:HD2	1.96	0.48
19:V:400:HIS:CD2	27:d:144:MET:HG3	2.48	0.48
20:W:454:ASN:OD1	23:Z:221:PRO:HG3	2.11	0.48
21:X:368:MET:HE2	21:X:374:PHE:CB	2.36	0.48
21:X:374:PHE:CD1	21:X:375:HIS:N	2.82	0.48
22:Y:228:MET:H	22:Y:228:MET:HG2	1.52	0.48
23:Z:112:MET:HE1	23:Z:119:SER:OG	2.14	0.48
24:a:254:ALA:HA	24:a:261:LEU:HD23	1.96	0.48
25:b:153:LEU:HB3	25:b:170:LEU:HD21	1.94	0.48
27:d:168:ASP:OD1	27:d:168:ASP:N	2.45	0.48
27:d:241:GLU:HA	27:d:244:LYS:HG2	1.96	0.48
7:h:4:ARG:HH12	8:i:2:SER:HA	1.79	0.48
7:h:49:GLU:OE1	7:h:51:LYS:NZ	2.47	0.48
1:A:263:MET:HE3	1:A:267:LYS:HZ3	1.77	0.48
1:A:417:ILE:HA	1:A:420:TYR:CE2	2.49	0.48
9:J:4:ASP:OD1	9:J:21:TYR:OH	2.32	0.48
21:X:415:TYR:CE1	22:Y:383:LEU:HB2	2.49	0.48
22:Y:372:LYS:O	22:Y:375:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:121:GLU:OE1	25:b:121:GLU:N	2.46	0.48
26:c:257:LYS:HZ3	26:c:261:GLU:HB2	1.79	0.48
27:d:10:ASN:OD1	27:d:10:ASN:N	2.47	0.48
8:i:233:VAL:HA	8:i:236:LEU:HD12	1.95	0.48
12:n:20:THR:O	12:n:20:THR:OG1	2.32	0.48
28:u:251:CYS:O	28:u:255:VAL:HG23	2.13	0.48
28:u:403:LYS:C	28:u:407:MET:HE1	2.39	0.48
29:U:218:GLN:HE22	29:U:752:THR:HB	1.78	0.48
29:U:757:MET:HE3	29:U:758:PRO:N	2.29	0.48
31:F:282:ILE:HB	31:F:329:ILE:HD11	1.96	0.48
1:A:225:CYS:O	1:A:229:VAL:HG22	2.13	0.48
1:A:353:HIS:HA	1:A:356:LYS:HD2	1.96	0.48
8:I:100:GLN:HG2	8:I:101:TYR:CD2	2.49	0.48
19:V:36:GLU:HA	19:V:39:GLU:CD	2.39	0.48
19:V:175:MET:HE1	19:V:216:ARG:HH22	1.78	0.48
20:W:425:LEU:HD23	20:W:425:LEU:HA	1.57	0.48
22:Y:184:GLN:NE2	22:Y:196:GLN:O	2.47	0.48
26:c:24:ALA:N	29:U:398:ASN:HD21	2.12	0.48
26:c:231:LEU:O	26:c:232:GLN:HG3	2.13	0.48
26:c:265:MET:SD	26:c:265:MET:O	2.72	0.48
26:c:302:ALA:O	26:c:306:THR:HG23	2.13	0.48
27:d:92:SER:O	27:d:95:MET:HG3	2.13	0.48
28:u:253:LEU:HD11	28:u:265:ALA:O	2.13	0.48
29:U:501:LEU:HD22	29:U:516:LEU:HD22	1.94	0.48
29:U:712:LEU:O	29:U:716:VAL:HG22	2.14	0.48
4:D:228:ILE:O	4:D:228:ILE:HG22	2.13	0.48
7:H:106:PRO:HG3	14:P:80:ARG:NH2	2.29	0.48
20:W:226:TYR:O	20:W:230:MET:HG2	2.14	0.48
23:Z:146:ASP:HB3	23:Z:149:THR:CG2	2.44	0.48
23:Z:288:LYS:HA	23:Z:288:LYS:HD2	1.74	0.48
26:c:278:GLN:HG2	26:c:282:ARG:HH21	1.78	0.48
27:d:132:TYR:HE1	27:d:160:ALA:HB2	1.78	0.48
11:m:229:LYS:O	11:m:233:GLU:N	2.47	0.48
29:U:82:LEU:HD21	29:U:130:LEU:HB3	1.94	0.48
29:U:137:MET:HE1	29:U:140:ARG:NH1	2.29	0.48
29:U:619:VAL:HA	29:U:622:LEU:HD23	1.95	0.48
1:A:254:ALA:H	1:A:298:THR:HG22	1.79	0.47
4:D:363:TYR:OH	4:D:400:GLU:HG3	2.14	0.47
8:I:163:CYS:SG	8:I:164:ILE:N	2.87	0.47
9:J:108:THR:HG21	9:J:145:TYR:HB2	1.95	0.47
14:P:125:ASP:OD2	14:P:125:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:142:CYS:HB2	14:P:145:GLN:OE1	2.14	0.47
19:V:224:LEU:HG	19:V:257:ASN:ND2	2.29	0.47
20:W:10:ASP:HA	20:W:13:ILE:HG12	1.96	0.47
20:W:78:LYS:HG2	20:W:82:LEU:HD23	1.96	0.47
21:X:190:LEU:HD21	21:X:214:SER:HA	1.95	0.47
22:Y:293:ARG:HA	30:e:57:ARG:CZ	2.44	0.47
22:Y:312:ARG:O	22:Y:355:GLU:HA	2.14	0.47
23:Z:78:MET:HE3	23:Z:78:MET:CA	2.43	0.47
24:a:205:LEU:O	24:a:271:LYS:NZ	2.43	0.47
11:m:8:ASP:O	11:m:22:GLN:NE2	2.46	0.47
1:A:236:CYS:HB3	1:A:270:CYS:CA	2.44	0.47
4:D:64:GLU:OE1	29:U:607:VAL:HG13	2.14	0.47
5:E:129:ASN:O	5:E:130:VAL:HG13	2.14	0.47
37:O:301:LDZ:H3	14:P:126:LEU:CD2	2.45	0.47
19:V:149:PRO:HG3	19:V:199:ASN:OD1	2.15	0.47
24:a:68:GLU:HG3	24:a:69:HIS:H	1.78	0.47
24:a:321:LYS:HE2	24:a:336:VAL:HG21	1.95	0.47
26:c:53:VAL:H	26:c:114:SER:HG	1.60	0.47
26:c:59:GLY:HA3	26:c:69:VAL:HA	1.95	0.47
27:d:94:TYR:O	27:d:98:LEU:HD13	2.14	0.47
15:q:49:GLU:HG3	15:q:50:ALA:H	1.79	0.47
15:q:186:ASN:HB2	15:q:189:HIS:CE1	2.49	0.47
29:U:24:LEU:HA	29:U:27:LEU:HB2	1.96	0.47
32:K:171:GLY:O	32:K:174:SER:HB3	2.14	0.47
1:A:274:PHE:N	1:A:274:PHE:CD1	2.80	0.47
3:C:25:LEU:O	3:C:29:GLU:HG2	2.13	0.47
5:E:287:PRO:HA	5:E:290:LEU:HB2	1.94	0.47
5:E:350:ALA:HB1	5:E:367:PHE:HD1	1.80	0.47
16:R:19:ARG:HE	16:R:29:GLN:NE2	2.13	0.47
19:V:203:LEU:HA	19:V:206:VAL:HB	1.95	0.47
19:V:323:GLY:C	30:e:6:GLN:HB3	2.39	0.47
22:Y:220:VAL:HA	22:Y:223:THR:HG22	1.96	0.47
23:Z:144:VAL:O	23:Z:145:HIS:CB	2.61	0.47
24:a:226:ARG:HH12	24:a:233:LEU:HB3	1.80	0.47
25:b:61:LEU:HD21	25:b:74:LYS:HD2	1.97	0.47
27:d:10:ASN:HB2	27:d:11:ARG:CZ	2.44	0.47
7:h:187:ALA:HA	7:h:190:THR:HG22	1.96	0.47
11:m:152:ASP:OD1	11:m:154:SER:OG	2.31	0.47
14:p:171:MET:HE3	14:p:175:VAL:CG1	2.44	0.47
17:s:145:LEU:HD22	17:s:178:VAL:HB	1.96	0.47
29:U:214:ILE:HD12	29:U:215:ASN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:32:GLU:C	31:F:36:MET:HE1	2.39	0.47
32:K:199:LEU:HG	32:K:210:LEU:HD11	1.95	0.47
5:E:16:LEU:O	5:E:21:GLU:OE1	2.32	0.47
5:E:173:TYR:CE1	5:E:298:LYS:HB3	2.49	0.47
5:E:216:ARG:O	5:E:220:ASN:ND2	2.47	0.47
5:E:349:GLU:HG3	5:E:373:LYS:HD2	1.95	0.47
13:O:163:ILE:HD12	13:O:169:SER:CB	2.44	0.47
13:O:170:GLY:O	13:O:171:SER:HB2	2.14	0.47
20:W:448:LYS:HZ3	23:Z:101:LEU:HD22	1.78	0.47
26:c:32:TYR:HB3	26:c:208:ARG:HG2	1.95	0.47
26:c:211:GLU:O	26:c:212:LEU:CB	2.60	0.47
26:c:232:GLN:NE2	26:c:298:GLN:OE1	2.47	0.47
7:h:130:PHE:O	7:h:151:PRO:HB3	2.14	0.47
17:s:151:ASN:ND2	17:s:156:LYS:O	2.47	0.47
29:U:24:LEU:HD21	29:U:59:PHE:C	2.39	0.47
29:U:130:LEU:HD12	29:U:131:GLU:H	1.79	0.47
29:U:135:ASN:HA	29:U:138:PHE:CD2	2.49	0.47
29:U:214:ILE:O	29:U:215:ASN:C	2.57	0.47
29:U:261:LEU:HD23	29:U:329:LEU:O	2.15	0.47
29:U:885:MET:HB2	29:U:888:GLN:HG2	1.96	0.47
31:F:272:PHE:O	31:F:276:LYS:HG2	2.14	0.47
3:C:44:ARG:HA	19:V:495:ARG:CG	2.45	0.47
3:C:110:PRO:HG2	3:C:130:LYS:HZ1	1.77	0.47
8:I:90:LEU:HG	8:I:114:LEU:HD13	1.97	0.47
13:O:198:ARG:NH1	14:P:152:SER:O	2.47	0.47
13:O:204:CYS:SG	14:P:165:GLU:HB3	2.55	0.47
16:R:9:ARG:HB2	16:R:145:TYR:O	2.14	0.47
19:V:314:ARG:NH1	22:Y:382:LYS:CE	2.78	0.47
24:a:363:MET:HE3	24:a:364:GLU:N	2.30	0.47
26:c:33:ILE:HG22	26:c:205:ILE:HD11	1.96	0.47
27:d:73:ARG:HG2	27:d:74:TYR:CD2	2.49	0.47
6:g:80:MET:SD	6:g:138:MET:HG3	2.54	0.47
9:j:8:THR:HB	32:k:135:ARG:HB3	1.95	0.47
9:j:171:PHE:HD2	9:j:171:PHE:O	1.98	0.47
13:o:146:MET:HE1	13:o:154:LEU:HD22	1.96	0.47
28:u:723:TYR:HB3	28:u:761:MET:CE	2.35	0.47
29:U:583:MET:O	29:U:586:VAL:HG22	2.13	0.47
31:F:292:GLY:C	31:F:310:MET:HE2	2.40	0.47
1:A:34:LYS:NZ	3:C:174:LEU:CD2	2.76	0.47
3:C:403:LYS:HD2	7:H:156:PHE:CD1	2.50	0.47
5:E:305:ASN:HB3	5:E:308:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:161:ALA:HB1	8:I:175:LEU:HD13	1.97	0.47
13:O:163:ILE:HD12	13:O:169:SER:HB2	1.97	0.47
19:V:108:LEU:HA	19:V:111:TYR:HD2	1.80	0.47
19:V:147:PHE:HB3	19:V:150:ARG:HG2	1.97	0.47
21:X:58:ALA:HA	21:X:99:MET:HE3	1.96	0.47
24:a:295:GLU:HG3	24:a:296:ILE:N	2.30	0.47
25:b:153:LEU:HD23	25:b:170:LEU:HD11	1.96	0.47
27:d:249:TYR:O	27:d:253:LEU:HG	2.14	0.47
6:g:217:VAL:HG12	6:g:230:LEU:HD13	1.96	0.47
8:i:31:ALA:O	8:i:166:ASN:HB2	2.15	0.47
10:l:5:GLN:NE2	10:l:5:GLN:H	2.12	0.47
15:q:43:LEU:HD12	15:q:183:ILE:HD11	1.96	0.47
29:U:475:HIS:CE1	29:U:507:VAL:HG22	2.49	0.47
29:U:497:LEU:HD12	29:U:516:LEU:HD13	1.95	0.47
29:U:836:THR:HB	29:U:840:LYS:NZ	2.30	0.47
31:F:188:ILE:HG13	31:F:235:LEU:O	2.15	0.47
31:F:370:SER:HB3	31:F:379:VAL:HG11	1.96	0.47
32:k:227:HIS:HE1	32:k:233:GLU:OE1	1.94	0.47
1:A:165:GLN:HE22	1:A:167:GLU:CD	2.23	0.47
1:A:252:GLU:OE2	1:A:256:MET:SD	2.72	0.47
2:B:387:LYS:HG2	2:B:390:LEU:HD23	1.97	0.47
3:C:345:ARG:NH1	3:C:345:ARG:HB2	2.29	0.47
3:C:391:MET:N	3:C:391:MET:SD	2.87	0.47
4:D:273:LYS:HB3	4:D:318:ASP:HA	1.97	0.47
4:D:338:ARG:C	4:D:340:GLN:N	2.52	0.47
5:E:81:VAL:HG21	5:E:107:ILE:CD1	2.30	0.47
5:E:153:LEU:O	5:E:156:PRO:HD3	2.15	0.47
5:E:175:PRO:HD2	5:E:301:ILE:O	2.15	0.47
6:G:129:ALA:O	6:G:130:GLU:CD	2.57	0.47
19:V:62:HIS:CE1	22:Y:389:MET:CE	2.75	0.47
19:V:294:ARG:HE	19:V:331:LEU:HD22	1.79	0.47
22:Y:53:TYR:HE2	22:Y:67:VAL:HG22	1.79	0.47
23:Z:192:THR:HG22	24:a:375:LEU:HD22	1.96	0.47
23:Z:278:ASN:HD21	23:Z:282:ASN:HD21	1.62	0.47
24:a:77:VAL:HG13	24:a:113:LEU:HD11	1.96	0.47
24:a:99:LYS:HB3	24:a:99:LYS:HE2	1.78	0.47
24:a:150:SER:HA	24:a:154:ARG:HH21	1.80	0.47
24:a:280:MET:HE1	24:a:299:SER:HB2	1.95	0.47
27:d:15:ASN:ND2	27:d:17:SER:H	2.12	0.47
8:i:38:LEU:HD12	8:i:43:VAL:HG22	1.97	0.47
9:j:175:ASN:OD1	9:j:175:ASN:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:366:ASP:O	28:u:370:MET:HE3	2.14	0.47
29:U:221:ILE:HG23	29:U:754:HIS:NE2	2.29	0.47
29:U:582:GLY:O	29:U:586:VAL:HG13	2.13	0.47
29:U:633:CYS:SG	29:U:659:CYS:CB	3.02	0.47
31:F:159:LEU:HD12	31:F:160:ILE:H	1.80	0.47
32:K:91:LYS:HG2	32:K:119:LEU:HD22	1.96	0.47
1:A:173:THR:HA	1:A:231:ASN:ND2	2.12	0.47
3:C:69:GLN:HG2	3:C:118:ASN:ND2	2.30	0.47
3:C:281:ASP:HB3	3:C:310:ARG:NH1	2.29	0.47
4:D:46:LYS:NZ	29:U:187:LEU:HD12	2.29	0.47
5:E:29:LEU:O	5:E:33:LEU:HD22	2.14	0.47
9:J:227:LYS:C	9:J:227:LYS:HD3	2.40	0.47
17:S:162:GLU:CD	17:S:162:GLU:H	2.23	0.47
19:V:18:PRO:HA	19:V:22:GLY:HA3	1.96	0.47
20:W:330:LYS:NZ	20:W:331:GLY:O	2.39	0.47
21:X:134:VAL:HB	21:X:149:LEU:HD23	1.96	0.47
21:X:244:SER:HA	21:X:247:ALA:HB3	1.97	0.47
21:X:337:ARG:HG2	21:X:337:ARG:HH11	1.80	0.47
22:Y:110:TYR:C	22:Y:110:TYR:CD2	2.92	0.47
23:Z:78:MET:HE3	23:Z:81:MET:HB3	1.97	0.47
13:o:191:VAL:O	13:o:194:LYS:NZ	2.37	0.47
17:s:144:MET:HE1	17:s:185:ARG:HB2	1.96	0.47
18:t:25:ASP:OD1	18:t:41:ARG:NH1	2.48	0.47
28:u:411:ALA:O	28:u:414:LEU:HD12	2.14	0.47
32:k:22:PHE:O	32:k:25:GLU:HG2	2.15	0.47
1:A:167:GLU:OE1	1:A:267:LYS:NZ	2.48	0.47
1:A:194:PRO:CB	1:A:316:LYS:HE3	2.44	0.47
2:B:167:THR:OG1	2:B:168:ASP:N	2.47	0.47
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.47	0.47
5:E:26:LEU:CD1	31:F:55:MET:HG2	2.44	0.47
5:E:84:ARG:HB2	5:E:87:LEU:HB2	1.97	0.47
5:E:376:ASP:HA	5:E:379:LYS:HG2	1.96	0.47
15:Q:152:SER:OG	15:Q:155:ARG:HG2	2.14	0.47
20:W:191:ARG:HD3	20:W:192:LEU:H	1.80	0.47
20:W:436:MET:CE	23:Z:236:LEU:HD22	2.42	0.47
21:X:307:THR:HA	21:X:310:ARG:HH11	1.80	0.47
22:Y:191:ILE:O	22:Y:191:ILE:CG2	2.62	0.47
24:a:69:HIS:ND1	24:a:70:ARG:HG2	2.29	0.47
26:c:211:GLU:HG3	26:c:212:LEU:N	2.30	0.47
8:i:206:LEU:HD13	8:i:206:LEU:O	2.15	0.47
12:n:103:TRP:CZ2	12:n:181:GLU:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:198:LEU:HG	29:U:219:CYS:HB3	1.95	0.47
29:U:341:PHE:HD1	29:U:881:PRO:HB2	1.80	0.47
29:U:872:GLU:HB2	29:U:873:PRO:HD3	1.96	0.47
1:A:258:ARG:O	1:A:262:GLU:HG2	2.15	0.47
2:B:313:LEU:HD12	2:B:341:LEU:HD22	1.96	0.47
3:C:251:ILE:HB	3:C:295:THR:HG21	1.95	0.47
4:D:238:LYS:HE2	5:E:207:TYR:CD2	2.50	0.47
5:E:101:ASP:OD1	5:E:108:MET:HE1	2.14	0.47
5:E:328:TYR:CE1	5:E:367:PHE:HE2	2.26	0.47
19:V:166:TYR:HA	19:V:168:GLN:HE21	1.78	0.47
23:Z:39:LEU:HD23	23:Z:53:SER:HB2	1.96	0.47
24:a:247:ARG:HH12	24:a:251:LEU:HD21	1.75	0.47
27:d:189:ILE:HD12	27:d:222:TYR:HB2	1.97	0.47
27:d:241:GLU:O	27:d:245:GLN:HB2	2.14	0.47
11:m:28:LYS:HA	11:m:31:GLU:HB2	1.96	0.47
17:s:114:ASP:C	17:s:114:ASP:OD2	2.58	0.47
28:u:284:SER:O	28:u:286:LYS:HD2	2.15	0.47
29:U:260:PHE:O	29:U:264:VAL:HG13	2.15	0.47
29:U:354:LYS:HD3	29:U:354:LYS:C	2.40	0.47
32:K:9:ASP:OD1	32:K:9:ASP:N	2.47	0.47
2:B:327:VAL:HG12	2:B:329:MET:HE2	1.97	0.46
4:D:335:LEU:O	4:D:336:PRO:C	2.58	0.46
5:E:261:LEU:HD11	5:E:294:ARG:NH1	2.30	0.46
5:E:354:ALA:HA	5:E:359:HIS:CD2	2.49	0.46
6:G:112:ASP:OD1	6:G:112:ASP:C	2.59	0.46
17:S:213:ASP:HB3	13:o:193:ASN:OD1	2.15	0.46
18:T:50:MET:HG2	18:T:113:GLY:O	2.14	0.46
23:Z:13:PRO:HA	23:Z:16:LEU:HD21	1.97	0.46
23:Z:78:MET:HA	23:Z:78:MET:CE	2.43	0.46
6:g:190:THR:O	6:g:194:THR:HG23	2.15	0.46
13:o:11:GLY:O	13:o:12:ILE:HD13	2.15	0.46
15:q:108:ASP:OD2	15:q:109:GLU:N	2.48	0.46
17:s:125:ASP:OD2	17:s:125:ASP:C	2.58	0.46
28:u:99:LEU:HD23	28:u:99:LEU:N	2.30	0.46
29:U:234:GLU:O	29:U:238:LYS:HG3	2.15	0.46
31:F:338:LEU:HD21	31:F:343:LEU:HD21	1.96	0.46
1:A:74:PRO:HG2	1:A:77:LEU:HB3	1.97	0.46
1:A:155:PRO:HD2	1:A:255:ARG:NH2	2.25	0.46
1:A:248:LYS:HA	1:A:248:LYS:HD3	1.74	0.46
1:A:366:ARG:NE	1:A:366:ARG:HA	2.30	0.46
1:A:400:ARG:HH22	28:u:867:THR:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:PHE:HD2	4:D:126:PRO:HA	1.80	0.46
4:D:311:THR:HG23	4:D:312:ASN:O	2.15	0.46
6:G:86:ASP:OD2	6:G:86:ASP:N	2.47	0.46
19:V:81:GLN:HB2	19:V:86:VAL:H	1.80	0.46
22:Y:274:SER:CA	22:Y:277:VAL:HG12	2.44	0.46
23:Z:185:GLY:H	23:Z:190:ARG:HH12	1.64	0.46
25:b:4:GLU:HA	25:b:106:LYS:N	2.30	0.46
26:c:96:LEU:O	26:c:100:LYS:HG3	2.14	0.46
26:c:210:ASN:N	26:c:210:ASN:OD1	2.46	0.46
9:j:71:MET:HE3	9:j:73:PHE:HB3	1.97	0.46
10:l:209:ASN:OD1	10:l:209:ASN:N	2.48	0.46
31:F:235:LEU:HA	31:F:238:ARG:HD3	1.96	0.46
6:G:36:GLY:O	6:G:37:LEU:HD23	2.15	0.46
8:I:100:GLN:HG2	8:I:101:TYR:CE2	2.50	0.46
19:V:77:GLU:OE1	19:V:161:PRO:HG3	2.14	0.46
21:X:156:GLU:O	21:X:160:MET:SD	2.73	0.46
23:Z:9:VAL:HG23	23:Z:48:LEU:HD22	1.96	0.46
26:c:184:LEU:HD13	26:c:184:LEU:H	1.79	0.46
16:r:191:ASN:HB3	16:r:194:ASP:OD2	2.15	0.46
31:F:413:THR:OG1	31:F:414:GLU:OE1	2.31	0.46
32:K:55:THR:HG22	32:K:59:MET:CE	2.46	0.46
2:B:98:LYS:HD2	2:B:98:LYS:C	2.41	0.46
3:C:83:LYS:O	3:C:83:LYS:HG2	2.16	0.46
3:C:186:VAL:HG22	3:C:313:ARG:HB2	1.96	0.46
5:E:195:PHE:CZ	5:E:197:LYS:HB2	2.50	0.46
20:W:448:LYS:NZ	23:Z:101:LEU:HD22	2.30	0.46
23:Z:103:LYS:O	23:Z:106:ILE:HG22	2.16	0.46
24:a:188:LEU:HD11	24:a:193:GLN:HG3	1.96	0.46
26:c:41:MET:HE3	26:c:145:VAL:HG21	1.98	0.46
26:c:123:SER:N	26:c:126:ASP:OD2	2.46	0.46
6:g:60:LEU:HD22	11:m:181:MET:HE1	1.96	0.46
9:j:117:ARG:O	9:j:121:SER:HB2	2.15	0.46
28:u:391:LEU:HD23	28:u:414:LEU:HD21	1.97	0.46
29:U:222:PHE:CD1	29:U:754:HIS:HE1	2.32	0.46
31:F:150:LEU:H	31:F:165:PRO:CB	2.28	0.46
1:A:303:ILE:HB	1:A:336:ARG:NH2	2.31	0.46
2:B:273:VAL:HG13	2:B:277:HIS:HD2	1.81	0.46
2:B:409:GLU:OE2	2:B:411:ARG:NH2	2.36	0.46
3:C:57:ARG:HH12	29:U:644:TYR:HB3	1.80	0.46
3:C:119:ASP:HB2	26:c:189:ILE:CD1	2.45	0.46
6:G:10:ASP:OD1	6:G:17:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:176:MET:SD	19:V:179:LYS:NZ	2.86	0.46
20:W:314:LEU:HD13	24:a:309:LEU:HD23	1.98	0.46
20:W:446:ILE:O	20:W:450:GLU:HG2	2.15	0.46
25:b:35:ILE:HD12	25:b:36:VAL:HG13	1.97	0.46
7:h:68:ILE:CD1	7:h:74:LEU:HD13	2.45	0.46
8:i:8:ARG:C	8:i:10:THR:H	2.24	0.46
10:l:148:CYS:SG	10:l:149:PRO:HD2	2.56	0.46
29:U:118:LEU:HD12	29:U:122:GLU:HG3	1.98	0.46
31:F:150:LEU:H	31:F:165:PRO:HB3	1.80	0.46
31:F:150:LEU:N	31:F:165:PRO:HB3	2.31	0.46
32:K:53:ARG:HG2	32:K:53:ARG:O	2.15	0.46
3:C:256:SER:O	3:C:302:ASP:N	2.49	0.46
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.97	0.46
4:D:176:GLU:HG2	4:D:331:ILE:HD11	1.98	0.46
5:E:101:ASP:OD1	5:E:108:MET:CE	2.63	0.46
8:I:10:THR:O	8:I:10:THR:CG2	2.63	0.46
19:V:54:LYS:O	19:V:54:LYS:HD2	2.15	0.46
19:V:470:ARG:HE	19:V:473:GLN:NE2	2.13	0.46
21:X:143:TYR:CE2	22:Y:252:SER:HB2	2.51	0.46
21:X:163:LYS:HA	21:X:163:LYS:HD3	1.79	0.46
22:Y:51:ALA:HB3	22:Y:52:PRO:HD3	1.97	0.46
22:Y:368:GLU:OE1	22:Y:368:GLU:HA	2.14	0.46
24:a:137:ASP:O	24:a:141:MET:HE3	2.16	0.46
15:q:38:MET:CE	15:q:64:VAL:HG21	2.44	0.46
29:U:68:PHE:HB2	29:U:77:SER:OG	2.15	0.46
29:U:796:LYS:HZ1	29:U:921:ILE:HB	1.81	0.46
32:K:206:MET:HE1	32:K:215:ILE:HG22	1.97	0.46
1:A:163:MET:SD	1:A:163:MET:N	2.89	0.46
1:A:167:GLU:HA	1:A:237:PHE:O	2.15	0.46
2:B:112:LEU:HD11	2:B:115:ILE:HG13	1.98	0.46
2:B:203:LEU:HD23	2:B:203:LEU:HA	1.79	0.46
2:B:365:PHE:HE1	2:B:395:ILE:HG12	1.81	0.46
3:C:171:HIS:HB2	3:C:174:LEU:CD2	2.45	0.46
3:C:398:ASN:C	3:C:400:SER:H	2.23	0.46
4:D:336:PRO:HG2	4:D:370:ILE:O	2.16	0.46
5:E:42:LYS:HB2	5:E:42:LYS:NZ	2.30	0.46
5:E:186:ALA:O	5:E:189:SER:OG	2.33	0.46
13:O:13:VAL:HG22	13:O:177:VAL:HG22	1.98	0.46
19:V:131:LEU:CD2	19:V:162:GLU:HG3	2.45	0.46
19:V:137:GLU:HA	19:V:140:ASP:HB2	1.97	0.46
19:V:455:LYS:HD2	19:V:457:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:470:ARG:HD3	23:Z:249:PHE:HE2	1.80	0.46
21:X:73:VAL:O	21:X:76:PHE:CE1	2.68	0.46
23:Z:34:ARG:HE	23:Z:102:HIS:CE1	2.34	0.46
23:Z:54:PHE:C	23:Z:54:PHE:HD2	2.20	0.46
26:c:32:TYR:HE1	26:c:66:THR:HB	1.80	0.46
9:j:99:GLU:OE1	16:r:120:ARG:NH2	2.48	0.46
15:q:101:ASN:HB3	15:q:132:HIS:CD2	2.50	0.46
17:s:16:ALA:HB2	17:s:121:VAL:HG23	1.96	0.46
18:t:208:ASN:CG	18:t:210:ASP:OD1	2.58	0.46
28:u:140:LEU:HD12	28:u:166:VAL:HG22	1.98	0.46
28:u:605:ASN:N	28:u:660:ILE:HD11	2.26	0.46
29:U:697:GLN:NE2	29:U:744:VAL:O	2.48	0.46
31:F:318:ASP:HB2	31:F:347:ARG:HD3	1.98	0.46
32:k:85:ALA:HB2	32:k:139:VAL:HG11	1.97	0.46
7:H:68:ILE:HG23	7:H:91:ARG:HG2	1.98	0.46
11:M:175:GLU:HA	11:M:178:LYS:HG3	1.98	0.46
22:Y:73:MET:SD	22:Y:74:LYS:N	2.88	0.46
23:Z:7:GLN:HB2	23:Z:46:LYS:HZ3	1.79	0.46
24:a:57:ILE:O	24:a:61:GLU:HG2	2.16	0.46
24:a:291:LEU:HD13	24:a:295:GLU:CD	2.41	0.46
24:a:325:ASP:HB3	24:a:330:ARG:CZ	2.45	0.46
26:c:111:TRP:HZ3	26:c:113:HIS:HD1	1.63	0.46
9:j:94:HIS:ND1	9:j:102:VAL:HG22	2.30	0.46
16:r:146:ASP:OD2	16:r:146:ASP:N	2.49	0.46
28:u:73:PRO:O	28:u:76:GLU:HG3	2.15	0.46
29:U:227:GLN:OE1	29:U:227:GLN:N	2.49	0.46
1:A:55:LEU:HA	1:A:58:LYS:HE2	1.98	0.46
1:A:97:ARG:HH22	1:A:144:ARG:HA	1.81	0.46
1:A:433:ASN:HD21	32:K:66:LYS:NZ	2.13	0.46
2:B:65:LEU:HA	2:B:68:ILE:HG13	1.98	0.46
2:B:204:PRO:O	28:u:740:ARG:NH2	2.49	0.46
2:B:385:MET:HB3	9:J:200:GLN:CB	2.46	0.46
4:D:56:VAL:HG22	29:U:600:ARG:HH21	1.81	0.46
22:Y:174:TRP:CG	22:Y:175:ASP:N	2.81	0.46
23:Z:138:TYR:O	23:Z:139:ILE:HD13	2.16	0.46
23:Z:272:LEU:O	23:Z:275:LEU:HB3	2.16	0.46
27:d:6:LYS:HG2	27:d:10:ASN:CG	2.41	0.46
27:d:74:TYR:CD2	27:d:74:TYR:N	2.82	0.46
6:g:206:LEU:HB2	6:g:208:ILE:HG12	1.97	0.46
7:h:199:PHE:HZ	7:h:207:ASN:HD22	1.62	0.46
10:l:5:GLN:H	10:l:5:GLN:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:210:VAL:CG1	10:l:229:VAL:HG11	2.44	0.46
13:o:199:LEU:HD23	13:o:199:LEU:HA	1.81	0.46
28:u:261:ARG:CZ	28:u:261:ARG:HA	2.46	0.46
29:U:567:ILE:HG23	29:U:586:VAL:HG12	1.98	0.46
31:F:250:LYS:HD3	31:F:250:LYS:N	2.30	0.46
31:F:282:ILE:HB	31:F:329:ILE:CD1	2.46	0.46
31:F:287:GLU:N	31:F:331:ALA:O	2.48	0.46
1:A:306:LEU:HB3	1:A:336:ARG:HH12	1.81	0.46
2:B:46:ALA:HB3	2:B:179:ALA:H	1.80	0.46
2:B:362:LYS:HZ3	2:B:366:GLN:HB2	1.79	0.46
4:D:173:GLN:HE22	4:D:334:PRO:CD	2.27	0.46
5:E:132:TYR:CD2	5:E:186:ALA:HB1	2.50	0.46
5:E:336:ASP:CB	5:E:338:PHE:CE1	2.99	0.46
7:H:6:TYR:OH	8:I:6:ASP:OD2	2.33	0.46
7:H:171:LYS:HE2	7:H:171:LYS:HB2	1.69	0.46
8:I:48:GLU:OE1	8:I:50:ARG:CD	2.64	0.46
9:J:71:MET:HE3	9:J:131:ALA:HB2	1.97	0.46
19:V:80:LYS:NZ	19:V:128:ARG:HA	2.29	0.46
20:W:16:MET:SD	20:W:17:GLU:HB2	2.56	0.46
20:W:125:ILE:HG13	20:W:129:ARG:HH11	1.81	0.46
20:W:191:ARG:NH1	20:W:192:LEU:HB2	2.31	0.46
20:W:335:SER:CB	20:W:336:PRO:HD3	2.45	0.46
24:a:105:LYS:HD3	24:a:105:LYS:H	1.81	0.46
26:c:118:PHE:CD2	26:c:121:TRP:CE2	3.04	0.46
27:d:44:THR:OG1	27:d:47:GLN:NE2	2.49	0.46
27:d:96:HIS:NE2	27:d:125:LYS:HE2	2.31	0.46
8:i:114:LEU:HD12	8:i:114:LEU:HA	1.82	0.46
8:i:171:ALA:HB2	8:i:200:THR:HG21	1.97	0.46
10:l:203:GLN:O	10:l:239:ARG:NH1	2.48	0.46
17:s:125:ASP:OD2	17:s:128:GLY:N	2.45	0.46
28:u:234:THR:O	28:u:237:VAL:HG22	2.16	0.46
31:F:63:THR:O	31:F:66:LEU:HB3	2.15	0.46
31:F:347:ARG:O	31:F:349:ASP:N	2.49	0.46
31:F:407:ALA:HA	31:F:410:ARG:NH1	2.31	0.46
1:A:432:TYR:OH	9:J:15:HIS:HA	2.15	0.45
3:C:377:HIS:HE1	22:Y:207:THR:HG22	1.81	0.45
5:E:312:ILE:HG22	5:E:316:HIS:CE1	2.51	0.45
5:E:368:MET:O	5:E:372:ARG:HG3	2.16	0.45
7:H:4:ARG:HA	7:H:4:ARG:HH11	1.79	0.45
17:S:24:ALA:HB1	17:S:193:LEU:HD11	1.98	0.45
19:V:265:ASP:HA	19:V:268:GLU:OE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:477:HIS:NE2	27:d:245:GLN:HG2	2.31	0.45
20:W:306:LEU:C	20:W:306:LEU:HD12	2.40	0.45
25:b:94:HIS:HD2	25:b:98:LYS:HE3	1.81	0.45
27:d:132:TYR:CE1	27:d:160:ALA:HB2	2.51	0.45
7:h:91:ARG:HD3	13:o:68:LEU:HD23	1.98	0.45
11:m:186:CYS:O	11:m:189:ILE:HG22	2.16	0.45
13:o:19:ARG:CB	13:o:169:SER:HA	2.45	0.45
18:t:150:LEU:HD23	18:t:168:LEU:HD23	1.99	0.45
29:U:89:ASN:OD1	29:U:129:ARG:NH1	2.49	0.45
29:U:255:SER:OG	29:U:754:HIS:HD2	2.00	0.45
29:U:556:MET:SD	29:U:556:MET:C	3.00	0.45
29:U:695:MET:HE2	29:U:695:MET:HB3	1.85	0.45
31:F:168:TYR:CD1	31:F:169:ASP:N	2.84	0.45
31:F:202:ILE:C	31:F:205:PRO:HD2	2.41	0.45
31:F:291:ILE:CG2	31:F:309:THR:HG21	2.46	0.45
31:F:376:SER:C	31:F:378:ASP:N	2.74	0.45
1:A:230:ALA:HB2	1:A:271:LEU:HD23	1.99	0.45
2:B:269:GLU:OE1	2:B:270:LEU:N	2.50	0.45
2:B:405:MET:CE	2:B:408:ARG:HD3	2.43	0.45
4:D:92:PHE:CD2	4:D:124:LEU:O	2.69	0.45
8:I:151:ASP:OD2	8:I:153:SER:N	2.49	0.45
10:L:41:LYS:HG3	10:L:180:MET:HG3	1.98	0.45
22:Y:176:ARG:O	22:Y:180:LEU:HG	2.16	0.45
24:a:84:VAL:HA	24:a:87:MET:HG2	1.97	0.45
24:a:193:GLN:HB3	24:a:225:LEU:HD13	1.98	0.45
24:a:270:ARG:HD2	24:a:271:LYS:HG3	1.98	0.45
26:c:189:ILE:HA	26:c:192:LEU:CD2	2.46	0.45
27:d:142:TYR:CD2	27:d:150:LYS:HG3	2.51	0.45
10:l:88:MET:HG2	10:l:112:ILE:HD11	1.98	0.45
12:n:190:LEU:O	12:n:193:GLN:NE2	2.49	0.45
2:B:317:ASP:OD2	2:B:346:ARG:HG2	2.16	0.45
2:B:362:LYS:NZ	2:B:366:GLN:OE1	2.49	0.45
3:C:399:MET:HG3	3:C:399:MET:O	2.15	0.45
4:D:92:PHE:CD2	4:D:126:PRO:HA	2.51	0.45
4:D:212:LYS:HA	4:D:333:PHE:HE2	1.82	0.45
4:D:214:MET:HE1	35:D:501:ATP:H2'	1.98	0.45
5:E:248:SER:OG	5:E:250:ASP:OD1	2.34	0.45
5:E:338:PHE:N	5:E:338:PHE:CD1	2.81	0.45
8:I:10:THR:O	8:I:10:THR:HG22	2.15	0.45
8:I:48:GLU:OE1	8:I:50:ARG:HD2	2.17	0.45
9:J:173:GLU:OE2	32:K:56:SER:OG	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:58:ALA:N	19:V:201:ARG:HH22	2.14	0.45
20:W:138:VAL:HG23	20:W:139:GLU:H	1.82	0.45
22:Y:43:ALA:HA	22:Y:46:ARG:NH1	2.27	0.45
22:Y:178:ASN:C	22:Y:180:LEU:N	2.73	0.45
26:c:137:SER:OG	26:c:138:GLU:N	2.49	0.45
27:d:95:MET:O	27:d:99:LEU:HG	2.16	0.45
9:j:79:ASP:HB3	9:j:127:PHE:HD1	1.82	0.45
11:m:170:GLN:HG3	11:m:171:ALA:N	2.32	0.45
29:U:198:LEU:O	29:U:202:VAL:HG23	2.16	0.45
29:U:328:ILE:N	29:U:333:MET:HE1	2.31	0.45
30:e:1:MET:C	30:e:1:MET:SD	3.00	0.45
31:F:395:GLN:O	31:F:399:VAL:HG23	2.17	0.45
1:A:101:ILE:HG13	1:A:138:MET:O	2.15	0.45
1:A:323:ARG:HG3	1:A:323:ARG:HH11	1.82	0.45
1:A:394:MET:HE2	1:A:394:MET:CA	2.33	0.45
3:C:201:ARG:HG3	4:D:299:PHE:CE1	2.51	0.45
5:E:10:GLN:O	5:E:14:LYS:HG2	2.17	0.45
5:E:26:LEU:HD13	31:F:55:MET:HG2	1.98	0.45
13:O:140:ASP:OD2	18:t:171:ARG:NH2	2.46	0.45
19:V:32:PRO:HA	19:V:36:GLU:OE2	2.17	0.45
19:V:62:HIS:ND1	19:V:201:ARG:HD3	2.31	0.45
19:V:488:ASN:HB2	19:V:489:MET:HE1	1.99	0.45
20:W:12:ARG:NE	20:W:12:ARG:O	2.49	0.45
20:W:328:LEU:HD23	20:W:341:PHE:CE2	2.51	0.45
21:X:129:LEU:HD23	21:X:129:LEU:O	2.16	0.45
21:X:377:ILE:HD12	21:X:378:LEU:H	1.81	0.45
23:Z:37:GLY:HA2	23:Z:56:VAL:HG12	1.97	0.45
24:a:279:GLU:HA	24:a:282:PHE:HB2	1.98	0.45
25:b:100:ARG:NH1	25:b:102:GLY:O	2.50	0.45
26:c:75:MET:HE3	26:c:87:VAL:HA	1.97	0.45
7:h:228:ASP:OD2	7:h:229:TYR:HD1	1.98	0.45
12:n:84:LYS:NZ	12:n:85:GLU:OE2	2.49	0.45
13:o:205:GLU:OE1	13:o:205:GLU:HA	2.15	0.45
29:U:563:ALA:O	29:U:567:ILE:HG12	2.17	0.45
31:F:169:ASP:O	31:F:173:LYS:HE3	2.17	0.45
31:F:251:LEU:O	31:F:286:ASP:N	2.33	0.45
1:A:238:ILE:HG21	1:A:272:ILE:HG23	1.99	0.45
2:B:202:GLU:O	2:B:206:THR:HG22	2.16	0.45
2:B:219:PRO:O	2:B:326:LYS:NZ	2.40	0.45
3:C:78:ARG:HA	3:C:108:VAL:HG23	1.98	0.45
3:C:88:LYS:HB3	3:C:94:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:ILE:HG12	3:C:198:LEU:HD22	1.98	0.45
4:D:146:GLU:CD	4:D:252:ARG:HD2	2.41	0.45
6:G:132:ARG:HH11	11:M:20:VAL:HG21	1.82	0.45
8:I:90:LEU:HD22	8:I:110:LEU:HG	1.99	0.45
11:M:64:LYS:H	11:M:64:LYS:HG2	1.57	0.45
15:Q:8:GLN:HG3	15:Q:113:PRO:HB2	1.99	0.45
22:Y:217:LYS:CD	22:Y:253:LEU:HD11	2.47	0.45
24:a:152:HIS:NE2	24:a:178:ARG:HB3	2.32	0.45
25:b:15:TYR:O	25:b:25:ARG:NH1	2.50	0.45
10:l:104:PRO:HB2	10:l:107:ARG:HG2	1.98	0.45
10:l:189:LYS:O	10:l:192:LEU:HD12	2.16	0.45
28:u:483:PHE:CE2	28:u:487:LEU:HD11	2.51	0.45
31:F:348:LEU:HB2	31:F:351:LYS:HE3	1.98	0.45
32:k:202:LEU:HA	32:k:202:LEU:HD23	1.81	0.45
32:k:227:HIS:CE1	32:k:233:GLU:OE2	2.69	0.45
2:B:272:ARG:HG2	2:B:272:ARG:HH11	1.80	0.45
5:E:26:LEU:CG	31:F:55:MET:HE3	2.47	0.45
5:E:168:LYS:NZ	5:E:294:ARG:HA	2.32	0.45
5:E:275:MET:HE3	5:E:275:MET:HB2	1.76	0.45
5:E:281:ARG:NH2	5:E:284:THR:HG22	2.32	0.45
13:O:49:ALA:HA	37:O:301:LDZ:H21	1.98	0.45
20:W:310:THR:HG23	20:W:311:THR:HG23	1.98	0.45
21:X:108:GLU:O	21:X:112:GLU:HG2	2.17	0.45
24:a:73:PRO:HB3	24:a:104:VAL:HG21	1.98	0.45
25:b:34:ASN:O	25:b:38:HIS:ND1	2.28	0.45
8:i:167:ASN:O	8:i:168:SER:OG	2.29	0.45
9:j:26:VAL:HG21	9:j:130:SER:HB2	1.99	0.45
13:o:48:THR:O	13:o:50:ALA:N	2.49	0.45
13:o:163:ILE:HD13	13:o:171:SER:OG	2.17	0.45
28:u:213:GLN:C	28:u:216:MET:HE3	2.41	0.45
29:U:185:MET:HE1	29:U:222:PHE:CZ	2.52	0.45
30:e:4:LYS:HA	30:e:6:GLN:HE21	1.82	0.45
31:F:70:LYS:O	31:F:74:LYS:HG2	2.17	0.45
31:F:342:LEU:HD23	31:F:342:LEU:H	1.81	0.45
32:K:107:MET:HE3	32:K:112:VAL:CG2	2.34	0.45
32:k:76:CYS:SG	32:k:77:ALA:N	2.90	0.45
2:B:46:ALA:HB2	2:B:178:LYS:HA	1.98	0.45
2:B:272:ARG:HG2	2:B:272:ARG:NH1	2.31	0.45
5:E:169:GLY:O	5:E:296:ASP:OD1	2.35	0.45
6:G:131:MET:HG3	11:M:125:TYR:CE1	2.52	0.45
8:I:151:ASP:OD2	8:I:151:ASP:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:184:ASP:OD2	15:Q:185:LYS:N	2.46	0.45
16:R:138:VAL:HG21	16:R:159:ALA:HA	1.99	0.45
20:W:141:GLU:OE1	20:W:144:ARG:HD3	2.17	0.45
20:W:271:VAL:HG23	20:W:305:LEU:HD22	1.98	0.45
21:X:216:ILE:HD11	21:X:253:TYR:CE2	2.51	0.45
23:Z:198:LEU:HD21	24:a:364:GLU:OE1	2.16	0.45
25:b:95:LEU:HA	25:b:98:LYS:HD2	1.99	0.45
26:c:158:ASP:OD1	26:c:158:ASP:C	2.59	0.45
26:c:278:GLN:HG3	26:c:282:ARG:NH2	2.32	0.45
27:d:22:GLU:CG	27:d:61:TRP:CZ3	2.89	0.45
27:d:73:ARG:HD2	29:U:10:SER:CB	2.47	0.45
7:h:119:GLN:HB2	8:i:81:SER:HG	1.80	0.45
11:m:87:LEU:HD23	11:m:87:LEU:HA	1.80	0.45
28:u:574:GLU:HA	28:u:577:LEU:HG	1.99	0.45
29:U:24:LEU:HG	29:U:63:VAL:HG21	1.99	0.45
29:U:222:PHE:HE1	29:U:754:HIS:CE1	2.30	0.45
29:U:243:LEU:HD12	29:U:244:MET:SD	2.56	0.45
29:U:371:ILE:HD11	29:U:732:LEU:HD11	1.99	0.45
29:U:620:GLU:OE2	29:U:654:MET:HE2	2.17	0.45
31:F:344:ARG:HE	31:F:347:ARG:HH21	1.65	0.45
31:F:392:ASN:OD1	31:F:395:GLN:HG3	2.17	0.45
1:A:78:TRP:HZ3	2:B:98:LYS:HZ1	1.64	0.45
1:A:164:MET:HG2	1:A:241:ILE:H	1.80	0.45
3:C:117:ARG:CZ	3:C:124:HIS:CD2	3.00	0.45
3:C:252:ASP:O	3:C:256:SER:OG	2.34	0.45
6:G:190:THR:O	6:G:194:THR:HG23	2.16	0.45
15:Q:35:MET:SD	15:Q:181:ARG:HG3	2.57	0.45
16:R:64:ARG:HG2	32:K:97:GLN:NE2	2.32	0.45
19:V:252:ASN:HD22	19:V:284:GLU:HG2	1.81	0.45
19:V:326:GLN:NE2	19:V:350:GLN:HG3	2.32	0.45
20:W:53:GLN:HG3	20:W:103:LYS:HD2	1.99	0.45
21:X:250:SER:O	21:X:254:MET:HG2	2.17	0.45
23:Z:21:ASP:O	23:Z:25:ARG:HG2	2.17	0.45
25:b:47:ASN:HA	25:b:105:HIS:HE1	1.82	0.45
17:s:81:LYS:HG3	17:s:82:ALA:N	2.31	0.45
29:U:98:GLU:HA	29:U:101:ILE:HG12	1.97	0.45
1:A:32:LEU:HD21	28:u:91:SER:O	2.17	0.45
1:A:125:LEU:HA	1:A:149:ILE:HB	1.99	0.45
1:A:274:PHE:CD2	1:A:319:MET:HE2	2.52	0.45
2:B:438:LEU:HD23	2:B:438:LEU:HA	1.85	0.45
3:C:70:GLY:HA3	4:D:113:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:LYS:HB2	5:E:42:LYS:HZ2	1.81	0.45
7:H:68:ILE:HD11	7:H:74:LEU:CG	2.29	0.45
11:M:66:LEU:HD23	11:M:66:LEU:HA	1.88	0.45
19:V:80:LYS:O	19:V:87:SER:N	2.50	0.45
19:V:258:TYR:CD2	19:V:258:TYR:N	2.82	0.45
19:V:492:LYS:C	19:V:494:MET:N	2.75	0.45
20:W:340:VAL:HG13	20:W:350:ARG:HD3	1.98	0.45
21:X:173:GLU:HA	21:X:176:THR:HG22	1.97	0.45
22:Y:191:ILE:HD11	22:Y:293:ARG:CZ	2.47	0.45
24:a:289:ARG:HE	24:a:332:HIS:HE1	1.64	0.45
25:b:72:LEU:HD12	25:b:73:SER:N	2.32	0.45
26:c:197:ASN:N	26:c:200:TYR:O	2.48	0.45
26:c:248:MET:CE	26:c:287:HIS:HB2	2.46	0.45
10:l:41:LYS:HG3	10:l:42:THR:HG23	1.97	0.45
10:l:188:VAL:O	10:l:192:LEU:HG	2.17	0.45
11:m:192:GLU:O	11:m:196:ILE:HG12	2.17	0.45
17:s:1:ARG:HG2	17:s:1:ARG:HH11	1.82	0.45
31:F:313:LEU:O	31:F:317:LEU:N	2.49	0.45
32:k:227:HIS:NE2	32:k:233:GLU:OE2	2.50	0.45
1:A:299:MET:O	1:A:303:ILE:HG23	2.17	0.45
2:B:248:LEU:HD12	2:B:282:VAL:HG22	1.99	0.45
3:C:174:LEU:N	3:C:174:LEU:CD2	2.79	0.45
4:D:64:GLU:CD	29:U:607:VAL:CG1	2.89	0.45
4:D:114:ARG:HB2	4:D:114:ARG:NH1	2.32	0.45
5:E:213:ARG:HA	5:E:216:ARG:HE	1.82	0.45
5:E:265:ASP:C	5:E:265:ASP:OD2	2.58	0.45
10:L:71:GLY:HA3	10:L:221:PHE:CZ	2.52	0.45
14:P:77:LYS:NZ	14:P:77:LYS:HB3	2.31	0.45
20:W:374:THR:CG2	24:a:327:VAL:HG22	2.47	0.45
21:X:368:MET:SD	21:X:374:PHE:HD2	2.38	0.45
22:Y:50:MET:HE2	22:Y:70:LEU:HD13	1.98	0.45
22:Y:180:LEU:HD22	22:Y:183:TYR:CE2	2.49	0.45
22:Y:237:ARG:O	22:Y:242:LYS:HG2	2.17	0.45
23:Z:7:GLN:HB2	23:Z:46:LYS:HG3	1.99	0.45
26:c:49:VAL:N	26:c:50:PRO:CD	2.80	0.45
8:i:249:ARG:HA	8:i:249:ARG:NE	2.32	0.45
9:j:7:ILE:HD13	9:j:119:THR:HA	1.99	0.45
11:m:180:GLN:HA	11:m:180:GLN:HE21	1.82	0.45
16:r:119:ASN:OD1	16:r:119:ASN:N	2.50	0.45
16:r:177:TYR:CE2	16:r:186:ARG:HG3	2.52	0.45
18:t:122:LEU:HG	18:t:137:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:289:VAL:HB	28:u:901:ARG:NH2	2.32	0.45
29:U:405:THR:HG23	29:U:441:GLY:HA3	1.99	0.45
29:U:564:ASP:HA	29:U:567:ILE:HB	1.99	0.45
29:U:837:ALA:HA	29:U:840:LYS:HG2	1.99	0.45
31:F:46:ARG:HD3	31:F:47:LEU:N	2.32	0.45
31:F:228:PRO:HD2	31:F:354:PHE:O	2.17	0.45
1:A:177:VAL:HG21	34:A:501:ADP:N1	2.31	0.44
1:A:193:THR:HA	1:A:200:ARG:NH2	2.32	0.44
1:A:221:GLY:HA2	1:A:224:LEU:HB3	1.98	0.44
1:A:272:ILE:HD12	1:A:272:ILE:N	2.33	0.44
3:C:80:MET:SD	3:C:81:ASP:O	2.74	0.44
5:E:122:MET:CE	5:E:198:VAL:HG22	2.46	0.44
6:G:132:ARG:NH1	11:M:20:VAL:HG21	2.33	0.44
16:R:191:ASN:HD21	14:p:203:ARG:HH12	1.65	0.44
17:S:37:THR:HG22	17:S:38:ARG:H	1.81	0.44
18:T:20:VAL:HG11	18:T:122:LEU:HD13	1.99	0.44
19:V:157:THR:OG1	19:V:158:PRO:HD3	2.17	0.44
19:V:447:ILE:HD13	19:V:449:ALA:HB3	1.99	0.44
19:V:448:GLU:O	19:V:448:GLU:HG2	2.17	0.44
24:a:222:LEU:HD23	24:a:223:GLU:N	2.32	0.44
24:a:346:ILE:HA	24:a:349:MET:HB3	1.99	0.44
9:j:62:ILE:HD12	9:j:62:ILE:N	2.32	0.44
9:j:175:ASN:O	9:j:177:THR:HG23	2.16	0.44
28:u:836:GLU:OE2	28:u:836:GLU:HA	2.17	0.44
28:u:862:ILE:CG2	28:u:865:PHE:HB3	2.47	0.44
29:U:137:MET:HE1	29:U:140:ARG:HH11	1.82	0.44
29:U:606:ALA:HB2	29:U:618:ALA:HB1	1.99	0.44
29:U:792:ASN:HB3	29:U:914:LEU:H	1.81	0.44
1:A:172:VAL:HB	1:A:227:ARG:HB2	2.00	0.44
4:D:139:LEU:HD23	4:D:139:LEU:HA	1.79	0.44
5:E:303:LEU:HD12	5:E:338:PHE:CB	2.43	0.44
6:G:117:ARG:HE	6:G:117:ARG:HB3	1.56	0.44
8:I:84:ASN:N	8:I:84:ASN:ND2	2.66	0.44
23:Z:68:TRP:CD1	23:Z:104:ASN:HD21	2.35	0.44
6:g:128:ASN:OD1	6:g:129:ALA:O	2.35	0.44
6:g:128:ASN:CG	6:g:131:MET:HE3	2.41	0.44
13:o:171:SER:HB2	13:o:193:ASN:HB2	1.99	0.44
29:U:792:ASN:HB3	29:U:914:LEU:HB3	1.99	0.44
29:U:832:VAL:HG13	29:U:832:VAL:O	2.17	0.44
30:e:57:ARG:O	30:e:59:GLU:HG2	2.18	0.44
31:F:86:LEU:HG	31:F:87:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:263:ASP:O	31:F:267:LEU:HB3	2.18	0.44
31:F:406:ILE:HG22	31:F:419:ASP:HB2	1.99	0.44
3:C:159:LYS:H	3:C:159:LYS:HG2	1.54	0.44
3:C:338:LEU:CD2	3:C:342:ILE:HG21	2.37	0.44
4:D:99:ASN:HA	4:D:115:ILE:HG13	1.99	0.44
5:E:183:LEU:CD1	5:E:301:ILE:HG12	2.47	0.44
19:V:452:ASN:HB3	19:V:457:TYR:HB2	1.99	0.44
22:Y:32:ARG:NH1	22:Y:32:ARG:O	2.50	0.44
22:Y:235:ASP:C	22:Y:235:ASP:OD1	2.60	0.44
23:Z:94:TRP:CD2	23:Z:121:LEU:HD23	2.53	0.44
23:Z:144:VAL:O	23:Z:145:HIS:HB2	2.18	0.44
24:a:17:GLY:O	24:a:21:VAL:HG22	2.17	0.44
24:a:208:GLU:HG3	24:a:209:GLY:H	1.82	0.44
25:b:18:ASN:CG	25:b:19:GLY:N	2.76	0.44
11:m:220:THR:HG22	11:m:225:GLU:OE2	2.18	0.44
11:m:243:LEU:HD13	11:m:243:LEU:C	2.39	0.44
29:U:253:TYR:CZ	29:U:331:GLY:HA3	2.52	0.44
29:U:592:GLY:HA3	29:U:628:ARG:HH21	1.82	0.44
29:U:619:VAL:HG23	29:U:651:GLY:HA3	1.98	0.44
29:U:792:ASN:OD1	29:U:793:LYS:N	2.50	0.44
31:F:188:ILE:O	31:F:188:ILE:CG2	2.64	0.44
1:A:113:ILE:HG13	1:A:123:VAL:HG22	1.99	0.44
1:A:268:LYS:HA	1:A:315:ILE:HG23	1.99	0.44
2:B:133:VAL:HG11	2:B:157:HIS:O	2.18	0.44
3:C:142:LYS:HD2	3:C:144:PRO:HD2	1.99	0.44
5:E:36:LEU:HA	5:E:39:GLN:HG2	2.00	0.44
8:I:244:GLU:OE2	8:I:244:GLU:HA	2.16	0.44
23:Z:153:LYS:HA	23:Z:153:LYS:HD2	1.69	0.44
24:a:8:LEU:HD11	24:a:26:GLU:HG3	2.00	0.44
25:b:161:ASN:ND2	25:b:167:GLY:H	2.15	0.44
15:q:18:ASP:C	15:q:18:ASP:OD1	2.60	0.44
28:u:55:GLU:HA	28:u:58:MET:HG2	2.00	0.44
28:u:79:ARG:HD3	28:u:121:PHE:HA	2.00	0.44
29:U:261:LEU:HA	29:U:264:VAL:HG22	1.98	0.44
29:U:401:LYS:O	29:U:405:THR:HG22	2.18	0.44
29:U:496:LEU:HA	29:U:499:THR:HG22	2.00	0.44
29:U:517:GLY:C	29:U:554:LEU:HD23	2.42	0.44
29:U:549:ALA:O	29:U:581:SER:OG	2.27	0.44
29:U:788:VAL:HA	29:U:910:GLY:O	2.17	0.44
31:F:35:LYS:C	31:F:36:MET:HE2	2.41	0.44
31:F:358:ASN:O	31:F:362:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:420:TYR:O	31:F:424:ILE:HG13	2.17	0.44
1:A:73:ALA:HB2	2:B:140:ASP:N	2.32	0.44
1:A:253:GLY:O	1:A:257:VAL:HG12	2.17	0.44
1:A:368:ILE:HD13	1:A:406:GLU:HB2	1.98	0.44
2:B:382:ASP:OD2	2:B:420:LYS:NZ	2.50	0.44
4:D:103:VAL:HG21	4:D:139:LEU:HD21	2.00	0.44
5:E:339:ASN:ND2	5:E:341:ALA:H	2.16	0.44
5:E:376:ASP:O	5:E:380:LEU:HG	2.17	0.44
10:L:225:ASP:OD2	10:L:225:ASP:N	2.50	0.44
19:V:444:ASP:OD2	19:V:444:ASP:N	2.39	0.44
21:X:374:PHE:CZ	21:X:376:GLY:HA3	2.53	0.44
23:Z:100:LYS:O	23:Z:100:LYS:HG2	2.17	0.44
27:d:41:THR:O	27:d:44:THR:HG22	2.18	0.44
11:m:99:ARG:HH12	18:t:72:ILE:HD12	1.83	0.44
13:o:19:ARG:HB2	13:o:170:GLY:H	1.81	0.44
37:o:301:LDZ:H6	14:p:127:ILE:HG12	2.00	0.44
28:u:585:GLU:N	28:u:586:PRO:HD2	2.33	0.44
28:u:657:ILE:HA	28:u:660:ILE:HG22	1.99	0.44
29:U:137:MET:HE2	29:U:137:MET:HA	2.00	0.44
29:U:633:CYS:HG	29:U:659:CYS:CB	2.29	0.44
29:U:877:LEU:O	29:U:878:LEU:HD23	2.17	0.44
30:e:67:MET:SD	30:e:68:GLU:N	2.91	0.44
31:F:282:ILE:O	31:F:283:ILE:HD12	2.17	0.44
1:A:38:GLN:OE1	1:A:40:THR:OG1	2.32	0.44
5:E:31:GLU:O	5:E:35:GLU:HG2	2.18	0.44
9:J:246:LYS:HG3	28:u:905:ASN:HB3	1.99	0.44
19:V:139:MET:SD	19:V:140:ASP:OD1	2.76	0.44
19:V:290:TYR:CD1	19:V:328:VAL:HB	2.53	0.44
19:V:309:MET:HG3	19:V:332:LEU:HD13	1.99	0.44
20:W:253:THR:HB	20:W:254:PRO:HD3	1.99	0.44
22:Y:297:ARG:O	22:Y:301:ILE:HG22	2.17	0.44
24:a:115:LYS:HA	24:a:118:ILE:HD12	2.00	0.44
24:a:246:GLU:OE1	24:a:249:GLN:HB3	2.17	0.44
26:c:196:LEU:HB3	26:c:197:ASN:HD22	1.83	0.44
26:c:250:GLU:OE2	26:c:250:GLU:C	2.60	0.44
27:d:63:ILE:HB	27:d:71:PHE:HE1	1.83	0.44
27:d:175:ARG:NH2	27:d:199:PHE:HD1	2.16	0.44
15:q:190:ASP:OD1	15:q:191:LEU:N	2.50	0.44
28:u:416:MET:HE3	28:u:819:TYR:HE1	1.83	0.44
29:U:222:PHE:CD1	29:U:754:HIS:CE1	3.05	0.44
29:U:645:ASN:OD1	29:U:645:ASN:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HG22	1:A:261:PHE:CD1	2.52	0.44
3:C:36:ASN:O	3:C:40:GLN:HG2	2.18	0.44
4:D:214:MET:HE1	35:D:501:ATP:C4	2.52	0.44
5:E:101:ASP:N	5:E:106:THR:O	2.51	0.44
5:E:134:GLU:H	5:E:134:GLU:CD	2.25	0.44
5:E:303:LEU:HB2	5:E:338:PHE:C	2.43	0.44
5:E:336:ASP:HB3	5:E:338:PHE:CE1	2.51	0.44
5:E:350:ALA:HB1	5:E:367:PHE:CD1	2.52	0.44
10:L:56:LEU:HD23	10:L:56:LEU:N	2.32	0.44
11:M:106:ILE:HG12	11:M:111:LEU:HB2	1.98	0.44
23:Z:7:GLN:CB	23:Z:46:LYS:HZ3	2.30	0.44
24:a:7:PHE:CZ	24:a:59:LEU:HD23	2.53	0.44
24:a:24:ARG:N	24:a:24:ARG:HD3	2.33	0.44
24:a:222:LEU:HD23	24:a:223:GLU:H	1.83	0.44
26:c:41:MET:HE1	26:c:112:TYR:CD2	2.51	0.44
26:c:156:VAL:CG2	26:c:156:VAL:O	2.66	0.44
27:d:107:LEU:HD12	27:d:115:PHE:CE1	2.53	0.44
28:u:192:VAL:HG23	28:u:193:PRO:CD	2.48	0.44
28:u:445:LEU:HD13	28:u:466:LEU:HD23	2.00	0.44
29:U:14:GLU:HG2	29:U:16:GLU:OE1	2.18	0.44
29:U:130:LEU:HD12	29:U:131:GLU:N	2.33	0.44
31:F:224:LEU:HD22	31:F:225:MET:H	1.83	0.44
31:F:381:TYR:CA	31:F:384:LEU:HG	2.36	0.44
32:K:199:LEU:HD11	32:K:215:ILE:HD13	1.99	0.44
32:k:204:GLN:OE1	32:k:204:GLN:O	2.35	0.44
2:B:144:LEU:HD22	2:B:144:LEU:H	1.82	0.44
3:C:145:ASP:OD1	3:C:145:ASP:N	2.49	0.44
4:D:116:LEU:HB2	4:D:119:ILE:CD1	2.48	0.44
4:D:121:ARG:HA	4:D:124:LEU:CD1	2.37	0.44
4:D:160:PRO:HB2	4:D:217:LYS:HB3	2.00	0.44
5:E:26:LEU:HD11	31:F:55:MET:CE	2.48	0.44
5:E:102:MET:O	5:E:102:MET:HE3	2.16	0.44
11:M:28:LYS:HE2	11:M:28:LYS:HB2	1.59	0.44
12:N:149:LYS:NZ	12:N:149:LYS:HB3	2.32	0.44
22:Y:43:ALA:CB	22:Y:46:ARG:NH2	2.78	0.44
22:Y:208:PHE:HZ	22:Y:214:MET:O	2.00	0.44
23:Z:79:TYR:CD1	23:Z:91:ILE:HD11	2.53	0.44
8:i:68:LEU:HD13	8:i:90:LEU:HD13	2.00	0.44
9:j:5:ARG:HD2	32:k:11:GLY:HA2	2.00	0.44
10:l:180:MET:HA	10:l:180:MET:HE3	1.99	0.44
11:m:215:TRP:CE3	11:m:219:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:t:208:ASN:OD1	18:t:208:ASN:C	2.61	0.44
28:u:72:ARG:CZ	28:u:72:ARG:HB3	2.47	0.44
28:u:412:ALA:CB	28:u:446:LEU:HD22	2.48	0.44
29:U:250:PHE:CD2	29:U:328:ILE:HD11	2.53	0.44
29:U:443:LEU:HA	29:U:446:LEU:CG	2.47	0.44
31:F:369:HIS:HA	31:F:372:LYS:HG2	2.00	0.44
32:K:10:ARG:HG2	32:K:10:ARG:HH11	1.82	0.44
32:K:239:LYS:HE3	32:K:239:LYS:HB2	1.80	0.44
32:k:18:GLU:O	32:k:20:ARG:NH1	2.51	0.44
1:A:251:GLY:H	1:A:294:GLU:HA	1.82	0.44
1:A:303:ILE:HA	1:A:336:ARG:NH1	2.32	0.44
5:E:100:LEU:H	5:E:100:LEU:HD12	1.82	0.44
5:E:303:LEU:CD1	5:E:338:PHE:CB	2.96	0.44
8:I:238:LYS:HA	8:I:238:LYS:HD2	1.88	0.44
19:V:100:MET:H	19:V:103:SER:HB2	1.83	0.44
19:V:199:ASN:C	19:V:203:LEU:HG	2.43	0.44
20:W:39:ARG:NH1	20:W:40:LEU:HB3	2.33	0.44
21:X:67:GLY:O	21:X:70:LEU:HG	2.17	0.44
24:a:11:SER:O	24:a:22:TRP:CH2	2.70	0.44
24:a:292:THR:HG23	24:a:295:GLU:H	1.82	0.44
6:g:117:ARG:O	6:g:121:ILE:HG12	2.18	0.44
13:o:64:GLU:OE1	13:o:68:LEU:HD22	2.17	0.44
14:p:11:VAL:HG12	14:p:24:ALA:HB2	2.00	0.44
28:u:827:PRO:HB2	28:u:829:MET:HG3	1.99	0.44
29:U:505:ASP:OD2	29:U:508:THR:HG22	2.18	0.44
29:U:650:TYR:HB2	29:U:683:VAL:HG12	1.99	0.44
31:F:96:LEU:HD12	31:F:145:LEU:HD11	2.00	0.44
31:F:163:THR:O	31:F:164:LEU:C	2.61	0.44
31:F:193:LYS:O	31:F:197:GLU:HG3	2.18	0.44
31:F:387:CYS:SG	31:F:424:ILE:HD13	2.57	0.44
32:K:50:VAL:HG11	32:K:66:LYS:CB	2.48	0.44
1:A:197:HIS:NE2	1:A:199:GLU:HB2	2.32	0.43
1:A:226:ALA:HA	1:A:229:VAL:HG22	1.99	0.43
1:A:299:MET:CE	1:A:330:ALA:HB3	2.43	0.43
1:A:360:ARG:O	1:A:361:SER:HB2	2.18	0.43
2:B:135:ILE:HG23	2:B:159:VAL:HB	1.99	0.43
5:E:287:PRO:O	5:E:291:ARG:N	2.51	0.43
5:E:322:LYS:HB2	5:E:362:VAL:O	2.18	0.43
5:E:348:THR:O	5:E:352:MET:SD	2.76	0.43
8:I:26:GLU:HG3	8:I:26:GLU:O	2.18	0.43
12:N:47:GLY:O	37:N:301:LDZ:H15	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:163:ILE:HD12	13:O:169:SER:OG	2.18	0.43
16:R:179:VAL:HA	16:R:184:TRP:HA	1.99	0.43
19:V:496:PHE:CG	19:V:497:PRO:HD3	2.52	0.43
22:Y:180:LEU:O	22:Y:183:TYR:CD2	2.63	0.43
22:Y:182:VAL:O	22:Y:185:GLY:N	2.41	0.43
23:Z:96:HIS:CD2	23:Z:123:ILE:HD13	2.53	0.43
24:a:28:LEU:HD23	24:a:37:LEU:HA	1.99	0.43
24:a:112:ILE:HD12	24:a:113:LEU:N	2.33	0.43
11:m:217:GLY:H	11:m:220:THR:HG1	1.61	0.43
13:o:104:ASP:OD1	13:o:106:THR:OG1	2.30	0.43
29:U:469:SER:N	29:U:473:VAL:HG21	2.32	0.43
29:U:768:GLN:O	29:U:775:LEU:HD12	2.18	0.43
29:U:837:ALA:HB1	29:U:841:LYS:HD3	2.00	0.43
31:F:65:GLU:O	31:F:66:LEU:C	2.60	0.43
31:F:81:LYS:HB3	31:F:81:LYS:HE2	1.84	0.43
31:F:258:GLN:HB2	31:F:263:ASP:OD2	2.18	0.43
31:F:364:ARG:NE	31:F:367:GLN:HE21	2.09	0.43
1:A:155:PRO:HB2	1:A:249:TYR:CE2	2.53	0.43
1:A:236:CYS:HB3	1:A:270:CYS:CB	2.48	0.43
1:A:343:PHE:CD1	1:A:343:PHE:N	2.86	0.43
3:C:83:LYS:NZ	3:C:98:ASP:HA	2.33	0.43
5:E:72:LYS:NZ	5:E:73:ALA:H	2.15	0.43
6:G:62:ASP:O	6:G:65:THR:HG22	2.18	0.43
6:G:179:LEU:O	6:G:183:VAL:HG13	2.17	0.43
16:R:1:THR:O	16:R:129:GLY:HA3	2.19	0.43
18:T:210:ASP:C	18:T:210:ASP:OD1	2.60	0.43
19:V:134:PHE:O	19:V:138:PRO:HG2	2.18	0.43
19:V:374:LYS:HD2	19:V:374:LYS:HA	1.88	0.43
20:W:10:ASP:O	20:W:14:VAL:HG13	2.17	0.43
21:X:336:ILE:HG23	21:X:368:MET:CE	2.48	0.43
22:Y:51:ALA:HB3	22:Y:115:GLY:HA2	2.00	0.43
23:Z:112:MET:O	23:Z:112:MET:SD	2.76	0.43
24:a:8:LEU:HD22	24:a:25:LEU:HD12	2.00	0.43
26:c:130:GLN:NE2	26:c:134:GLU:HB3	2.33	0.43
26:c:278:GLN:HA	26:c:283:HIS:CD2	2.53	0.43
7:h:145:TYR:HB3	7:h:147:PHE:HE1	1.81	0.43
28:u:166:VAL:HG13	28:u:184:LEU:HD22	2.01	0.43
29:U:616:ARG:HD3	29:U:647:HIS:HD2	1.82	0.43
