



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:06 PM UTC

PDB ID : 7ML1 / pdb_00007ml1
EMDB ID : EMD-23905
Title : RNA polymerase II pre-initiation complex (PIC2)
Authors : Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on : 2021-04-27
Resolution : 4.00 Å(reported)
Based on initial model : 5OQJ

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:

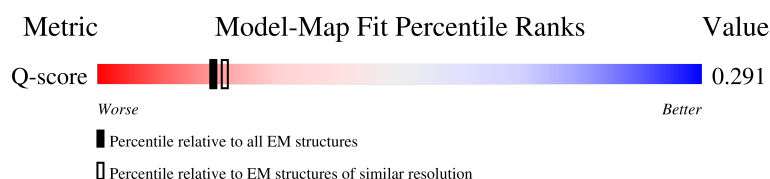
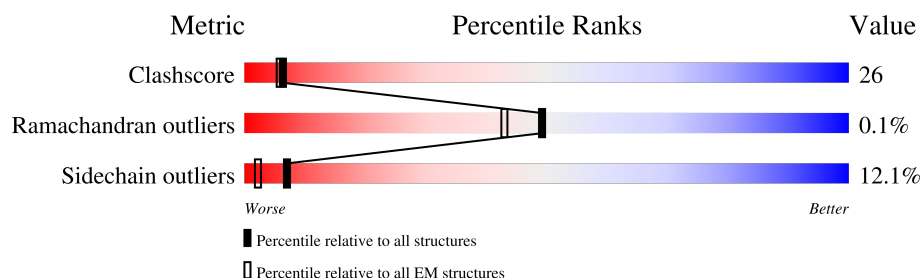
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1	542	17% 37% 27% 32%
2	4	338	9% 40% 39% 5% 16%
3	0	778	20% 32% 58% 8%
4	6	461	7% 29% 40% 7% 24%

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Mol	Chain	Length	Quality of chain
5	2	513	
6	5	72	
7	7	843	
8	3	321	
9	O	240	
10	N	57	
11	T	57	
12	A	1733	
13	B	1224	
14	C	318	
15	D	221	
16	E	215	
17	F	155	
18	G	171	
19	H	146	
20	I	122	
21	J	70	
22	K	120	
23	L	70	
24	M	345	
25	Q	735	
26	R	400	
27	U	286	
28	V	122	
29	W	482	

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Mol	Chain	Length	Quality of chain
30	X	328	25% 38% 9% 52%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	SF4	0	801	-	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 64538 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 Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	367	Total	C	N	O	S	0	0
			2411	1536	438	430	7		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

- Molecule 5 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 8 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

- Molecule 9 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 10 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	57	Total	C	N	O	P	0	0
			1178	562	227	332	57		

- Molecule 11 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	57	Total	C	N	O	P	0	0
			1159	559	191	352	57		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	1147	Total	C	N	O	S	0	0
			9132	5775	1602	1700	55		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 17 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 21 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 23 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 25 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 26 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	44	Total	C	N	O	S	0	0
			366	233	64	66	3		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	50	Total	C	N	O	S	0	0
			389	245	65	76	3		

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

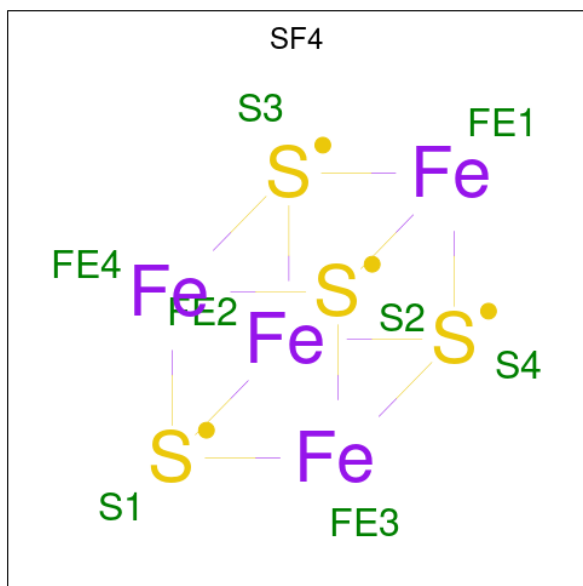
- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	4	1	Total	Zn	0
			1	1	
31	6	4	Total	Zn	0
			4	4	
31	3	2	Total	Zn	0
			2	2	
31	A	3	Total	Zn	0
			3	3	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	W	1	Total	Zn	0
			1	1	
31	X	1	Total	Zn	0
			1	1	

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
32	0	1	Total	Fe	S	0
			8	4	4	

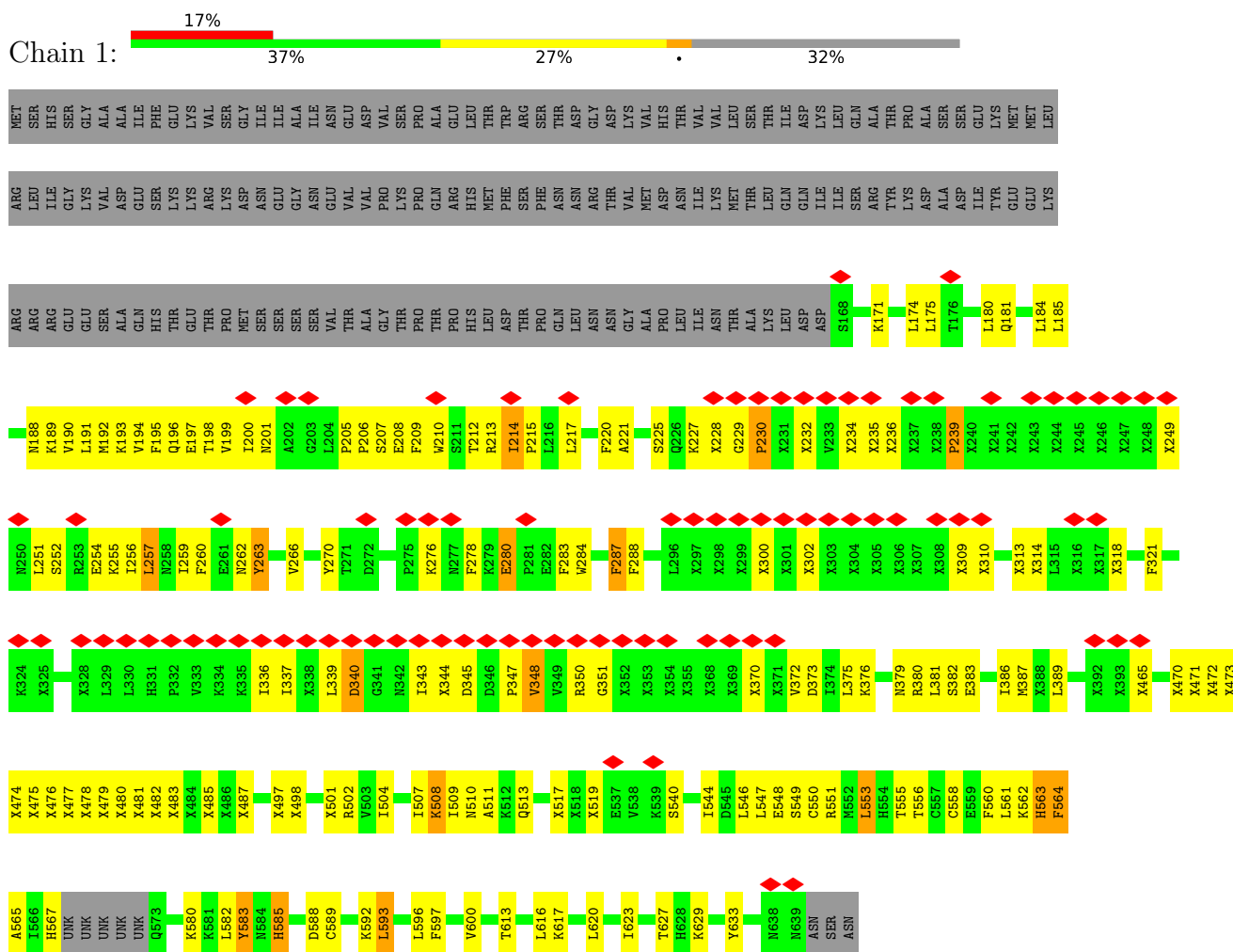
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

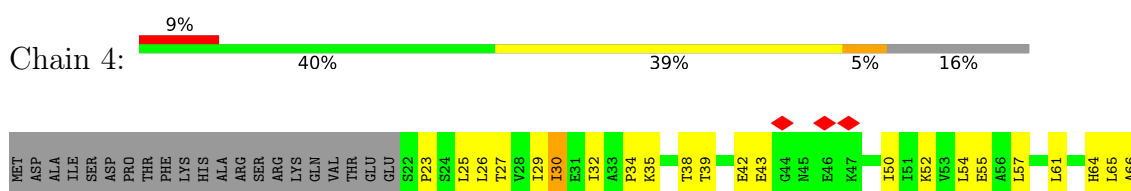
3 Residue-property plots

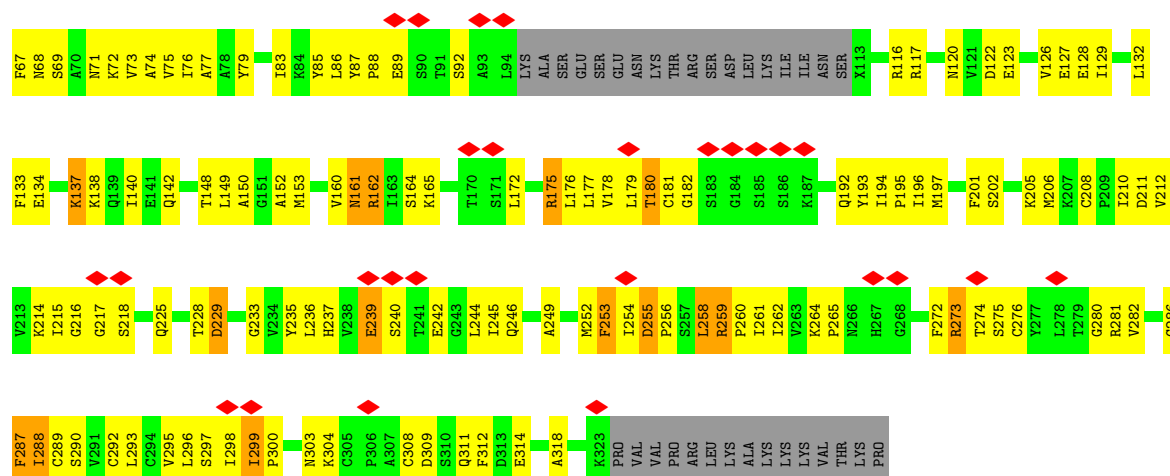
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tfb1

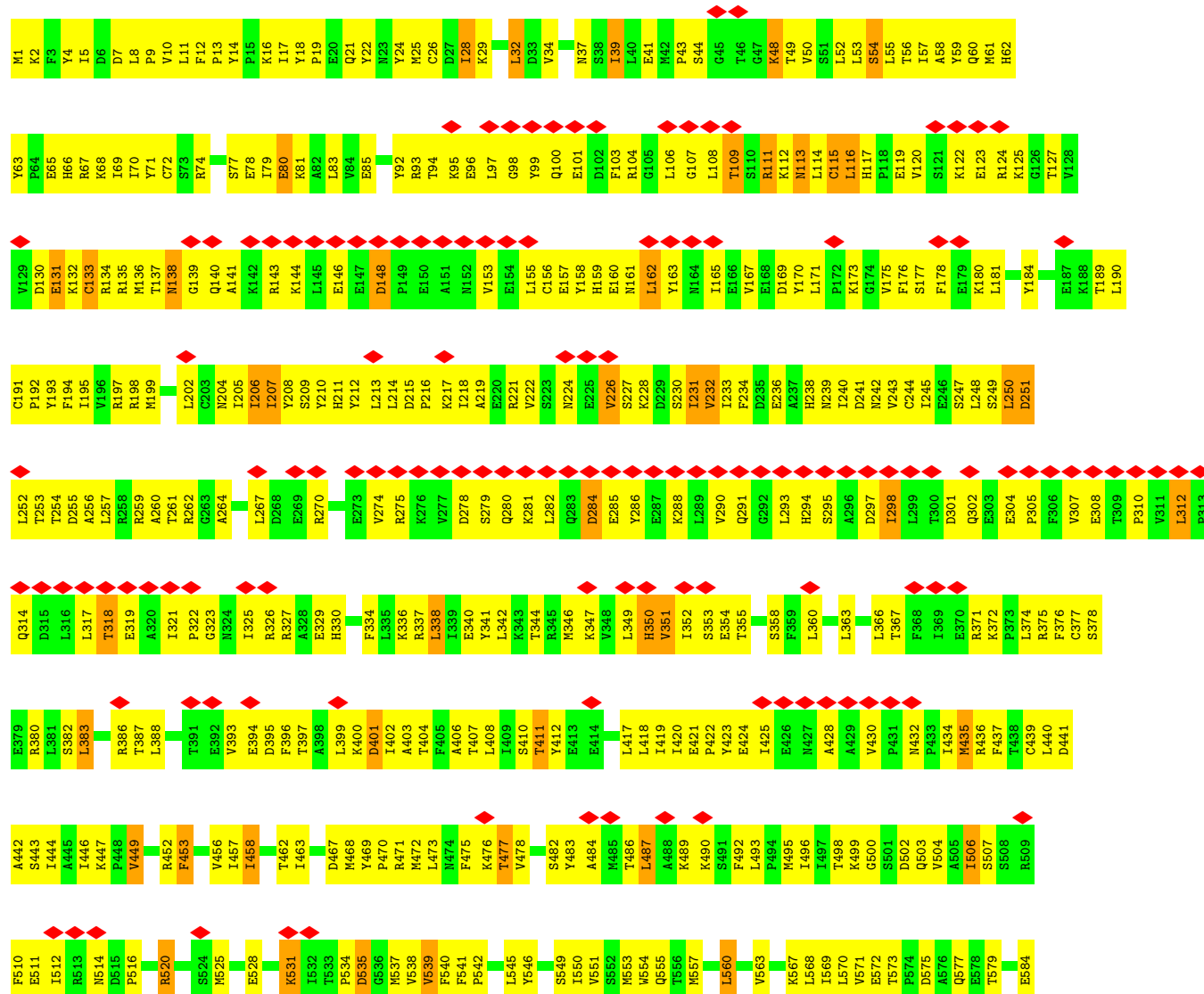


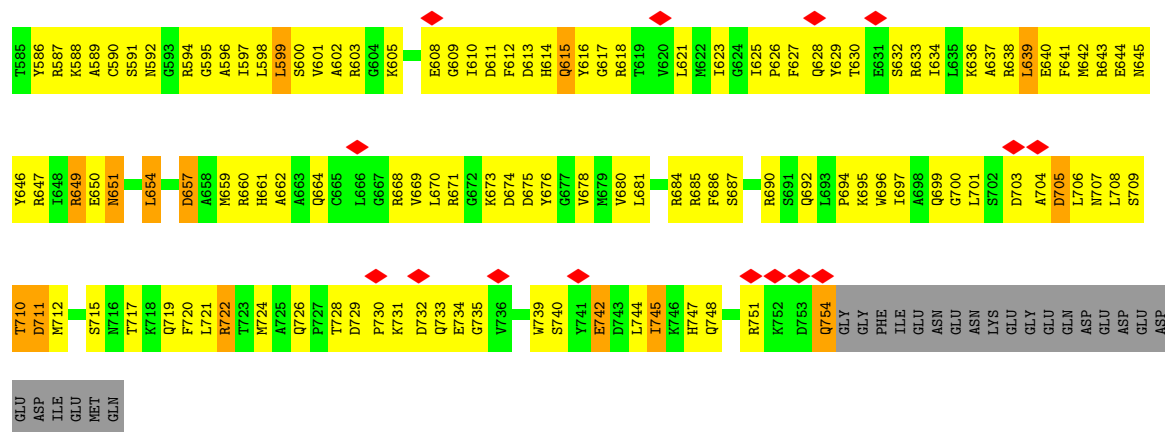
• Molecule 2: General transcription and DNA repair factor IIH subunit TFB4



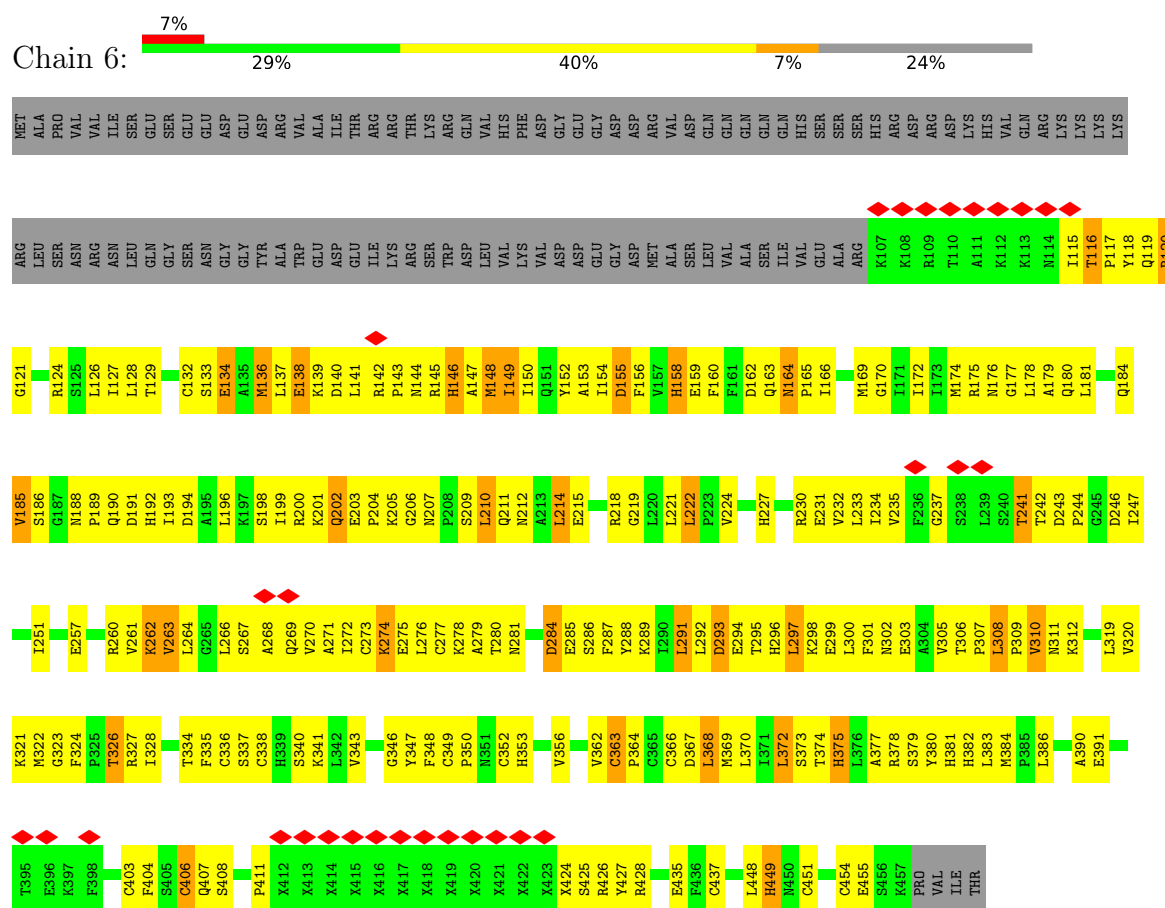


• Molecule 3: General transcription and DNA repair factor IIH helicase subunit XPD