29:U:802:TYR:HB3	29:U:895:PRO:HD3	2.00	0.43
31:F:208:HIS:CG	31:F:211:LYS:HB3	2.53	0.43
1:A:92:PRO:HD2	1:A:93:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:274:LEU:HA	3:C:277:LEU:HD12	2.00	0.43
4:D:245:ARG:HA	4:D:248:ARG:HH11	1.82	0.43
5:E:67:GLU:O	5:E:82:GLY:HA2	2.19	0.43
6:G:9:PHE:HE2	7:H:8:PHE:CD1	2.37	0.43
8:I:179:TYR:CD2	8:I:181:GLU:HG3	2.54	0.43
15:Q:108:ASP:HB3	15:Q:111:GLU:HB2	1.99	0.43
15:Q:164:LEU:HB3	15:Q:196:PHE:HE2	1.83	0.43
16:R:47:GLY:H	37:R:301:LDZ:H23	1.83	0.43
18:T:127:MET:HE2	18:T:127:MET:HB3	1.79	0.43
20:W:177:MET:HG2	20:W:181:GLU:CB	2.43	0.43
20:W:272:LEU:HD21	20:W:341:PHE:CE2	2.53	0.43
20:W:316:ARG:NH1	20:W:383:ASP:OD1	2.51	0.43
25:b:1:MET:SD	25:b:1:MET:N	2.88	0.43
25:b:12:ASN:HB2	25:b:80:PRO:HA	2.00	0.43
26:c:179:SER:HB3	29:U:770:TRP:NE1	2.34	0.43
27:d:120:GLU:H	27:d:121:ARG:HH11	1.66	0.43
6:g:37:LEU:H	6:g:37:LEU:HD22	1.82	0.43
7:h:107:THR:O	7:h:111:VAL:HG23	2.19	0.43
28:u:294:MET:HA	28:u:297:MET:HG3	2.00	0.43
28:u:326:LEU:HD11	28:u:420:TRP:CD2	2.53	0.43
28:u:829:MET:HE3	28:u:831:VAL:CG2	2.47	0.43
29:U:780:SER:HA	29:U:783:TYR:CD2	2.53	0.43
31:F:39:GLU:HB3	31:F:43:GLN:HB2	1.99	0.43
3:C:172:PRO:HG2	3:C:173:GLU:OE1	2.18	0.43
20:W:435:LEU:HD23	23:Z:236:LEU:HD11	2.00	0.43
21:X:161:ASP:O	21:X:163:LYS:HE2	2.17	0.43
22:Y:100:ILE:O	22:Y:104:MET:SD	2.76	0.43
23:Z:81:MET:HE3	23:Z:81:MET:O	2.18	0.43
27:d:105:PHE:HB2	27:d:166:PHE:CE1	2.52	0.43
11:m:221:ASN:HB2	11:m:223:ARG:NH2	2.31	0.43
29:U:152:GLY:O	29:U:156:GLU:HG2	2.18	0.43
29:U:757:MET:HE3	29:U:757:MET:C	2.43	0.43
1:A:30:ILE:HG22	1:A:34:LYS:HG2	2.00	0.43
1:A:54:GLN:HG3	1:A:58:LYS:HZ1	1.82	0.43
2:B:220:LYS:HE2	2:B:220:LYS:HB2	1.69	0.43
3:C:149:GLU:C	3:C:149:GLU:CD	2.86	0.43
4:D:213:THR:O	4:D:217:LYS:HG3	2.19	0.43
4:D:388:ARG:NH1	4:D:388:ARG:HA	2.33	0.43
5:E:35:GLU:O	5:E:39:GLN:HG2	2.18	0.43
5:E:128:GLY:O	5:E:129:ASN:ND2	2.51	0.43
7:H:91:ARG:HD3	13:O:68:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:176:LEU:HD23	16:R:187:VAL:HG11	2.01	0.43
19:V:348:PHE:CE2	19:V:350:GLN:NE2	2.87	0.43
22:Y:174:TRP:O	22:Y:177:ARG:N	2.52	0.43
22:Y:220:VAL:HG13	22:Y:246:ILE:CD1	2.47	0.43
26:c:115:HIS:ND1	26:c:118:PHE:CE2	2.87	0.43
27:d:155:LYS:HG3	27:d:156:GLY:N	2.33	0.43
10:l:65:HIS:O	10:l:89:ARG:NH1	2.51	0.43
11:m:215:TRP:CZ3	11:m:219:LEU:HD11	2.54	0.43
28:u:151:LEU:HD12	28:u:162:LEU:HD21	2.00	0.43
28:u:740:ARG:O	28:u:744:MET:SD	2.76	0.43
29:U:543:LYS:HG2	29:U:546:ARG:NH2	2.33	0.43
1:A:426:THR:HB	1:A:428:ARG:HG2	1.99	0.43
2:B:329:MET:HE1	2:B:347:ILE:HD11	2.01	0.43
2:B:394:ASP:OD1	2:B:394:ASP:N	2.51	0.43
3:C:113:ARG:NH2	3:C:129:ASN:O	2.51	0.43
3:C:156:LYS:HB3	3:C:156:LYS:HE3	1.77	0.43
3:C:326:LEU:HG	3:C:330:LYS:HE3	2.00	0.43
5:E:20:LYS:HG3	5:E:21:GLU:OE1	2.19	0.43
5:E:149:ILE:HG22	5:E:150:GLU:HG2	2.01	0.43
7:H:207:ASN:O	7:H:208:ILE:HD13	2.19	0.43
8:I:238:LYS:HZ1	8:I:242:GLU:HB2	1.84	0.43
10:L:22:ILE:O	10:L:26:MET:HG2	2.18	0.43
37:N:301:LDZ:H19	37:N:301:LDZ:H13	1.85	0.43
14:P:15:LYS:HE3	14:P:121:ILE:HG12	2.00	0.43
16:R:191:ASN:HD22	16:R:193:ALA:H	1.66	0.43
17:S:68:ILE:HD11	17:S:92:LEU:HD13	2.00	0.43
18:T:45:VAL:HB	18:T:49:THR:HG23	2.01	0.43
19:V:368:ARG:O	19:V:368:ARG:NE	2.35	0.43
19:V:433:ASP:O	19:V:437:ILE:HG12	2.18	0.43
21:X:114:ILE:CD1	21:X:129:LEU:HD22	2.49	0.43
22:Y:352:GLU:CD	22:Y:352:GLU:N	2.76	0.43
24:a:282:PHE:CD1	24:a:335:TRP:CH2	3.07	0.43
26:c:183:HIS:O	26:c:185:ASN:N	2.52	0.43
6:g:118:ILE:HG13	6:g:138:MET:HE1	2.01	0.43
7:h:38:ILE:HD13	7:h:191:ALA:HB2	2.00	0.43
28:u:759:LEU:HA	28:u:762:VAL:HG22	2.00	0.43
29:U:57:ARG:HG3	29:U:58:GLN:H	1.83	0.43
29:U:218:GLN:NE2	29:U:752:THR:HB	2.34	0.43
29:U:623:GLY:HA3	29:U:658:ILE:HG13	2.00	0.43
29:U:688:LEU:HD13	29:U:730:ALA:HB2	2.01	0.43
29:U:731:ILE:HA	29:U:734:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:29:ILE:O	31:F:33:VAL:HG23	2.19	0.43
32:K:210:LEU:HD23	32:K:210:LEU:C	2.43	0.43
32:k:78:MET:HB2	32:k:78:MET:HE2	1.75	0.43
2:B:133:VAL:HG11	2:B:157:HIS:C	2.42	0.43
2:B:288:ASP:OD1	2:B:288:ASP:N	2.49	0.43
4:D:60:TYR:CD2	4:D:64:GLU:HG2	2.54	0.43
4:D:115:ILE:HD12	4:D:115:ILE:C	2.44	0.43
4:D:264:ILE:HG23	4:D:264:ILE:O	2.17	0.43
11:M:88:ALA:O	11:M:92:ARG:HG3	2.18	0.43
18:T:23:ALA:CB	18:T:173:MET:HE3	2.49	0.43
18:T:110:MET:HB2	18:T:110:MET:HE3	1.70	0.43
19:V:26:PRO:O	19:V:30:PRO:HD3	2.18	0.43
19:V:216:ARG:HH21	19:V:217:VAL:HG22	1.83	0.43
20:W:425:LEU:HD12	23:Z:251:LEU:HD22	2.01	0.43
21:X:114:ILE:HD13	21:X:114:ILE:HA	1.57	0.43
22:Y:109:GLU:C	22:Y:113:ARG:HH12	2.26	0.43
24:a:233:LEU:HA	24:a:236:THR:HG22	2.01	0.43
27:d:29:VAL:HG21	27:d:54:ILE:CD1	2.48	0.43
27:d:176:ASP:HA	27:d:179:ALA:HB3	2.00	0.43
27:d:194:ALA:O	27:d:199:PHE:N	2.52	0.43
10:l:72:ILE:HG21	10:l:88:MET:HE1	2.00	0.43
29:U:358:ASP:OD1	29:U:358:ASP:N	2.51	0.43
29:U:374:SER:HB3	29:U:407:SER:HB3	2.01	0.43
31:F:418:GLU:O	31:F:421:MET:N	2.51	0.43
1:A:143:ASP:OD2	1:A:146:LYS:N	2.45	0.43
3:C:281:ASP:OD2	3:C:307:ARG:NH2	2.49	0.43
4:D:64:GLU:OE1	29:U:607:VAL:CG2	2.66	0.43
5:E:165:ILE:C	5:E:165:ILE:HD12	2.44	0.43
5:E:328:TYR:CE1	5:E:367:PHE:CE2	3.01	0.43
11:M:117:MET:HE2	11:M:117:MET:HA	2.00	0.43
14:P:14:MET:HE3	14:P:14:MET:HB3	1.72	0.43
17:S:114:ASP:OD1	17:S:116:GLU:N	2.51	0.43
19:V:324:PHE:CD2	30:e:5:LYS:HE3	2.54	0.43
19:V:345:ARG:HG3	19:V:346:LEU:N	2.32	0.43
22:Y:133:ALA:HB3	22:Y:136:HIS:CD2	2.54	0.43
9:j:121:SER:OG	9:j:124:ARG:NH2	2.43	0.43
10:l:199:LEU:O	10:l:239:ARG:NH2	2.51	0.43
11:m:152:ASP:OD1	11:m:154:SER:N	2.52	0.43
15:q:155:ARG:HA	15:q:155:ARG:HD3	1.78	0.43
29:U:324:LYS:HZ2	29:U:794:ASP:HB3	1.84	0.43
29:U:680:VAL:HB	29:U:683:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:813:TYR:HB2	29:U:883:ARG:CZ	2.49	0.43
1:A:141:GLY:HA3	1:A:151:ILE:H	1.82	0.43
1:A:187:LEU:HD12	1:A:229:VAL:HG11	2.00	0.43
1:A:312:ARG:HA	1:A:312:ARG:HD2	1.79	0.43
2:B:133:VAL:HG12	2:B:156:VAL:O	2.19	0.43
8:I:41:ASP:OD1	8:I:186:LEU:HG	2.18	0.43
10:L:26:MET:SD	10:L:150:SER:HB3	2.59	0.43
13:O:193:ASN:ND2	17:s:213:ASP:HB3	2.33	0.43
20:W:45:GLU:OE2	20:W:94:ARG:NE	2.39	0.43
20:W:444:HIS:CE1	23:Z:204:LYS:O	2.71	0.43
21:X:74:ARG:N	21:X:75:PRO:HD3	2.34	0.43
22:Y:101:ARG:CZ	22:Y:105:MET:HE2	2.49	0.43
23:Z:13:PRO:HG2	26:c:221:HIS:CE1	2.54	0.43
23:Z:114:ARG:NH1	23:Z:114:ARG:HB2	2.34	0.43
26:c:56:LEU:HD11	26:c:75:MET:HE1	2.00	0.43
27:d:135:HIS:HB3	27:d:136:PRO:HD3	2.01	0.43
27:d:175:ARG:CZ	27:d:199:PHE:CD1	3.02	0.43
15:q:118:MET:HE2	15:q:118:MET:HB2	1.90	0.43
29:U:148:LYS:O	29:U:151:ILE:HG22	2.19	0.43
29:U:541:HIS:HB2	29:U:544:ILE:HG22	2.01	0.43
1:A:168:GLU:O	1:A:170:PRO:HD3	2.18	0.43
1:A:197:HIS:HB3	1:A:200:ARG:HH21	1.84	0.43
3:C:273:MET:O	3:C:277:LEU:HD12	2.18	0.43
5:E:16:LEU:HG	5:E:20:LYS:HB3	1.99	0.43
5:E:231:PHE:CG	5:E:276:ILE:HD11	2.53	0.43
8:I:28:ILE:O	8:I:28:ILE:HG22	2.19	0.43
19:V:168:GLN:HE22	19:V:175:MET:HE1	1.83	0.43
20:W:12:ARG:HD3	20:W:24:VAL:HA	2.00	0.43
20:W:12:ARG:NH2	20:W:15:LYS:HE2	2.33	0.43
20:W:345:GLU:OE1	20:W:345:GLU:N	2.50	0.43
20:W:353:ASP:O	20:W:357:ARG:HG2	2.19	0.43
23:Z:104:ASN:O	23:Z:108:ILE:HG12	2.19	0.43
23:Z:220:LEU:HD12	23:Z:221:PRO:O	2.19	0.43
24:a:148:VAL:C	24:a:150:SER:H	2.27	0.43
24:a:215:GLU:HA	24:a:218:MET:HG2	2.01	0.43
24:a:252:LYS:HA	24:a:255:TRP:HD1	1.84	0.43
26:c:54:MET:HE3	26:c:54:MET:HB3	1.85	0.43
26:c:196:LEU:HD23	26:c:196:LEU:HA	1.82	0.43
26:c:284:LEU:HD23	26:c:284:LEU:HA	1.83	0.43
11:m:179:LEU:HD21	11:m:192:GLU:HB3	1.99	0.43
28:u:192:VAL:CG2	28:u:193:PRO:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:226:PRO:HA	29:U:264:VAL:HG12	2.00	0.43
29:U:660:CYS:SG	29:U:665:ASN:ND2	2.92	0.43
29:U:923:GLU:O	29:U:923:GLU:HG2	2.19	0.43
31:F:238:ARG:H	31:F:238:ARG:NH1	2.17	0.43
32:K:192:LYS:HE3	32:K:192:LYS:HB3	1.57	0.43
1:A:232:ARG:HG3	1:A:232:ARG:H	1.59	0.42
4:D:114:ARG:NH1	4:D:114:ARG:CB	2.82	0.42
4:D:388:ARG:HA	4:D:388:ARG:CZ	2.49	0.42
6:G:130:GLU:OE1	6:G:130:GLU:O	2.37	0.42
8:I:38:LEU:O	8:I:39:ALA:HB3	2.19	0.42
8:I:124:PHE:HE1	9:J:118:TYR:HE2	1.67	0.42
19:V:136:GLU:O	19:V:140:ASP:N	2.52	0.42
20:W:446:ILE:HG22	23:Z:226:ILE:HD12	2.01	0.42
22:Y:201:PHE:HD1	22:Y:219:PHE:CE1	2.36	0.42
23:Z:54:PHE:HD1	23:Z:82:PHE:HE2	1.64	0.42
23:Z:246:VAL:O	23:Z:250:TYR:CD2	2.72	0.42
16:r:138:VAL:HG11	16:r:159:ALA:HA	2.00	0.42
31:F:188:ILE:N	31:F:188:ILE:CD1	2.82	0.42
31:F:222:GLY:C	31:F:348:LEU:HG	2.44	0.42
31:F:418:GLU:HA	31:F:421:MET:CG	2.49	0.42
32:k:52:LYS:HE3	32:k:61:PRO:O	2.19	0.42
1:A:216:GLY:H	1:A:222:LYS:NZ	2.17	0.42
3:C:251:ILE:C	3:C:253:SER:N	2.76	0.42
3:C:254:ILE:HG13	3:C:254:ILE:O	2.19	0.42
5:E:23:ASP:OD2	5:E:27:LYS:NZ	2.51	0.42
6:G:123:GLN:NE2	7:H:82:ASP:OD1	2.52	0.42
10:L:55:GLU:OE1	32:K:182:GLN:NE2	2.52	0.42
11:M:62:SER:C	11:M:63:ASN:OD1	2.62	0.42
19:V:62:HIS:CE1	19:V:201:ARG:CZ	3.01	0.42
19:V:216:ARG:HH21	19:V:217:VAL:CG2	2.31	0.42
20:W:314:LEU:HD21	24:a:313:LYS:HD3	2.01	0.42
20:W:445:LEU:HD23	20:W:445:LEU:HA	1.76	0.42
21:X:166:LEU:HG	21:X:170:GLN:NE2	2.34	0.42
22:Y:293:ARG:H	22:Y:293:ARG:HG3	1.57	0.42
23:Z:235:ASN:ND2	24:a:335:TRP:O	2.52	0.42
23:Z:237:LEU:HD23	23:Z:237:LEU:H	1.84	0.42
24:a:34:TRP:O	24:a:38:THR:OG1	2.29	0.42
25:b:35:ILE:H	25:b:35:ILE:HG13	1.69	0.42
25:b:41:THR:HG23	25:b:42:ARG:HD2	2.00	0.42
26:c:139:ARG:HB3	26:c:161:ARG:CZ	2.49	0.42
26:c:186:LYS:O	26:c:187:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:9:PHE:HB2	6:g:13:ILE:HG22	2.02	0.42
6:g:144:ASP:HB3	6:g:147:GLN:HB2	2.00	0.42
9:j:11:SER:H	9:j:15:HIS:H	1.66	0.42
9:j:134:VAL:HG22	9:j:144:LEU:HD12	2.01	0.42
9:j:171:PHE:HE2	9:j:175:ASN:ND2	2.11	0.42
15:q:167:LEU:HD12	15:q:167:LEU:HA	1.91	0.42
28:u:888:LEU:HD23	28:u:888:LEU:HA	1.82	0.42
29:U:580:ARG:HG3	29:U:617:ALA:CB	2.49	0.42
31:F:154:ASN:C	31:F:154:ASN:OD1	2.61	0.42
2:B:67:ARG:NH1	28:u:664:GLU:OE1	2.48	0.42
4:D:336:PRO:O	4:D:340:GLN:HB2	2.19	0.42
5:E:3:ASP:OD1	5:E:3:ASP:N	2.52	0.42
8:I:72:MET:HE2	8:I:72:MET:HB3	1.96	0.42
15:Q:28:MET:HE2	15:Q:28:MET:HB3	1.86	0.42
20:W:135:LYS:HZ2	20:W:137:TYR:HB3	1.84	0.42
20:W:272:LEU:O	20:W:275:ILE:HG22	2.19	0.42
20:W:444:HIS:HE1	23:Z:204:LYS:CB	2.26	0.42
21:X:114:ILE:HD11	21:X:129:LEU:HD22	2.01	0.42
21:X:319:ILE:H	21:X:319:ILE:HG13	1.62	0.42
22:Y:178:ASN:C	22:Y:180:LEU:H	2.27	0.42
23:Z:25:ARG:HB3	26:c:103:GLY:HA2	2.01	0.42
24:a:192:GLU:O	24:a:196:ARG:HG3	2.19	0.42
27:d:251:ARG:HB3	27:d:251:ARG:CZ	2.49	0.42
6:g:58:ASP:OD2	6:g:59:LYS:N	2.52	0.42
7:h:11:THR:HG22	7:h:19:LEU:HD22	2.01	0.42
12:n:49:ALA:HB2	37:n:301:LDZ:H21	2.01	0.42
15:q:54:VAL:O	15:q:58:GLU:HG3	2.19	0.42
29:U:470:ASN:CG	29:U:471:ASP:N	2.78	0.42
29:U:475:HIS:HE1	29:U:507:VAL:HG22	1.84	0.42
29:U:619:VAL:CG2	29:U:651:GLY:HA3	2.49	0.42
29:U:833:LEU:HA	29:U:836:THR:HG21	2.00	0.42
31:F:185:TYR:CZ	31:F:240:CYS:HA	2.54	0.42
31:F:402:GLU:O	31:F:406:ILE:HG12	2.20	0.42
1:A:186:LYS:HD3	1:A:186:LYS:HA	1.71	0.42
1:A:410:LEU:O	1:A:414:ASN:ND2	2.53	0.42
3:C:213:ARG:CZ	4:D:299:PHE:CB	2.97	0.42
3:C:242:ALA:HB3	3:C:243:PRO:HD3	2.02	0.42
3:C:251:ILE:O	3:C:253:SER:N	2.53	0.42
5:E:199:VAL:C	5:E:201:SER:H	2.27	0.42
5:E:231:PHE:CB	5:E:276:ILE:HD11	2.48	0.42
5:E:249:ALA:O	5:E:253:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:123:GLN:HG3	9:J:125:ARG:HH21	1.84	0.42
13:O:10:ASP:OD2	13:O:10:ASP:N	2.52	0.42
15:Q:177:THR:HG22	15:Q:195:SER:HB3	2.02	0.42
19:V:288:TYR:CD1	19:V:288:TYR:O	2.71	0.42
20:W:1:MET:CG	20:W:42:GLU:HB3	2.47	0.42
23:Z:212:LEU:CD2	24:a:353:LEU:HD13	2.50	0.42
24:a:129:GLN:OE1	24:a:130:VAL:N	2.52	0.42
27:d:189:ILE:HD11	27:d:215:TRP:HZ3	1.84	0.42
28:u:45:LEU:HD12	28:u:50:LYS:HD3	2.01	0.42
28:u:391:LEU:HD22	28:u:414:LEU:HG	2.02	0.42
28:u:404:ASP:O	28:u:407:MET:HE2	2.19	0.42
29:U:24:LEU:CD1	29:U:60:ALA:HA	2.49	0.42
29:U:353:LEU:HD12	29:U:385:PHE:CZ	2.54	0.42
31:F:208:HIS:HB3	31:F:211:LYS:HB3	2.01	0.42
1:A:124:ASP:OD2	1:A:124:ASP:N	2.52	0.42
2:B:360:THR:O	2:B:364:ILE:HG13	2.19	0.42
3:C:103:ILE:HD11	3:C:123:LEU:HB3	2.01	0.42
5:E:291:ARG:HD2	5:E:294:ARG:HG3	2.00	0.42
13:O:143:ARG:HB2	13:O:143:ARG:NH1	2.34	0.42
17:S:158:MET:HE2	17:S:158:MET:HB2	1.88	0.42
18:T:103:MET:HE3	18:T:103:MET:HB3	1.78	0.42
19:V:179:LYS:HA	19:V:182:LYS:NZ	2.33	0.42
19:V:495:ARG:HD2	19:V:497:PRO:HD2	2.00	0.42
20:W:373:ILE:HG21	20:W:378:MET:HE3	2.01	0.42
22:Y:204:THR:C	22:Y:206:SER:H	2.27	0.42
6:g:22:LEU:O	6:g:26:GLU:HG3	2.19	0.42
8:i:92:LEU:HD12	8:i:92:LEU:HA	1.93	0.42
8:i:115:CYS:SG	8:i:156:TYR:HB3	2.59	0.42
37:n:301:LDZ:H33	37:n:301:LDZ:H11	1.89	0.42
14:p:135:ASP:OD1	14:p:135:ASP:N	2.46	0.42
29:U:347:ASN:HB2	29:U:813:TYR:CZ	2.54	0.42
32:K:206:MET:HE1	32:K:214:ASN:O	2.19	0.42
32:k:202:LEU:HA	32:k:205:VAL:HG12	2.02	0.42
1:A:199:GLU:O	1:A:203:ASN:ND2	2.52	0.42
1:A:264:ALA:O	1:A:315:ILE:HD13	2.19	0.42
2:B:49:LEU:HD21	28:u:666:ILE:HG12	2.02	0.42
3:C:70:GLY:O	3:C:118:ASN:ND2	2.52	0.42
3:C:80:MET:HE3	3:C:80:MET:HB3	1.90	0.42
3:C:118:ASN:N	3:C:118:ASN:OD1	2.50	0.42
4:D:74:HIS:O	4:D:78:GLU:HG2	2.20	0.42
4:D:154:LEU:HD22	4:D:158:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:403:TYR:O	4:D:407:ILE:HG13	2.20	0.42
4:D:418:LYS:NZ	6:G:159:TYR:CE1	2.88	0.42
7:H:106:PRO:HG2	7:H:109:GLN:HG3	2.01	0.42
8:I:105:ILE:HD12	8:I:106:PRO:HD2	2.01	0.42
20:W:252:ASP:OD1	20:W:253:THR:N	2.52	0.42
23:Z:54:PHE:HD2	23:Z:55:ALA:N	2.18	0.42
24:a:214:GLY:HA3	24:a:339:ARG:HH22	1.85	0.42
24:a:280:MET:SD	24:a:295:GLU:OE2	2.78	0.42
26:c:173:GLU:O	26:c:175:ARG:HD3	2.20	0.42
7:h:74:LEU:HD23	7:h:83:TYR:CE1	2.55	0.42
9:j:41:VAL:HG11	9:j:134:VAL:CG1	2.47	0.42
18:t:38:ASN:OD1	18:t:38:ASN:C	2.62	0.42
29:U:188:MET:HE1	29:U:193:PHE:CE2	2.55	0.42
29:U:415:HIS:CD2	29:U:418:GLU:HB2	2.54	0.42
29:U:418:GLU:H	29:U:418:GLU:CD	2.27	0.42
29:U:458:ILE:HG21	29:U:490:ARG:NH1	2.35	0.42
31:F:282:ILE:O	31:F:282:ILE:HD12	2.20	0.42
1:A:362:MET:HE2	1:A:362:MET:HB3	1.91	0.42
2:B:188:GLY:HA2	2:B:367:ILE:HD12	2.01	0.42
2:B:264:PRO:O	2:B:268:ARG:HG3	2.19	0.42
2:B:329:MET:HB2	2:B:329:MET:HE3	1.87	0.42
3:C:159:LYS:HB3	3:C:159:LYS:HE2	1.76	0.42
5:E:363:VAL:HG12	5:E:366:ASP:OD2	2.20	0.42
6:G:86:ASP:OD1	6:G:134:LEU:HD22	2.19	0.42
9:J:100:ASP:OD1	16:R:75:SER:OG	2.32	0.42
19:V:409:MET:HA	19:V:409:MET:HE3	2.01	0.42
20:W:225:LYS:HE2	20:W:225:LYS:N	2.35	0.42
22:Y:169:GLU:CD	22:Y:180:LEU:HD11	2.45	0.42
22:Y:204:THR:C	22:Y:206:SER:N	2.77	0.42
23:Z:44:GLN:HE21	23:Z:47:VAL:HG13	1.84	0.42
25:b:51:LEU:HG	25:b:62:THR:HG22	2.02	0.42
26:c:150:SER:HB2	26:c:156:VAL:H	1.85	0.42
26:c:284:LEU:HB3	26:c:285:GLU:H	1.67	0.42
27:d:168:ASP:OD1	27:d:169:ILE:HD12	2.19	0.42
27:d:174:ILE:O	27:d:178:ILE:HG12	2.20	0.42
6:g:54:LYS:HB3	6:g:54:LYS:HE3	1.86	0.42
8:i:230:GLN:O	8:i:234:GLU:HG2	2.20	0.42
13:o:67:SER:HB3	13:o:74:PRO:HG3	2.01	0.42
28:u:266:LEU:CD2	28:u:297:MET:HE3	2.37	0.42
29:U:131:GLU:HA	29:U:134:VAL:HB	2.01	0.42
29:U:596:ASN:HA	29:U:599:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:145:GLY:HA2	32:k:220:VAL:HG21	2.02	0.42
3:C:119:ASP:OD2	26:c:189:ILE:HG23	2.19	0.42
3:C:251:ILE:H	3:C:295:THR:HB	1.84	0.42
3:C:339:THR:HG23	3:C:340:ARG:O	2.19	0.42
3:C:364:THR:O	3:C:368:MET:HG2	2.20	0.42
5:E:253:ILE:HD13	5:E:253:ILE:N	2.34	0.42
19:V:86:VAL:HA	19:V:89:LYS:HG3	2.00	0.42
20:W:137:TYR:CG	20:W:138:VAL:N	2.88	0.42
20:W:372:ARG:HG2	24:a:325:ASP:OD1	2.20	0.42
22:Y:109:GLU:O	22:Y:113:ARG:NH1	2.53	0.42
22:Y:174:TRP:CG	22:Y:175:ASP:H	2.37	0.42
23:Z:263:ALA:CB	26:c:292:MET:CE	2.96	0.42
24:a:273:GLN:HE22	24:a:302:ILE:HD13	1.83	0.42
26:c:191:ALA:C	26:c:196:LEU:HB2	2.44	0.42
7:h:92:LYS:HB3	7:h:92:LYS:HE2	1.82	0.42
8:i:140:ASP:OD1	8:i:144:GLY:N	2.41	0.42
13:o:63:LEU:HD23	13:o:63:LEU:HA	1.88	0.42
28:u:57:GLU:O	28:u:61:GLU:HG2	2.20	0.42
28:u:583:VAL:O	28:u:588:ARG:HD3	2.20	0.42
29:U:27:LEU:HB3	29:U:63:VAL:HG11	2.02	0.42
29:U:93:ASN:OD1	29:U:93:ASN:N	2.52	0.42
29:U:694:ILE:HG23	29:U:695:MET:CE	2.33	0.42
1:A:55:LEU:HD23	2:B:72:LEU:HB3	2.01	0.42
1:A:213:LEU:HD11	1:A:321:THR:HG22	2.01	0.42
2:B:388:ASP:OD1	2:B:388:ASP:N	2.53	0.42
4:D:400:GLU:OE1	4:D:400:GLU:N	2.52	0.42
5:E:300:HIS:HD2	5:E:301:ILE:H	1.68	0.42
6:G:18:PRO:HD3	7:H:24:TYR:CE2	2.54	0.42
12:N:165:GLU:OE2	18:t:37:ARG:NH2	2.53	0.42
13:O:22:GLU:HA	37:O:301:LDZ:O31	2.20	0.42
19:V:337:LEU:HD22	19:V:367:VAL:HG11	2.02	0.42
20:W:137:TYR:O	20:W:144:ARG:CZ	2.68	0.42
20:W:167:GLN:H	20:W:167:GLN:HG3	1.63	0.42
24:a:174:LYS:O	24:a:178:ARG:HG3	2.20	0.42
24:a:304:VAL:O	24:a:307:VAL:HG22	2.20	0.42
25:b:180:ALA:O	25:b:184:ILE:HD13	2.20	0.42
10:l:189:LYS:HA	10:l:192:LEU:HD11	2.02	0.42
17:s:148:LEU:HD12	17:s:178:VAL:HG12	2.02	0.42
28:u:881:GLU:HA	28:u:894:LEU:HD12	2.02	0.42
29:U:266:GLN:HA	29:U:269:ARG:NH1	2.35	0.42
29:U:624:PHE:CE2	29:U:764:LEU:HD23	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:230:GLY:H	31:F:233:LYS:HD2	1.85	0.42
31:F:317:LEU:HD12	31:F:317:LEU:HA	1.77	0.42
32:K:232:GLU:N	32:K:232:GLU:OE2	2.53	0.42
3:C:232:ARG:NH1	3:C:275:GLU:OE2	2.46	0.42
5:E:204:VAL:HG23	5:E:238:ILE:HD11	2.02	0.42
11:M:202:ASP:HB2	11:M:209:PHE:CE1	2.55	0.42
12:N:84:LYS:HD3	12:N:120:MET:HE2	2.02	0.42
13:O:209:THR:N	14:P:165:GLU:OE2	2.53	0.42
15:Q:150:THR:O	15:Q:150:THR:OG1	2.34	0.42
20:W:140:ILE:O	20:W:140:ILE:HG13	2.20	0.42
20:W:284:SER:O	20:W:287:VAL:HG22	2.19	0.42
23:Z:164:ALA:HB1	23:Z:169:GLU:OE2	2.20	0.42
24:a:236:THR:HA	24:a:249:GLN:HE22	1.83	0.42
24:a:270:ARG:HH12	24:a:271:LYS:HE3	1.85	0.42
26:c:176:GLN:HB3	26:c:177:THR:H	1.65	0.42
26:c:179:SER:HB3	29:U:770:TRP:CD1	2.55	0.42
27:d:150:LYS:HE2	27:d:150:LYS:HA	2.02	0.42
8:i:135:LEU:HD23	8:i:135:LEU:HA	1.92	0.42
13:o:20:ALA:HB1	37:o:301:LDZ:H38	2.00	0.42
15:q:4:LEU:HD13	15:q:45:LEU:HB3	2.01	0.42
28:u:253:LEU:CD1	28:u:265:ALA:O	2.68	0.42
1:A:69:ASP:C	1:A:71:GLY:H	2.28	0.41
2:B:435:PRO:HG2	2:B:439:TYR:HE2	1.85	0.41
3:C:399:MET:HE2	3:C:399:MET:HB2	1.94	0.41
4:D:237:GLN:HE21	4:D:242:GLU:HG3	1.85	0.41
5:E:142:ILE:O	5:E:146:ARG:HG3	2.20	0.41
8:I:170:ALA:O	8:I:199:LYS:NZ	2.53	0.41
9:J:236:LYS:O	9:J:236:LYS:HD3	2.19	0.41
12:N:29:ARG:NE	13:O:139:GLU:OE1	2.53	0.41
15:Q:167:LEU:HD23	15:Q:167:LEU:HA	1.87	0.41
16:R:45:MET:HE2	37:R:301:LDZ:H20	2.02	0.41
16:R:73:ARG:HE	16:R:73:ARG:HB2	1.72	0.41
22:Y:332:GLN:HG3	22:Y:336:ARG:NH2	2.34	0.41
26:c:96:LEU:HG	26:c:100:LYS:HE2	2.02	0.41
26:c:191:ALA:O	26:c:196:LEU:HB2	2.20	0.41
27:d:11:ARG:N	27:d:11:ARG:HD3	2.34	0.41
6:g:211:LYS:H	6:g:211:LYS:HG2	1.70	0.41
28:u:482:ILE:HG22	28:u:517:VAL:HG12	2.02	0.41
29:U:62:LEU:HA	29:U:88:PHE:CZ	2.55	0.41
31:F:154:ASN:OD1	31:F:156:ASP:N	2.53	0.41
31:F:188:ILE:CG1	31:F:235:LEU:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:289:ASP:HB3	31:F:337:ILE:HB	2.01	0.41
31:F:373:MET:HB2	31:F:374:ASN:H	1.71	0.41
31:F:424:ILE:O	31:F:427:VAL:HG13	2.20	0.41
32:K:149:LYS:HB3	32:K:149:LYS:HE3	1.69	0.41
32:K:181:LEU:HA	32:K:184:VAL:HG22	2.02	0.41
32:k:167:ALA:HB1	32:k:181:LEU:HD21	2.02	0.41
1:A:138:MET:HB3	1:A:155:PRO:HD3	2.02	0.41
3:C:47:ALA:HB2	19:V:495:ARG:HH22	1.85	0.41
3:C:201:ARG:CG	4:D:299:PHE:CD1	3.01	0.41
4:D:64:GLU:OE2	4:D:64:GLU:CA	2.64	0.41
5:E:7:LYS:HA	5:E:7:LYS:HD2	1.78	0.41
5:E:229:ILE:HD12	5:E:274:LYS:O	2.20	0.41
5:E:251:ARG:O	5:E:255:ARG:HG3	2.19	0.41
5:E:339:ASN:O	5:E:343:LEU:HG	2.20	0.41
10:L:100:ASP:OD1	10:L:100:ASP:O	2.38	0.41
11:M:150:MET:HB3	11:M:160:TYR:HE2	1.85	0.41
16:R:5:ALA:HA	16:R:13:ILE:O	2.20	0.41
37:R:301:LDZ:H11	37:R:301:LDZ:H33	1.66	0.41
17:S:145:LEU:HD22	17:S:178:VAL:HB	2.01	0.41
18:T:46:ASN:OD1	18:T:47:ASN:N	2.53	0.41
20:W:1:MET:HG2	20:W:42:GLU:OE1	2.20	0.41
22:Y:274:SER:C	22:Y:277:VAL:HG12	2.44	0.41
24:a:68:GLU:C	24:a:70:ARG:H	2.29	0.41
24:a:100:THR:O	24:a:103:LYS:HG2	2.20	0.41
25:b:94:HIS:O	25:b:98:LYS:HG3	2.20	0.41
26:c:54:MET:SD	26:c:55:GLY:N	2.93	0.41
10:l:36:VAL:HG13	10:l:172:LEU:HD11	2.02	0.41
11:m:88:ALA:O	11:m:92:ARG:HG3	2.20	0.41
12:n:116:MET:HE2	12:n:116:MET:HB3	1.99	0.41
28:u:771:LEU:HD11	28:u:825:MET:SD	2.60	0.41
29:U:872:GLU:CB	29:U:873:PRO:HD3	2.50	0.41
31:F:365:ILE:HA	31:F:368:ILE:HD12	2.01	0.41
1:A:165:GLN:NE2	1:A:167:GLU:CD	2.78	0.41
1:A:170:PRO:HD2	1:A:231:ASN:HB3	2.03	0.41
2:B:39:LYS:HE2	2:B:276:GLU:OE2	2.20	0.41
3:C:120:SER:OG	26:c:193:ILE:HD11	2.20	0.41
3:C:150:MET:H	3:C:150:MET:HG2	1.68	0.41
3:C:377:HIS:CE1	22:Y:207:THR:CG2	3.03	0.41
5:E:63:GLN:CB	5:E:69:PHE:CE1	3.04	0.41
9:J:183:THR:O	9:J:185:ASP:N	2.52	0.41
15:Q:184:ASP:CG	15:Q:185:LYS:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:115:ASP:HB3	16:R:117:GLU:OE2	2.20	0.41
19:V:36:GLU:HG2	19:V:76:LYS:HE2	2.02	0.41
19:V:477:HIS:CD2	27:d:249:TYR:HH	2.36	0.41
20:W:141:GLU:O	20:W:142:ARG:C	2.62	0.41
20:W:435:LEU:HD12	20:W:435:LEU:C	2.44	0.41
21:X:344:ARG:HG3	21:X:384:VAL:CG2	2.49	0.41
22:Y:99:GLU:CD	22:Y:99:GLU:N	2.78	0.41
24:a:37:LEU:O	24:a:41:VAL:HG23	2.20	0.41
25:b:23:PRO:O	25:b:24:THR:OG1	2.37	0.41
27:d:234:ASP:OD2	27:d:237:ILE:CD1	2.66	0.41
8:i:72:MET:HE2	8:i:107:CYS:SG	2.60	0.41
14:p:113:ASP:OD1	14:p:115:LYS:N	2.54	0.41
16:r:68:LEU:HD23	16:r:68:LEU:HA	1.90	0.41
17:s:49:LYS:HB2	17:s:49:LYS:HE2	1.75	0.41
28:u:887:PHE:HD1	28:u:901:ARG:O	2.03	0.41
29:U:68:PHE:CE2	29:U:80:TYR:HD2	2.37	0.41
29:U:144:ASP:C	29:U:146:LYS:H	2.28	0.41
29:U:182:LYS:HE3	29:U:182:LYS:HB3	1.78	0.41
29:U:199:ARG:O	29:U:203:LYS:HG2	2.21	0.41
29:U:340:GLN:HA	29:U:343:ILE:HG22	2.02	0.41
29:U:397:THR:OG1	29:U:401:LYS:NZ	2.52	0.41
29:U:446:LEU:CD1	29:U:461:LEU:HD21	2.50	0.41
29:U:631:GLU:OE1	29:U:631:GLU:N	2.46	0.41
31:F:212:PHE:CE2	31:F:219:PRO:HB3	2.55	0.41
31:F:243:GLN:H	31:F:243:GLN:CD	2.28	0.41
32:k:121:LEU:C	32:k:121:LEU:HD12	2.44	0.41
1:A:73:ALA:HB3	1:A:78:TRP:CD1	2.55	0.41
1:A:97:ARG:HG2	2:B:130:GLU:O	2.20	0.41
1:A:433:ASN:OD1	32:K:66:LYS:HD3	2.20	0.41
2:B:403:GLY:HA3	3:C:180:ILE:HD13	2.02	0.41
4:D:414:HIS:ND1	6:G:26:GLU:HB2	2.35	0.41
9:J:70:CYS:SG	9:J:217:LEU:HD13	2.61	0.41
13:O:43:CYS:SG	13:O:98:LEU:HB3	2.61	0.41
17:S:26:ASP:OD2	17:S:26:ASP:C	2.63	0.41
19:V:24:GLN:C	19:V:27:PRO:HD2	2.45	0.41
19:V:236:ARG:NH2	29:U:35:TRP:HE1	2.17	0.41
19:V:324:PHE:HB3	30:e:6:GLN:HG3	2.02	0.41
19:V:348:PHE:CZ	19:V:350:GLN:NE2	2.88	0.41
20:W:363:ILE:HD11	20:W:382:LEU:HD11	2.01	0.41
23:Z:68:TRP:CH2	23:Z:111:LEU:HD13	2.55	0.41
23:Z:208:ILE:HD13	23:Z:208:ILE:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:30:GLN:HE22	25:b:76:HIS:CE1	2.38	0.41
11:m:231:ILE:HD12	11:m:231:ILE:N	2.35	0.41
15:q:103:LEU:HD12	15:q:103:LEU:O	2.20	0.41
28:u:159:VAL:HA	28:u:162:LEU:HG	2.02	0.41
28:u:177:GLU:O	28:u:181:ARG:NH1	2.50	0.41
29:U:41:SER:HA	29:U:44:LYS:HD2	2.02	0.41
29:U:256:ALA:HB3	29:U:261:LEU:HD11	2.03	0.41
29:U:444:TYR:HB2	29:U:476:GLY:HA2	2.02	0.41
30:e:43:TRP:C	30:e:43:TRP:CD1	2.98	0.41
31:F:197:GLU:O	31:F:350:ARG:NH1	2.52	0.41
32:K:24:VAL:O	32:K:28:ILE:HG12	2.20	0.41
1:A:43:ARG:HD2	1:A:43:ARG:O	2.20	0.41
1:A:114:ASN:OD1	1:A:114:ASN:N	2.54	0.41
1:A:267:LYS:HG3	1:A:270:CYS:SG	2.60	0.41
3:C:119:ASP:HB2	26:c:189:ILE:HD11	2.02	0.41
3:C:215:SER:OG	3:C:218:GLU:OE1	2.35	0.41
5:E:170:CYS:SG	5:E:297:ARG:HB2	2.61	0.41
5:E:193:CYS:SG	5:E:194:ASN:ND2	2.94	0.41
5:E:336:ASP:C	5:E:338:PHE:CD1	2.99	0.41
6:G:91:VAL:O	6:G:95:ARG:HG3	2.21	0.41
9:J:4:ASP:OD2	9:J:4:ASP:N	2.52	0.41
10:L:61:LYS:H	10:L:61:LYS:HG2	1.57	0.41
11:M:215:TRP:HZ2	11:M:219:LEU:HD11	1.83	0.41
14:P:61:GLN:HB2	15:Q:85:ARG:NH2	2.35	0.41
19:V:37:MET:HA	19:V:40:GLU:OE2	2.21	0.41
20:W:278:PRO:HG3	20:W:357:ARG:NH2	2.35	0.41
20:W:433:ASN:CG	20:W:434:SER:N	2.79	0.41
23:Z:92:VAL:O	23:Z:120:VAL:HG12	2.20	0.41
23:Z:236:LEU:C	23:Z:236:LEU:CD2	2.92	0.41
25:b:20:ASP:OD1	25:b:21:PHE:N	2.48	0.41
27:d:52:ARG:CZ	27:d:92:SER:HB3	2.51	0.41
8:i:108:GLU:O	8:i:112:THR:HG23	2.20	0.41
9:j:5:ARG:O	9:j:7:ILE:N	2.52	0.41
10:l:43:HIS:CD2	10:l:216:GLY:HA3	2.55	0.41
11:m:233:GLU:H	11:m:233:GLU:HG2	1.61	0.41
13:o:18:THR:OG1	13:o:172:ASN:HB2	2.21	0.41
29:U:580:ARG:HG2	29:U:584:TYR:CE2	2.55	0.41
29:U:763:VAL:O	29:U:767:THR:HG23	2.19	0.41
31:F:62:VAL:CG2	31:F:63:THR:N	2.83	0.41
31:F:166:THR:O	31:F:167:GLU:HB2	2.20	0.41
31:F:380:ASN:O	31:F:382:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:O	1:A:239:ARG:HB3	2.21	0.41
1:A:191:VAL:HG13	1:A:195:LEU:HD23	2.02	0.41
1:A:328:ASP:C	1:A:332:MET:SD	3.04	0.41
1:A:343:PHE:N	1:A:343:PHE:HD1	2.18	0.41
1:A:350:GLY:O	1:A:354:ILE:HG13	2.21	0.41
5:E:81:VAL:HG11	5:E:100:LEU:HD23	2.02	0.41
5:E:99:ALA:O	5:E:108:MET:N	2.50	0.41
5:E:138:LEU:HA	5:E:141:GLN:CD	2.46	0.41
12:N:187:GLN:HE21	12:N:189:LEU:HD21	1.85	0.41
19:V:214:HIS:CE1	19:V:218:TYR:CE1	3.09	0.41
19:V:336:GLU:HG2	19:V:341:GLU:O	2.20	0.41
20:W:130:MET:SD	20:W:131:VAL:HG23	2.60	0.41
20:W:262:LYS:HB2	20:W:262:LYS:HE3	1.89	0.41
23:Z:195:VAL:O	23:Z:199:LYS:HG2	2.19	0.41
23:Z:243:GLN:OE1	23:Z:243:GLN:N	2.45	0.41
24:a:69:HIS:O	24:a:70:ARG:HD2	2.20	0.41
25:b:7:MET:HB2	25:b:97:LEU:HD11	2.01	0.41
25:b:20:ASP:OD1	25:b:25:ARG:NE	2.49	0.41
26:c:163:ILE:HD12	26:c:201:TYR:CD1	2.55	0.41
27:d:50:LEU:HD12	27:d:51:ALA:N	2.35	0.41
8:i:124:PHE:HB3	9:j:124:ARG:HG3	2.02	0.41
8:i:167:ASN:C	8:i:169:ALA:H	2.28	0.41
9:j:130:SER:OG	9:j:149:PRO:HD3	2.21	0.41
11:m:197:ILE:O	11:m:200:VAL:HG12	2.20	0.41
15:q:164:LEU:HB3	15:q:196:PHE:CZ	2.55	0.41
28:u:742:ALA:O	28:u:746:ARG:HG3	2.20	0.41
29:U:214:ILE:HD13	29:U:218:GLN:CG	2.49	0.41
29:U:524:LYS:NZ	29:U:562:GLU:O	2.54	0.41
31:F:313:LEU:HA	31:F:316:GLN:HB3	2.02	0.41
1:A:157:ILE:HB	1:A:255:ARG:NH1	2.36	0.41
1:A:289:ALA:HB1	1:A:292:ASP:O	2.21	0.41
8:I:82:ASP:HB3	8:I:130:PHE:CD1	2.55	0.41
8:I:155:ASN:ND2	9:J:77:THR:OG1	2.54	0.41
11:M:202:ASP:HB2	11:M:209:PHE:CD1	2.56	0.41
13:O:30:ASN:C	13:O:30:ASN:HD22	2.26	0.41
19:V:495:ARG:HD2	19:V:495:ARG:C	2.43	0.41
20:W:306:LEU:HA	20:W:309:PHE:CE2	2.55	0.41
22:Y:173:ASP:OD1	22:Y:174:TRP:N	2.52	0.41
22:Y:220:VAL:HG13	22:Y:246:ILE:HD12	2.03	0.41
23:Z:9:VAL:HA	23:Z:48:LEU:HB3	2.02	0.41
23:Z:247:LYS:CD	23:Z:247:LYS:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:82:TYR:OH	27:d:95:MET:HG2	2.20	0.41
8:i:174:MET:HE2	8:i:174:MET:HB2	1.90	0.41
29:U:265:ILE:HA	29:U:268:LEU:HB2	2.02	0.41
29:U:841:LYS:HE3	29:U:841:LYS:HB3	1.91	0.41
31:F:208:HIS:CD2	31:F:211:LYS:NZ	2.89	0.41
31:F:327:LYS:N	31:F:327:LYS:HD2	2.36	0.41
31:F:363:ALA:O	31:F:367:GLN:HG3	2.21	0.41
31:F:409:ARG:HA	31:F:409:ARG:HD3	1.96	0.41
1:A:293:ASN:O	1:A:297:ARG:NE	2.50	0.41
1:A:332:MET:HB2	1:A:332:MET:HE2	1.69	0.41
2:B:214:MET:HG3	2:B:216:ILE:CD1	2.51	0.41
3:C:31:LEU:O	3:C:35:VAL:HG23	2.20	0.41
4:D:212:LYS:HG2	4:D:333:PHE:HD2	1.86	0.41
4:D:363:TYR:CD1	4:D:366:ARG:HD2	2.55	0.41
9:J:57:ARG:O	9:J:57:ARG:HG2	2.21	0.41
11:M:202:ASP:OD1	11:M:202:ASP:N	2.52	0.41
19:V:489:MET:N	19:V:489:MET:CE	2.76	0.41
21:X:96:PHE:CE2	21:X:109:LEU:HD12	2.56	0.41
21:X:171:LEU:HD21	21:X:209:THR:HG22	2.03	0.41
22:Y:31:HIS:ND1	22:Y:31:HIS:N	2.66	0.41
23:Z:12:HIS:O	23:Z:14:LEU:N	2.47	0.41
23:Z:206:LEU:HA	23:Z:209:ARG:HB3	2.03	0.41
23:Z:263:ALA:HB1	26:c:288:VAL:HG13	2.01	0.41
23:Z:267:ARG:HA	23:Z:270:VAL:HG12	2.01	0.41
24:a:125:ILE:O	24:a:125:ILE:HG13	2.20	0.41
9:j:45:VAL:CG2	9:j:62:ILE:CD1	2.98	0.41
13:o:219:LEU:HD11	14:p:195:ILE:HD12	2.02	0.41
28:u:344:VAL:HG22	28:u:345:PRO:HD2	2.02	0.41
28:u:404:ASP:HB2	28:u:405:HIS:H	1.65	0.41
28:u:538:ILE:HG23	28:u:558:LEU:HB3	2.02	0.41
28:u:610:GLN:HA	28:u:613:LEU:CD1	2.51	0.41
29:U:328:ILE:CA	29:U:333:MET:HE1	2.50	0.41
31:F:163:THR:HG22	31:F:165:PRO:HG3	2.01	0.41
31:F:181:PRO:O	31:F:242:ALA:HB1	2.20	0.41
1:A:347:ASP:OD1	1:A:349:GLU:N	2.53	0.41
2:B:60:LEU:HD11	28:u:232:TYR:CE1	2.55	0.41
2:B:365:PHE:CD2	2:B:380:LEU:HB3	2.56	0.41
3:C:155:ASP:O	3:C:159:LYS:HG2	2.20	0.41
3:C:340:ARG:HD2	22:Y:175:ASP:CG	2.46	0.41
3:C:406:LYS:HE2	3:C:406:LYS:HB3	1.86	0.41
4:D:160:PRO:O	4:D:161:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:GLY:HA2	5:E:291:ARG:NH2	2.35	0.41
4:D:266:GLU:HA	4:D:310:ALA:O	2.21	0.41
4:D:313:ARG:HB3	4:D:313:ARG:CZ	2.51	0.41
4:D:341:LYS:HG2	4:D:375:ILE:HD11	2.02	0.41
5:E:56:ILE:HG22	5:E:57:VAL:N	2.36	0.41
7:H:14:SER:OG	7:H:15:PRO:HD2	2.21	0.41
9:J:174:LYS:O	9:J:175:ASN:HB2	2.20	0.41
11:M:71:ARG:HH21	18:T:72:ILE:HG12	1.86	0.41
16:R:141:ARG:NE	16:R:141:ARG:HA	2.36	0.41
18:T:25:ASP:C	18:T:25:ASP:OD2	2.63	0.41
19:V:120:PHE:C	19:V:121:PHE:CD2	2.99	0.41
19:V:121:PHE:CD2	19:V:121:PHE:N	2.88	0.41
19:V:192:MET:SD	19:V:192:MET:C	3.04	0.41
20:W:89:LEU:HD23	20:W:91:SER:O	2.21	0.41
20:W:177:MET:O	20:W:177:MET:CG	2.69	0.41
21:X:407:MET:HA	21:X:407:MET:CE	2.43	0.41
22:Y:101:ARG:NH2	22:Y:105:MET:HE2	2.36	0.41
23:Z:54:PHE:HD1	23:Z:82:PHE:CD2	2.39	0.41
23:Z:165:GLU:O	23:Z:168:GLU:HG2	2.21	0.41
24:a:80:ILE:HA	24:a:83:VAL:HB	2.02	0.41
24:a:83:VAL:HG12	24:a:87:MET:HE1	2.03	0.41
24:a:289:ARG:HE	24:a:332:HIS:CE1	2.39	0.41
24:a:290:GLN:HG3	24:a:330:ARG:HD3	2.03	0.41
25:b:107:MET:HB3	25:b:136:VAL:HG22	2.03	0.41
26:c:213:GLU:O	26:c:217:LEU:N	2.54	0.41
26:c:277:LYS:HA	26:c:282:ARG:HE	1.85	0.41
27:d:120:GLU:H	27:d:121:ARG:NH1	2.19	0.41
27:d:131:VAL:HG12	27:d:134:LYS:HE2	2.02	0.41
27:d:215:TRP:CH2	27:d:224:SER:HB2	2.55	0.41
27:d:251:ARG:HB3	27:d:251:ARG:NH1	2.36	0.41
11:m:215:TRP:CD2	11:m:219:LEU:HD11	2.56	0.41
14:p:116:THR:O	14:p:117:PHE:HB2	2.19	0.41
14:p:189:ILE:HD12	14:p:189:ILE:H	1.85	0.41
15:q:13:VAL:HG23	15:q:113:PRO:HB2	2.03	0.41
28:u:211:ILE:HD12	28:u:213:GLN:H	1.86	0.41
28:u:591:ALA:O	28:u:595:VAL:HG23	2.21	0.41
29:U:775:LEU:HA	29:U:778:PHE:CE1	2.56	0.41
31:F:163:THR:C	31:F:164:LEU:HD12	2.46	0.41
31:F:292:GLY:HA3	31:F:310:MET:HG2	2.02	0.41
32:k:121:LEU:HD12	32:k:121:LEU:O	2.21	0.41
1:A:51:ASP:C	1:A:54:GLN:HG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:PRO:CA	3:C:175:PHE:HE1	2.31	0.41
4:D:265:ASP:O	4:D:266:GLU:C	2.63	0.41
5:E:26:LEU:HD11	31:F:55:MET:SD	2.60	0.41
5:E:199:VAL:O	5:E:234:GLU:HB3	2.20	0.41
5:E:307:GLN:OE1	5:E:307:GLN:N	2.44	0.41
7:H:79:MET:HB3	7:H:79:MET:HE3	1.75	0.41
17:S:73:LYS:HE3	17:S:73:LYS:HB3	1.88	0.41
18:T:124:TYR:HB2	18:T:137:LEU:HD13	2.02	0.41
19:V:74:ASP:OD2	19:V:74:ASP:N	2.53	0.41
20:W:1:MET:HG3	20:W:43:VAL:HG13	2.02	0.41
20:W:312:MET:HB2	20:W:365:ILE:CD1	2.50	0.41
22:Y:375:LEU:O	22:Y:379:ARG:HG2	2.21	0.41
26:c:176:GLN:O	26:c:178:THR:N	2.54	0.41
26:c:278:GLN:H	26:c:282:ARG:HH21	1.68	0.41
27:d:241:GLU:OE1	27:d:241:GLU:N	2.41	0.41
27:d:254:GLU:HB2	27:d:255:MET:SD	2.60	0.41
7:h:177:ARG:HB2	7:h:177:ARG:NH1	2.32	0.41
7:h:191:ALA:HA	7:h:194:THR:HG22	2.02	0.41
8:i:106:PRO:O	8:i:140:ASP:HB3	2.21	0.41
18:t:154:LEU:HD12	18:t:154:LEU:HA	1.90	0.41
28:u:731:MET:HE3	28:u:731:MET:C	2.41	0.41
28:u:761:MET:H	28:u:761:MET:HG2	1.57	0.41
29:U:793:LYS:HE3	29:U:796:LYS:HB2	2.02	0.41
1:A:302:LEU:HA	1:A:305:GLN:HB2	2.03	0.40
2:B:346:ARG:O	2:B:347:ILE:HD13	2.21	0.40
3:C:252:ASP:OD2	3:C:297:ARG:HB2	2.21	0.40
4:D:248:ARG:HA	4:D:295:GLN:HE22	1.86	0.40
5:E:206:LYS:HB3	31:F:261:ILE:HG13	2.02	0.40
5:E:222:ALA:O	5:E:224:ASP:N	2.54	0.40
6:G:182:LYS:HE2	6:G:182:LYS:HA	2.03	0.40
9:J:246:LYS:O	28:u:905:ASN:HB3	2.22	0.40
10:L:212:ILE:HD12	10:L:229:VAL:HG13	2.03	0.40
16:R:17:ASP:O	16:R:33:LYS:HD2	2.21	0.40
20:W:428:TRP:CZ3	23:Z:238:PRO:HG2	2.55	0.40
21:X:313:LEU:O	21:X:314:ARG:C	2.63	0.40
23:Z:147:ASP:N	23:Z:147:ASP:OD1	2.53	0.40
24:a:12:GLN:CA	24:a:22:TRP:CZ3	2.93	0.40
27:d:42:LYS:HA	27:d:45:LYS:HD2	2.02	0.40
11:m:200:VAL:HG22	11:m:200:VAL:O	2.20	0.40
13:o:178:ILE:HG12	13:o:183:LEU:HD13	2.03	0.40
14:p:14:MET:HG2	14:p:136:PHE:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:t:51:LEU:HD11	18:t:110:MET:HB3	2.03	0.40
29:U:112:CYS:SG	29:U:157:THR:OG1	2.76	0.40
29:U:522:GLY:O	29:U:559:ARG:NH2	2.54	0.40
2:B:250:VAL:O	2:B:284:ILE:HA	2.21	0.40
3:C:143:VAL:HG23	3:C:205:HIS:ND1	2.36	0.40
3:C:253:SER:O	3:C:254:ILE:O	2.39	0.40
4:D:158:GLN:OE1	4:D:158:GLN:HA	2.20	0.40
5:E:30:ARG:CA	5:E:33:LEU:HD22	2.49	0.40
5:E:62:LYS:HB3	5:E:62:LYS:HE2	1.91	0.40
5:E:87:LEU:O	5:E:91:LYS:HD2	2.21	0.40
5:E:247:THR:HA	5:E:251:ARG:NH2	2.37	0.40
6:G:72:ILE:HG21	6:G:114:LEU:HD11	2.02	0.40
14:P:107:PRO:HG2	14:P:124:LEU:HD13	2.02	0.40
14:P:164:PHE:HB2	14:P:189:ILE:CD1	2.51	0.40
15:Q:38:MET:HE3	15:Q:38:MET:HB3	1.84	0.40
19:V:37:MET:HE3	19:V:92:ARG:NH2	2.34	0.40
19:V:144:ASP:HB3	19:V:146:GLN:HG3	2.03	0.40
19:V:462:GLU:HG2	19:V:463:MET:H	1.86	0.40
19:V:481:SER:O	19:V:485:ASP:OD2	2.40	0.40
20:W:130:MET:O	20:W:134:GLY:HA3	2.21	0.40
21:X:87:ARG:NH1	21:X:87:ARG:HA	2.36	0.40
21:X:258:LYS:HD2	21:X:270:LEU:HD11	2.03	0.40
21:X:398:GLU:O	21:X:402:GLU:HG2	2.21	0.40
25:b:26:LEU:HD21	25:b:80:PRO:HD3	2.03	0.40
26:c:75:MET:HG3	26:c:76:PRO:HD2	2.03	0.40
6:g:50:ILE:HD13	6:g:79:VAL:HG12	2.04	0.40
8:i:59:VAL:O	8:i:59:VAL:CG2	2.69	0.40
10:l:192:LEU:HD22	10:l:233:LEU:HD23	2.03	0.40
10:l:233:LEU:HD23	10:l:233:LEU:HA	1.94	0.40
12:n:81:SER:O	12:n:85:GLU:OE1	2.39	0.40
14:p:138:VAL:HG11	14:p:146:MET:HB3	2.03	0.40
29:U:475:HIS:NE2	29:U:507:VAL:O	2.55	0.40
29:U:583:MET:HE3	29:U:583:MET:HB2	1.85	0.40
29:U:592:GLY:HA3	29:U:628:ARG:NH2	2.37	0.40
29:U:775:LEU:HA	29:U:778:PHE:HE1	1.86	0.40
1:A:115:VAL:HB	1:A:119:ALA:O	2.22	0.40
1:A:325:ASP:OD2	1:A:325:ASP:C	2.64	0.40
2:B:60:LEU:HD21	28:u:232:TYR:CZ	2.56	0.40
2:B:107:MET:H	2:B:107:MET:HG3	1.68	0.40
2:B:227:PRO:O	2:B:230:THR:OG1	2.36	0.40
2:B:362:LYS:HZ2	2:B:366:GLN:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:ARG:H	5:E:85:ARG:CD	2.34	0.40
5:E:235:ILE:HD12	5:E:235:ILE:HA	1.70	0.40
6:G:113:MET:HE3	6:G:113:MET:HB3	1.90	0.40
6:G:114:LEU:HD23	6:G:118:ILE:HG12	2.03	0.40
8:I:79:ILE:HG22	8:I:81:SER:H	1.86	0.40
8:I:174:MET:HE3	8:I:199:LYS:CE	2.50	0.40
10:L:204:ASP:OD1	10:L:239:ARG:NH1	2.42	0.40
21:X:306:LEU:HD12	21:X:313:LEU:HD23	2.03	0.40
22:Y:215:ASP:OD2	22:Y:217:LYS:HB3	2.20	0.40
23:Z:177:ARG:HH22	26:c:207:TYR:HD2	1.68	0.40
24:a:65:SER:HA	24:a:68:GLU:OE1	2.21	0.40
24:a:333:MET:SD	24:a:333:MET:N	2.94	0.40
25:b:20:ASP:O	25:b:176:GLY:HA2	2.21	0.40
26:c:278:GLN:HG3	26:c:282:ARG:HH21	1.82	0.40
27:d:175:ARG:CZ	27:d:199:PHE:HD1	2.34	0.40
9:j:43:LEU:HD11	9:j:62:ILE:CG1	2.46	0.40
28:u:829:MET:HE2	28:u:830:LEU:C	2.46	0.40
29:U:32:ASN:O	29:U:35:TRP:NE1	2.54	0.40
29:U:45:ILE:HG21	29:U:64:ALA:HB2	2.03	0.40
29:U:675:MET:HA	29:U:675:MET:CE	2.39	0.40
29:U:801:GLN:HA	29:U:878:LEU:O	2.21	0.40
30:e:40:GLU:CD	30:e:43:TRP:HB3	2.46	0.40
1:A:78:TRP:O	1:A:78:TRP:HE3	2.05	0.40
1:A:157:ILE:HG13	1:A:255:ARG:HD3	2.03	0.40
2:B:292:THR:HG23	2:B:336:THR:O	2.21	0.40
3:C:110:PRO:HG2	3:C:130:LYS:HZ3	1.84	0.40
3:C:251:ILE:HD13	3:C:251:ILE:HA	1.97	0.40
5:E:175:PRO:HD3	5:E:300:HIS:NE2	2.35	0.40
7:H:107:THR:O	7:H:111:VAL:HG23	2.21	0.40
10:L:4:ASN:OD1	10:L:4:ASN:N	2.54	0.40
11:M:179:LEU:HD21	11:M:192:GLU:HB3	2.03	0.40
11:M:192:GLU:HA	11:M:195:LYS:HG2	2.03	0.40
12:N:167:ASP:OD1	12:N:168:GLY:N	2.55	0.40
17:S:160:ASN:N	17:S:160:ASN:HD22	2.18	0.40
19:V:33:GLN:HA	19:V:37:MET:HE2	2.03	0.40
20:W:16:MET:SD	20:W:16:MET:C	3.04	0.40
20:W:413:ILE:HD11	20:W:415:PHE:CZ	2.57	0.40
21:X:190:LEU:O	21:X:194:ARG:HG2	2.20	0.40
22:Y:41:LEU:O	22:Y:41:LEU:HD23	2.22	0.40
22:Y:194:PHE:CD1	22:Y:195:LYS:HB3	2.57	0.40
22:Y:217:LYS:O	22:Y:221:THR:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:312:MET:HG2	24:a:312:MET:H	1.58	0.40
25:b:106:LYS:C	25:b:107:MET:SD	3.05	0.40
25:b:161:ASN:OD1	25:b:161:ASN:N	2.53	0.40
26:c:280:PRO:C	26:c:281:LYS:HD2	2.47	0.40
6:g:208:ILE:HD13	6:g:208:ILE:N	2.36	0.40
10:l:163:ALA:C	10:l:164:ARG:HG2	2.47	0.40
11:m:66:LEU:HD13	11:m:214:SER:OG	2.21	0.40
11:m:150:MET:HE3	11:m:163:CYS:SG	2.61	0.40
13:o:43:CYS:HB2	13:o:100:LEU:HD12	2.03	0.40
15:q:110:HIS:HB2	15:q:111:GLU:OE2	2.21	0.40
29:U:757:MET:HE3	29:U:758:PRO:CA	2.51	0.40
30:e:56:LEU:HD12	30:e:56:LEU:O	2.22	0.40
31:F:28:GLY:O	31:F:32:GLU:HG2	2.21	0.40
32:K:88:LEU:HD13	32:K:156:MET:HE1	2.04	0.40
3:C:188:LEU:HB3	3:C:317:PHE:HE2	1.87	0.40
4:D:45:LYS:HG2	29:U:187:LEU:HD21	2.04	0.40
4:D:363:TYR:HA	4:D:366:ARG:HD2	2.04	0.40
5:E:303:LEU:HG	5:E:304:PRO:HD3	2.04	0.40
7:H:119:GLN:O	7:H:122:THR:HG22	2.22	0.40
11:M:75:MET:HE2	11:M:135:PHE:CD2	2.56	0.40
14:P:31:GLN:HB3	14:P:32:ALA:H	1.67	0.40
16:R:160:ILE:HA	16:R:160:ILE:HD13	1.86	0.40
20:W:131:VAL:O	20:W:136:ILE:HG23	2.22	0.40
20:W:137:TYR:HD1	20:W:139:GLU:HG2	1.78	0.40
22:Y:104:MET:HB3	22:Y:104:MET:HE3	1.66	0.40
22:Y:349:LYS:O	22:Y:352:GLU:OE2	2.38	0.40
24:a:249:GLN:HA	24:a:252:LYS:HD3	2.04	0.40
24:a:252:LYS:HA	24:a:255:TRP:CD1	2.57	0.40
25:b:35:ILE:HD13	25:b:184:ILE:CD1	2.51	0.40
26:c:198:ARG:H	26:c:198:ARG:HG2	1.68	0.40
27:d:6:LYS:HB2	27:d:6:LYS:HE2	1.87	0.40
8:i:58:GLU:O	8:i:58:GLU:HG3	2.21	0.40
10:l:52:ALA:HB2	10:l:59:HIS:NE2	2.37	0.40
29:U:340:GLN:HB3	29:U:344:ARG:HH22	1.86	0.40
29:U:745:THR:O	29:U:784:THR:N	2.49	0.40
31:F:333:ASN:HB2	31:F:334:ARG:HH21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	411/433 (95%)	346 (84%)	58 (14%)	7 (2%)	7	24
2	B	409/440 (93%)	359 (88%)	50 (12%)	0	100	100
3	C	394/398 (99%)	345 (88%)	42 (11%)	7 (2%)	6	23
4	D	378/418 (90%)	327 (86%)	47 (12%)	4 (1%)	11	35
5	E	379/403 (94%)	344 (91%)	32 (8%)	3 (1%)	16	43
6	G	235/245 (96%)	219 (93%)	13 (6%)	3 (1%)	9	30
6	g	238/245 (97%)	225 (94%)	12 (5%)	1 (0%)	30	58
7	H	229/233 (98%)	217 (95%)	10 (4%)	2 (1%)	14	40
7	h	230/233 (99%)	218 (95%)	11 (5%)	1 (0%)	30	58
8	I	246/260 (95%)	227 (92%)	18 (7%)	1 (0%)	30	58
8	i	248/260 (95%)	230 (93%)	17 (7%)	1 (0%)	30	58
9	J	245/247 (99%)	224 (91%)	17 (7%)	4 (2%)	7	25
9	j	237/247 (96%)	208 (88%)	27 (11%)	2 (1%)	16	43
10	L	236/268 (88%)	229 (97%)	7 (3%)	0	100	100
10	l	236/268 (88%)	225 (95%)	10 (4%)	1 (0%)	30	58
11	M	238/254 (94%)	227 (95%)	10 (4%)	1 (0%)	30	58
11	m	238/254 (94%)	221 (93%)	15 (6%)	2 (1%)	16	43
12	N	195/238 (82%)	188 (96%)	6 (3%)	1 (0%)	24	53
12	n	195/238 (82%)	189 (97%)	6 (3%)	0	100	100
13	O	218/276 (79%)	209 (96%)	8 (4%)	1 (0%)	24	53
13	o	218/276 (79%)	202 (93%)	16 (7%)	0	100	100
14	P	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
14	p	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	53
15	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
15	q	197/201 (98%)	188 (95%)	8 (4%)	1 (0%)	24	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	R	199/262 (76%)	190 (96%)	8 (4%)	1 (0%)	24	53
16	r	199/262 (76%)	189 (95%)	10 (5%)	0	100	100
17	S	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	53
17	s	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	53
18	T	213/263 (81%)	205 (96%)	7 (3%)	1 (0%)	24	53
18	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
19	V	478/533 (90%)	425 (89%)	51 (11%)	2 (0%)	30	58
20	W	453/456 (99%)	415 (92%)	34 (8%)	4 (1%)	14	40
21	X	378/422 (90%)	360 (95%)	17 (4%)	1 (0%)	36	64
22	Y	375/389 (96%)	339 (90%)	35 (9%)	1 (0%)	36	64
23	Z	284/324 (88%)	245 (86%)	38 (13%)	1 (0%)	30	58
24	a	371/376 (99%)	343 (92%)	26 (7%)	2 (0%)	24	53
25	b	189/377 (50%)	166 (88%)	23 (12%)	0	100	100
26	c	285/309 (92%)	244 (86%)	37 (13%)	4 (1%)	9	29
27	d	248/349 (71%)	208 (84%)	40 (16%)	0	100	100
28	u	838/908 (92%)	799 (95%)	39 (5%)	0	100	100
29	U	829/953 (87%)	747 (90%)	77 (9%)	5 (1%)	21	50
30	e	36/70 (51%)	29 (81%)	7 (19%)	0	100	100
31	F	378/439 (86%)	328 (87%)	46 (12%)	4 (1%)	11	35
32	K	226/240 (94%)	219 (97%)	7 (3%)	0	100	100
32	k	224/240 (93%)	215 (96%)	9 (4%)	0	100	100
All	All	13289/14859 (89%)	12219 (92%)	998 (8%)	72 (0%)	26	53

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	PRO
1	A	160	THR
1	A	164	MET
1	A	284	ARG
1	A	361	SER
4	D	339	ARG
5	E	130	VAL
6	G	9	PHE
7	H	8	PHE

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Mol	Chain	Res	Type
8	I	107	CYS
9	J	175	ASN
9	J	199	VAL
9	J	213	ARG
20	W	335	SER
6	g	19	GLU
8	i	107	CYS
9	j	9	VAL
9	j	52	LYS
11	m	216	VAL
17	s	191	ASP
29	U	213	PHE
29	U	834	SER
3	C	130	LYS
3	C	254	ILE
4	D	149	SER
4	D	162	VAL
6	G	146	GLU
7	H	180	GLU
9	J	6	ALA
12	N	19	ARG
16	R	38	ASN
17	S	191	ASP
18	T	46	ASN
19	V	495	ARG
20	W	137	TYR
23	Z	145	HIS
24	a	343	LEU
26	c	183	HIS
26	c	212	LEU
14	p	31	GLN
15	q	24	ASN
31	F	417	HIS
3	C	90	HIS
5	E	223	ARG
13	O	172	ASN
24	a	69	HIS
26	c	280	PRO
29	U	875	PHE
31	F	167	GLU
31	F	337	ILE
31	F	377	PRO