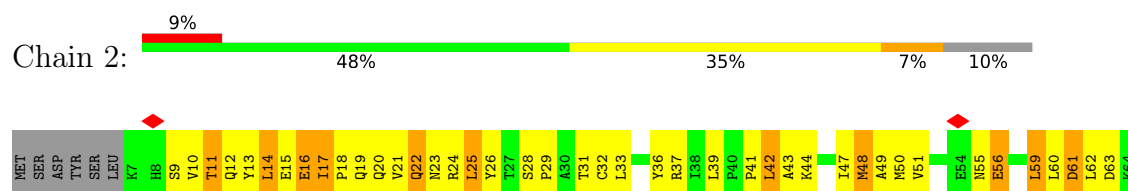


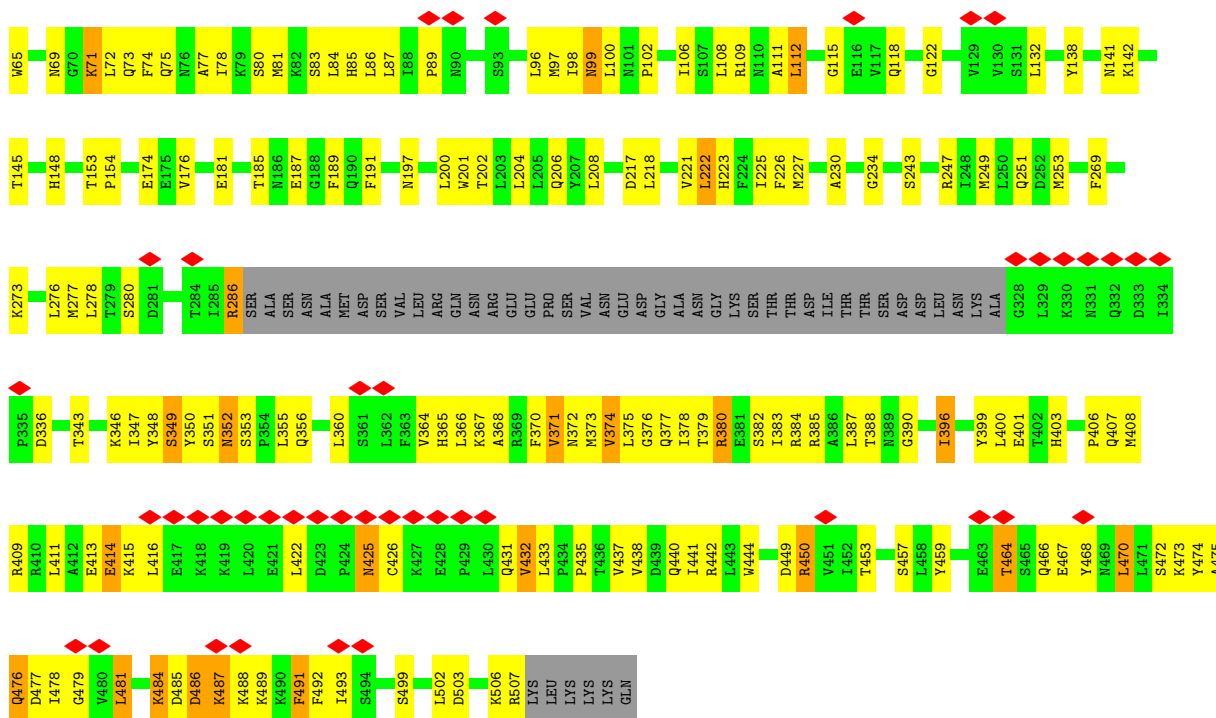


• Molecule 4: General transcription and DNA repair factor IIH subunit SSL1

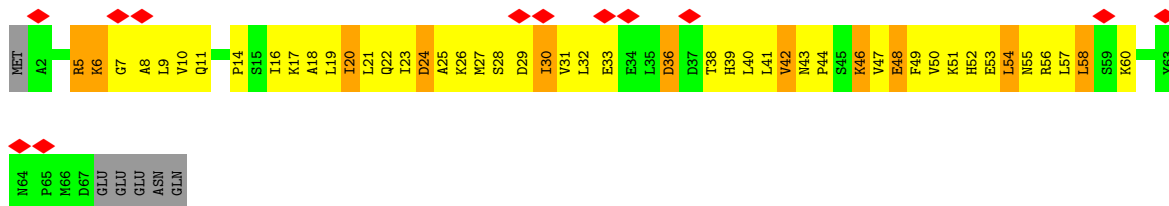


• Molecule 5: RNA polymerase II transcription factor B subunit 2

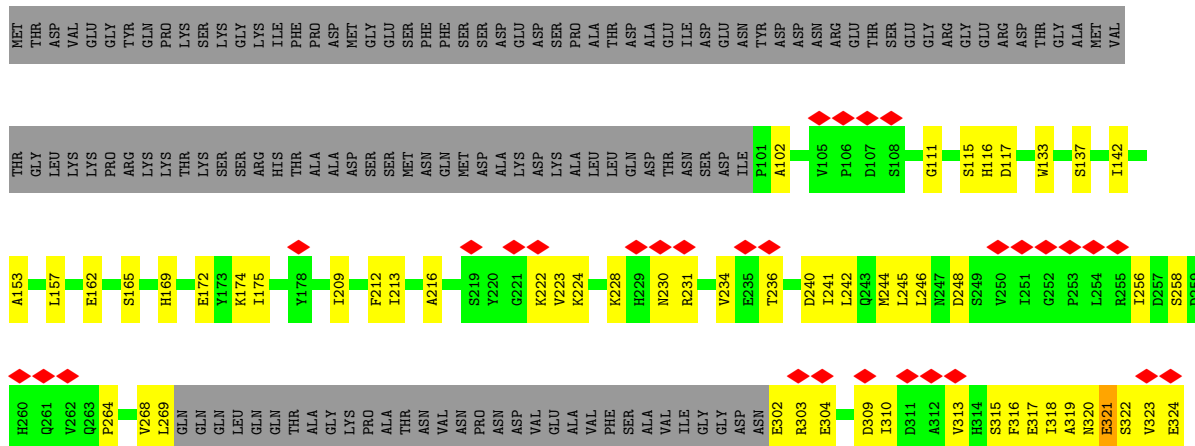
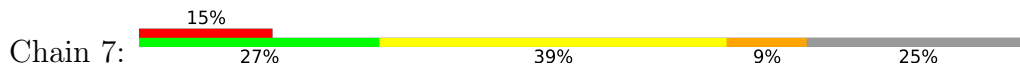




- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

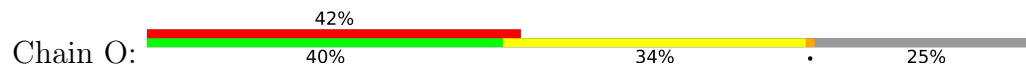


- Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB



THR
GLU
ALA
PHE
MET
GLY
LEU
GLY
CYS
VAL
ILE
SER
GLU
LEU

• Molecule 9: TATA-box-binding protein



MET
ALA
ASP
GLU
GLU
ARG
LYS
PHE
GLU
ASN
ALA
LYS
ILE
VAL
PHE
ASP
PRO
ASN
THR
ARG
GLN
VAL
TRP
GLU
ASN
GLN
ASN
ARG
ASP
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THR
LYS
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ALA
THR
THR
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SER
GLU
GLU
ASP
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ALA
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SER
GLU
LYS
ASP
THR
SER
ALA
THR

S61
G62
I63
V64
P65
T66
L67
Q68
N69
I70
V71
A72
T73
Y74
T75
L76
G77
C78
R79
L80
D81
L82
K83
T84
V85
A86
L87
A88
A89
R90
N91
A92
E93
Y94
N95
P96
K97
R98
A101
V102
I103
M104
I105
I106
I107
E108
K109
K110
T111
T112
A113
L114
I115
F116
A117
S118
G119
K120
M121

V122
V123
T124
G125
A126
K127
S128
E129
D130
P131
D132
L133
K134
A135
S136
R137
K138
Y139
A140
R141
I142
I143
Q144
K145
I146
F147
G148
A149
A150
K151
F152
T153
D154
F155
K156
I157
Q158
N159
I160
V161
G162
S163
C164
D165
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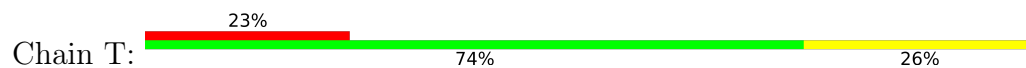
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I206
F207
V208
S209
G210
K211
I212
V213
L214
T215
Q219
R220
E221
E222
I223
Y224
Q225
A226
F227
E228
A229
I230
V231
P232
V233
L234
S235
E236
F237
R238
K239
M240

• Molecule 10: non-template strand DNA



A2
A3
A4
A5
A6
A7
A8
A9
A10
A11
G12
G13
C14
G15
C16
G17
T20
A21
A22
A23
A24
A25
A26
G27
T28
T29
C30
G31
A32
A33
T34
G35
T36
C37
G38
C39
G40
A41
A42
T43
T44
C45
G46
G47
G50
T51
T55
A56
C57
A58

• Molecule 11: template strand DNA



T108
C120
T124
A130
C132
T133
T134
G135
A136
A137
A138
A144
A145
G150
C151
G152
C153
C154
T155
T156
T157
T158
T159
T160
T161
T162
T163
T164

• Molecule 12: DNA-directed RNA polymerase subunit

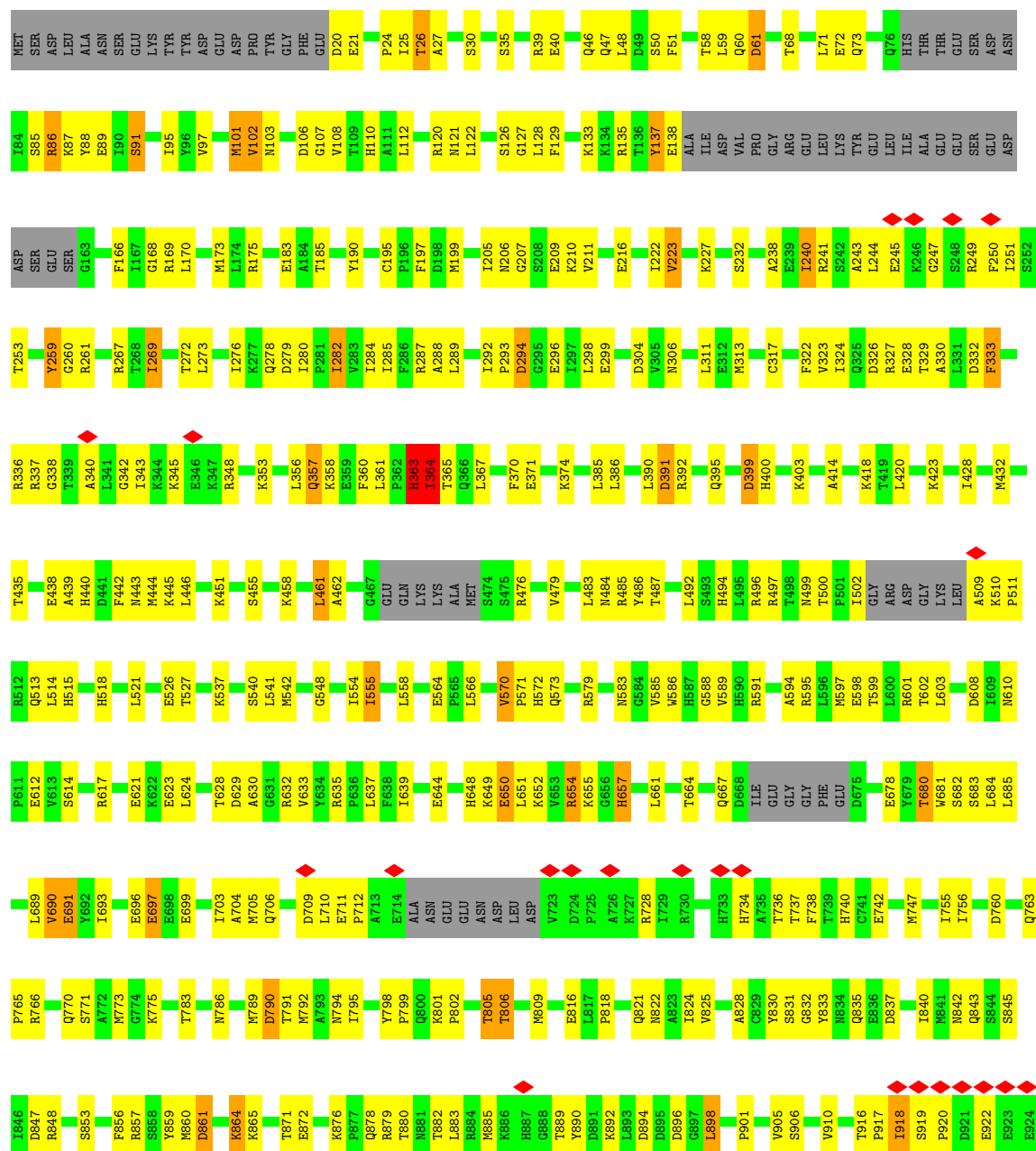


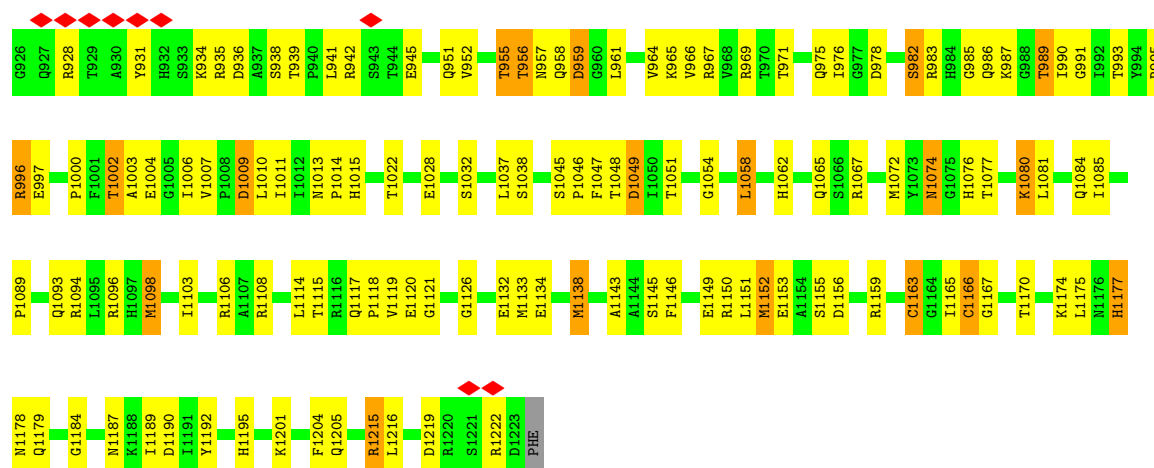
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E26
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R28
A29
I30
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D42
T46
R47
A48
K49
L53
N54
D55
L58
G59
S60
I61
D62
L65
K66
T69
C70
Q71
E72
G73
M74
N75
E76
C77
P78
G79
H80
F81
I84
K88
P89
V90

F91
F95
V106
G107
M108
H109
L114
E120
R123
Q124
I128
K129
D130
S131
K132
R133
R134
T140
L141
C142
K143
T144
K145
M146
V147
C148
E149
T150
D151
V152
P153
S154
ASP
ASP
PRO
THR
GLN
LEU
SER
R164
G165
G166
C167
T170
Q171
T172
T173
I174
R175
K176

D177
L181
V182
G183
S184
H185
K186
K187
ASP
ARG
ALA
THR
GLY
ASP
ALA
ASP
GLU
P197
E198
L199
R200
V201
L202
S203
E205
E206
I207
L208
N209
I210
K211
K212
H213
V216
K217
D218
F219
S221
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L239

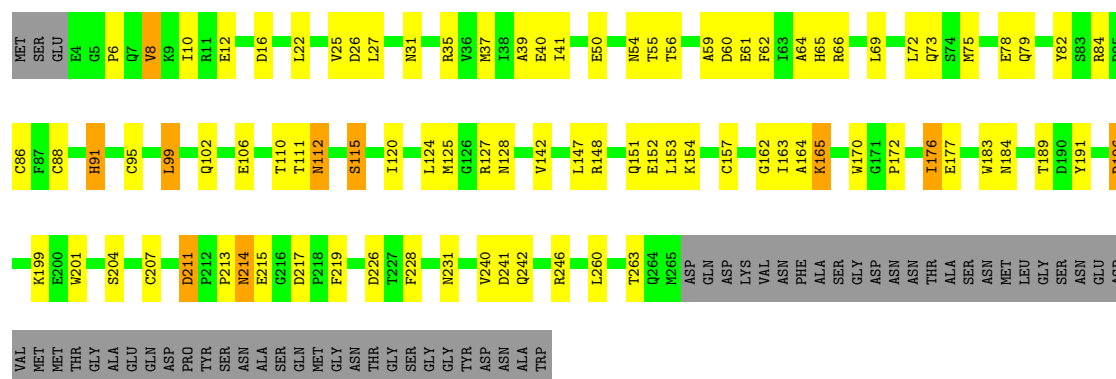






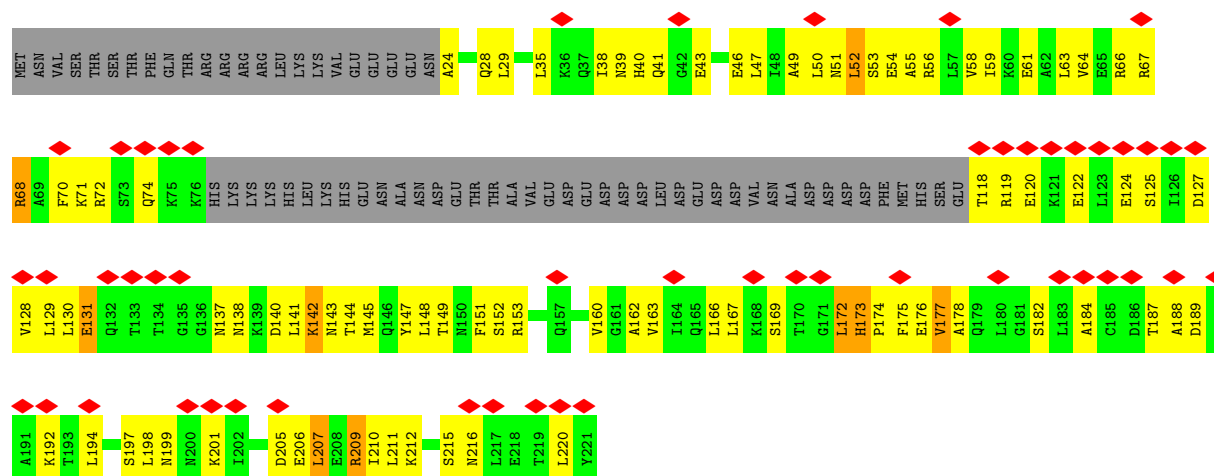
• Molecule 14: DNA-directed RNA polymerase II subunit RPB3