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Mol	Chain	Res	Type
6	G	130	GLU
11	M	201	HIS
19	V	493	ALA
20	W	261	GLU
7	h	232	ALA
10	l	226	ASP
11	m	201	HIS
5	E	89	LYS
20	W	139	GLU
22	Y	183	TYR
26	c	184	LEU
3	C	221	GLN
3	C	252	ASP
1	A	157	ILE
4	D	151	ILE
29	U	832	VAL
1	A	158	ASP
3	C	91	PRO
29	U	881	PRO
21	X	318	ILE
3	C	89	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	348/372 (94%)	332 (95%)	16 (5%)	24	56
2	B	356/385 (92%)	353 (99%)	3 (1%)	73	89
3	C	340/346 (98%)	326 (96%)	14 (4%)	27	60
4	D	332/366 (91%)	318 (96%)	14 (4%)	26	59
5	E	333/353 (94%)	319 (96%)	14 (4%)	26	59
6	G	191/209 (91%)	190 (100%)	1 (0%)	81	93
6	g	194/209 (93%)	190 (98%)	4 (2%)	47	76
7	H	164/190 (86%)	161 (98%)	3 (2%)	51	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	167/190 (88%)	165 (99%)	2 (1%)	63	85
8	I	191/220 (87%)	186 (97%)	5 (3%)	40	72
8	i	193/220 (88%)	191 (99%)	2 (1%)	68	87
9	J	179/210 (85%)	172 (96%)	7 (4%)	28	61
9	j	152/210 (72%)	146 (96%)	6 (4%)	28	61
10	L	198/229 (86%)	193 (98%)	5 (2%)	42	73
10	l	198/229 (86%)	190 (96%)	8 (4%)	28	61
11	M	192/211 (91%)	188 (98%)	4 (2%)	47	76
11	m	193/211 (92%)	185 (96%)	8 (4%)	27	60
12	N	154/180 (86%)	150 (97%)	4 (3%)	40	72
12	n	154/180 (86%)	151 (98%)	3 (2%)	50	78
13	O	177/227 (78%)	173 (98%)	4 (2%)	44	74
13	o	177/227 (78%)	176 (99%)	1 (1%)	78	92
14	P	173/173 (100%)	172 (99%)	1 (1%)	78	92
14	p	173/173 (100%)	171 (99%)	2 (1%)	63	85
15	Q	164/171 (96%)	161 (98%)	3 (2%)	51	79
15	q	165/171 (96%)	162 (98%)	3 (2%)	51	79
16	R	153/201 (76%)	149 (97%)	4 (3%)	40	72
16	r	153/201 (76%)	149 (97%)	4 (3%)	40	72
17	S	174/198 (88%)	170 (98%)	4 (2%)	44	74
17	s	174/198 (88%)	173 (99%)	1 (1%)	78	92
18	T	175/214 (82%)	175 (100%)	0	100	100
18	t	176/214 (82%)	175 (99%)	1 (1%)	78	92
19	V	414/459 (90%)	407 (98%)	7 (2%)	53	80
20	W	413/416 (99%)	402 (97%)	11 (3%)	39	71
21	X	326/362 (90%)	320 (98%)	6 (2%)	51	79
22	Y	333/344 (97%)	321 (96%)	12 (4%)	31	63
23	Z	256/295 (87%)	248 (97%)	8 (3%)	35	67
24	a	333/336 (99%)	328 (98%)	5 (2%)	57	82
25	b	167/312 (54%)	165 (99%)	2 (1%)	63	85
26	c	251/267 (94%)	241 (96%)	10 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	d	226/293 (77%)	220 (97%)	6 (3%)	39	71
28	u	709/763 (93%)	700 (99%)	9 (1%)	61	84
29	U	714/816 (88%)	697 (98%)	17 (2%)	43	73
30	e	38/63 (60%)	37 (97%)	1 (3%)	40	72
31	F	330/379 (87%)	322 (98%)	8 (2%)	43	73
32	K	190/202 (94%)	189 (100%)	1 (0%)	81	93
32	k	186/202 (92%)	181 (97%)	5 (3%)	39	71
All	All	11149/12597 (88%)	10890 (98%)	259 (2%)	44	74