Chain C: 54% 25% 18%

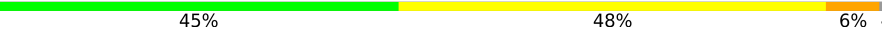


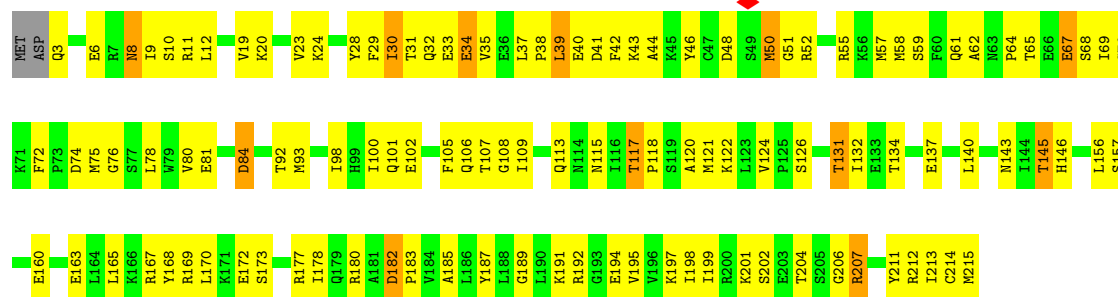
• Molecule 15: DNA-directed RNA polymerase II subunit RPB4

Chain D: 23% 30% 37% 29%



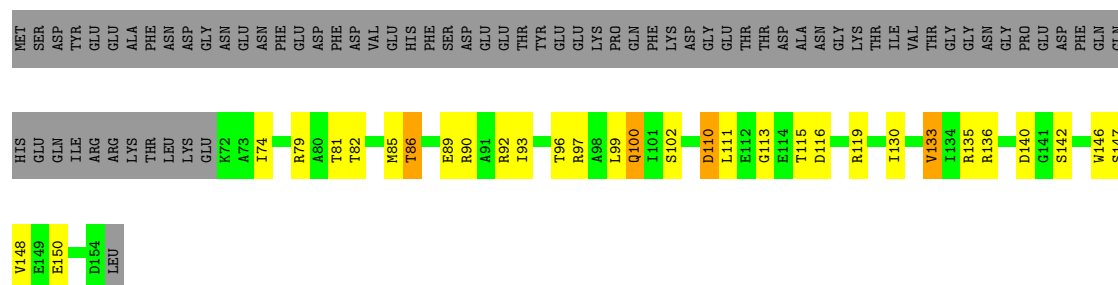
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



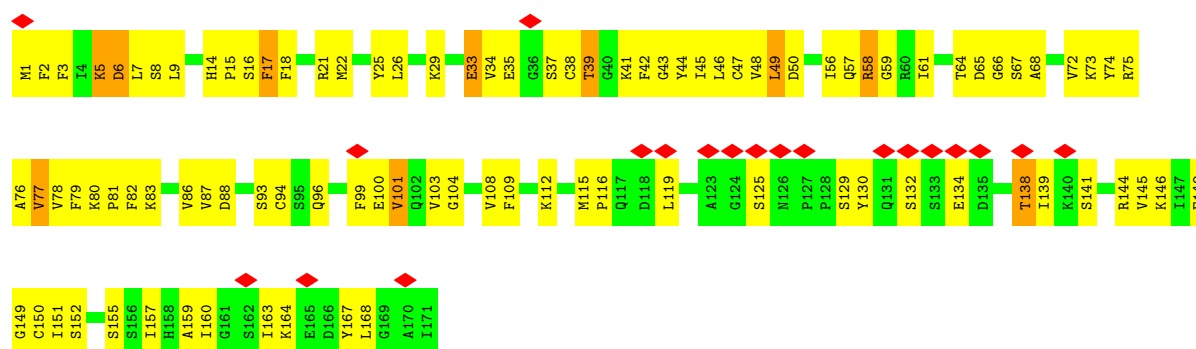
- Molecule 17: DNA-directed RNA polymerases I,II,and III subunit RPABC2

Chain F: 



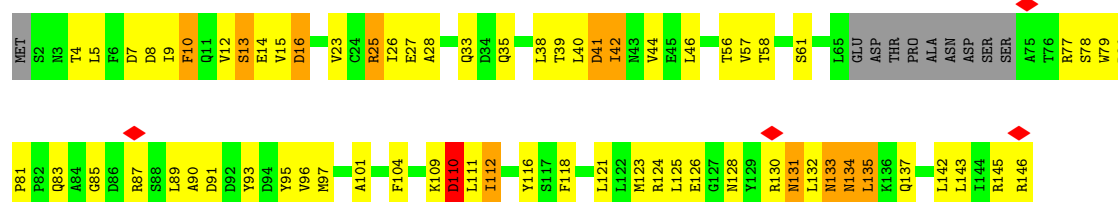
- Molecule 18: DNA-directed RNA polymerase II subunit RPB7

Chain G: 

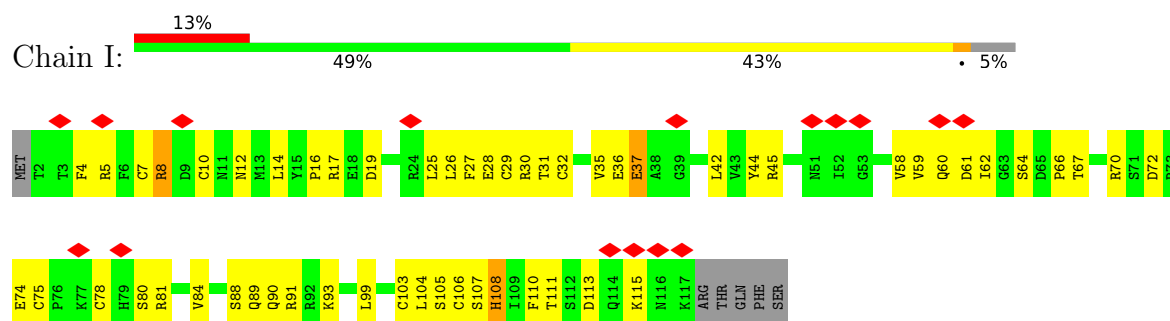


- Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC3

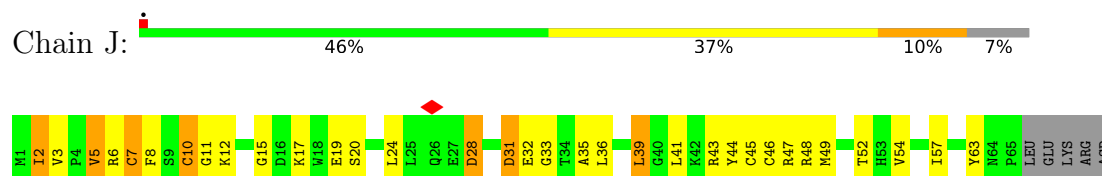
Chain H: 



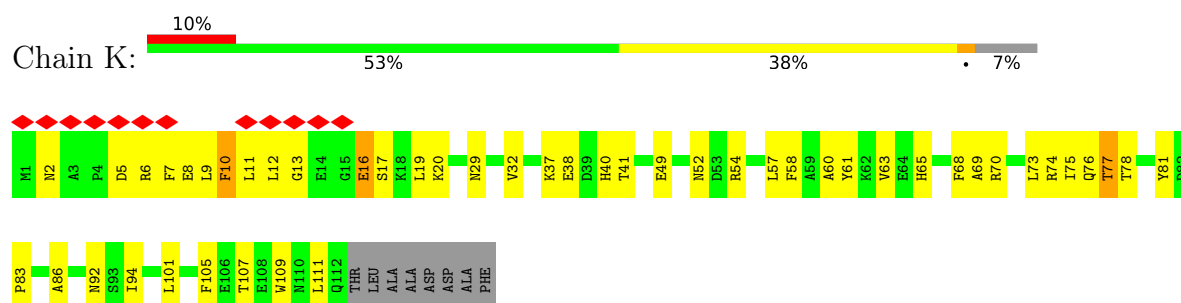
- Molecule 20: DNA-directed RNA polymerase II subunit RPB9



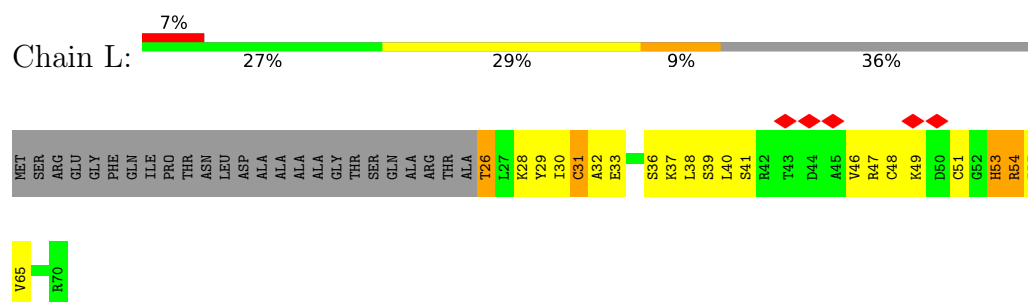
- Molecule 21: DNA-directed RNA polymerases II subunit RPABC5



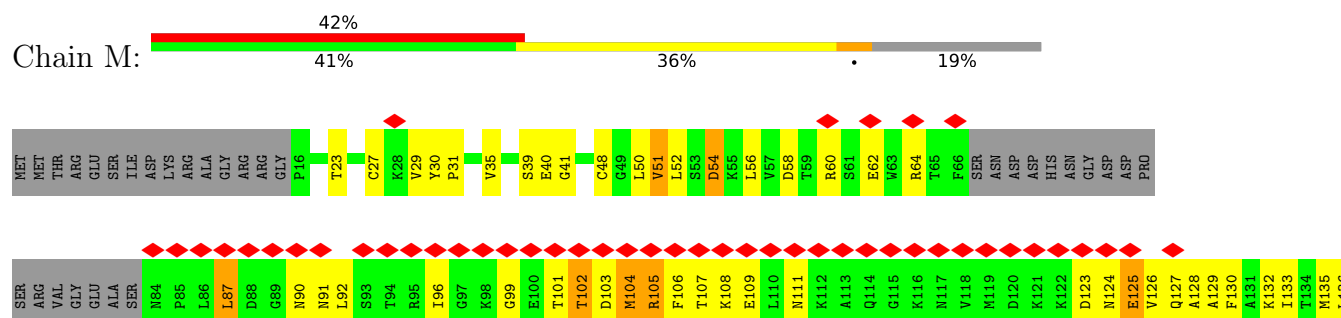
- Molecule 22: DNA-directed RNA polymerase II subunit RPB11

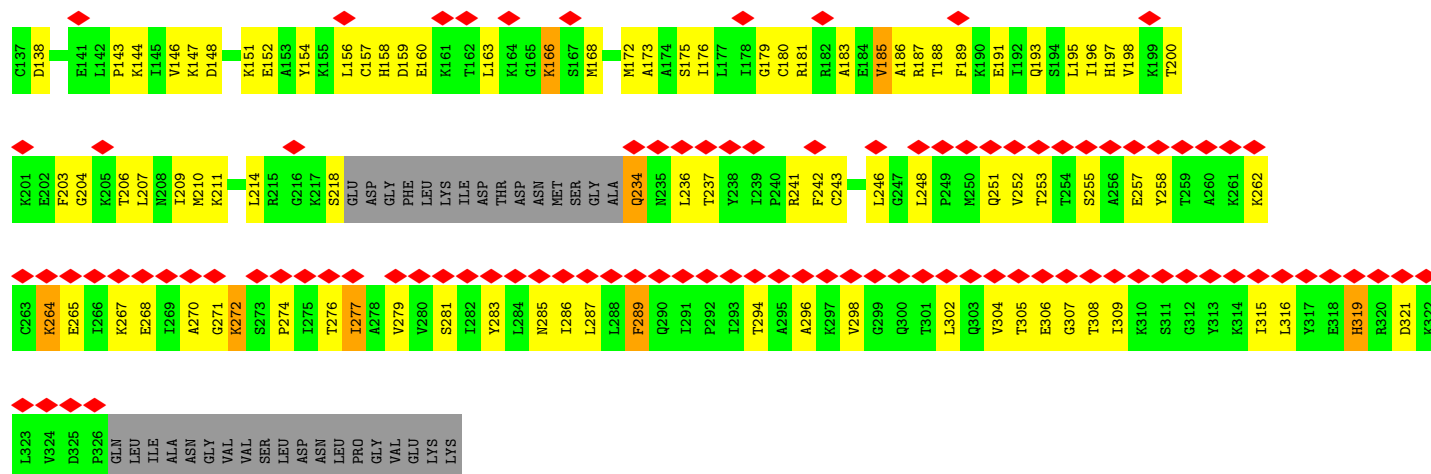


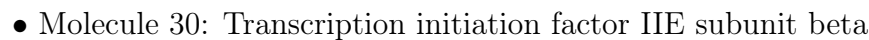
- Molecule 23: DNA-directed RNA polymerases II subunit RPABC4



- Molecule 24: Transcription initiation factor IIB







A272	E273	L274	P275	R276	K277	L278	Q279	D280	L281	G282	L283	LYS	PRO	ALA	SER	VAL	ASP	PRO	ALA	THR	ILE	LYS	ARG	GLN	THR	LYS	ARG	VAL	GLU	VAL	LYS	LYS	ARG	GLN	ARG	LYS	GLY	GLY	LYS	ILE	THR	ASN	THR	HIS	MET	THR	GLY	ILE	LEU	LYS	ASP	TYR	SER	HIS	ARG	VAL	L196	R197	S198	T201	G204	I205	S206	C207	K208	D209	L210	K211	D212	G213	W214	P215	Q216	C217	D218	E219	T220	I221	N222	L233	R234	T235	K236	K237	D238	K239	T240	W245	Y246	N247	N251	L252	K253	C254	I255	D256	E257	E258	F259	V260	K261	M262	W263	E264	N265	V266	Q267	L268	P269	Q270	F271	LYS	SER	H123	D124	E133	Y134	K137	L143	V144	N145	E146	L147	L148	S152	M153	K154	K155	D156	D157	K158	E161	L162	L163	K164	K165	L166	D167	R168	I169	E170	F171	D172	P173	K174	K175	G176	T177	F178	K179	Y180	L181	SER	THR	TYR	ASP	VAL	H187	S188	P189	S190	E191	L192	L193	K194	L195

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	453.67996, 405.97998, 419.75998	wwPDB
Map dimensions	428, 383, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

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	1	0.14	0/1896	0.35	1/2543 (0.0%)
2	4	0.17	0/2062	0.46	3/2805 (0.1%)
3	0	0.14	0/6226	0.38	0/8407
4	6	0.16	0/2506	0.41	0/3402
5	2	0.16	0/3057	0.39	0/4071
6	5	0.18	0/502	0.46	0/677
7	7	0.19	0/4521	0.47	0/6036
8	3	0.13	0/870	0.36	0/1190
9	O	0.12	0/1443	0.31	0/1942
10	N	0.24	0/1326	0.48	0/2045
11	T	0.21	0/1294	0.42	0/1994
12	A	0.27	0/11192	0.39	0/15128
13	B	0.29	0/9311	0.38	0/12558
14	C	0.31	0/2099	0.39	0/2845
15	D	0.15	0/1262	0.37	0/1693
16	E	0.26	0/1780	0.37	0/2395
17	F	0.30	0/682	0.41	0/922
18	G	0.18	0/1368	0.36	0/1844
19	H	0.26	0/1107	0.42	0/1499
20	I	0.20	0/962	0.41	0/1295
21	J	0.34	0/541	0.51	0/727
22	K	0.28	0/922	0.40	0/1244
23	L	0.25	0/360	0.55	0/478
24	M	0.16	0/2204	0.42	0/2963
25	Q	0.20	0/1168	0.37	0/1579
26	R	0.17	0/1312	0.37	0/1777
27	U	0.12	0/372	0.33	0/500
28	V	0.11	0/392	0.27	0/529
29	W	0.11	0/1490	0.28	0/2014
30	X	0.10	0/993	0.31	0/1357
All	All	0.22	0/65220	0.40	4/88459 (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
2	4	0	1
4	6	0	1
7	7	0	1
12	A	0	2
13	B	0	2
24	M	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	4	298	ILE	CA-C-N	8.43	125.55	120.24
2	4	298	ILE	C-N-CA	8.43	125.55	120.24
1	1	336	ILE	N-CA-C	-5.28	107.45	111.62
2	4	299	ILE	CB-CA-C	-5.14	108.90	114.35

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	255	ASP	Peptide
4	6	116	THR	Peptide
7	7	321	GLU	Peptide
12	A	465	TYR	Peptide
12	A	71	GLN	Peptide
13	B	137	TYR	Peptide
13	B	363	HIS	Peptide
24	M	272	LYS	Peptide

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	1	2411	0	1880	132	0
2	4	2041	0	1954	120	0
3	0	6108	0	6168	433	0
4	6	2527	0	2322	187	0
5	2	3011	0	2600	184	0
6	5	498	0	506	49	0
7	7	4447	0	3905	440	0
8	3	860	0	622	34	0
9	O	1416	0	1493	79	0
10	N	1178	0	642	52	0
11	T	1159	0	652	17	0
12	A	10997	0	11081	434	0
13	B	9132	0	9146	346	0
14	C	2061	0	2029	63	0
15	D	1253	0	1275	67	0
16	E	1744	0	1772	83	0
17	F	670	0	690	21	0
18	G	1340	0	1357	79	0
19	H	1089	0	1062	58	0
20	I	944	0	899	45	0
21	J	532	0	542	34	0
22	K	904	0	911	34	0
23	L	358	0	381	29	0
24	M	2175	0	2283	98	0
25	Q	1144	0	1034	65	0
26	R	1303	0	1110	60	0
27	U	366	0	372	41	0
28	V	389	0	394	31	0
29	W	1469	0	1432	78	0
30	X	984	0	722	27	0
31	3	2	0	0	0	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	3	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	W	1	0	0	0	0
31	X	1	0	0	0	0
32	0	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A	1	0	0	0	0
All	All	64538	0	61236	3180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (3180) 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)
3:0:133:CYS:HB2	32:0:801:SF4:S4	1.97	1.03
7:7:303:ARG:H	7:7:323:VAL:HG13	1.29	0.97
7:7:477:LEU:HA	7:7:482:TRP:HE1	1.36	0.91
7:7:592:GLN:HE22	7:7:747:ASN:HB3	1.38	0.89
7:7:234:VAL:H	7:7:316:PHE:H	1.20	0.88
12:A:70:CYS:SG	12:A:80:HIS:CE1	2.64	0.86
12:A:1239:ARG:HH12	12:A:1241:ARG:HH21	1.23	0.86
13:B:794:ASN:HD22	13:B:1096:ARG:HE	1.25	0.84
20:I:75:CYS:SG	20:I:103:CYS:HB2	2.18	0.83
10:N:11:DA:H5'	10:N:11:DA:C8	2.15	0.82
10:N:10:DA:H1'	10:N:11:DA:N7	1.95	0.82
7:7:428:CYS:SG	7:7:429:THR:N	2.53	0.81
26:R:277:PHE:H	26:R:279:LYS:HE2	1.45	0.81
29:W:17:VAL:HG22	29:W:25:PHE:HB3	1.61	0.81
29:W:132:THR:HG22	29:W:135:GLU:HG2	1.62	0.81
3:0:63:TYR:O	3:0:67:ARG:NH2	2.14	0.81
7:7:403:ILE:HG13	7:7:405:LYS:H	1.44	0.81
3:0:719:GLN:HA	3:0:722:ARG:HD3	1.61	0.80
9:O:158:GLN:HB3	10:N:23:DA:H4'	1.62	0.80
12:A:60:SER:HB2	12:A:65:LEU:HB2	1.64	0.80
13:B:959:ASP:N	13:B:959:ASP:OD1	2.15	0.80
25:Q:378:VAL:O	26:R:66:ARG:NH1	2.14	0.80
1:1:251:LEU:HB3	1:1:254:GLU:HB2	1.64	0.79
7:7:411:CYS:SG	7:7:412:THR:N	2.53	0.79
9:O:114:LEU:HB2	9:O:122:VAL:HB	1.64	0.79
16:E:100:ILE:HG23	16:E:105:PHE:HB2	1.64	0.79
27:U:248:TYR:HB3	28:V:115:ALA:HB1	1.64	0.79
7:7:487:LEU:HB2	7:7:512:GLY:HA2	1.63	0.79
7:7:343:PHE:HD2	7:7:380:ARG:HB2	1.47	0.78
7:7:604:LYS:HG2	7:7:666:GLU:HB2	1.63	0.78
7:7:389:GLY:HA2	7:7:692:ARG:HG2	1.66	0.78
7:7:682:GLN:NE2	7:7:685:GLN:OE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:370:PHE:HB2	5:2:373:MET:H	1.49	0.77
7:7:302:GLU:O	7:7:321:GLU:N	2.17	0.77
7:7:604:LYS:HD3	7:7:694:LYS:HZ1	1.50	0.77
12:A:326:ARG:HG2	12:A:1406:VAL:HG11	1.67	0.76
12:A:1128:GLN:NE2	12:A:1284:MET:SD	2.56	0.76
7:7:554:CYS:HA	7:7:705:PHE:HB3	1.67	0.76
12:A:268:ASP:OD2	12:A:299:HIS:NE2	2.18	0.76
5:2:75:GLN:NE2	5:2:503:ASP:OD2	2.18	0.76
7:7:303:ARG:HB3	7:7:323:VAL:HG22	1.68	0.76
7:7:613:TYR:O	7:7:617:GLU:N	2.15	0.76
23:L:47:ARG:NH2	23:L:48:CYS:O	2.19	0.76
7:7:365:TYR:H	7:7:548:HIS:HB2	1.50	0.76
7:7:425:LEU:HB3	7:7:430:LEU:HB3	1.67	0.76
2:4:116:ARG:O	2:4:120:ASN:ND2	2.18	0.76
25:Q:127:ILE:O	26:R:133:TYR:OH	2.04	0.75
12:A:1209:MET:N	12:A:1209:MET:SD	2.59	0.75
7:7:302:GLU:HB2	7:7:321:GLU:H	1.51	0.75
28:V:78:PHE:HB2	28:V:113:ILE:HB	1.69	0.75
7:7:668:THR:OG1	7:7:694:LYS:NZ	2.18	0.75
13:B:894:ASP:OD2	23:L:58:LYS:NZ	2.19	0.75
5:2:343:THR:OG1	5:2:415:LYS:NZ	2.18	0.75
24:M:281:SER:O	24:M:285:ASN:ND2	2.19	0.75
3:0:297:ASP:O	3:0:386:ARG:NH1	2.18	0.74
5:2:373:MET:HE3	5:2:375:LEU:HA	1.68	0.74
7:7:698:ASP:OD1	7:7:698:ASP:N	2.18	0.74
3:0:259:ARG:HG2	3:0:262:ARG:HH21	1.51	0.74
4:6:286:SER:O	4:6:289:LYS:NZ	2.21	0.74
16:E:197:LYS:HG3	16:E:211:TYR:HE1	1.53	0.74
12:A:55:ASP:N	12:A:55:ASP:OD1	2.20	0.74
4:6:211:GLN:HB3	4:6:244:PRO:HD2	1.70	0.74
7:7:407:VAL:HG13	7:7:484:PHE:HB3	1.69	0.74
15:D:144:THR:O	15:D:148:LEU:N	2.20	0.74
2:4:289:CYS:SG	2:4:290:SER:N	2.61	0.73
7:7:579:LEU:HD13	7:7:766:LYS:HB3	1.69	0.73
3:0:535:ASP:HB3	3:0:595:GLY:HA2	1.70	0.73
7:7:343:PHE:HB2	7:7:344:ARG:HH21	1.53	0.73
12:A:269:ILE:HG12	12:A:299:HIS:HB3	1.70	0.73
4:6:156:PHE:HB2	4:6:301:PHE:HD2	1.52	0.73
2:4:275:SER:HA	2:4:282:VAL:HA	1.70	0.73
3:0:167:VAL:HG22	3:0:198:ARG:HD2	1.71	0.73
12:A:451:HIS:HB2	12:A:454:SER:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:368:LYS:HE3	7:7:543:LEU:HD23	1.70	0.73
12:A:882:SER:O	12:A:1025:ARG:NH2	2.22	0.73
20:I:88:SER:O	20:I:91:ARG:NH2	2.17	0.73
3:0:535:ASP:HB2	3:0:590:CYS:HA	1.70	0.73
5:2:69:ASN:HA	5:2:71:LYS:HE3	1.69	0.73
26:R:138:GLN:HB2	26:R:211:LYS:HB2	1.69	0.73
4:6:141:LEU:HD23	4:6:145:ARG:HA	1.71	0.73
7:7:536:TYR:OH	7:7:540:TRP:NE1	2.21	0.73
13:B:706:GLN:HB2	13:B:709:ASP:HB3	1.70	0.72
12:A:862:ASN:OD1	12:A:862:ASN:N	2.23	0.72
29:W:65:ARG:NH2	30:X:270:GLN:O	2.22	0.72
7:7:372:LYS:O	7:7:380:ARG:NH2	2.23	0.72
10:N:43:DT:N3	11:T:124:DT:O2	2.23	0.72
14:C:211:ASP:OD1	14:C:211:ASP:N	2.16	0.72
4:6:127:ILE:HG13	4:6:170:GLY:H	1.53	0.72
3:0:111:ARG:NE	3:0:133:CYS:SG	2.62	0.72
5:2:102:PRO:O	5:2:106:ILE:N	2.23	0.72
14:C:142:VAL:HG13	21:J:15:GLY:HA3	1.71	0.72
2:4:228:THR:O	2:4:233:GLY:N	2.20	0.72
5:2:59:LEU:HD13	5:2:96:LEU:HD12	1.72	0.72
7:7:739:LEU:HB2	7:7:742:MET:HB3	1.71	0.72
7:7:370:LEU:HD21	7:7:395:VAL:HG13	1.71	0.72
16:E:180:ARG:HH21	16:E:191:LYS:HA	1.54	0.72
9:O:70:ILE:HG13	9:O:160:ILE:HG12	1.71	0.72
1:1:210:TRP:HB3	1:1:217:LEU:HD11	1.72	0.71
13:B:367:LEU:HB2	13:B:370:PHE:HE1	1.54	0.71
3:0:687:SER:HA	3:0:706:LEU:HD12	1.72	0.71
28:V:81:LYS:HE2	28:V:110:LYS:HG3	1.70	0.71
4:6:224:VAL:O	4:6:230:ARG:NH2	2.24	0.71
12:A:456:MET:HE2	12:A:507:VAL:HG22	1.72	0.71
7:7:572:GLU:O	7:7:577:ARG:NH2	2.23	0.71
13:B:24:PRO:O	13:B:655:LYS:NZ	2.22	0.71
13:B:919:SER:HB3	13:B:922:GLU:HB2	1.73	0.71
7:7:302:GLU:HB3	7:7:319:ALA:HB3	1.71	0.71
13:B:399:ASP:OD1	13:B:399:ASP:N	2.24	0.71
14:C:56:THR:HG22	14:C:147:LEU:HD21	1.71	0.71
19:H:56:THR:OG1	19:H:146:ARG:NH1	2.23	0.71
5:2:109:ARG:HA	5:2:112:LEU:HD22	1.73	0.71
3:0:108:LEU:HB3	3:0:208:TYR:HB3	1.72	0.71
1:1:379:ASN:HD21	3:0:571:VAL:H	1.37	0.71
7:7:363:ARG:HB2	7:7:548:HIS:CG	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:624:LYS:NZ	7:7:648:GLN:O	2.24	0.71
25:Q:375:LEU:HG	26:R:70:LEU:HD13	1.72	0.71
3:0:295:SER:HA	3:0:298:ILE:HG22	1.73	0.70
13:B:103:ASN:O	13:B:958:GLN:NE2	2.23	0.70
5:2:384:ARG:NH1	5:2:444:TRP:O	2.24	0.70
12:A:636:GLU:OE2	12:A:962:ARG:NH1	2.23	0.70
7:7:309:ASP:OD1	7:7:309:ASP:N	2.24	0.70
3:0:252:LEU:HD12	3:0:435:MET:HB3	1.73	0.70
8:3:46:ILE:HG23	8:3:52:ALA:HB3	1.72	0.70
29:W:5:ILE:HD11	29:W:189:ILE:HA	1.71	0.70
7:7:434:ASN:HB3	7:7:451:GLY:HA3	1.73	0.70
12:A:53:LEU:O	12:A:247:ARG:NH2	2.23	0.70
12:A:406:ILE:HB	12:A:431:LYS:HB2	1.74	0.70
2:4:64:HIS:O	2:4:71:ASN:ND2	2.23	0.70
12:A:346:ASP:OD1	12:A:346:ASP:N	2.24	0.70
13:B:199:MET:N	13:B:199:MET:SD	2.64	0.70
12:A:451:HIS:HB3	12:A:453:MET:HE2	1.74	0.70
12:A:881:GLN:NE2	12:A:957:PRO:O	2.24	0.70
1:1:174:LEU:O	1:1:181:GLN:NE2	2.24	0.70
7:7:407:VAL:HB	7:7:452:LEU:HD13	1.73	0.70
3:0:1:MET:HE3	3:0:742:GLU:H	1.57	0.69
3:0:587:ARG:NH2	3:0:611:ASP:O	2.25	0.69
5:2:486:ASP:OD1	5:2:486:ASP:N	2.24	0.69
12:A:592:ASP:OD1	12:A:592:ASP:N	2.26	0.69
13:B:20:ASP:OD1	13:B:21:GLU:N	2.25	0.69
29:W:121:GLY:HA2	29:W:132:THR:HA	1.74	0.69
7:7:256:ILE:N	7:7:317:GLU:O	2.25	0.69
9:O:203:VAL:HG11	10:N:21:DA:H4'	1.74	0.69
29:W:172:LEU:HB3	29:W:176:MET:HE3	1.73	0.69
24:M:195:LEU:HD23	24:M:196:ILE:HG13	1.73	0.69
25:Q:141:ARG:HH22	25:Q:343:ARG:HH12	1.40	0.69
7:7:477:LEU:HB3	7:7:505:ILE:HG13	1.73	0.69
13:B:232:SER:O	13:B:261:ARG:NH1	2.24	0.69
1:1:597:PHE:HA	1:1:600:VAL:HB	1.74	0.69
29:W:44:LYS:NZ	29:W:49:ILE:O	2.24	0.69
2:4:23:PRO:HG2	2:4:172:LEU:HG	1.73	0.69
3:0:484:ALA:HA	3:0:696:TRP:HB3	1.72	0.69
7:7:642:ASN:HA	7:7:646:ASN:HB3	1.74	0.69
19:H:12:VAL:HG11	19:H:15:VAL:HG23	1.73	0.69
27:U:260:CYS:HB3	27:U:281:VAL:HB	1.74	0.69
7:7:556:GLU:HG3	7:7:707:SER:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:879:GLU:OE2	12:A:962:ARG:NH2	2.26	0.69
13:B:842:ASN:OD1	13:B:845:SER:N	2.19	0.69
15:D:172:LEU:HB3	15:D:177:VAL:HG12	1.75	0.69
27:U:246:CYS:SG	27:U:247:LEU:N	2.63	0.69
25:Q:386:MET:N	25:Q:386:MET:SD	2.65	0.69
18:G:57:GLN:OE1	18:G:57:GLN:N	2.23	0.69
2:4:162:ARG:NH2	4:6:407:GLN:O	2.26	0.68
5:2:22:GLN:O	5:2:26:TYR:N	2.26	0.68
12:A:1386:ARG:O	12:A:1391:ARG:NH1	2.26	0.68
24:M:264:LYS:HE3	24:M:265:GLU:HG3	1.74	0.68
4:6:132:CYS:HB2	4:6:175:ARG:HG2	1.75	0.68
7:7:674:SER:O	7:7:686:ARG:NH1	2.26	0.68
13:B:801:LYS:O	21:J:52:THR:OG1	2.10	0.68
16:E:48:ASP:OD1	16:E:52:ARG:N	2.26	0.68
3:0:496:ILE:HD12	3:0:686:PHE:HB3	1.73	0.68
7:7:264:PRO:O	7:7:268:VAL:N	2.26	0.68
7:7:344:ARG:NH2	7:7:379:ALA:O	2.26	0.68
7:7:554:CYS:HB2	7:7:733:PHE:HA	1.73	0.68
13:B:363:HIS:O	13:B:365:THR:N	2.26	0.68
13:B:443:ASN:HD22	13:B:446:LEU:HG	1.57	0.68
14:C:86:CYS:HB2	14:C:88:CYS:SG	2.33	0.68
15:D:52:LEU:HG	15:D:182:SER:HB2	1.74	0.68
16:E:182:ASP:OD1	16:E:185:ALA:N	2.20	0.68
12:A:544:ASP:OD1	12:A:544:ASP:N	2.24	0.68
12:A:603:ASN:N	12:A:603:ASN:OD1	2.25	0.68
15:D:153:ARG:NH2	15:D:182:SER:O	2.26	0.68
18:G:94:CYS:SG	18:G:130:TYR:OH	2.51	0.68
2:4:292:CYS:HB2	2:4:308:CYS:SG	2.33	0.68
3:0:221:ARG:HD3	3:0:221:ARG:H	1.58	0.68
12:A:1423:GLY:O	12:A:1427:ASN:ND2	2.26	0.68
13:B:364:ILE:HG22	13:B:585:VAL:HG13	1.75	0.68
7:7:473:VAL:O	7:7:477:LEU:N	2.22	0.68
3:0:476:LYS:NZ	3:0:477:THR:O	2.24	0.68
12:A:898:ARG:O	12:A:1029:ARG:NH2	2.27	0.68
7:7:209:ILE:O	7:7:213:ILE:N	2.25	0.68
7:7:370:LEU:O	7:7:374:PHE:N	2.18	0.68
9:O:74:VAL:HB	9:O:121:MET:HB3	1.76	0.68
24:M:54:ASP:OD1	24:M:54:ASP:N	2.25	0.68
7:7:696:ARG:HB3	7:7:702:ASN:HB3	1.75	0.68
10:N:9:DA:H1'	10:N:10:DA:H5'	1.76	0.68
4:6:262:LYS:HE2	4:6:289:LYS:HE2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:61:ASP:N	5:2:61:ASP:OD1	2.26	0.67
23:L:36:SER:OG	23:L:48:CYS:SG	2.50	0.67
3:0:215:ASP:HB3	3:0:218:ILE:HG12	1.75	0.67
3:0:722:ARG:HH21	4:6:292:LEU:HB2	1.59	0.67