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	63	THR
1	A	123	VAL
1	A	124	ASP
1	A	157	ILE
1	A	213	LEU
1	A	234	ASP
1	A	261	PHE
1	A	268	LYS
1	A	277	ILE
1	A	294	GLU
1	A	302	LEU
1	A	344	SER
1	A	373	LEU
1	A	397	ILE
1	A	403	ILE
2	B	125	THR
2	B	191	ASP
2	B	380	LEU
3	C	64	GLN
3	C	80	MET
3	C	98	ASP
3	C	123	LEU
3	C	126	ILE
3	C	142	LYS
3	C	148	TYR
3	C	171	HIS
3	C	210	THR

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Mol	Chain	Res	Type
3	C	240	GLU
3	C	244	SER
3	C	254	ILE
3	C	287	LYS
3	C	338	LEU
4	D	60	TYR
4	D	110	ASN
4	D	115	ILE
4	D	154	LEU
4	D	162	VAL
4	D	164	TYR
4	D	261	ILE
4	D	270	ILE
4	D	302	ASN
4	D	337	ASP
4	D	339	ARG
4	D	360	LEU
4	D	382	SER
4	D	409	LYS
5	E	33	LEU
5	E	63	GLN
5	E	85	ARG
5	E	92	LEU
5	E	104	THR
5	E	129	ASN
5	E	130	VAL
5	E	148	VAL
5	E	171	LEU
5	E	181	THR
5	E	199	VAL
5	E	204	VAL
5	E	250	ASP
5	E	284	THR
6	G	112	ASP
7	H	61	SER
7	H	122	THR
7	H	156	PHE
8	I	71	ASP
8	I	75	SER
8	I	107	CYS
8	I	200	THR
8	I	206	LEU

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Mol	Chain	Res	Type
9	J	43	LEU
9	J	45	VAL
9	J	70	CYS
9	J	71	MET
9	J	167	SER
9	J	173	GLU
9	J	236	LYS
10	L	64	LEU
10	L	78	THR
10	L	118	ILE
10	L	140	MET
10	L	225	ASP
11	M	28	LYS
11	M	34	SER
11	M	229	LYS
11	M	230	ASP
12	N	1	THR
12	N	72	GLU
12	N	98	ILE
12	N	144	ARG
13	O	10	ASP
13	O	12	ILE
13	O	73	LEU
13	O	167	LEU
14	P	150	CYS
15	Q	20	VAL
15	Q	28	MET
15	Q	102	LEU
16	R	41	LEU
16	R	102	CYS
16	R	146	ASP
16	R	191	ASN
17	S	6	VAL
17	S	69	GLU
17	S	169	ASP
17	S	201	GLU
19	V	74	ASP
19	V	226	VAL
19	V	276	PHE
19	V	333	ILE
19	V	336	GLU
19	V	338	LEU

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Mol	Chain	Res	Type
19	V	495	ARG
20	W	47	LEU
20	W	107	GLN
20	W	213	PHE
20	W	219	THR
20	W	261	GLU
20	W	263	TRP
20	W	334	GLU
20	W	386	VAL
20	W	413	ILE
20	W	451	MET
20	W	455	LEU
21	X	51	LEU
21	X	93	LEU
21	X	114	ILE
21	X	160	MET
21	X	185	LYS
21	X	319	ILE
22	Y	41	LEU
22	Y	53	TYR
22	Y	86	GLU
22	Y	104	MET
22	Y	169	GLU
22	Y	176	ARG
22	Y	181	LYS
22	Y	202	LEU
22	Y	203	ASP
22	Y	204	THR
22	Y	215	ASP
22	Y	228	MET
23	Z	53	SER
23	Z	125	ASP
23	Z	126	VAL
23	Z	179	ILE
23	Z	198	LEU
23	Z	208	ILE
23	Z	220	LEU
23	Z	272	LEU
24	a	91	ASN
24	a	151	VAL
24	a	315	LEU
24	a	372	HIS