9:O:67:LEU:HA	9:O:162:GLY:HA2	1.76	0.67
16:E:67:GLU:OE1	16:E:68:SER:N	2.28	0.67
18:G:34:VAL:HG12	18:G:45:ILE:HG21	1.75	0.67
5:2:364:VAL:HA	5:2:382:SER:HB3	1.76	0.67
3:0:77:SER:OG	3:0:81:LYS:NZ	2.28	0.67
7:7:615:LEU:O	7:7:619:ALA:N	2.24	0.67
13:B:71:LEU:HD22	13:B:432:MET:HE3	1.76	0.67
13:B:1074:ASN:OD1	13:B:1077:THR:N	2.25	0.67
3:0:259:ARG:HH22	3:0:395:ASP:HA	1.60	0.67
4:6:134:GLU:HA	4:6:137:LEU:HD12	1.76	0.67
4:6:175:ARG:HH21	4:6:205:LYS:HB2	1.58	0.67
5:2:352:ASN:ND2	5:2:370:PHE:O	2.27	0.67
12:A:443:LEU:HD21	12:A:455:MET:HE3	1.75	0.67
12:A:746:MET:HE1	13:B:1015:HIS:HA	1.75	0.67
24:M:270:ALA:HB1	24:M:277:ILE:HG21	1.77	0.67
1:1:510:ASN:OD1	1:1:513:GLN:NE2	2.28	0.67
3:0:563:VAL:HG22	3:0:569:ILE:HD11	1.77	0.67
4:6:272:ILE:O	4:6:276:LEU:N	2.25	0.67
29:W:69:ILE:HA	29:W:87:TYR:HA	1.77	0.67
3:0:232:VAL:O	3:0:457:ILE:N	2.25	0.66
5:2:48:MET:HE3	5:2:49:ALA:HA	1.78	0.66
3:0:157:GLU:O	3:0:161:ASN:ND2	2.27	0.66
26:R:71:VAL:HG13	26:R:223:GLN:HA	1.75	0.66
4:6:237:GLY:HA2	4:6:266:LEU:HG	1.77	0.66
1:1:351:GLY:O	3:0:436:ARG:NH1	2.28	0.66
5:2:218:LEU:O	5:2:222:LEU:N	2.27	0.66
12:A:974:ASP:HB2	12:A:977:LYS:HD3	1.77	0.66
14:C:61:GLU:OE1	14:C:61:GLU:N	2.26	0.66
24:M:316:LEU:HD13	24:M:319:HIS:HD2	1.60	0.66
29:W:28:VAL:HG21	29:W:57:LEU:HB3	1.78	0.66
1:1:560:PHE:O	1:1:563:HIS:ND1	2.28	0.66
7:7:577:ARG:HA	7:7:580:LEU:HB2	1.78	0.66
7:7:663:ASP:OD1	7:7:663:ASP:N	2.21	0.66
19:H:101:ALA:HA	19:H:116:TYR:HA	1.78	0.66
1:1:232:UNK:O	1:1:236:UNK:N	2.28	0.66
2:4:153:MET:HE1	2:4:196:ILE:HG12	1.76	0.66
4:6:188:ASN:HD21	4:6:190:GLN:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:416:ARG:NH2	24:M:40:GLU:OE2	2.28	0.66
14:C:41:ILE:HB	14:C:172:PRO:HG3	1.75	0.66
19:H:110:ASP:OD2	19:H:130:ARG:NH2	2.28	0.66
3:O:499:LYS:HB3	3:O:503:GLN:HA	1.77	0.66
4:6:262:LYS:HB2	4:6:287:PHE:HD2	1.61	0.66
13:B:496:ARG:NH2	13:B:540:SER:O	2.28	0.66
13:B:728:ARG:NH1	13:B:1048:THR:O	2.29	0.66
15:D:127:ASP:HB3	15:D:142:LYS:HE2	1.76	0.66
19:H:90:ALA:HA	19:H:93:TYR:HB2	1.77	0.66
25:Q:141:ARG:NH2	25:Q:346:GLU:O	2.29	0.66
4:6:124:ARG:NH2	4:6:306:THR:O	2.25	0.66
4:6:128:LEU:HG	4:6:233:LEU:HB3	1.76	0.66
12:A:804:TYR:OH	12:A:816:HIS:NE2	2.28	0.66
16:E:40:GLU:HA	16:E:43:LYS:HE2	1.77	0.66
16:E:67:GLU:O	16:E:70:SER:OG	2.11	0.66
20:I:19:ASP:HB2	20:I:26:LEU:HG	1.77	0.66
21:J:33:GLY:O	21:J:47:ARG:NH2	2.28	0.66
23:L:26:THR:OG1	23:L:39:SER:O	2.14	0.66
11:T:136:DA:H2'	11:T:137:DA:C8	2.31	0.66
12:A:818:MET:HG2	13:B:514:LEU:HB3	1.78	0.66
12:A:908:LEU:HD11	12:A:912:LEU:HD12	1.78	0.66
13:B:705:MET:HG3	13:B:706:GLN:HG3	1.78	0.66
2:4:150:ALA:HB2	2:4:192:GLN:HB2	1.78	0.66
5:2:346:LYS:NZ	5:2:347:ILE:O	2.29	0.66
7:7:303:ARG:N	7:7:323:VAL:HG13	2.06	0.66
13:B:996:ARG:HD2	13:B:1007:VAL:HG21	1.78	0.66
4:6:174:MET:HA	4:6:179:ALA:HA	1.78	0.65
7:7:344:ARG:HD2	7:7:378:ARG:HD2	1.77	0.65
7:7:409:VAL:HB	7:7:454:VAL:HA	1.78	0.65
7:7:464:ARG:HH21	7:7:466:ARG:HH12	1.44	0.65
12:A:997:LEU:O	12:A:1011:GLN:NE2	2.29	0.65
18:G:47:CYS:H	18:G:77:VAL:HG22	1.61	0.65
29:W:141:ASN:OD1	29:W:141:ASN:N	2.28	0.65
3:O:211:HIS:O	3:O:215:ASP:N	2.29	0.65
4:6:169:MET:O	4:6:192:HIS:NE2	2.30	0.65
4:6:347:TYR:N	4:6:356:VAL:O	2.29	0.65
7:7:594:LEU:O	7:7:598:HIS:ND1	2.28	0.65
21:J:10:CYS:SG	21:J:12:LYS:N	2.68	0.65
2:4:258:LEU:HB2	2:4:260:PRO:HD3	1.79	0.65
3:O:117:HIS:N	32:O:801:SF4:S3	2.69	0.65
12:A:446:ARG:HB2	12:A:487:MET:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:445:LYS:NZ	26:R:267:GLY:O	2.28	0.65
6:5:32:LEU:N	6:5:41:LEU:O	2.29	0.65
15:D:119:ARG:NH1	15:D:149:THR:O	2.28	0.65
24:M:91:ASN:ND2	24:M:123:ASP:OD2	2.29	0.65
3:0:711:ASP:OD1	3:0:711:ASP:N	2.24	0.65
7:7:541:MET:SD	7:7:545:GLN:NE2	2.61	0.65
8:3:39:CYS:SG	8:3:41:SER:OG	2.54	0.65
3:0:37:ASN:ND2	3:0:476:LYS:O	2.30	0.65
3:0:643:ARG:HH11	3:0:650:GLU:HG3	1.61	0.65
6:5:16:ILE:HG23	6:5:19:LEU:HD12	1.77	0.65
7:7:111:GLY:N	7:7:175:ILE:O	2.30	0.65
10:N:5:DA:H2"	10:N:6:DA:H8	1.60	0.65
13:B:241:ARG:HH21	13:B:251:ILE:HA	1.62	0.65
13:B:802:PRO:HG3	13:B:809:MET:HE1	1.79	0.65
18:G:96:GLN:OE1	29:W:145:THR:OG1	2.14	0.65
27:U:267:VAL:HB	27:U:274:TYR:HB2	1.77	0.65
29:W:14:LYS:NZ	29:W:30:ASP:OD1	2.28	0.65
1:1:593:LEU:HD21	1:1:620:LEU:HD12	1.78	0.65
2:4:150:ALA:HA	2:4:153:MET:HE2	1.78	0.65
2:4:217:GLY:O	2:4:237:HIS:NE2	2.30	0.65
3:0:215:ASP:O	3:0:219:ALA:N	2.29	0.65
25:Q:127:ILE:HG23	25:Q:129:PRO:HD3	1.79	0.65
3:0:363:LEU:O	3:0:367:THR:N	2.30	0.65
30:X:187:HIS:HA	30:X:214:TRP:HB2	1.79	0.65
3:0:74:ARG:HH21	3:0:236:GLU:HB3	1.60	0.65
4:6:116:THR:O	4:6:118:TYR:N	2.30	0.65
5:2:353:SER:HB2	5:2:356:GLN:HB3	1.77	0.65
7:7:583:MET:O	7:7:618:TYR:OH	2.15	0.65
12:A:537:ARG:NE	12:A:602:ASP:OD2	2.30	0.65
13:B:392:ARG:HG2	20:I:90:GLN:HE22	1.62	0.65
7:7:363:ARG:HG2	7:7:695:ARG:HB2	1.79	0.65
7:7:386:LEU:O	7:7:392:LYS:NZ	2.29	0.65
14:C:115:SER:OG	14:C:142:VAL:N	2.29	0.65
1:1:227:LYS:O	4:6:212:ASN:ND2	2.25	0.64
3:0:191:CYS:SG	3:0:194:PHE:HB2	2.37	0.64
3:0:371:ARG:O	3:0:410:SER:OG	2.15	0.64
5:2:132:LEU:O	5:2:286:ARG:NH2	2.30	0.64
7:7:578:MET:SD	7:7:581:TYR:OH	2.55	0.64
8:3:128:LYS:O	8:3:132:LYS:N	2.26	0.64
13:B:763:GLN:HG2	13:B:765:PRO:HD2	1.79	0.64
14:C:177:GLU:HB2	14:C:231:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:114:MET:HB2	26:R:138:GLN:HG2	1.79	0.64
2:4:52:LYS:NZ	2:4:240:SER:O	2.30	0.64
5:2:370:PHE:N	5:2:373:MET:O	2.30	0.64
12:A:90:VAL:O	12:A:236:LEU:N	2.30	0.64
13:B:287:ARG:NE	13:B:292:ILE:O	2.29	0.64
20:I:29:CYS:SG	20:I:31:THR:OG1	2.55	0.64
7:7:614:ALA:HA	7:7:617:GLU:HB3	1.79	0.64
12:A:526:ASP:OD1	12:A:526:ASP:N	2.17	0.64
27:U:281:VAL:HG13	28:V:62:VAL:HB	1.79	0.64
1:1:343:ILE:O	1:1:345:ASP:N	2.26	0.64
1:1:507:ILE:HG23	2:4:264:LYS:HG2	1.80	0.64
3:0:322:PRO:HB2	3:0:325:ILE:HB	1.78	0.64
13:B:121:ASN:HA	13:B:207:GLY:HA3	1.78	0.64
24:M:175:SER:O	24:M:179:GLY:N	2.30	0.64
2:4:29:ILE:HB	2:4:178:VAL:HG22	1.78	0.64
4:6:293:ASP:O	4:6:297:LEU:N	2.30	0.64
12:A:767:GLN:NE2	12:A:768:GLN:O	2.25	0.64
13:B:101:MET:HE1	13:B:127:GLY:H	1.62	0.64
3:0:353:SER:HA	3:0:419:ILE:HA	1.77	0.64
3:0:375:ARG:HA	3:0:407:THR:HA	1.79	0.64
4:6:451:CYS:O	4:6:455:GLU:N	2.30	0.64
5:2:396:ILE:HA	5:2:399:TYR:HB3	1.78	0.64
9:O:76:LEU:HD12	9:O:80:LEU:HD11	1.80	0.64
19:H:13:SER:N	19:H:27:GLU:O	2.30	0.64
3:0:148:ASP:N	3:0:148:ASP:OD1	2.30	0.64
12:A:198:GLU:OE1	12:A:200:ARG:NH1	2.31	0.64
12:A:1386:ARG:HB3	12:A:1403:GLU:HG3	1.80	0.64
17:F:110:ASP:OD1	17:F:110:ASP:N	2.30	0.64
5:2:349:SER:OG	5:2:373:MET:SD	2.51	0.64
7:7:347:HIS:O	7:7:405:LYS:NZ	2.23	0.64
7:7:489:GLU:OE1	7:7:685:GLN:NE2	2.29	0.64
12:A:351:THR:OG1	12:A:352:VAL:N	2.28	0.64
13:B:287:ARG:HD3	13:B:292:ILE:HA	1.80	0.64
21:J:10:CYS:SG	21:J:11:GLY:N	2.71	0.64
25:Q:359:ASN:N	25:Q:359:ASN:OD1	2.31	0.64
3:0:217:LYS:HB2	3:0:308:GLU:HG3	1.80	0.64
3:0:360:LEU:HD11	3:0:371:ARG:HB2	1.80	0.64
6:5:8:ALA:HB3	6:5:42:VAL:H	1.63	0.64
12:A:362:ASP:OD2	12:A:459:ARG:NE	2.29	0.64
12:A:931:GLU:OE2	12:A:991:LYS:NZ	2.30	0.64
20:I:108:HIS:CE1	20:I:110:PHE:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:343:ILE:HG21	3:0:605:LYS:HD3	1.80	0.64
3:0:112:LYS:NZ	3:0:123:GLU:O	2.31	0.64
7:7:469:ASP:N	7:7:469:ASP:OD1	2.28	0.64
12:A:1013:ASP:OD1	16:E:207:ARG:NH1	2.31	0.64
12:A:1334:ASP:N	12:A:1334:ASP:OD1	2.27	0.64
15:D:148:LEU:O	15:D:152:SER:N	2.31	0.64
9:O:184:SER:HB3	9:O:194:ILE:HB	1.79	0.63
10:N:15:DG:OP1	27:U:257:ARG:NH2	2.31	0.63
13:B:205:ILE:HD11	13:B:461:LEU:HD23	1.80	0.63
18:G:108:VAL:HG22	18:G:159:ALA:HB3	1.80	0.63
7:7:222:LYS:N	7:7:336:PRO:O	2.30	0.63
7:7:302:GLU:HA	7:7:318:ILE:HG22	1.79	0.63
7:7:495:ALA:HA	7:7:498:PHE:HB3	1.79	0.63
16:E:76:GLY:N	16:E:106:GLN:OE1	2.29	0.63
18:G:88:ASP:HA	18:G:144:ARG:HA	1.79	0.63
1:1:582:LEU:O	1:1:585:HIS:ND1	2.31	0.63
2:4:255:ASP:O	2:4:259:ARG:NH1	2.31	0.63
3:0:224:ASN:OD1	3:0:452:ARG:NH2	2.31	0.63
9:O:66:THR:N	9:O:163:SER:O	2.22	0.63
10:N:24:DA:H2'	10:N:25:DA:C8	2.33	0.63
14:C:40:GLU:OE2	14:C:165:LYS:NZ	2.31	0.63
26:R:65:ASN:O	26:R:67:GLN:NE2	2.31	0.63
3:0:420:ILE:HG12	3:0:435:MET:HG3	1.80	0.63
3:0:424:GLU:OE1	3:0:432:ASN:ND2	2.30	0.63
4:6:158:HIS:O	4:6:162:ASP:N	2.31	0.63
6:5:24:ASP:HA	6:5:27:MET:HG3	1.80	0.63
24:M:271:GLY:HA3	24:M:274:PRO:HA	1.80	0.63
2:4:75:VAL:HG12	2:4:86:LEU:HD23	1.80	0.63
3:0:111:ARG:HD2	3:0:130:ASP:HA	1.79	0.63
9:O:162:GLY:N	9:O:214:LEU:O	2.27	0.63
12:A:968:GLN:HA	12:A:973:ILE:HG12	1.79	0.63
13:B:336:ARG:HD2	13:B:348:ARG:HD3	1.80	0.63
1:1:214:ILE:HG23	1:1:215:PRO:HD3	1.81	0.63
3:0:83:LEU:HB3	3:0:177:SER:HA	1.81	0.63
3:0:507:SER:HB2	3:0:684:ARG:HG2	1.79	0.63
7:7:223:VAL:N	7:7:336:PRO:O	2.31	0.63
7:7:519:ARG:NH2	7:7:521:ASP:OD2	2.32	0.63
12:A:107:CYS:SG	12:A:171:GLN:NE2	2.71	0.63
3:0:307:VAL:HB	3:0:382:SER:HB3	1.81	0.63
3:0:534:PRO:O	3:0:567:LYS:NZ	2.30	0.63
4:6:149:ILE:O	4:6:153:ALA:N	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:516:THR:OG1	7:7:681:ARG:O	2.16	0.63
13:B:885:MET:HG2	13:B:936:ASP:HB2	1.81	0.63
15:D:66:ARG:NH2	18:G:35:GLU:OE2	2.29	0.63
19:H:130:ARG:O	19:H:133:ASN:ND2	2.26	0.63
3:0:109:THR:OG1	3:0:113:ASN:ND2	2.30	0.63
7:7:365:TYR:HB3	7:7:548:HIS:HB3	1.81	0.63
9:O:91:ASN:OD1	9:O:107:ARG:NH2	2.32	0.63
1:1:209:PHE:O	1:1:213:ARG:NH1	2.32	0.62
3:0:326:ARG:O	3:0:380:ARG:NH2	2.32	0.62
3:0:327:ARG:HD2	3:0:329:GLU:HG2	1.81	0.62
3:0:377:CYS:HG	3:0:407:THR:HG1	1.39	0.62
3:0:407:THR:O	3:0:411:THR:OG1	2.14	0.62
10:N:23:DA:H2'	10:N:24:DA:C8	2.33	0.62
12:A:218:ASP:O	12:A:221:SER:OG	2.16	0.62
29:W:122:TYR:O	29:W:131:TYR:N	2.28	0.62
1:1:259:ILE:HG22	1:1:266:VAL:HG11	1.81	0.62
7:7:162:GLU:O	7:7:174:LYS:N	2.32	0.62
12:A:355:GLY:O	12:A:469:ARG:NH1	2.31	0.62
13:B:361:LEU:HD22	13:B:363:HIS:HE1	1.64	0.62
19:H:109:LYS:O	19:H:111:LEU:N	2.31	0.62
19:H:112:ILE:HG23	19:H:132:LEU:HD12	1.80	0.62
2:4:304:LYS:HG3	2:4:309:ASP:HA	1.81	0.62
12:A:225:ASN:OD1	12:A:228:PHE:N	2.33	0.62
12:A:399:HIS:O	12:A:435:HIS:ND1	2.33	0.62
12:A:1345:ARG:NE	12:A:1373:ASP:OD1	2.31	0.62
7:7:685:GLN:HG3	7:7:689:ARG:HD2	1.80	0.62