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Mol	Chain	Res	Type
24	a	375	LEU
25	b	35	ILE
25	b	137	ASN
26	c	51	MET
26	c	53	VAL
26	c	64	ASP
26	c	69	VAL
26	c	87	VAL
26	c	184	LEU
26	c	193	ILE
26	c	196	LEU
26	c	226	MET
26	c	229	LEU
27	d	16	LEU
27	d	27	LYS
27	d	173	THR
27	d	187	GLU
27	d	190	LEU
27	d	235	THR
6	g	81	THR
6	g	112	ASP
6	g	115	CYS
6	g	131	MET
7	h	124	SER
7	h	205	GLU
8	i	43	VAL
8	i	213	ILE
9	j	35	VAL
9	j	91	CYS
9	j	130	SER
9	j	134	VAL
9	j	184	ASP
9	j	219	ILE
10	l	9	ASP
10	l	38	LEU
10	l	74	ILE
10	l	114	SER
10	l	156	CYS
10	l	182	CYS
10	l	204	ASP
10	l	206	THR
11	m	5	THR

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Mol	Chain	Res	Type
11	m	75	MET
11	m	133	CYS
11	m	142	VAL
11	m	206	ASP
11	m	218	GLU
11	m	223	ARG
11	m	233	GLU
12	n	20	THR
12	n	46	SER
12	n	182	SER
13	o	127	MET
14	p	116	THR
14	p	122	CYS
15	q	47	VAL
15	q	94	SER
15	q	148	THR
16	r	100	MET
16	r	102	CYS
16	r	138	VAL
16	r	182	ASP
17	s	12	ILE
18	t	155	GLU
28	u	140	LEU
28	u	151	LEU
28	u	333	LEU
28	u	416	MET
28	u	524	MET
28	u	744	MET
28	u	851	ASP
28	u	870	THR
28	u	887	PHE
29	U	41	SER
29	U	54	PHE
29	U	239	GLU
29	U	350	LEU
29	U	459	ASP
29	U	497	LEU
29	U	578	LEU
29	U	586	VAL
29	U	629	THR
29	U	663	THR
29	U	754	HIS

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Mol	Chain	Res	Type
29	U	788	VAL
29	U	830	THR
29	U	872	GLU
29	U	880	ASN
29	U	913	ILE
29	U	921	ILE
30	e	6	GLN
31	F	69	MET
31	F	145	LEU
31	F	164	LEU
31	F	202	ILE
31	F	238	ARG
31	F	306	VAL
31	F	329	ILE
31	F	373	MET
32	K	47	CYS
32	k	10	ARG
32	k	16	SER
32	k	47	CYS
32	k	148	GLU
32	k	229	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (242) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	247	GLN
1	A	305	GLN
1	A	358	HIS
1	A	379	ASN
1	A	414	ASN
1	A	433	ASN
2	B	82	GLN
2	B	119	ASN
2	B	277	HIS
2	B	425	ASN
3	C	90	HIS
3	C	124	HIS
3	C	171	HIS
3	C	205	HIS
3	C	377	HIS
4	D	110	ASN

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Mol	Chain	Res	Type
4	D	137	ASN
4	D	173	GLN
4	D	237	GLN
4	D	257	ASN
4	D	295	GLN
4	D	304	ASN
4	D	340	GLN
5	E	10	GLN
5	E	129	ASN
5	E	194	ASN
5	E	263	GLN
5	E	305	ASN
5	E	323	HIS
5	E	339	ASN
5	E	345	ASN
5	E	359	HIS
6	G	53	GLN
6	G	92	GLN
6	G	100	ASN
6	G	172	GLN
7	H	71	HIS
7	H	95	GLN
7	H	119	GLN
7	H	148	GLN
7	H	189	HIS
7	H	207	ASN
8	I	40	ASN
8	I	84	ASN
8	I	95	GLN
8	I	100	GLN
8	I	102	GLN
8	I	109	GLN
8	I	146	GLN
8	I	155	ASN
8	I	240	HIS
9	J	23	GLN
9	J	175	ASN
9	J	244	GLN
10	L	53	GLN
10	L	60	GLN
10	L	90	GLN
10	L	117	GLN

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Mol	Chain	Res	Type
11	M	97	ASN
11	M	101	ASN
12	N	28	ASN
12	N	53	GLN
12	N	62	GLN
12	N	106	GLN
12	N	110	GLN
12	N	187	GLN
12	N	193	GLN
13	O	30	ASN
13	O	35	HIS
13	O	62	ASN
13	O	116	HIS
13	O	193	ASN
14	P	72	ASN
14	P	93	ASN
14	P	157	ASN
14	P	162	HIS
14	P	169	GLN
14	P	173	ASN
15	Q	27	GLN
15	Q	55	GLN
15	Q	82	ASN
15	Q	87	ASN
15	Q	101	ASN
15	Q	193	ASN
16	R	29	GLN
16	R	38	ASN
16	R	85	ASN
16	R	191	ASN
17	S	36	HIS
17	S	108	ASN
17	S	160	ASN
18	T	47	ASN
18	T	108	ASN
18	T	162	GLN
19	V	168	GLN
19	V	232	HIS
19	V	319	HIS
19	V	453	HIS
19	V	473	GLN
20	W	203	GLN

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Mol	Chain	Res	Type
20	W	210	ASN
20	W	265	GLN
20	W	362	ASN
20	W	422	ASN
20	W	423	ASN
20	W	433	ASN
21	X	44	GLN
21	X	262	ASN
21	X	329	ASN
21	X	333	GLN
21	X	405	GLN
21	X	416	ASN
22	Y	77	ASN
22	Y	178	ASN
22	Y	184	GLN
22	Y	196	GLN
22	Y	251	HIS
22	Y	357	ASN
23	Z	12	HIS
23	Z	145	HIS
23	Z	157	HIS
23	Z	254	ASN
23	Z	273	HIS
23	Z	277	ASN
23	Z	282	ASN
24	a	46	GLN
24	a	86	GLN
24	a	143	ASN
24	a	169	HIS
24	a	193	GLN
24	a	227	ASN
24	a	273	GLN
24	a	290	GLN
24	a	332	HIS
24	a	369	HIS
24	a	370	GLN
25	b	18	ASN
25	b	76	HIS
25	b	137	ASN
25	b	161	ASN
26	c	92	GLN
26	c	130	GLN

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Mol	Chain	Res	Type
26	c	149	GLN
26	c	197	ASN
26	c	232	GLN
26	c	240	HIS
26	c	274	ASN
27	d	96	HIS
27	d	128	GLN
6	g	34	GLN
6	g	53	GLN
6	g	75	ASN
6	g	100	ASN
7	h	21	GLN
7	h	207	ASN
8	i	95	GLN
8	i	142	HIS
8	i	146	GLN
8	i	155	ASN
8	i	167	ASN
9	j	122	ASN
10	l	4	ASN
10	l	5	GLN
10	l	8	ASN
10	l	21	GLN
10	l	53	GLN
10	l	69	HIS
10	l	86	ASN
10	l	117	GLN
10	l	190	HIS
11	m	32	ASN
11	m	97	ASN
11	m	101	ASN
11	m	105	ASN
11	m	180	GLN
11	m	221	ASN
12	n	77	HIS
12	n	110	GLN
12	n	123	GLN
12	n	193	GLN
13	o	80	ASN
14	p	7	ASN
14	p	72	ASN
14	p	169	GLN

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Mol	Chain	Res	Type
15	q	8	GLN
15	q	27	GLN
15	q	63	ASN
15	q	101	ASN
15	q	132	HIS
15	q	193	ASN
16	r	70	ASN
16	r	89	GLN
17	s	151	ASN
17	s	152	GLN
17	s	160	ASN
17	s	163	HIS
18	t	46	ASN
18	t	89	HIS
18	t	185	ASN
18	t	213	HIS
28	u	112	ASN
28	u	327	ASN
28	u	405	HIS
28	u	493	ASN
28	u	566	HIS
28	u	737	ASN
28	u	808	ASN
28	u	876	HIS
29	U	28	ASN
29	U	115	ASN
29	U	189	GLN
29	U	192	GLN
29	U	218	GLN
29	U	366	HIS
29	U	464	GLN
29	U	647	HIS
29	U	665	ASN
29	U	685	GLN
29	U	718	ASN
29	U	880	ASN
29	U	888	GLN
30	e	6	GLN
30	e	55	GLN
31	F	321	GLN
31	F	325	GLN
31	F	367	GLN

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Mol	Chain	Res	Type
32	K	13	ASN
32	K	23	GLN
32	K	97	GLN
32	K	98	ASN
32	K	104	ASN
32	K	114	GLN
32	K	164	GLN
32	K	182	GLN
32	K	186	HIS
32	K	204	GLN
32	k	13	ASN
32	k	98	ASN
32	k	155	HIS
32	k	178	GLN
32	k	214	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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
34	ADP	E	401	-	28,29,29	1.45	4 (14%)	43,45,45	1.80	9 (20%)
34	ADP	F	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
37	LDZ	N	301	-	33,34,34	0.40	0	42,44,44	0.78	2 (4%)
35	ATP	C	501	36	32,33,33	0.37	0	48,52,52	0.42	0
37	LDZ	n	301	-	33,34,34	0.51	1 (3%)	42,44,44	1.69	4 (9%)
35	ATP	B	501	36	32,33,33	1.88	1 (3%)	48,52,52	0.86	2 (4%)
37	LDZ	r	301	-	33,34,34	0.46	0	42,44,44	0.83	2 (4%)
37	LDZ	O	301	-	33,34,34	0.18	0	42,44,44	0.38	0
34	ADP	A	501	-	28,29,29	1.42	5 (17%)	43,45,45	1.83	8 (18%)
37	LDZ	o	301	-	33,34,34	0.45	0	42,44,44	1.22	4 (9%)
37	LDZ	R	301	-	33,34,34	0.55	1 (3%)	42,44,44	1.05	2 (4%)
35	ATP	D	501	36	32,33,33	0.32	0	48,52,52	0.30	0

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
34	ADP	E	401	-	-	5/16/32/32	0/3/3/3
34	ADP	F	501	-	-	5/16/32/32	0/3/3/3
37	LDZ	N	301	-	-	9/38/39/39	0/1/1/1
35	ATP	C	501	36	-	6/22/38/38	0/3/3/3
37	LDZ	n	301	-	-	24/38/39/39	0/1/1/1
35	ATP	B	501	36	-	3/22/38/38	0/3/3/3
37	LDZ	r	301	-	-	14/38/39/39	0/1/1/1
37	LDZ	O	301	-	-	15/38/39/39	0/1/1/1
34	ADP	A	501	-	-	4/16/32/32	0/3/3/3
37	LDZ	o	301	-	-	16/38/39/39	0/1/1/1
37	LDZ	R	301	-	-	10/38/39/39	0/1/1/1
35	ATP	D	501	36	-	2/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ATP	PA-O3A	10.41	1.70	1.59
34	E	401	ADP	C5-C4	4.82	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	501	ADP	C5-C4	4.75	1.47	1.39
34	A	501	ADP	C5-C4	4.72	1.47	1.39
34	F	501	ADP	C5-C6	2.75	1.48	1.41
34	E	401	ADP	C5-C6	2.64	1.48	1.41
34	A	501	ADP	C5-C6	2.61	1.48	1.41
34	E	401	ADP	C5-N7	-2.46	1.34	1.39
34	A	501	ADP	C5-N7	-2.41	1.34	1.39
34	F	501	ADP	C8-N7	2.32	1.36	1.31
37	R	301	LDZ	C17-N16	-2.31	1.43	1.46
34	F	501	ADP	C5-N7	-2.28	1.34	1.39
34	A	501	ADP	C8-N7	2.22	1.35	1.31
34	E	401	ADP	C8-N7	2.20	1.35	1.31
34	A	501	ADP	PA-O3A	2.04	1.61	1.59
37	n	301	LDZ	C17-N16	-2.03	1.43	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	301	LDZ	C14-N13-C12	8.22	139.31	121.65
34	F	501	ADP	C5-C4-N3	-5.95	118.53	126.72
34	E	401	ADP	C5-C4-N3	-5.92	118.56	126.72
34	A	501	ADP	C5-C4-N3	-5.82	118.70	126.72
34	E	401	ADP	N3-C4-N9	4.77	135.28	127.17
34	F	501	ADP	N3-C4-N9	4.75	135.24	127.17
34	A	501	ADP	N3-C4-N9	4.69	135.14	127.17
35	B	501	ATP	O2B-PB-O3A	4.68	119.93	107.27
37	o	301	LDZ	C14-N13-C12	4.67	131.68	121.65
37	R	301	LDZ	C18-C17-N16	-4.47	103.94	110.69
37	n	301	LDZ	C24-C14-N13	4.42	120.56	110.58
34	F	501	ADP	C2-N3-C4	3.75	120.99	111.83
34	A	501	ADP	C2-N3-C4	3.64	120.73	111.83
34	E	401	ADP	C2-N3-C4	3.59	120.60	111.83
34	A	501	ADP	C4-C5-N7	-3.35	106.75	110.58
34	F	501	ADP	C4-C5-N7	-3.34	106.76	110.58
34	E	401	ADP	C4-C5-N7	-3.29	106.83	110.58
34	A	501	ADP	N3-C2-N1	-3.24	123.68	128.58
34	F	501	ADP	N3-C2-N1	-3.23	123.69	128.58
37	o	301	LDZ	C15-C14-N13	-3.20	102.45	111.11
34	E	401	ADP	N3-C2-N1	-3.14	123.82	128.58
37	r	301	LDZ	C18-C17-N16	3.10	115.36	110.69
37	R	301	LDZ	C15-C14-N13	-2.95	103.13	111.11
37	n	301	LDZ	C11-C12-N13	2.80	122.61	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	501	ADP	C3'-C2'-C1'	2.68	106.53	101.46
37	r	301	LDZ	C14-N13-C12	2.65	127.34	121.65
34	A	501	ADP	C4-N9-C8	2.60	108.47	105.74
34	F	501	ADP	C4-N9-C8	2.50	108.37	105.74
34	A	501	ADP	C5-N7-C8	2.47	107.34	103.45
34	F	501	ADP	C5-N7-C8	2.47	107.33	103.45
34	E	401	ADP	C3'-C2'-C1'	2.41	106.02	101.46
37	o	301	LDZ	C24-C14-N13	2.40	115.99	110.58
37	o	301	LDZ	O32-C12-N13	2.38	127.21	122.96
34	A	501	ADP	C3'-C2'-C1'	2.30	105.82	101.46
34	E	401	ADP	C4-N9-C8	2.30	108.15	105.74
34	E	401	ADP	C5-N7-C8	2.23	106.96	103.45
37	n	301	LDZ	C18-C17-N16	2.20	114.00	110.69
37	N	301	LDZ	C22-C17-N16	2.14	113.64	109.50
35	B	501	ATP	O3B-PB-O1B	-2.09	104.41	110.70
37	N	301	LDZ	C14-N13-C12	2.02	125.99	121.65
34	E	401	ADP	C2-N1-C6	2.01	122.02	118.73
34	F	501	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ADP	C5'-O5'-PA-O3A
34	E	401	ADP	C5'-O5'-PA-O1A
34	E	401	ADP	C5'-O5'-PA-O3A
34	F	501	ADP	C5'-O5'-PA-O1A
34	F	501	ADP	C5'-O5'-PA-O2A
34	F	501	ADP	C5'-O5'-PA-O3A
34	F	501	ADP	O4'-C4'-C5'-O5'
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	PB-O3B-PG-O2G
35	C	501	ATP	C5'-O5'-PA-O1A
35	C	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O3A
37	N	301	LDZ	N10-C11-C30-C31
37	N	301	LDZ	C22-C17-C18-C19
37	O	301	LDZ	C14-C15-N16-C17
37	O	301	LDZ	O34-C15-N16-C17
37	O	301	LDZ	C22-C17-N16-C15

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Mol	Chain	Res	Type	Atoms
37	O	301	LDZ	C18-C17-N16-C15
37	R	301	LDZ	O31-C9-O8-C7
37	R	301	LDZ	N10-C9-O8-C7
37	n	301	LDZ	N10-C9-O8-C7
37	n	301	LDZ	C24-C14-N13-C12
37	o	301	LDZ	C24-C14-N13-C12
37	o	301	LDZ	C22-C17-N16-C15
37	r	301	LDZ	C18-C17-C22-O33
37	r	301	LDZ	N16-C17-C18-C19
37	r	301	LDZ	C22-C17-C18-C19
37	O	301	LDZ	O8-C9-N10-C11
37	n	301	LDZ	O8-C9-N10-C11
37	O	301	LDZ	O31-C9-O8-C7
37	n	301	LDZ	O31-C9-O8-C7
37	O	301	LDZ	N10-C9-O8-C7
37	O	301	LDZ	O31-C9-N10-C11
37	n	301	LDZ	O31-C9-N10-C11
34	F	501	ADP	C3'-C4'-C5'-O5'
37	N	301	LDZ	N16-C17-C18-C19
37	R	301	LDZ	N13-C14-C24-C25
37	R	301	LDZ	C15-C14-C24-C25
37	R	301	LDZ	N10-C11-C30-C31
37	n	301	LDZ	C12-C11-N10-C9
37	R	301	LDZ	C12-C11-C30-C31
37	n	301	LDZ	N10-C11-C30-C31
37	r	301	LDZ	C12-C11-C30-C31
37	o	301	LDZ	C30-C11-C12-O32
34	A	501	ADP	O4'-C4'-C5'-O5'
34	A	501	ADP	C3'-C4'-C5'-O5'
34	E	401	ADP	O4'-C4'-C5'-O5'
34	E	401	ADP	C3'-C4'-C5'-O5'
35	C	501	ATP	O4'-C4'-C5'-O5'
37	n	301	LDZ	C15-C14-C24-C25
37	n	301	LDZ	C17-C18-C19-C21
37	O	301	LDZ	C14-C24-C25-C26
37	n	301	LDZ	C11-C30-C31-C33
37	n	301	LDZ	O32-C12-N13-C14
37	n	301	LDZ	N13-C14-C24-C25
37	r	301	LDZ	N10-C11-C30-C31
37	n	301	LDZ	C11-C12-N13-C14
37	o	301	LDZ	C30-C11-C12-N13
37	O	301	LDZ	C14-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
37	n	301	LDZ	C11-C30-C31-C32
37	n	301	LDZ	C17-C18-C19-C20
37	r	301	LDZ	C17-C18-C19-C21
37	o	301	LDZ	C17-C18-C19-C20
37	o	301	LDZ	C15-C14-C24-C25
37	R	301	LDZ	C17-C18-C19-C21
37	o	301	LDZ	C17-C18-C19-C21
37	R	301	LDZ	C17-C18-C19-C20
37	r	301	LDZ	C17-C18-C19-C20
37	N	301	LDZ	C14-C24-C25-C27
37	R	301	LDZ	C14-C24-C25-C27
37	N	301	LDZ	C12-C11-C30-C31
37	n	301	LDZ	C12-C11-C30-C31
37	r	301	LDZ	C14-C24-C25-C27
37	r	301	LDZ	C14-C24-C25-C26
37	N	301	LDZ	C14-C24-C25-C26
35	C	501	ATP	C3'-C4'-C5'-O5'
37	o	301	LDZ	N13-C14-C24-C25
37	O	301	LDZ	N13-C14-C15-O34
37	o	301	LDZ	N10-C11-C12-O32
37	n	301	LDZ	N13-C14-C15-N16
37	o	301	LDZ	N13-C14-C15-O34
37	o	301	LDZ	N13-C14-C15-N16
37	n	301	LDZ	N13-C14-C15-O34
37	R	301	LDZ	C14-C24-C25-C26
37	o	301	LDZ	N10-C11-C12-N13
37	n	301	LDZ	C22-C17-N16-C15
37	n	301	LDZ	C30-C11-N10-C9
37	O	301	LDZ	C24-C14-C15-O34
37	O	301	LDZ	C24-C14-C15-N16
37	O	301	LDZ	N13-C14-C15-N16
37	n	301	LDZ	N10-C11-C12-O32
37	n	301	LDZ	N10-C11-C12-N13
37	o	301	LDZ	C11-C30-C31-C32
37	o	301	LDZ	C11-C30-C31-C33
37	O	301	LDZ	C15-C14-N13-C12
34	A	501	ADP	C5'-O5'-PA-O1A
34	E	401	ADP	C5'-O5'-PA-O2A
37	r	301	LDZ	N13-C14-C15-O34
35	D	501	ATP	PG-O3B-PB-O1B
37	r	301	LDZ	N13-C14-C24-C25
37	r	301	LDZ	C15-C14-C24-C25

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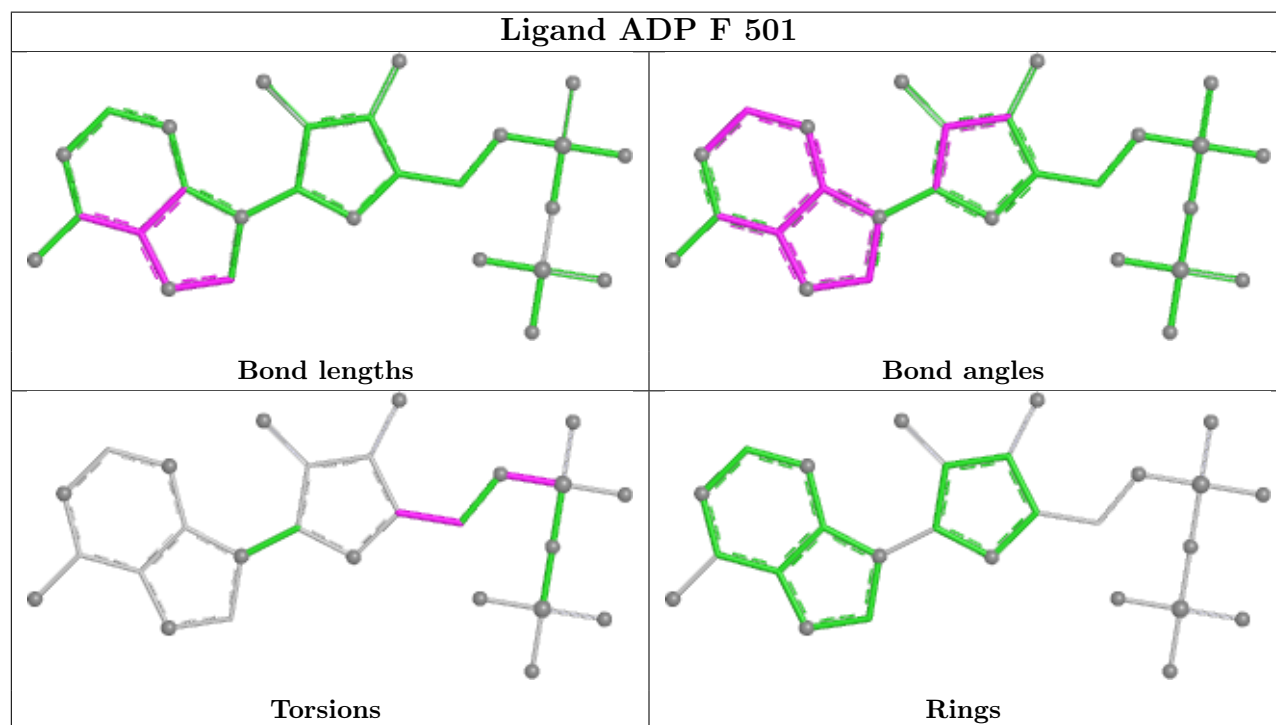
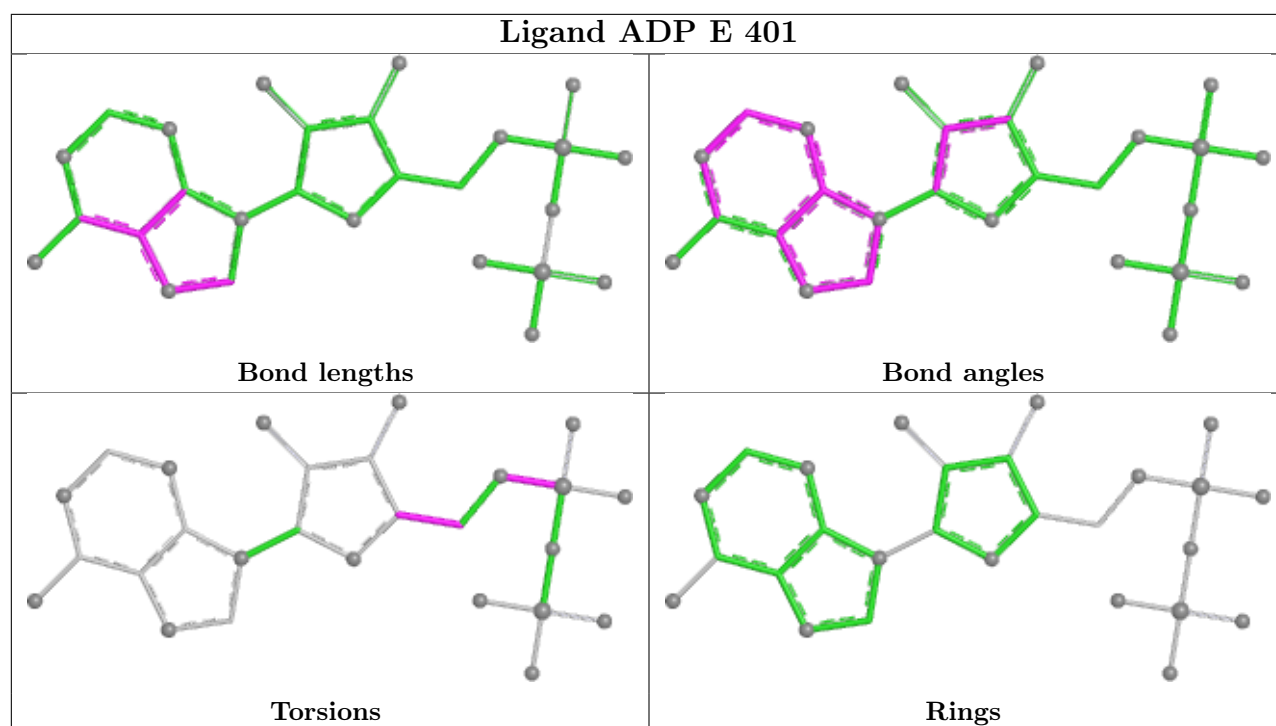
Mol	Chain	Res	Type	Atoms
37	r	301	LDZ	N13-C14-C15-N16
37	N	301	LDZ	C22-C17-N16-C15
37	N	301	LDZ	C18-C17-N16-C15
37	n	301	LDZ	C18-C17-N16-C15
37	o	301	LDZ	C18-C17-N16-C15
35	D	501	ATP	PG-O3B-PB-O2B
37	r	301	LDZ	C15-C14-N13-C12
37	n	301	LDZ	N16-C17-C18-C19
37	N	301	LDZ	C24-C14-C15-O34
37	o	301	LDZ	C24-C14-C15-O34

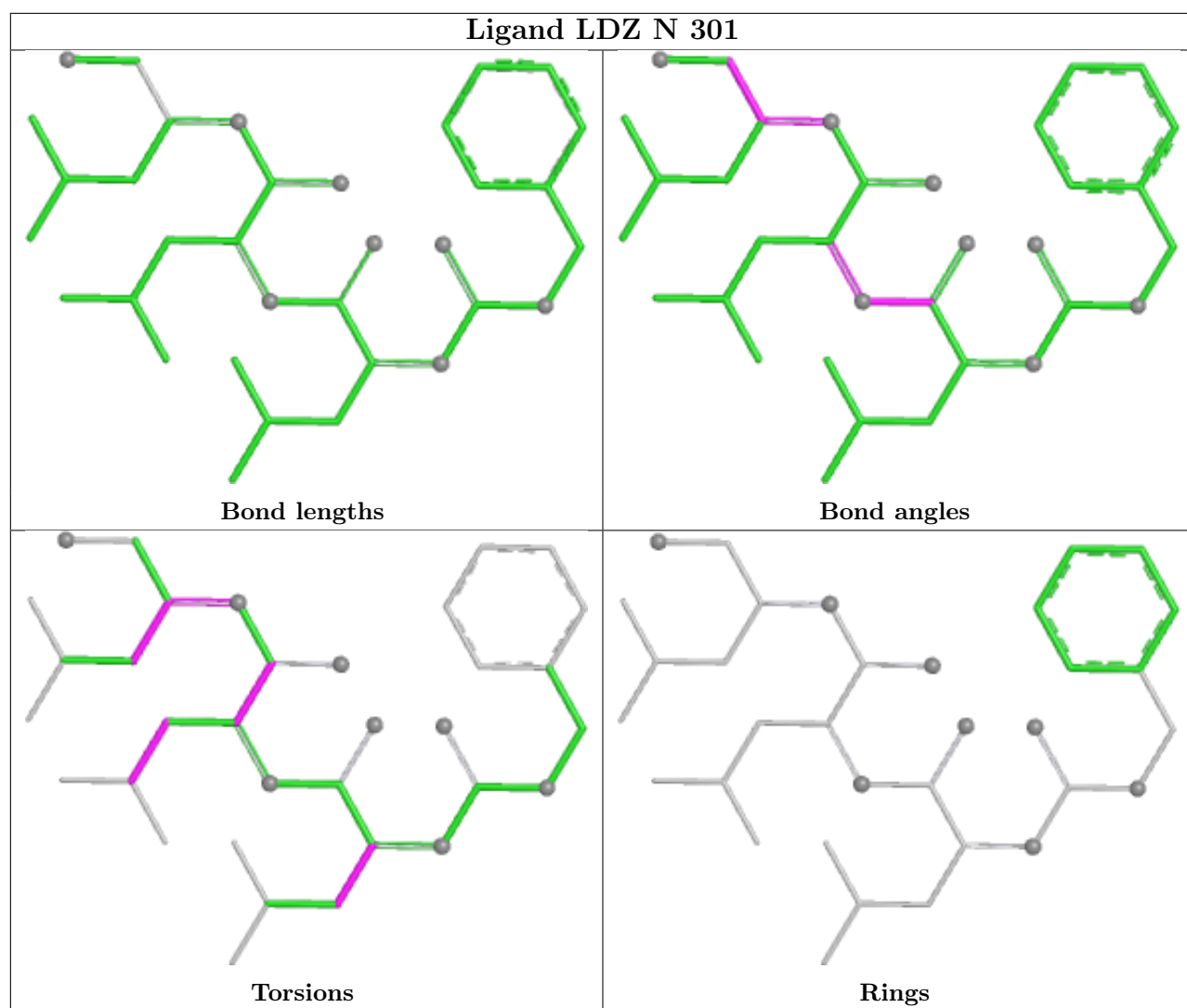
There are no ring outliers.