13:B:860:MET:HB2	13:B:965:LYS:HG2	1.81	0.62
16:E:98:ILE:O	16:E:102:GLU:N	2.25	0.62
29:W:19:GLY:HA2	30:X:252:LEU:HD12	1.80	0.62
8:3:136:TYR:O	8:3:140:ASN:N	2.27	0.62
12:A:526:ASP:OD2	13:B:1013:ASN:ND2	2.31	0.62
12:A:1188:GLN:HA	12:A:1243:VAL:HA	1.82	0.62
18:G:9:LEU:N	18:G:72:VAL:O	2.30	0.62
8:3:79:GLU:O	8:3:83:ASP:N	2.25	0.62
12:A:76:GLU:OE2	13:B:1159:ARG:NH2	2.32	0.62
13:B:365:THR:HG21	13:B:370:PHE:HB2	1.79	0.62
15:D:211:LEU:O	15:D:215:SER:N	2.30	0.62
3:0:304:GLU:HB3	3:0:386:ARG:HD3	1.80	0.62
3:0:443:SER:HB3	3:0:473:LEU:HA	1.80	0.62
5:2:379:THR:H	5:2:382:SER:HB2	1.63	0.62
7:7:456:THR:HG23	7:7:459:MET:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:5:DA:H2"	10:N:6:DA:C8	2.34	0.62
10:N:8:DA:C2	10:N:9:DA:C6	2.88	0.62
3:0:286:TYR:HE1	3:0:380:ARG:HH22	1.48	0.62
7:7:423:GLN:NE2	7:7:663:ASP:O	2.31	0.62
7:7:568:GLU:HG3	7:7:577:ARG:HD3	1.82	0.62
7:7:707:SER:OG	7:7:722:ARG:NH1	2.33	0.62
7:7:752:SER:HG	7:7:754:ARG:HG3	1.64	0.62
9:O:227:PHE:HA	9:O:230:ILE:HG22	1.82	0.62
12:A:88:LYS:HG2	12:A:293:GLU:HG3	1.80	0.62
12:A:368:LYS:HD2	22:K:2:ASN:HB3	1.81	0.62
12:A:457:ALA:HB2	12:A:501:LEU:HD12	1.82	0.62
13:B:486:TYR:HA	13:B:1096:ARG:HH22	1.63	0.62
3:0:120:VAL:HG22	3:0:132:LYS:HD2	1.82	0.62
5:2:99:ASN:N	5:2:99:ASN:OD1	2.32	0.62
7:7:359:SER:OG	7:7:427:TRP:O	2.15	0.62
13:B:771:SER:O	13:B:775:LYS:NZ	2.32	0.62
4:6:262:LYS:HD2	4:6:287:PHE:HA	1.81	0.62
5:2:73:GLN:O	5:2:77:ALA:N	2.31	0.62
7:7:348:ARG:HA	7:7:348:ARG:HE	1.63	0.62
13:B:195:CYS:SG	13:B:783:THR:OG1	2.57	0.62
3:0:742:GLU:HA	3:0:745:ILE:HD11	1.82	0.61
4:6:221:LEU:HD23	4:6:230:ARG:HB3	1.82	0.61
4:6:262:LYS:HA	4:6:287:PHE:HB3	1.82	0.61
7:7:407:VAL:H	7:7:452:LEU:HD22	1.65	0.61
29:W:127:CYS:SG	29:W:129:THR:OG1	2.52	0.61
2:4:286:GLY:N	4:6:322:MET:O	2.33	0.61
13:B:1163:CYS:SG	13:B:1166:CYS:N	2.67	0.61
20:I:74:GLU:HA	20:I:81:ARG:HA	1.82	0.61
2:4:57:LEU:O	2:4:61:LEU:N	2.31	0.61
3:0:5:ILE:O	3:0:29:LYS:NZ	2.34	0.61
3:0:567:LYS:HE3	3:0:597:ILE:HD11	1.82	0.61
4:6:277:CYS:O	4:6:281:ASN:ND2	2.26	0.61
5:2:62:LEU:HA	5:2:65:TRP:HD1	1.66	0.61
7:7:568:GLU:HG2	7:7:580:LEU:HD22	1.80	0.61
7:7:628:TYR:O	7:7:631:THR:OG1	2.14	0.61
7:7:634:GLN:HA	7:7:637:MET:HB2	1.81	0.61
7:7:720:THR:HA	7:7:723:GLN:HB3	1.81	0.61
9:O:191:PRO:HG3	24:M:272:LYS:HA	1.82	0.61
12:A:1342:GLU:OE2	16:E:212:ARG:NE	2.32	0.61
13:B:211:VAL:HG21	13:B:483:LEU:HD13	1.82	0.61
13:B:901:PRO:HG3	23:L:58:LYS:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:85:GLY:O	19:H:87:ARG:NH2	2.33	0.61
7:7:617:GLU:OE2	7:7:621:LYS:NZ	2.32	0.61
14:C:99:LEU:O	14:C:157:CYS:N	2.33	0.61
15:D:184:ALA:H	18:G:144:ARG:HH22	1.48	0.61
5:2:475:ALA:HA	5:2:478:ILE:HG12	1.81	0.61
7:7:630:SER:H	7:7:657:VAL:HG21	1.66	0.61
7:7:726:LEU:HD12	7:7:733:PHE:HD1	1.65	0.61
12:A:871:ASP:OD2	12:A:1366:ARG:NH2	2.34	0.61
1:1:283:PHE:HD1	1:1:284:TRP:HD1	1.48	0.61
4:6:137:LEU:HA	4:6:144:ASN:HD22	1.66	0.61
13:B:818:PRO:HG3	21:J:54:VAL:HG21	1.82	0.61
14:C:75:MET:SD	14:C:246:ARG:NH2	2.74	0.61
1:1:510:ASN:O	1:1:513:GLN:NE2	2.32	0.61
3:0:17:ILE:HG13	3:0:18:TYR:H	1.65	0.61
7:7:577:ARG:HG2	7:7:580:LEU:HB2	1.83	0.61
15:D:67:ARG:HG2	15:D:71:LYS:HE3	1.83	0.61
1:1:251:LEU:HD22	1:1:255:LYS:HE3	1.83	0.61
5:2:222:LEU:HA	5:2:225:ILE:HB	1.82	0.61
13:B:650:GLU:HB3	13:B:654:ARG:HH22	1.64	0.61
2:4:288:ILE:HG13	2:4:293:LEU:HA	1.83	0.61
4:6:177:GLY:N	4:6:207:ASN:O	2.29	0.61
4:6:196:LEU:O	4:6:200:ARG:N	2.25	0.61
4:6:406:CYS:SG	4:6:407:GLN:N	2.74	0.61
7:7:595:ILE:O	7:7:599:GLU:N	2.31	0.61
12:A:337:ARG:NE	13:B:1132:GLU:OE2	2.27	0.61
12:A:926:GLN:NE2	12:A:930:ASP:OD1	2.34	0.61
2:4:182:GLY:N	2:4:215:ILE:O	2.29	0.60
3:0:111:ARG:NH1	3:0:130:ASP:OD1	2.33	0.60
6:5:53:GLU:HA	6:5:56:ARG:HB2	1.83	0.60
7:7:384:ILE:HG23	7:7:536:TYR:HD2	1.65	0.60
7:7:541:MET:HE1	7:7:552:VAL:HG11	1.83	0.60
12:A:427:GLN:HB2	12:A:430:TRP:CE2	2.36	0.60
12:A:791:ASP:OD1	12:A:793:SER:OG	2.19	0.60
12:A:1152:ILE:HB	20:I:44:TYR:HB3	1.83	0.60
13:B:901:PRO:HD3	23:L:58:LYS:HG3	1.82	0.60
21:J:7:CYS:HB2	21:J:49:MET:HG3	1.82	0.60
3:0:19:PRO:HB2	3:0:486:THR:HG21	1.83	0.60
7:7:115:SER:N	7:7:137:SER:O	2.31	0.60
7:7:551:ASN:ND2	7:7:702:ASN:OD1	2.32	0.60
8:3:27:LYS:HB3	8:3:29:LEU:HG	1.82	0.60
9:O:68:GLN:O	9:O:127:LYS:NZ	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:130:DA:H2''	11:T:131:DC:H5''	1.83	0.60
13:B:120:ARG:NH2	13:B:956:THR:OG1	2.35	0.60
1:1:284:TRP:HA	1:1:287:PHE:HB3	1.83	0.60
4:6:328:ILE:N	4:6:346:GLY:O	2.29	0.60
4:6:175:ARG:NH2	4:6:203:GLU:O	2.35	0.60
4:6:336:CYS:N	4:6:341:LYS:O	2.34	0.60
7:7:722:ARG:O	7:7:726:LEU:N	2.33	0.60
12:A:860:LEU:HD11	12:A:1394:THR:HA	1.83	0.60
13:B:260:GLY:O	13:B:267:ARG:NH2	2.30	0.60
15:D:71:LYS:HA	15:D:74:GLN:HB3	1.82	0.60
16:E:8:ASN:OD1	16:E:8:ASN:N	2.34	0.60
5:2:80:SER:O	5:2:83:SER:OG	2.14	0.60
7:7:351:ASP:HA	7:7:405:LYS:HG2	1.83	0.60
1:1:478:UNK:O	1:1:482:UNK:N	2.34	0.60
5:2:399:TYR:O	5:2:403:HIS:N	2.24	0.60
7:7:497:MET:HA	7:7:500:ARG:HE	1.65	0.60
11:T:131:DC:OP1	25:Q:327:ARG:N	2.35	0.60
12:A:951:GLU:OE2	12:A:953:ASN:ND2	2.34	0.60
13:B:1134:GLU:OE1	13:B:1134:GLU:N	2.30	0.60
14:C:8:VAL:HG11	22:K:105:PHE:HD1	1.66	0.60
15:D:39:ASN:ND2	15:D:43:GLU:OE1	2.35	0.60
7:7:421:ARG:HG3	7:7:454:VAL:HG11	1.83	0.60
7:7:556:GLU:HB2	7:7:733:PHE:CE1	2.36	0.60
12:A:306:ASN:HB2	12:A:324:SER:HB3	1.82	0.60
12:A:506:ALA:HB3	12:A:509:LEU:HG	1.81	0.60
14:C:69:LEU:O	21:J:6:ARG:NH2	2.34	0.60
3:0:97:LEU:O	3:0:100:GLN:NE2	2.33	0.60
3:0:439:CYS:SG	3:0:440:LEU:N	2.75	0.60
5:2:221:VAL:O	5:2:225:ILE:N	2.30	0.60
7:7:353:ASP:OD1	7:7:404:LYS:NZ	2.35	0.60
7:7:674:SER:O	7:7:722:ARG:NH2	2.34	0.60
12:A:475:THR:OG1	12:A:480:ALA:O	2.18	0.60
20:I:14:LEU:HB3	20:I:27:PHE:HB3	1.84	0.60
20:I:59:VAL:HG23	20:I:61:ASP:H	1.66	0.60
1:1:194:VAL:O	1:1:198:THR:OG1	2.17	0.60
1:1:382:SER:O	1:1:386:ILE:N	2.32	0.60
3:0:21:GLN:O	3:0:25:MET:N	2.30	0.60
7:7:391:GLY:HA2	7:7:394:LEU:HD13	1.84	0.60
7:7:515:ALA:HB1	7:7:685:GLN:HB2	1.84	0.60
12:A:250:ILE:O	12:A:258:GLY:N	2.35	0.60
13:B:652:LYS:HB3	13:B:689:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:198:LEU:HD23	15:D:201:LYS:HG3	1.83	0.60
16:E:28:TYR:HA	16:E:64:PRO:HA	1.82	0.60
18:G:45:ILE:HG13	18:G:78:VAL:HG12	1.82	0.60
24:M:298:VAL:HG13	24:M:302:LEU:HD13	1.84	0.60
6:5:42:VAL:HB	6:5:47:VAL:HG22	1.82	0.60
7:7:371:SER:HA	7:7:374:PHE:HB2	1.84	0.60
7:7:597:TYR:HA	7:7:600:ARG:HH21	1.67	0.60
12:A:335:ARG:HH21	13:B:1114:LEU:HD21	1.66	0.60
20:I:103:CYS:SG	20:I:105:SER:N	2.75	0.60
1:1:498:UNK:O	1:1:502:ARG:N	2.34	0.59
3:0:644:GLU:O	3:0:647:ARG:NH1	2.35	0.59
21:J:32:GLU:OE1	21:J:32:GLU:N	2.30	0.59
27:U:269:ILE:HG12	28:V:111:LEU:HD21	1.82	0.59
3:0:44:SER:HA	3:0:48:LYS:HZ3	1.67	0.59
3:0:675:ASP:OD1	3:0:676:TYR:N	2.36	0.59
3:0:751:ARG:O	3:0:754:GLN:NE2	2.35	0.59
7:7:598:HIS:CD2	7:7:603:ASP:HB2	2.37	0.59
11:T:135:DG:H2'	11:T:136:DA:C8	2.37	0.59
12:A:250:ILE:HG23	24:M:62:GLU:HB2	1.84	0.59
18:G:100:GLU:HA	18:G:109:PHE:HA	1.84	0.59
24:M:39:SER:OG	24:M:40:GLU:OE1	2.19	0.59
29:W:143:ASP:OD1	29:W:143:ASP:N	2.29	0.59
2:4:52:LYS:NZ	2:4:242:GLU:O	2.31	0.59
7:7:242:LEU:O	7:7:246:LEU:N	2.27	0.59
7:7:345:ASN:O	7:7:508:HIS:NE2	2.35	0.59
12:A:999:VAL:H	12:A:1011:GLN:HE22	1.50	0.59
13:B:975:GLN:N	13:B:978:ASP:OD2	2.30	0.59
15:D:197:SER:O	15:D:201:LYS:NZ	2.28	0.59
16:E:192:ARG:NH1	16:E:215:MET:O	2.35	0.59
3:0:68:LYS:HG3	3:0:226:VAL:HA	1.84	0.59
3:0:210:TYR:O	3:0:214:LEU:N	2.32	0.59
3:0:274:VAL:O	3:0:278:ASP:N	2.32	0.59
3:0:573:THR:OG1	3:0:575:ASP:O	2.19	0.59
5:2:484:LYS:NZ	5:2:486:ASP:OD1	2.35	0.59
12:A:175:ARG:HH22	12:A:184:SER:HB2	1.67	0.59
3:0:692:GLN:OE1	3:0:692:GLN:N	2.35	0.59
7:7:461:ALA:HB1	7:7:500:ARG:HB3	1.83	0.59
7:7:669:CYS:HA	7:7:704:PHE:HB2	1.84	0.59
13:B:68:THR:HG22	13:B:91:SER:HB3	1.85	0.59
16:E:61:GLN:HG3	16:E:105:PHE:HE1	1.68	0.59
6:5:14:PRO:HA	6:5:17:LYS:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:699:GLU:O	7:7:702:ASN:ND2	2.36	0.59
3:0:489:LYS:NZ	3:0:728:THR:OG1	2.33	0.59
7:7:303:ARG:HG2	7:7:304:GLU:H	1.68	0.59
7:7:366:GLN:O	7:7:370:LEU:N	2.29	0.59
7:7:593:PHE:HA	7:7:596:GLN:HG2	1.83	0.59
12:A:491:VAL:O	13:B:1150:ARG:NH2	2.34	0.59
12:A:1444:MET:HB2	17:F:133:VAL:HG13	1.84	0.59
14:C:75:MET:O	14:C:246:ARG:NH2	2.31	0.59
18:G:33:GLU:HG3	18:G:34:VAL:HG23	1.84	0.59
4:6:162:ASP:O	4:6:378:ARG:NH2	2.35	0.59
4:6:176:ASN:HA	4:6:206:GLY:HA3	1.85	0.59
5:2:50:MET:HB3	5:2:100:LEU:HG	1.83	0.59
7:7:386:LEU:HD12	7:7:513:LEU:HD22	1.85	0.59
7:7:409:VAL:O	7:7:455:SER:N	2.35	0.59
7:7:474:MET:HA	7:7:477:LEU:HB2	1.85	0.59
7:7:477:LEU:HA	7:7:482:TRP:NE1	2.12	0.59
7:7:603:ASP:OD1	7:7:696:ARG:NH1	2.36	0.59
7:7:635:GLU:O	7:7:638:ASN:ND2	2.36	0.59
13:B:46:GLN:OE1	13:B:46:GLN:N	2.36	0.59
13:B:324:ILE:HG21	13:B:330:ALA:HB2	1.83	0.59
3:0:227:SER:OG	3:0:452:ARG:NH2	2.30	0.59
3:0:250:LEU:N	3:0:437:PHE:O	2.35	0.59
4:6:260:ARG:HG2	4:6:281:ASN:HA	1.85	0.59
5:2:352:ASN:N	5:2:352:ASN:OD1	2.35	0.59
7:7:331:GLN:HE22	7:7:523:LYS:HB2	1.68	0.59
7:7:387:PRO:HG2	7:7:540:TRP:HZ2	1.68	0.59
7:7:439:THR:O	7:7:440:SER:OG	2.18	0.59
12:A:525:GLN:HG3	13:B:835:GLN:HB3	1.83	0.59
19:H:110:ASP:OD1	19:H:110:ASP:N	2.31	0.59
3:0:50:VAL:O	3:0:54:SER:OG	2.17	0.59
5:2:32:CYS:HB3	5:2:108:LEU:HB2	1.85	0.59
12:A:438:ASP:OD1	12:A:438:ASP:N	2.33	0.59
12:A:767:GLN:NE2	12:A:798:GLY:O	2.36	0.59
13:B:843:GLN:NE2	13:B:847:ASP:OD1	2.34	0.59
19:H:8:ASP:OD1	19:H:9:ILE:N	2.36	0.59
25:Q:102:PRO:O	25:Q:383:SER:OG	2.19	0.59
28:V:62:VAL:HA	28:V:85:VAL:HA	1.84	0.59
3:0:625:ILE:HD12	3:0:626:PRO:HD2	1.84	0.58
5:2:378:ILE:HD11	5:2:383:ILE:HG22	1.84	0.58
7:7:413:SER:O	7:7:417:VAL:HG23	2.03	0.58
12:A:326:ARG:NH2	12:A:1407:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:413:ILE:HG12	24:M:50:LEU:HD12	1.85	0.58
12:A:417:TYR:HE2	24:M:35:VAL:HG21	1.68	0.58
12:A:782:ARG:NH2	13:B:699:GLU:O	2.36	0.58
12:A:1209:MET:HB2	12:A:1228:TRP:CD1	2.38	0.58
13:B:451:LYS:O	13:B:455:SER:OG	2.16	0.58
15:D:151:PHE:O	15:D:153:ARG:NH1	2.36	0.58