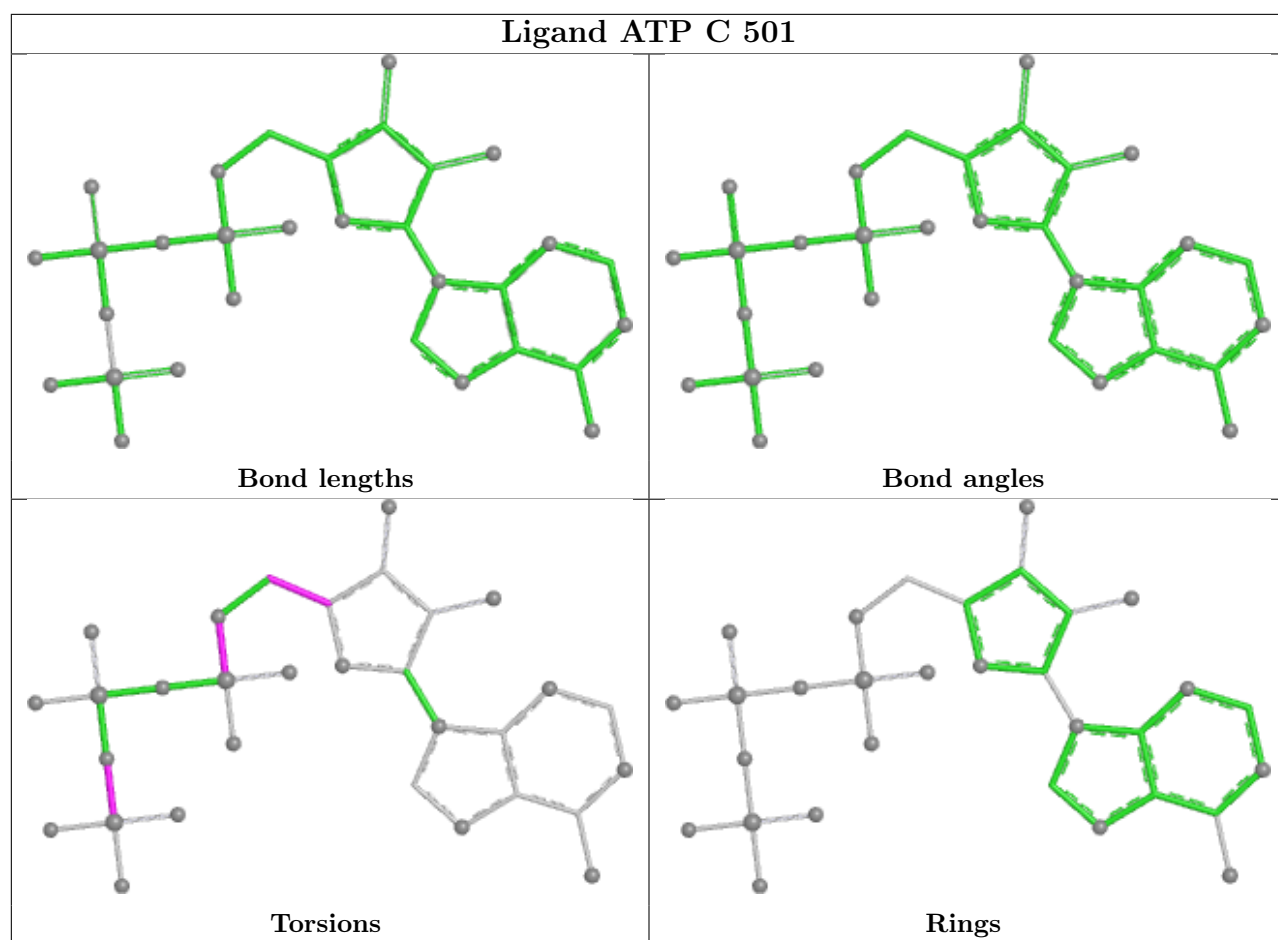
11 monomers are involved in 29 short contacts:

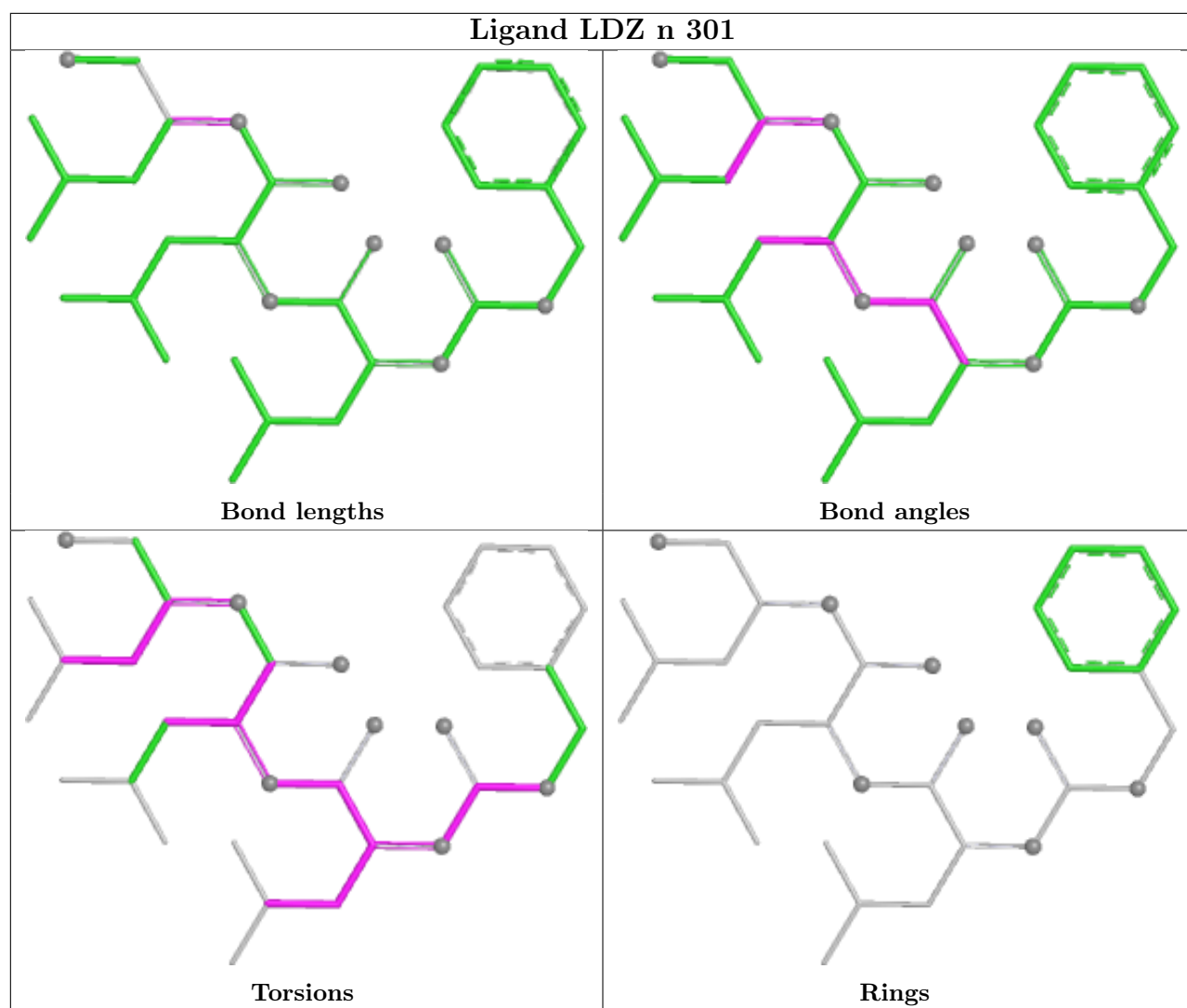
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	E	401	ADP	3	0
34	F	501	ADP	2	0
37	N	301	LDZ	2	0
37	n	301	LDZ	2	0
35	B	501	ATP	1	0
37	r	301	LDZ	1	0
37	O	301	LDZ	5	0
34	A	501	ADP	2	0
37	o	301	LDZ	4	0
37	R	301	LDZ	4	0
35	D	501	ATP	3	0

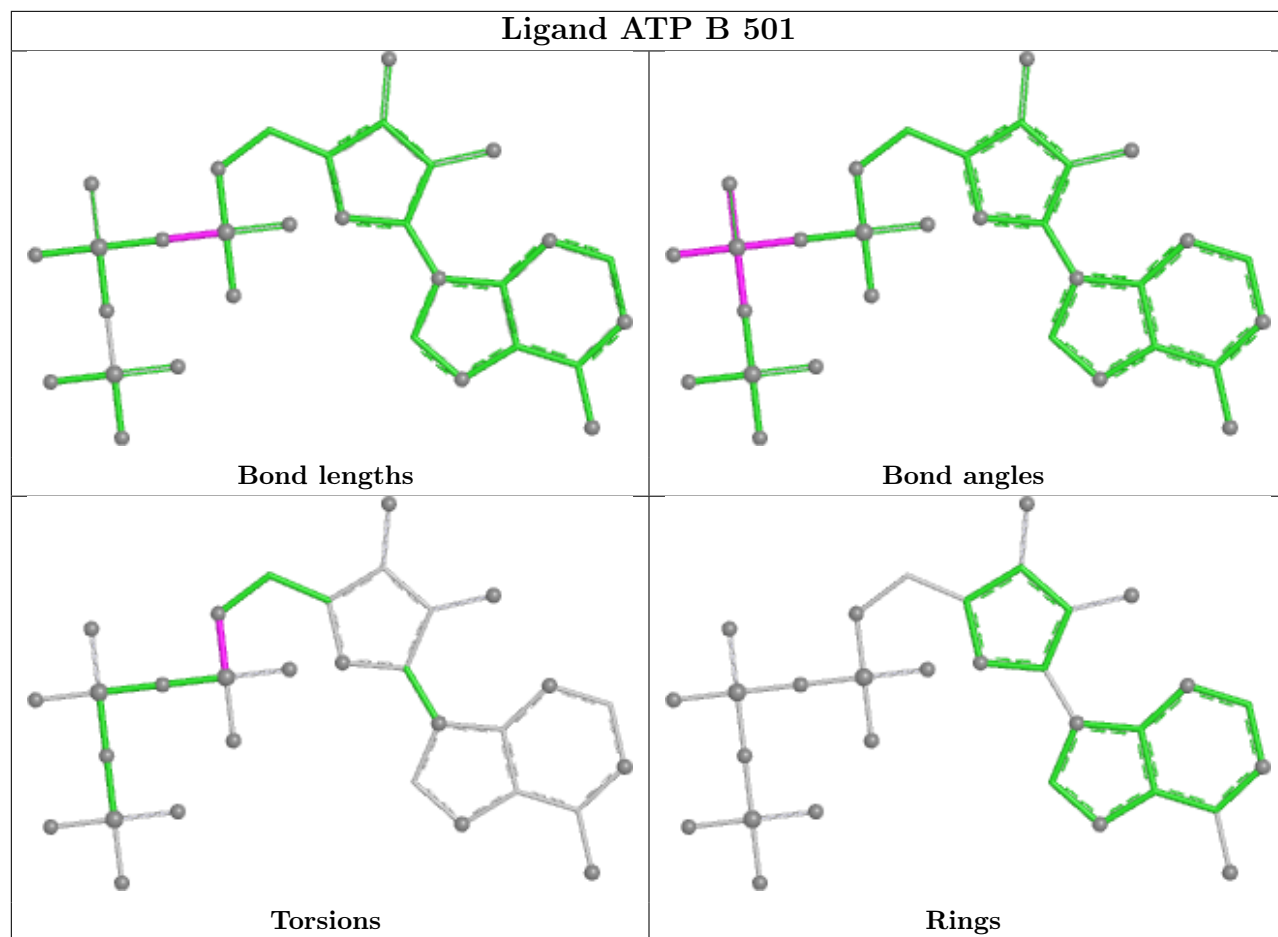
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

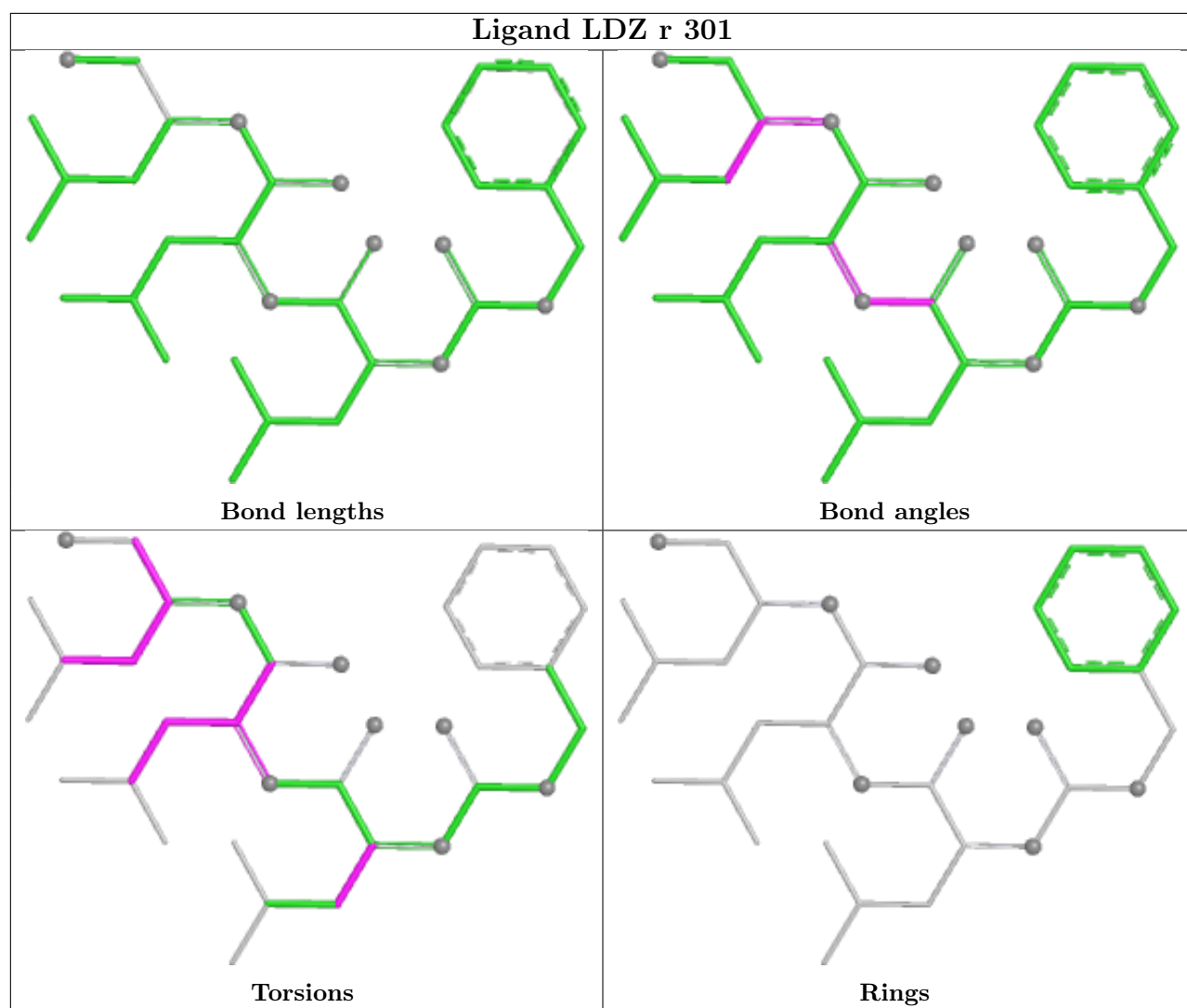


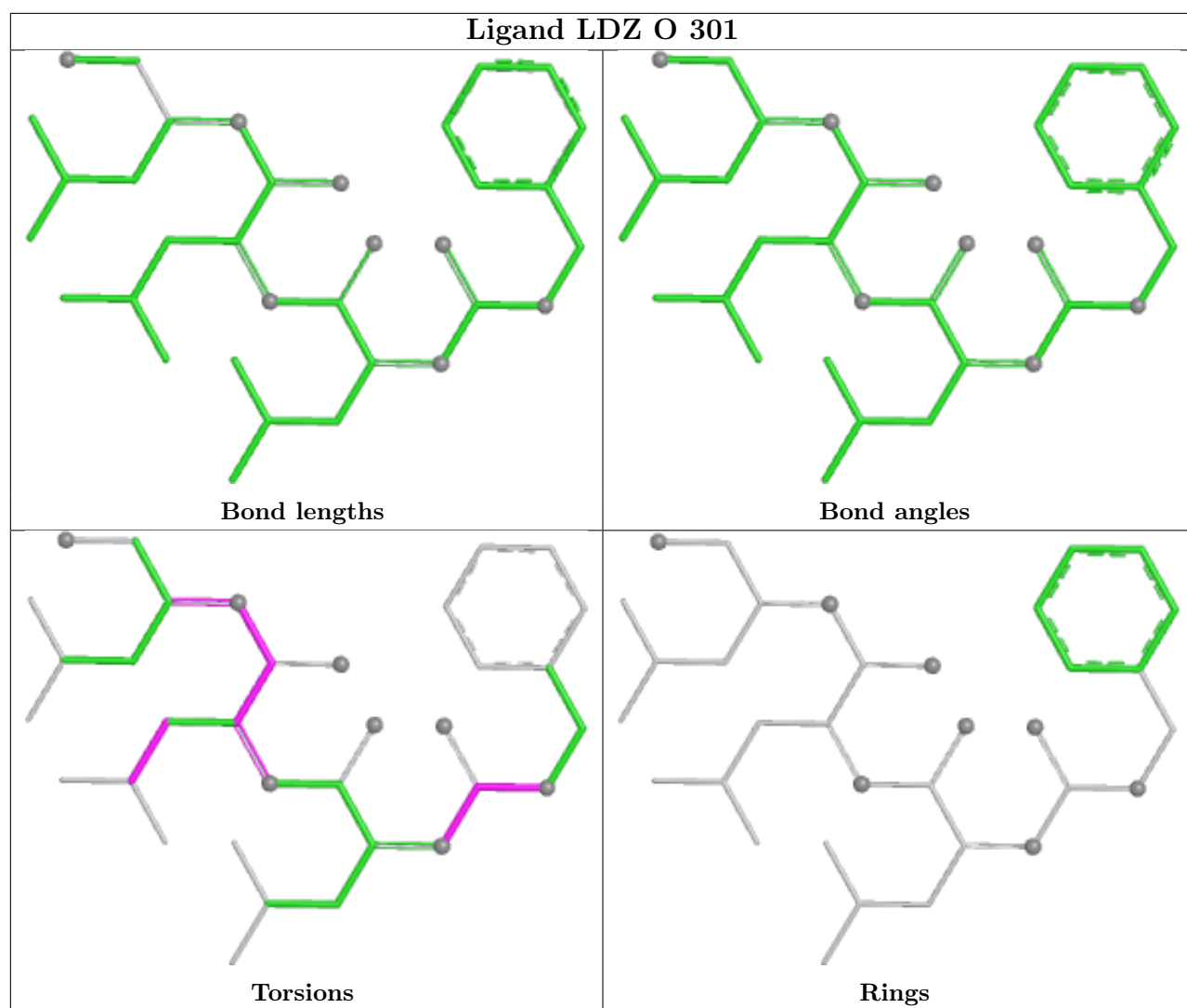


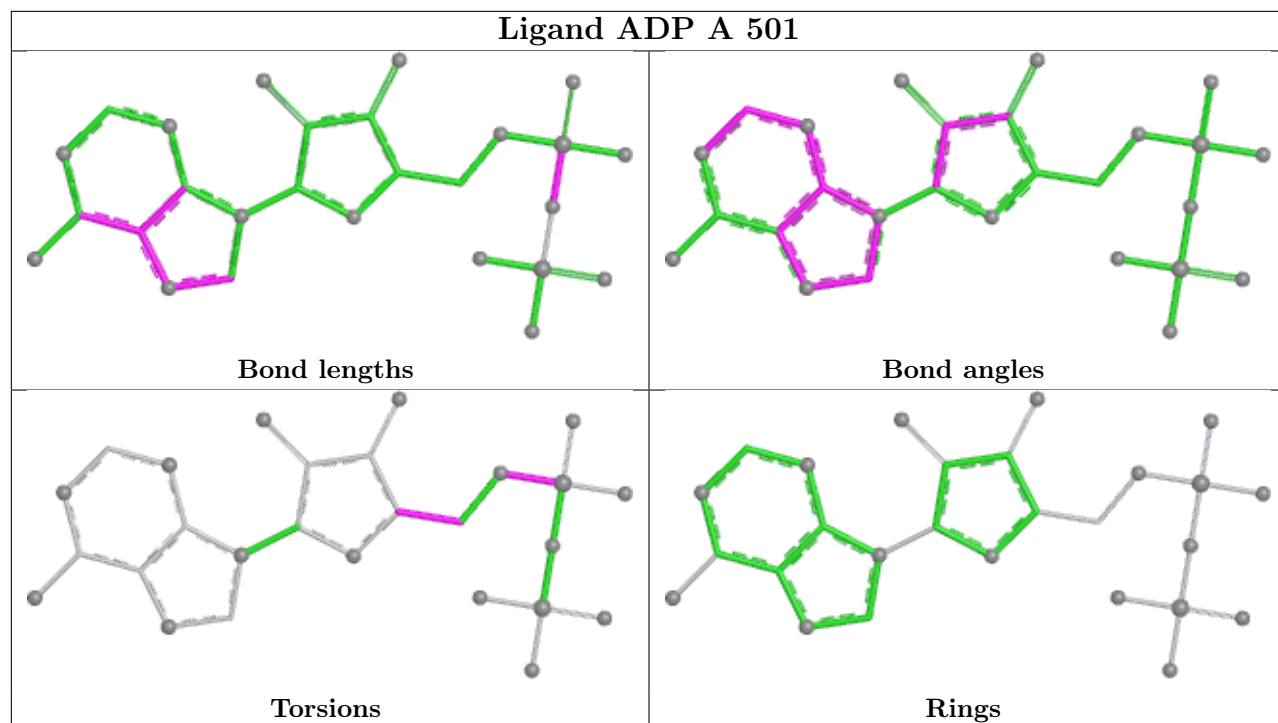


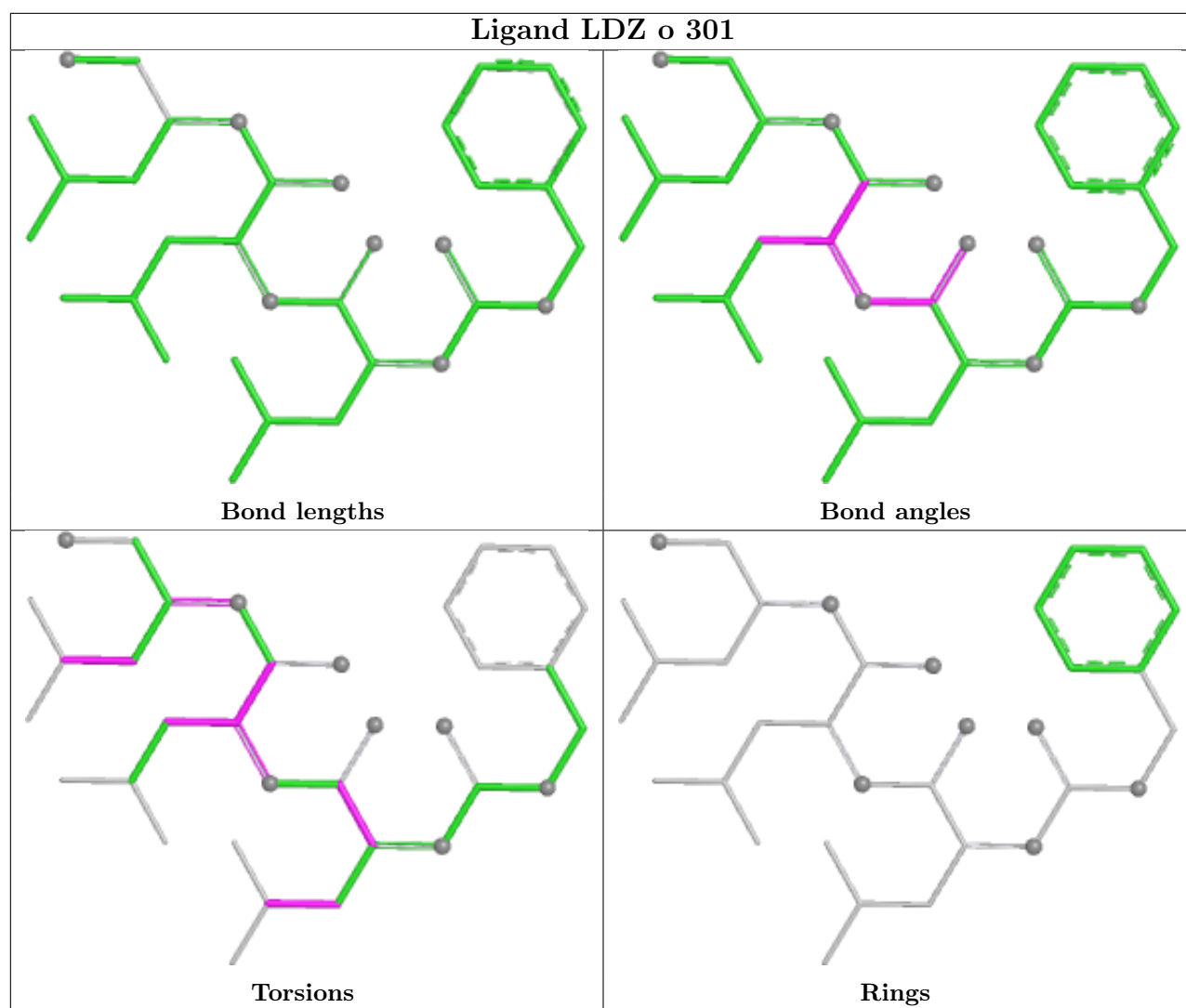


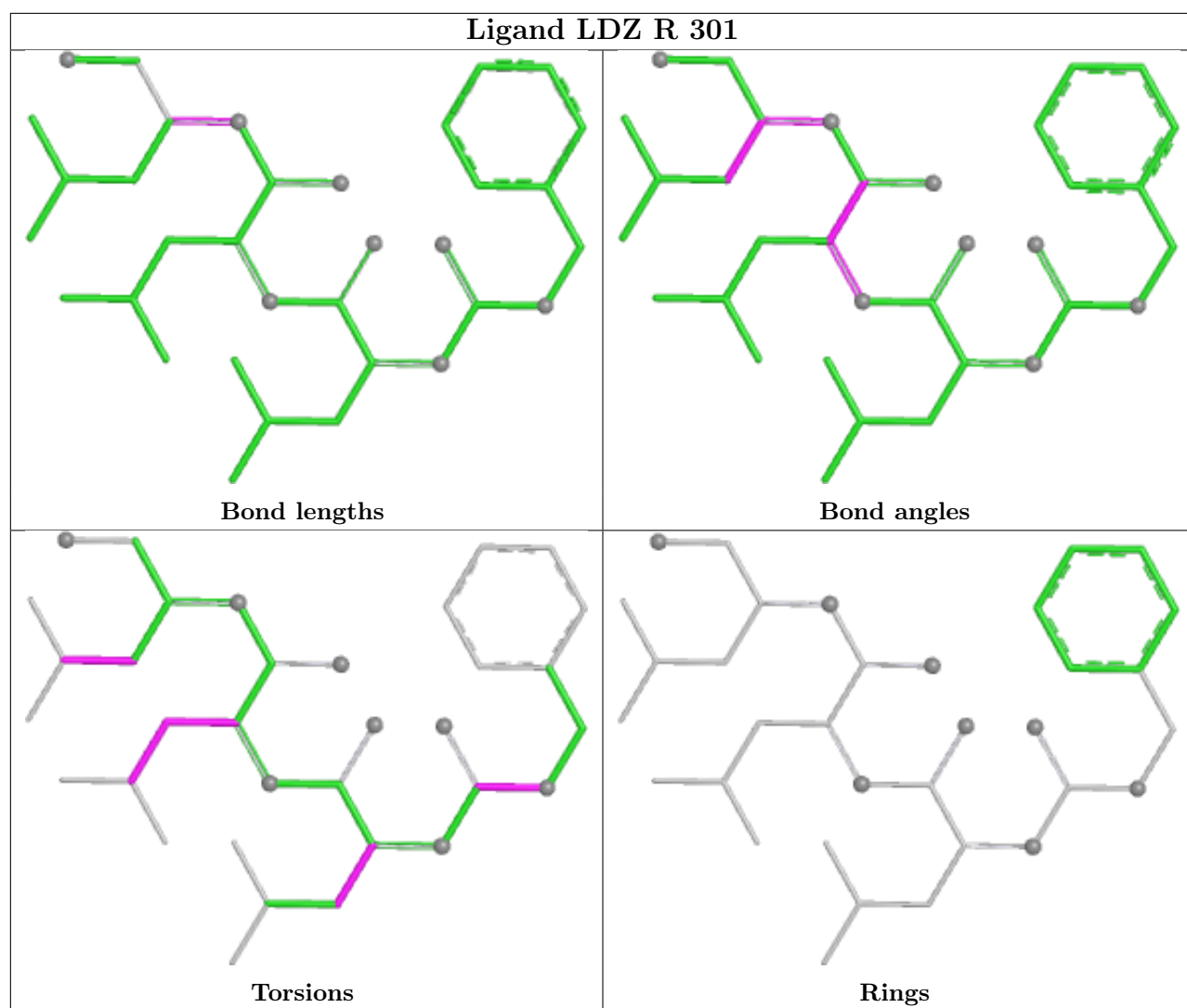


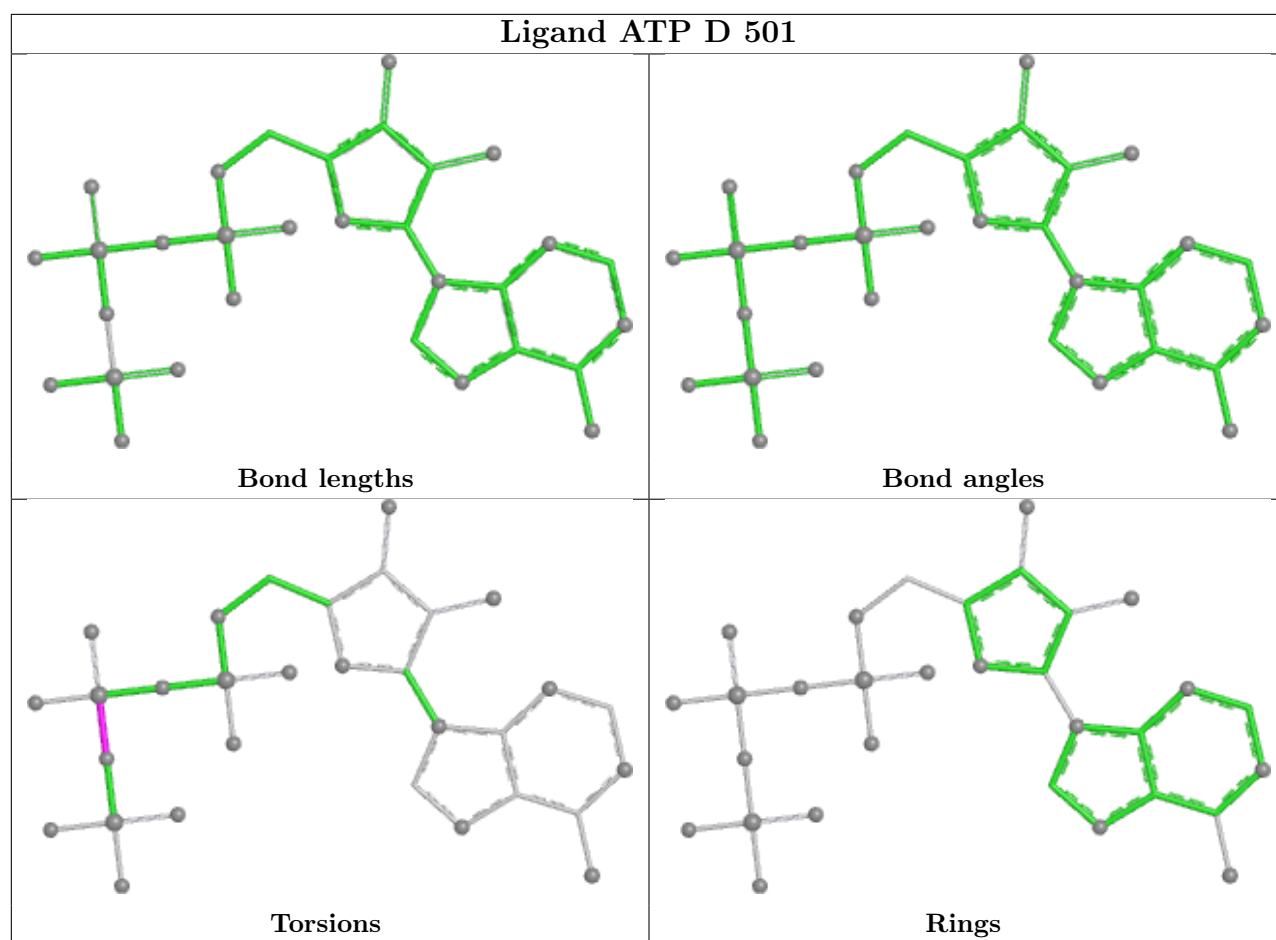












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

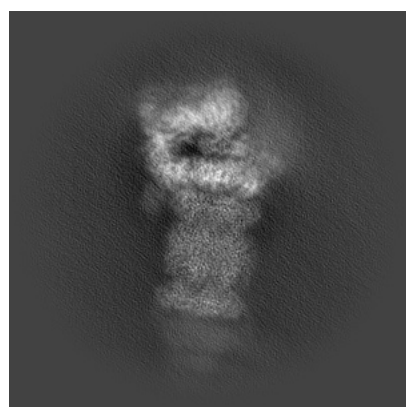
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63817. These allow visual inspection of the internal detail of the map and identification of artifacts.