16:E:191:LYS:N	16:E:194:GLU:OE1	2.36	0.58
7:7:443:LYS:NZ	7:7:444:GLU:O	2.36	0.58
7:7:757:ARG:O	7:7:761:GLN:NE2	2.35	0.58
18:G:152:SER:HA	18:G:157:ILE:HG12	1.85	0.58
23:L:30:ILE:HB	23:L:57:LEU:HB2	1.85	0.58
24:M:251:GLN:OE1	24:M:251:GLN:N	2.33	0.58
25:Q:141:ARG:NE	25:Q:348:TYR:O	2.35	0.58
29:W:110:LYS:HZ2	29:W:172:LEU:HD13	1.68	0.58
1:1:249:UNK:O	1:1:252:SER:OG	2.20	0.58
3:0:169:ASP:O	3:0:198:ARG:NH1	2.26	0.58
5:2:453:THR:HG23	6:5:10:VAL:HA	1.85	0.58
12:A:42:ASP:HB3	12:A:46:THR:H	1.68	0.58
13:B:629:ASP:O	13:B:632:ARG:NH2	2.35	0.58
25:Q:343:ARG:O	25:Q:343:ARG:NH2	2.35	0.58
3:0:92:TYR:OH	3:0:96:GLU:OE2	2.20	0.58
4:6:200:ARG:NH1	5:2:425:ASN:O	2.36	0.58
5:2:450:ARG:HH11	6:5:16:ILE:HG13	1.69	0.58
9:O:93:GLU:O	9:O:103:ILE:N	2.30	0.58
12:A:261:ASP:HB3	12:A:322:VAL:HG13	1.84	0.58
12:A:433:GLU:OE2	13:B:1108:ARG:NH2	2.36	0.58
12:A:1010:ALA:O	12:A:1014:ALA:N	2.36	0.58
14:C:120:ILE:HD13	14:C:124:LEU:HD21	1.85	0.58
18:G:125:SER:OG	18:G:129:SER:N	2.36	0.58
20:I:7:CYS:HB3	20:I:12:ASN:H	1.68	0.58
4:6:277:CYS:HB3	4:6:287:PHE:HB2	1.85	0.58
6:5:55:ASN:HA	6:5:58:LEU:HD23	1.84	0.58
13:B:21:GLU:HA	13:B:655:LYS:HB2	1.85	0.58
25:Q:366:GLU:OE1	25:Q:366:GLU:N	2.36	0.58
2:4:161:ASN:O	2:4:165:LYS:N	2.35	0.58
3:0:238:HIS:O	3:0:660:ARG:NH1	2.37	0.58
4:6:136:MET:O	4:6:144:ASN:ND2	2.37	0.58
4:6:218:ARG:NH1	4:6:257:GLU:OE2	2.36	0.58
9:O:144:GLN:NE2	9:O:150:ALA:O	2.36	0.58
18:G:86:VAL:HA	18:G:146:LYS:HA	1.85	0.58
21:J:17:LYS:HG2	21:J:41:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:28:LYS:HA	23:L:39:SER:HA	1.86	0.58
27:U:281:VAL:HG21	28:V:113:ILE:HG12	1.86	0.58
2:4:193:TYR:HA	2:4:196:ILE:HD12	1.84	0.58
5:2:485:ASP:HB2	5:2:487:LYS:HG2	1.84	0.58
7:7:584:ASN:HB3	7:7:587:LYS:HB3	1.85	0.58
9:O:68:GLN:N	9:O:161:VAL:O	2.29	0.58
12:A:47:ARG:H	12:A:47:ARG:HD3	1.68	0.58
12:A:731:ARG:NH1	12:A:734:GLU:OE1	2.37	0.58
15:D:66:ARG:O	15:D:70:PHE:N	2.34	0.58
28:V:78:PHE:O	28:V:113:ILE:N	2.33	0.58
30:X:196:LEU:HD22	30:X:245:TRP:H	1.69	0.58
1:1:548:GLU:HA	1:1:551:ARG:HB3	1.86	0.58
3:0:722:ARG:HG2	4:6:267:SER:HB2	1.85	0.58
7:7:224:LYS:H	7:7:337:VAL:HG12	1.68	0.58
7:7:412:THR:HA	7:7:457:TYR:CD2	2.37	0.58
8:3:83:ASP:O	8:3:87:ARG:N	2.26	0.58
9:O:102:VAL:HB	9:O:115:ILE:HB	1.86	0.58
15:D:39:ASN:ND2	15:D:41:GLN:OE1	2.36	0.58
19:H:93:TYR:HA	19:H:145:ARG:HB3	1.85	0.58
30:X:218:ASP:OD1	30:X:218:ASP:N	2.36	0.58
3:0:353:SER:HB2	3:0:417:LEU:HD11	1.86	0.58
4:6:159:GLU:O	4:6:163:GLN:NE2	2.37	0.58
4:6:210:LEU:HB3	4:6:241:THR:HB	1.86	0.58
4:6:293:ASP:OD2	4:6:295:THR:OG1	2.16	0.58
5:2:384:ARG:O	5:2:388:THR:N	2.36	0.58
6:5:43:ASN:HB3	6:5:46:LYS:HG3	1.84	0.58
9:O:195:TYR:HB3	9:O:204:LEU:HB2	1.86	0.58
12:A:526:ASP:O	12:A:530:GLY:N	2.27	0.58
12:A:771:GLU:N	12:A:822:GLU:OE2	2.32	0.58
12:A:1111:MET:SD	12:A:1330:ASN:ND2	2.77	0.58
12:A:1293:SER:N	12:A:1297:GLU:O	2.37	0.58
24:M:133:ILE:HA	24:M:136:LEU:HB2	1.85	0.58
1:1:207:SER:OG	1:1:208:GLU:OE1	2.19	0.58
1:1:483:UNK:O	1:1:485:UNK:N	2.37	0.58
10:N:37:DC:H2'	10:N:38:DG:C8	2.38	0.58
12:A:672:ASP:OD1	12:A:672:ASP:N	2.37	0.58
12:A:1079:MET:HE3	12:A:1359:ASP:HB3	1.86	0.58
12:A:1141:THR:OG1	12:A:1274:ARG:N	2.36	0.58
3:0:99:TYR:OH	3:0:173:LYS:NZ	2.34	0.57
3:0:286:TYR:O	3:0:326:ARG:NH1	2.28	0.57
3:0:690:ARG:NH2	3:0:701:LEU:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:378:ARG:O	4:6:382:HIS:ND1	2.37	0.57
7:7:582:ILE:HG12	7:7:673:ILE:HG22	1.86	0.57
7:7:654:LEU:HD22	7:7:662:ILE:HD11	1.86	0.57
13:B:298:LEU:HD23	13:B:311:LEU:HD22	1.84	0.57
18:G:138:THR:O	18:G:141:SER:OG	2.21	0.57
29:W:32:ILE:HD11	29:W:58:ILE:HD12	1.86	0.57
2:4:66:ALA:O	5:2:37:ARG:NE	2.37	0.57
3:0:354:GLU:N	3:0:418:LEU:O	2.37	0.57
4:6:188:ASN:ND2	4:6:191:ASP:OD1	2.37	0.57
5:2:11:THR:HA	5:2:14:LEU:HD22	1.86	0.57
7:7:682:GLN:O	7:7:686:ARG:N	2.37	0.57
14:C:102:GLN:HG3	14:C:154:LYS:HG2	1.85	0.57
1:1:475:UNK:O	1:1:479:UNK:N	2.38	0.57
3:0:288:LYS:O	3:0:291:GLN:NE2	2.37	0.57
5:2:42:LEU:H	5:2:42:LEU:HD22	1.69	0.57
6:5:27:MET:HE2	6:5:49:PHE:HD2	1.67	0.57
7:7:234:VAL:N	7:7:316:PHE:H	1.95	0.57
7:7:244:MET:O	7:7:248:ASP:N	2.38	0.57
12:A:658:LEU:HD12	13:B:831:SER:HA	1.84	0.57
13:B:1049:ASP:OD1	13:B:1049:ASP:N	2.35	0.57
20:I:10:CYS:SG	20:I:31:THR:OG1	2.62	0.57
2:4:288:ILE:HD12	2:4:293:LEU:HD13	1.85	0.57
5:2:350:TYR:H	5:2:407:GLN:CD	2.11	0.57
7:7:712:ASP:N	7:7:716:MET:SD	2.72	0.57
12:A:1044:TRP:O	12:A:1048:ASN:ND2	2.33	0.57
12:A:1141:THR:HG22	12:A:1205:LYS:HD2	1.84	0.57
13:B:323:VAL:HG23	13:B:324:ILE:HG13	1.86	0.57
1:1:547:LEU:O	1:1:551:ARG:N	2.30	0.57
1:1:558:CYS:O	1:1:562:LYS:N	2.33	0.57
3:0:647:ARG:O	3:0:649:ARG:NH2	2.28	0.57
7:7:576:LYS:HG2	7:7:579:LEU:HD12	1.86	0.57
7:7:724:ALA:O	7:7:728:ASP:N	2.38	0.57
12:A:41:MET:O	24:M:90:ASN:ND2	2.37	0.57
13:B:861:ASP:OD2	13:B:939:THR:OG1	2.16	0.57
13:B:1219:ASP:N	13:B:1219:ASP:OD1	2.38	0.57
16:E:118:PRO:O	16:E:122:LYS:N	2.34	0.57
3:0:645:ASN:O	3:0:647:ARG:NH2	2.37	0.57
5:2:384:ARG:HA	5:2:387:LEU:HB2	1.86	0.57
13:B:356:LEU:O	13:B:374:LYS:NZ	2.32	0.57
22:K:58:PHE:HE2	22:K:74:ARG:HD3	1.69	0.57
24:M:189:PHE:O	24:M:193:GLN:N	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:83:ILE:HG21	2:4:152:ALA:HB2	1.86	0.57
6:5:14:PRO:O	6:5:18:ALA:N	2.30	0.57
7:7:343:PHE:CD2	7:7:380:ARG:HB2	2.34	0.57
7:7:366:GLN:HE22	7:7:394:LEU:HB2	1.69	0.57
7:7:608:PHE:HB2	7:7:690:ILE:HG21	1.87	0.57
15:D:66:ARG:NH2	18:G:48:VAL:O	2.36	0.57
23:L:53:HIS:O	23:L:54:ARG:NH1	2.37	0.57
29:W:109:LEU:HD21	29:W:171:LYS:HB3	1.87	0.57
8:3:86:LYS:O	8:3:90:ASN:N	2.36	0.57
14:C:55:THR:HG1	14:C:152:GLU:H	1.53	0.57
18:G:87:VAL:N	18:G:145:VAL:O	2.26	0.57
24:M:315:ILE:O	24:M:319:HIS:NE2	2.38	0.57
1:1:544:ILE:O	1:1:548:GLU:N	2.30	0.57
3:0:1:MET:HB2	3:0:12:PHE:HB3	1.87	0.57
3:0:78:GLU:HA	3:0:81:LYS:HD2	1.87	0.57
3:0:117:HIS:CE1	3:0:119:GLU:HB3	2.39	0.57
6:5:24:ASP:HB3	6:5:29:ASP:CG	2.29	0.57
7:7:434:ASN:OD1	7:7:450:SER:OG	2.23	0.57
7:7:461:ALA:HB3	7:7:501:VAL:HG12	1.87	0.57
12:A:1287:TYR:OH	12:A:1307:GLU:OE2	2.22	0.57
13:B:364:ILE:HG13	13:B:365:THR:HG22	1.85	0.57
14:C:184:ASN:ND2	14:C:189:THR:O	2.34	0.57
25:Q:100:GLU:HG3	26:R:94:LYS:HG2	1.87	0.57
3:0:104:ARG:O	3:0:204:ASN:N	2.37	0.57
3:0:212:TYR:HA	3:0:218:ILE:HG13	1.87	0.57
5:2:59:LEU:HD11	5:2:507:ARG:HH12	1.70	0.57
7:7:361:GLN:HG2	7:7:424:PHE:HE1	1.69	0.57
7:7:396:GLY:O	7:7:400:ALA:N	2.24	0.57
13:B:756:ILE:HG12	13:B:770:GLN:HG2	1.87	0.57
20:I:78:CYS:SG	20:I:105:SER:OG	2.62	0.57
5:2:200:LEU:O	5:2:204:LEU:N	2.31	0.56
5:2:351:SER:N	5:2:407:GLN:OE1	2.29	0.56
5:2:437:VAL:O	5:2:441:ILE:N	2.33	0.56
7:7:212:PHE:O	7:7:216:ALA:N	2.32	0.56
7:7:625:PRO:HB2	7:7:639:ILE:HG12	1.86	0.56
12:A:54:ASN:OD1	12:A:54:ASN:N	2.37	0.56
12:A:1193:LEU:HD23	12:A:1240:CYS:HB3	1.87	0.56
13:B:101:MET:N	13:B:101:MET:SD	2.77	0.56
19:H:40:LEU:HD13	19:H:123:MET:HB2	1.86	0.56
3:0:8:LEU:HD23	3:0:62:HIS:HB3	1.86	0.56
3:0:80:GLU:HB3	3:0:178:PHE:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:489:GLU:HB2	7:7:491:HIS:CE1	2.40	0.56
7:7:725:PHE:O	7:7:729:GLN:NE2	2.37	0.56
14:C:6:PRO:HG2	22:K:101:LEU:HD13	1.87	0.56
15:D:39:ASN:HD21	15:D:41:GLN:HB2	1.70	0.56
25:Q:337:GLU:CD	25:Q:340:LYS:H	2.12	0.56
26:R:75:MET:SD	26:R:76:PHE:N	2.78	0.56
2:4:32:ILE:HD11	2:4:79:TYR:HD1	1.70	0.56
3:0:116:LEU:N	32:0:801:SF4:S3	2.78	0.56
3:0:208:TYR:CD2	3:0:212:TYR:HB2	2.40	0.56
3:0:587:ARG:HH21	3:0:612:PHE:HA	1.69	0.56
12:A:340:LEU:HD13	12:A:1429:ILE:HG23	1.87	0.56
12:A:690:VAL:O	12:A:694:THR:OG1	2.23	0.56
12:A:890:ASP:O	12:A:894:GLU:N	2.32	0.56
22:K:29:ASN:ND2	22:K:77:THR:OG1	2.38	0.56
24:M:181:ARG:NH1	24:M:234:GLN:OE1	2.38	0.56
1:1:561:LEU:HA	1:1:564:PHE:HB2	1.85	0.56
2:4:122:ASP:O	2:4:126:VAL:N	2.38	0.56
4:6:379:SER:O	4:6:383:LEU:N	2.35	0.56
4:6:403:CYS:HB2	4:6:437:CYS:HB3	1.86	0.56
6:5:20:ILE:HA	6:5:23:ILE:HB	1.88	0.56
7:7:258:SER:O	7:7:317:GLU:N	2.28	0.56
10:N:6:DA:C2	10:N:7:DA:C5	2.94	0.56
12:A:114:LEU:HD13	12:A:145:LYS:HB3	1.87	0.56
13:B:216:GLU:OE1	13:B:537:LYS:NZ	2.39	0.56
16:E:55:ARG:NH1	16:E:113:GLN:OE1	2.39	0.56
16:E:173:SER:O	16:E:177:ARG:NH1	2.36	0.56
2:4:274:THR:HG23	2:4:295:VAL:HG11	1.87	0.56
2:4:303:ASN:HA	2:4:312:PHE:H	1.71	0.56
4:6:310:VAL:HG13	4:6:311:ASN:H	1.70	0.56
4:6:390:ALA:N	4:6:428:ARG:O	2.38	0.56
6:5:27:MET:O	6:5:28:SER:OG	2.21	0.56
7:7:372:LYS:HB3	7:7:535:LEU:HD12	1.88	0.56
7:7:670:LEU:N	7:7:704:PHE:O	2.35	0.56
7:7:752:SER:HG	7:7:755:GLU:H	1.51	0.56
16:E:19:VAL:HG22	16:E:140:LEU:HD13	1.88	0.56
5:2:197:ASN:O	5:2:201:TRP:N	2.35	0.56
7:7:315:SER:OG	7:7:316:PHE:N	2.33	0.56
7:7:348:ARG:H	7:7:508:HIS:CE1	2.23	0.56
7:7:383:ILE:HG13	7:7:528:ASN:HA	1.85	0.56
7:7:457:TYR:HH	7:7:488:ASP:H	1.53	0.56
19:H:5:LEU:HD11	19:H:61:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:370:SER:HB3	25:Q:392:VAL:HG12	1.88	0.56
2:4:117:ARG:HA	2:4:120:ASN:HD21	1.70	0.56
3:0:32:LEU:HB3	3:0:59:TYR:CZ	2.40	0.56
3:0:394:GLU:O	3:0:397:THR:OG1	2.22	0.56
5:2:50:MET:HE2	5:2:100:LEU:H	1.70	0.56
7:7:491:HIS:CG	7:7:681:ARG:HH11	2.23	0.56
7:7:554:CYS:O	7:7:734:LYS:N	2.39	0.56
7:7:566:TYR:O	7:7:570:LEU:N	2.34	0.56
12:A:146:MET:HA	12:A:171:GLN:HB2	1.88	0.56
12:A:809:THR:OG1	12:A:812:GLU:OE2	2.23	0.56
13:B:969:ARG:NH2	14:C:60:ASP:OD2	2.39	0.56
13:B:1187:ASN:ND2	13:B:1190:ASP:O	2.39	0.56
18:G:101:VAL:N	18:G:108:VAL:O	2.25	0.56
2:4:162:ARG:HD2	4:6:406:CYS:HB2	1.87	0.56
3:0:291:GLN:HE22	3:0:294:HIS:HA	1.70	0.56
3:0:690:ARG:HG3	3:0:701:LEU:HD23	1.87	0.56
3:0:740:SER:H	3:0:744:LEU:HD22	1.69	0.56
7:7:485:ILE:HB	7:7:510:LYS:HA	1.87	0.56
12:A:405:VAL:HG23	12:A:415:LEU:HD21	1.86	0.56
12:A:1143:LEU:HB2	12:A:1273:LEU:HD21	1.88	0.56
13:B:71:LEU:O	13:B:88:TYR:N	2.27	0.56
13:B:693:ILE:HG23	13:B:697:GLU:HB3	1.87	0.56
13:B:983:ARG:NH2	13:B:1028:GLU:OE2	2.35	0.56
3:0:744:LEU:O	3:0:748:GLN:N	2.32	0.56
4:6:200:ARG:HH21	4:6:201:LYS:HE3	1.70	0.56
6:5:49:PHE:HA	6:5:52:HIS:CD2	2.41	0.56
7:7:363:ARG:HA	7:7:695:ARG:CZ	2.35	0.56
7:7:476:PHE:O	7:7:480:ARG:N	2.33	0.56
13:B:294:ASP:OD1	13:B:294:ASP:N	2.38	0.56