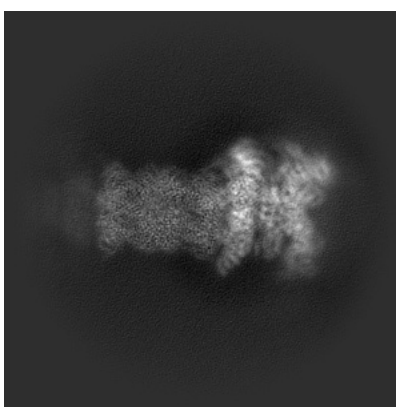
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

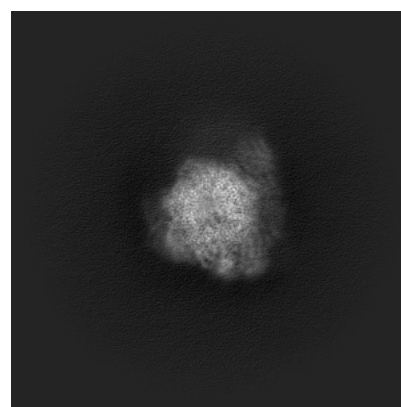
6.1.1 Primary map



X



Y

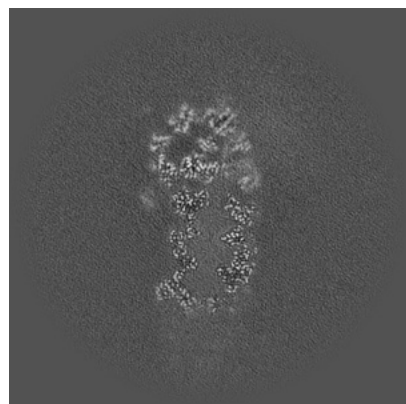


Z

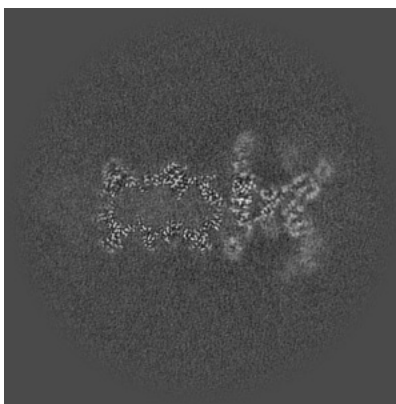
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

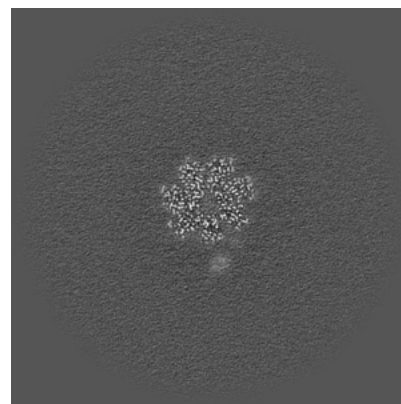
6.2.1 Primary map



X Index: 300



Y Index: 300

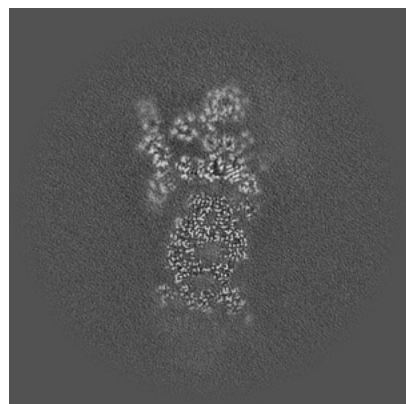


Z Index: 300

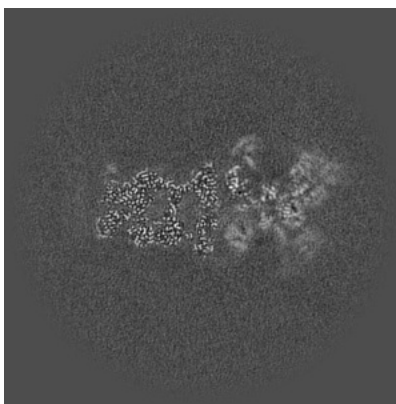
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

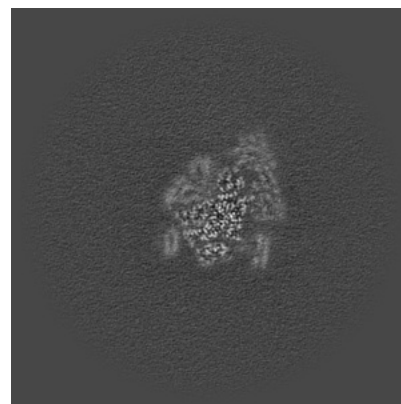
6.3.1 Primary map



X Index: 326



Y Index: 324

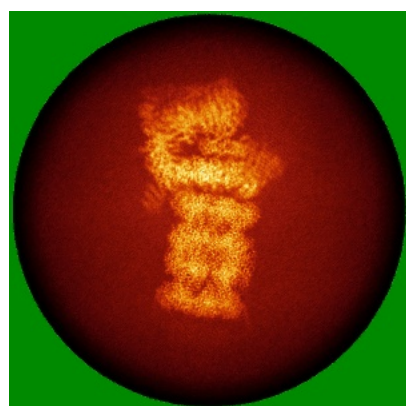


Z Index: 356

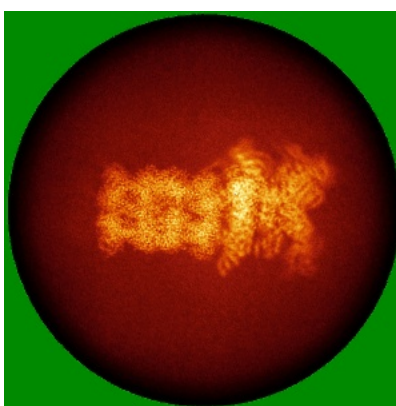
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

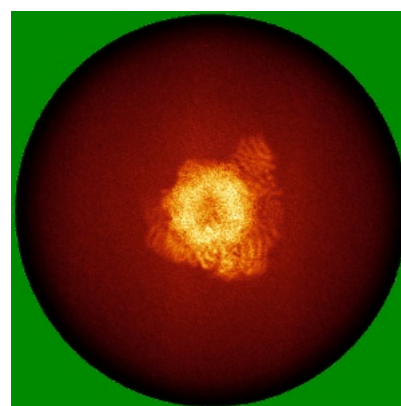
6.4.1 Primary map



X



Y

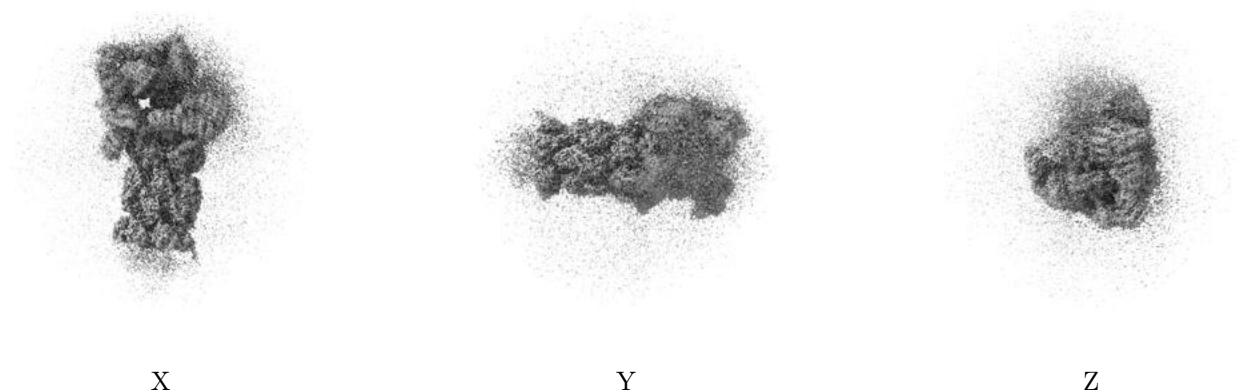


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

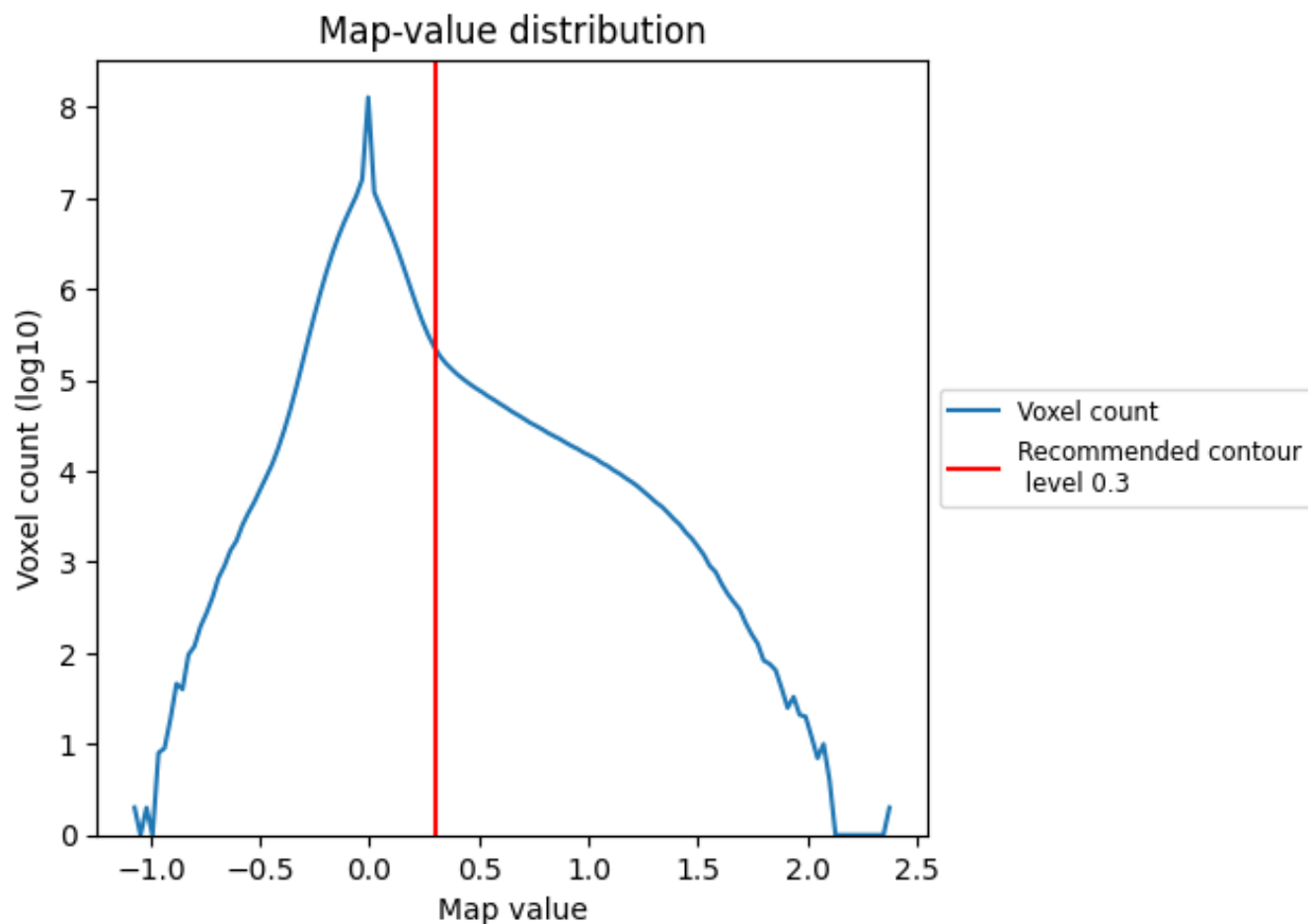
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

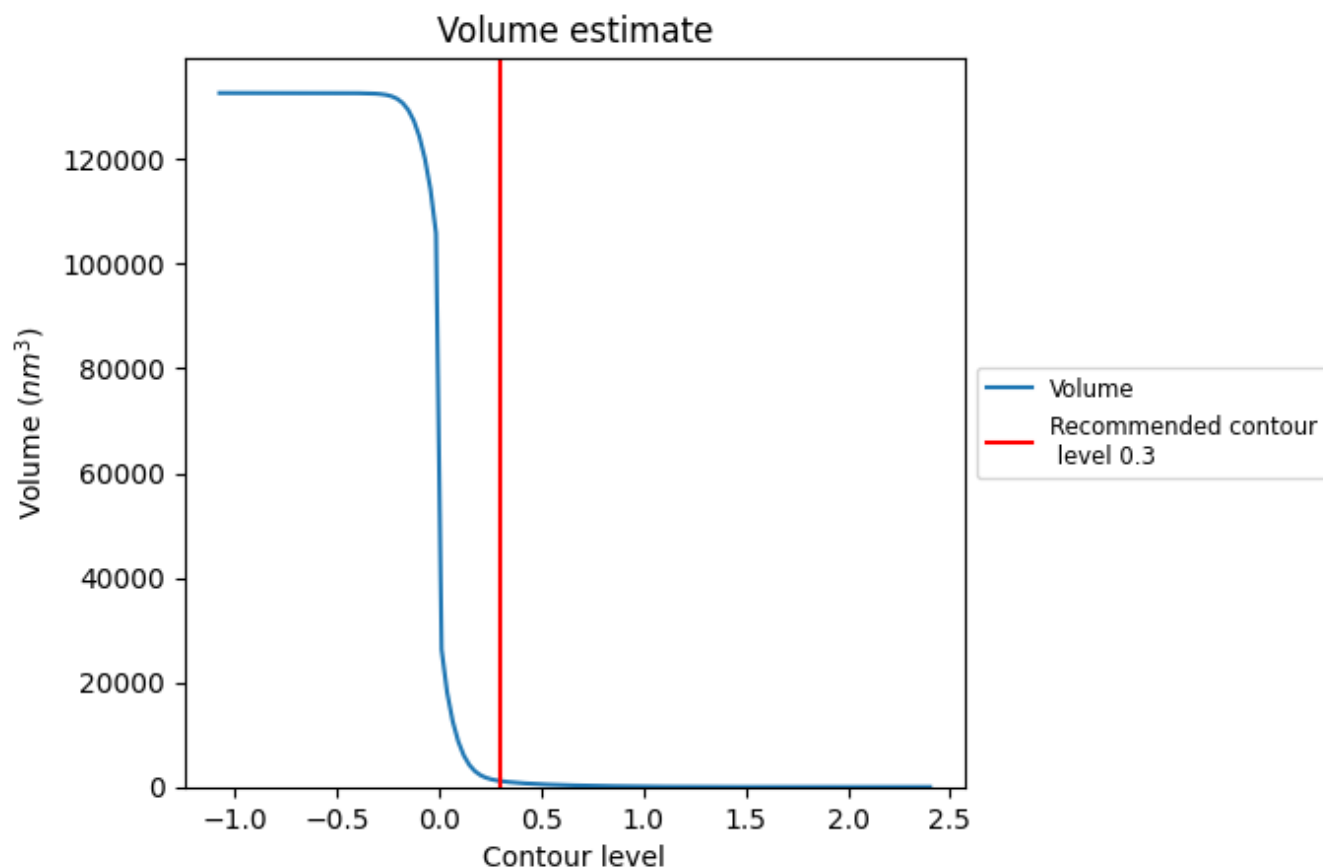
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

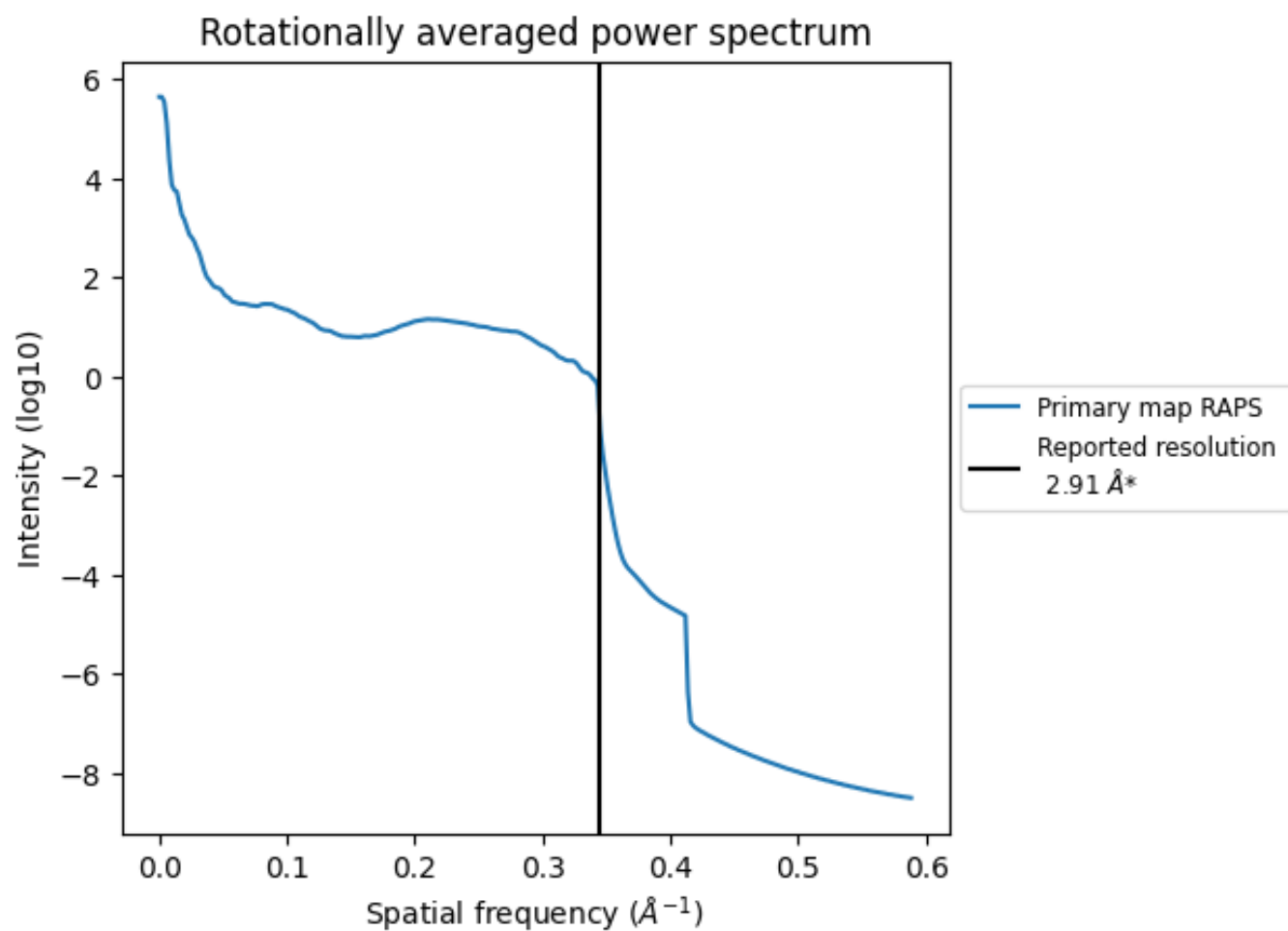
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1137 nm^3 ; this corresponds to an approximate mass of 1027 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

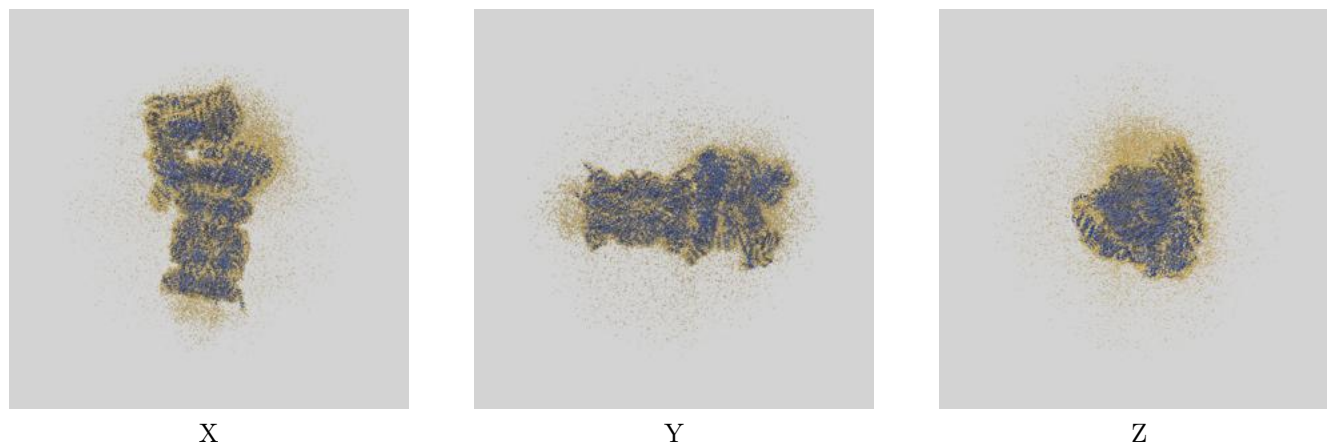
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

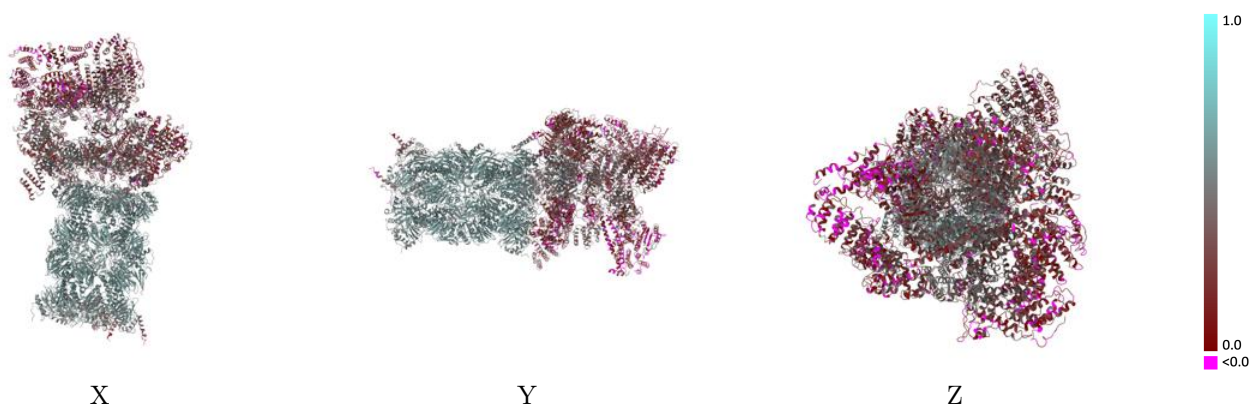
This section contains information regarding the fit between EMDB map EMD-63817 and PDB model 9U3L. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

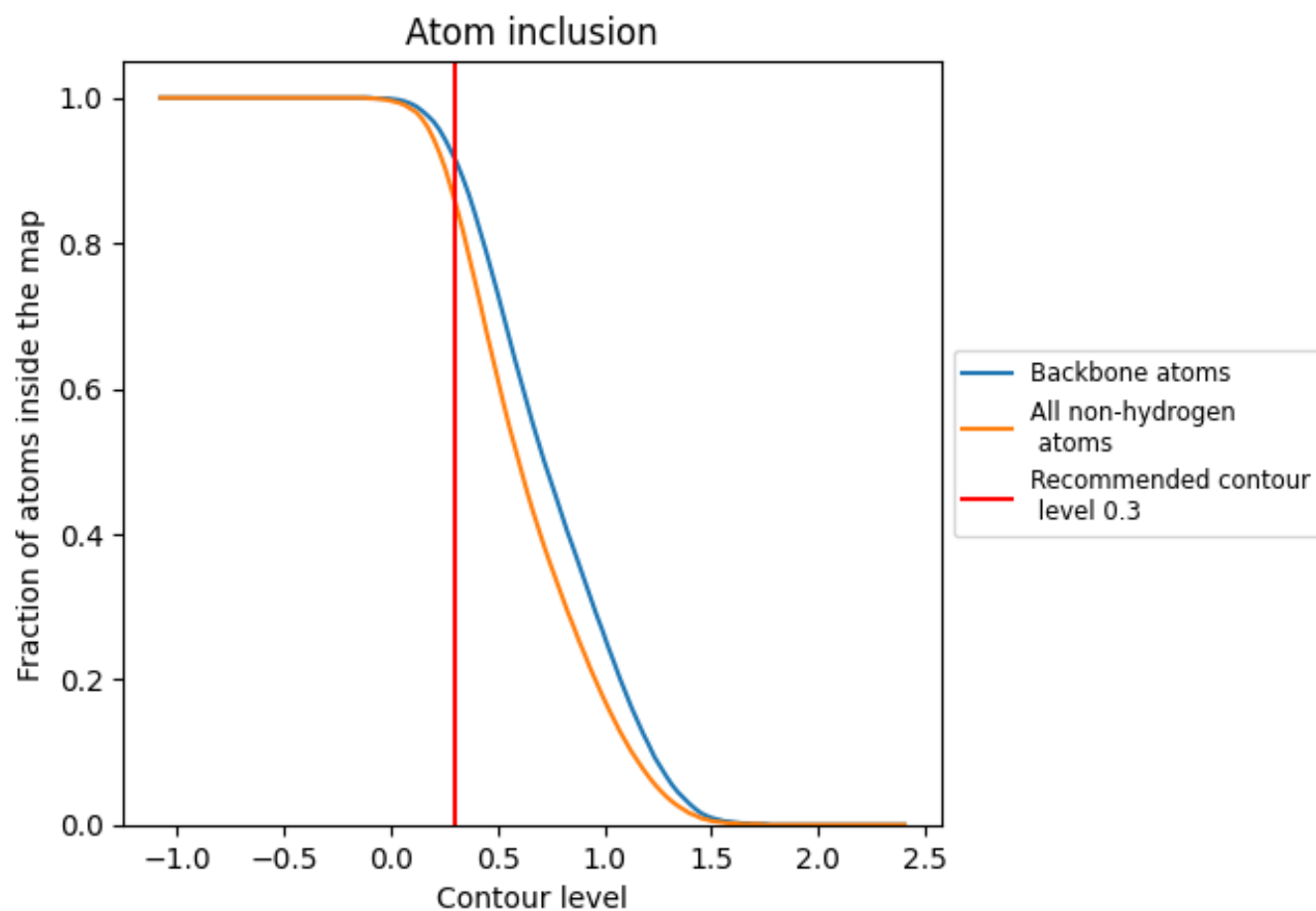


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



























The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.4110
A	 0.8260	 0.2470
B	 0.8430	 0.3650
C	 0.9010	 0.4170
D	 0.9170	 0.4150
E	 0.8190	 0.2480
F	 0.7640	 0.1870
G	 0.9320	 0.5600
H	 0.9350	 0.5660
I	 0.9080	 0.5420
J	 0.8940	 0.5270
K	 0.9090	 0.5640
L	 0.9550	 0.5840
M	 0.9250	 0.5630
N	 0.9470	 0.5880
O	 0.9210	 0.5720
P	 0.9520	 0.5850
Q	 0.9480	 0.5810
R	 0.9470	 0.5850
S	 0.9410	 0.5870
T	 0.9560	 0.5900
U	 0.7880	 0.2500
V	 0.7140	 0.2030
W	 0.8640	 0.3020
X	 0.9180	 0.3930
Y	 0.9300	 0.3820
Z	 0.8560	 0.2600
a	 0.6650	 0.1430
b	 0.5800	 0.1500
c	 0.8900	 0.3620
d	 0.5940	 0.1730
e	 0.8730	 0.2710
g	 0.9020	 0.5460
h	 0.9050	 0.5540
i	 0.8220	 0.5090



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Chain	Atom inclusion	Q-score
j	 0.8150	 0.4720
k	 0.8350	 0.5150
l	 0.8740	 0.5450
m	 0.8910	 0.5490
n	 0.9540	 0.5890
o	 0.9390	 0.5750
p	 0.9460	 0.5870
q	 0.9340	 0.5850
r	 0.9410	 0.5800
s	 0.9330	 0.5860
t	 0.9470	 0.5860
u	 0.8040	 0.2810
v	 0.9870	 0.5280