13:B:603:LEU:HB3	13:B:608:ASP:HB2	1.88	0.56
18:G:49:LEU:HD21	18:G:75:ARG:HG2	1.87	0.56
19:H:80:ARG:HG2	22:K:57:LEU:HD22	1.88	0.56
24:M:253:THR:O	24:M:257:GLU:N	2.34	0.56
25:Q:374:VAL:HG22	25:Q:388:PRO:HB3	1.88	0.56
26:R:258:THR:HG22	26:R:261:VAL:HG22	1.88	0.56
1:1:350:ARG:NH1	3:0:401:ASP:OD1	2.38	0.56
2:4:258:LEU:H	2:4:258:LEU:HD12	1.69	0.56
5:2:473:LYS:O	5:2:477:ASP:N	2.39	0.56
7:7:468:HIS:ND1	7:7:471:GLN:OE1	2.39	0.56
7:7:591:CYS:HA	7:7:594:LEU:HD12	1.87	0.56
12:A:225:ASN:N	12:A:229:SER:OG	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:849:MET:HE2	12:A:1061:GLY:HA2	1.87	0.56
13:B:982:SER:OG	13:B:983:ARG:N	2.37	0.56
25:Q:340:LYS:O	25:Q:344:PHE:N	2.36	0.56
1:1:348:VAL:HG12	3:0:127:THR:HG22	1.87	0.55
3:0:314:GLN:HA	3:0:317:LEU:HD13	1.88	0.55
5:2:56:GLU:HB2	5:2:99:ASN:HB3	1.88	0.55
7:7:637:MET:N	7:7:637:MET:SD	2.79	0.55
8:3:31:ASN:HB3	8:3:34:CYS:HB2	1.87	0.55
12:A:599:SER:O	12:A:599:SER:OG	2.17	0.55
13:B:805:THR:OG1	13:B:806:THR:N	2.40	0.55
18:G:35:GLU:OE2	18:G:48:VAL:N	2.32	0.55
19:H:81:PRO:O	19:H:83:GLN:NE2	2.38	0.55
3:0:256:ALA:O	3:0:260:ALA:N	2.36	0.55
3:0:378:SER:OG	3:0:403:ALA:O	2.23	0.55
3:0:625:ILE:HG22	3:0:685:ARG:HH21	1.72	0.55
4:6:156:PHE:HB2	4:6:301:PHE:CD2	2.40	0.55
5:2:62:LEU:HA	5:2:65:TRP:CD1	2.41	0.55
5:2:202:THR:O	5:2:206:GLN:N	2.33	0.55
5:2:222:LEU:HD22	5:2:225:ILE:HD12	1.87	0.55
12:A:217:LYS:O	12:A:217:LYS:NZ	2.38	0.55
12:A:230:ARG:HB2	12:A:233:TRP:CD2	2.41	0.55
13:B:573:GLN:OE1	13:B:573:GLN:N	2.39	0.55
15:D:140:ASP:O	15:D:144:THR:N	2.26	0.55
19:H:87:ARG:NH1	19:H:91:ASP:OD2	2.39	0.55
25:Q:123:SER:HB3	25:Q:361:TRP:HH2	1.71	0.55
25:Q:351:VAL:HG22	25:Q:362:VAL:HG22	1.87	0.55
1:1:510:ASN:HB3	2:4:264:LYS:HG3	1.88	0.55
6:5:22:GLN:H	6:5:22:GLN:CD	2.13	0.55
7:7:580:LEU:HD11	7:7:764:LEU:HA	1.87	0.55
7:7:596:GLN:HA	7:7:599:GLU:HB2	1.88	0.55
12:A:900:ASP:N	12:A:900:ASP:OD1	2.39	0.55
16:E:157:SER:N	16:E:160:GLU:OE1	2.39	0.55
25:Q:374:VAL:HA	25:Q:388:PRO:HA	1.87	0.55
5:2:234:GLY:O	5:2:269:PHE:N	2.40	0.55
7:7:365:TYR:HB2	7:7:543:LEU:O	2.06	0.55
7:7:694:LYS:HG3	7:7:696:ARG:HB2	1.88	0.55
12:A:367:PRO:HB3	12:A:466:SER:HA	1.87	0.55
12:A:840:ARG:NH1	12:A:1106:ASN:OD1	2.36	0.55
13:B:766:ARG:NH1	13:B:985:GLY:O	2.39	0.55
24:M:41:GLY:HA2	24:M:56:LEU:HD23	1.87	0.55
29:W:65:ARG:HB3	29:W:93:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:185:LEU:HD12	1:1:191:LEU:HB3	1.89	0.55
12:A:78:PRO:O	13:B:1201:LYS:NZ	2.29	0.55
16:E:24:LYS:NZ	16:E:32:GLN:OE1	2.38	0.55
25:Q:361:TRP:HB3	25:Q:395:PHE:HD2	1.72	0.55
1:1:195:PHE:O	1:1:199:VAL:N	2.39	0.55
3:0:131:GLU:OE2	3:0:135:ARG:NH2	2.40	0.55
3:0:573:THR:OG1	3:0:579:THR:OG1	2.22	0.55
7:7:366:GLN:HG3	7:7:548:HIS:HE1	1.72	0.55
7:7:495:ALA:N	7:7:521:ASP:OD1	2.39	0.55
9:O:129:GLU:HB2	9:O:157:ILE:HD11	1.88	0.55
10:N:5:DA:C2	10:N:6:DA:C5	2.95	0.55
22:K:83:PRO:HA	22:K:86:ALA:HB3	1.89	0.55
24:M:132:LYS:HA	24:M:135:MET:HE2	1.88	0.55
25:Q:369:ASN:OD1	26:R:72:ARG:NH2	2.39	0.55
2:4:202:SER:O	2:4:206:MET:N	2.34	0.55
7:7:372:LYS:HE2	7:7:543:LEU:HD21	1.87	0.55
7:7:446:PHE:HB3	7:7:473:VAL:HG22	1.89	0.55
7:7:757:ARG:HH11	7:7:758:GLU:HA	1.72	0.55
9:O:158:GLN:HE21	10:N:23:DA:H4'	1.70	0.55
12:A:585:GLY:N	12:A:609:ASP:OD1	2.34	0.55
13:B:1074:ASN:ND2	13:B:1076:HIS:H	2.04	0.55
14:C:196:ASP:OD2	14:C:199:LYS:N	2.36	0.55
19:H:35:GLN:OE1	19:H:35:GLN:N	2.39	0.55
19:H:38:LEU:HB2	19:H:125:LEU:HD13	1.89	0.55
22:K:58:PHE:HB3	22:K:76:GLN:HB3	1.88	0.55
22:K:68:PHE:HB2	22:K:70:ARG:HG2	1.88	0.55
1:1:550:CYS:HA	1:1:553:LEU:HB3	1.88	0.55
3:0:116:LEU:HB3	3:0:158:TYR:CE2	2.42	0.55
9:O:66:THR:O	9:O:163:SER:N	2.39	0.55
13:B:120:ARG:NH2	13:B:957:ASN:O	2.39	0.55
15:D:63:LEU:HB3	15:D:130:LEU:HD22	1.89	0.55
15:D:212:LYS:O	15:D:216:ASN:N	2.38	0.55
2:4:182:GLY:HA3	2:4:216:GLY:HA3	1.88	0.55
5:2:176:VAL:O	5:2:181:GLU:N	2.37	0.55
5:2:187:GLU:O	5:2:191:PHE:N	2.40	0.55
6:5:51:LYS:HA	6:5:54:LEU:HB3	1.89	0.55
12:A:469:ARG:NH2	13:B:991:GLY:O	2.39	0.55
13:B:122:LEU:O	13:B:207:GLY:N	2.40	0.55
19:H:96:VAL:HA	19:H:142:LEU:O	2.06	0.55
3:0:137:THR:HG23	3:0:156:CYS:H	1.72	0.55
5:2:226:PHE:O	5:2:230:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:538:ASP:OD1	12:A:538:ASP:N	2.39	0.55
13:B:238:ALA:HB2	13:B:385:LEU:HD13	1.89	0.55
16:E:55:ARG:HG2	16:E:58:MET:HE2	1.89	0.55
16:E:84:ASP:O	16:E:113:GLN:NE2	2.39	0.55
18:G:39:THR:OG1	18:G:42:PHE:N	2.40	0.55
30:X:187:HIS:N	30:X:191:GLU:OE1	2.40	0.55
4:6:172:ILE:HA	4:6:181:LEU:HA	1.88	0.54
7:7:329:ARG:O	7:7:333:ILE:N	2.26	0.54
7:7:403:ILE:O	7:7:405:LYS:HG3	2.07	0.54
12:A:1323:ASP:OD1	12:A:1325:THR:OG1	2.20	0.54
13:B:127:GLY:HA2	13:B:169:ARG:HA	1.90	0.54
13:B:952:VAL:O	23:L:58:LYS:HB2	2.08	0.54
15:D:64:VAL:HG22	15:D:67:ARG:HH12	1.72	0.54
15:D:212:LYS:HA	15:D:215:SER:HB3	1.88	0.54
19:H:132:LEU:HA	19:H:135:LEU:HD21	1.89	0.54
24:M:40:GLU:OE1	24:M:40:GLU:N	2.40	0.54
29:W:101:LYS:NZ	30:X:263:TRP:O	2.30	0.54
4:6:189:PRO:O	4:6:193:ILE:N	2.34	0.54
6:5:24:ASP:O	6:5:29:ASP:N	2.40	0.54
7:7:384:ILE:HG23	7:7:536:TYR:CD2	2.41	0.54
7:7:544:SER:HB2	7:7:549:ILE:HB	1.90	0.54
13:B:806:THR:HG23	13:B:1045:SER:HA	1.88	0.54
14:C:54:ASN:ND2	14:C:60:ASP:OD1	2.34	0.54
19:H:28:ALA:HB3	19:H:38:LEU:HB3	1.89	0.54
1:1:254:GLU:OE1	1:1:254:GLU:N	2.34	0.54
1:1:375:LEU:HB3	3:0:571:VAL:HG11	1.89	0.54
2:4:137:LYS:H	2:4:140:ILE:HB	1.70	0.54
3:0:601:VAL:HG12	3:0:603:ARG:H	1.71	0.54
3:0:729:ASP:O	3:0:731:LYS:NZ	2.41	0.54
5:2:352:ASN:HB3	5:2:374:VAL:HG22	1.88	0.54
8:3:53:GLN:HG3	8:3:60:ASP:HA	1.89	0.54
13:B:129:PHE:HE2	26:R:266:THR:HG21	1.72	0.54
15:D:178:ALA:O	15:D:182:SER:N	2.31	0.54
24:M:58:ASP:OD1	24:M:60:ARG:N	2.33	0.54
27:U:282:GLU:N	28:V:62:VAL:O	2.40	0.54
2:4:180:THR:HG23	2:4:214:LYS:HA	1.89	0.54
3:0:419:ILE:HG23	3:0:436:ARG:HB3	1.89	0.54
6:5:36:ASP:HB2	6:5:39:HIS:CE1	2.42	0.54
9:O:161:VAL:HA	9:O:215:THR:HA	1.88	0.54
12:A:1364:ASN:HD21	12:A:1366:ARG:HH11	1.55	0.54
14:C:79:GLN:HB3	14:C:127:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:118:THR:OG1	15:D:120:GLU:OE1	2.25	0.54
25:Q:140:HIS:HB3	26:R:209:PRO:HB3	1.89	0.54
3:0:139:GLY:HA3	3:0:302:GLN:HE21	1.73	0.54
3:0:337:ARG:HB3	3:0:367:THR:HG21	1.89	0.54
4:6:209:SER:HA	4:6:242:THR:HB	1.89	0.54
4:6:390:ALA:O	4:6:428:ARG:N	2.26	0.54
7:7:719:SER:O	7:7:723:GLN:N	2.40	0.54
9:O:76:LEU:O	9:O:151:LYS:N	2.36	0.54
24:M:283:TYR:HA	24:M:286:ILE:HG22	1.89	0.54
1:1:228:UNK:C	4:6:244:PRO:HG3	2.38	0.54
4:6:262:LYS:HZ3	4:6:287:PHE:C	2.14	0.54
5:2:370:PHE:CD2	5:2:373:MET:HB3	2.42	0.54
11:T:150:DG:H5"	24:M:276:THR:HG21	1.89	0.54
12:A:866:PHE:HE2	16:E:211:TYR:H	1.56	0.54
18:G:149:GLY:O	18:G:160:ILE:N	2.33	0.54
27:U:247:LEU:HB3	28:V:118:SER:HB3	1.90	0.54
2:4:27:THR:HG21	2:4:160:VAL:HG22	1.90	0.54
4:6:176:ASN:HA	4:6:207:ASN:H	1.72	0.54
5:2:21:VAL:HA	5:2:24:ARG:HB2	1.89	0.54
5:2:349:SER:HA	5:2:407:GLN:HE22	1.72	0.54
8:3:82:VAL:O	8:3:86:LYS:N	2.30	0.54
12:A:1239:ARG:NH1	12:A:1241:ARG:HH21	1.99	0.54
13:B:1174:LYS:O	13:B:1178:ASN:N	2.41	0.54
21:J:31:ASP:OD1	21:J:31:ASP:N	2.41	0.54
3:0:137:THR:HG21	3:0:159:HIS:HB3	1.89	0.54
4:6:121:GLY:H	4:6:308:LEU:H	1.55	0.54
7:7:553:GLN:HB2	7:7:701:PHE:HB3	1.89	0.54
8:3:75:ASP:O	8:3:79:GLU:N	2.29	0.54
13:B:955:THR:HG21	23:L:55:ILE:HG12	1.88	0.54
3:0:103:PHE:O	3:0:104:ARG:NH1	2.41	0.54
3:0:171:LEU:HD22	3:0:184:TYR:HE2	1.72	0.54
7:7:354:ILE:HG22	7:7:355:ASP:H	1.73	0.54
7:7:725:PHE:HA	7:7:728:ASP:HB2	1.90	0.54
12:A:439:ASN:OD1	12:A:459:ARG:NH1	2.36	0.54
12:A:587:HIS:CD2	12:A:969:GLN:HG3	2.43	0.54
13:B:667:GLN:NE2	13:B:667:GLN:O	2.41	0.54
13:B:853:SER:OG	13:B:1094:ARG:NH1	2.41	0.54
2:4:129:ILE:O	2:4:133:PHE:N	2.41	0.54
3:0:1:MET:N	3:0:92:TYR:OH	2.41	0.54
3:0:487:LEU:HD12	3:0:489:LYS:H	1.72	0.54
5:2:111:ALA:HA	5:2:115:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:406:SER:HB2	7:7:482:TRP:CE3	2.43	0.54
7:7:540:TRP:O	7:7:544:SER:N	2.41	0.54
7:7:582:ILE:HG23	7:7:673:ILE:HG21	1.89	0.54
12:A:1393:ASN:OD1	12:A:1393:ASN:N	2.37	0.54
13:B:816:GLU:OE1	13:B:816:GLU:N	2.41	0.54
20:I:7:CYS:SG	20:I:8:ARG:N	2.81	0.54
29:W:95:ILE:HB	29:W:99:LYS:HE2	1.90	0.54
3:0:215:ASP:OD1	3:0:217:LYS:NZ	2.29	0.53
4:6:428:ARG:HA	4:6:435:GLU:HA	1.88	0.53
20:I:103:CYS:SG	20:I:107:SER:N	2.81	0.53
1:1:623:ILE:O	1:1:627:THR:N	2.32	0.53
6:5:7:GLY:HA3	6:5:41:LEU:HD23	1.90	0.53
6:5:20:ILE:O	6:5:24:ASP:N	2.28	0.53
7:7:556:GLU:HB2	7:7:733:PHE:HE1	1.73	0.53
7:7:584:ASN:ND2	7:7:710:SER:OG	2.28	0.53
9:O:71:VAL:HB	9:O:159:ASN:HB3	1.91	0.53
9:O:94:TYR:HB2	9:O:102:VAL:HG22	1.90	0.53
12:A:401:GLY:O	12:A:435:HIS:ND1	2.41	0.53
12:A:1420:ASP:N	12:A:1420:ASP:OD1	2.34	0.53
13:B:273:LEU:HB2	13:B:276:ILE:HG13	1.90	0.53
14:C:125:MET:SD	14:C:125:MET:N	2.82	0.53
19:H:131:ASN:OD1	19:H:131:ASN:N	2.33	0.53
26:R:273:ASP:HA	26:R:279:LYS:HE3	1.90	0.53
28:V:76:TRP:HB2	28:V:115:ALA:HB3	1.91	0.53
3:0:115:CYS:SG	3:0:120:VAL:HB	2.48	0.53
5:2:467:GLU:HA	5:2:470:LEU:HB2	1.90	0.53
9:O:183:SER:HB3	9:O:193:LEU:HD11	1.88	0.53
12:A:344:ARG:NH2	13:B:1120:GLU:OE1	2.41	0.53
13:B:279:ASP:OD1	13:B:279:ASP:N	2.35	0.53
13:B:326:ASP:O	13:B:329:THR:OG1	2.27	0.53
13:B:661:LEU:HD11	13:B:684:LEU:HD11	1.90	0.53
18:G:8:SER:HA	18:G:73:LYS:HA	1.89	0.53
22:K:8:GLU:O	22:K:37:LYS:HD2	2.09	0.53
3:0:37:ASN:HD22	3:0:475:PHE:HD2	1.56	0.53
3:0:553:MET:SD	3:0:554:TRP:N	2.82	0.53
7:7:341:TYR:CE2	7:7:343:PHE:HA	2.44	0.53
7:7:351:ASP:OD1	7:7:351:ASP:N	2.42	0.53
12:A:494:SER:O	12:A:497:THR:OG1	2.23	0.53
12:A:590:ARG:NH2	12:A:621:THR:OG1	2.31	0.53
12:A:1100:ARG:NH2	12:A:1351:GLU:OE2	2.33	0.53
13:B:299:GLU:HG2	13:B:571:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:586:TRP:CD1	13:B:588:GLY:H	2.26	0.53
20:I:103:CYS:SG	20:I:106:CYS:N	2.81	0.53
24:M:246:LEU:HB2	24:M:248:LEU:HD11	1.91	0.53
25:Q:346:GLU:OE1	25:Q:391:LYS:NZ	2.40	0.53
29:W:136:ALA:O	29:W:140:LEU:N	2.42	0.53
3:O:176:PHE:HA	3:O:180:LYS:HD3	1.91	0.53
3:O:539:VAL:HB	3:O:623:ILE:HD11	1.89	0.53
7:7:556:GLU:HB3	7:7:735:VAL:HG22	1.90	0.53
12:A:25:GLU:OE1	12:A:25:GLU:N	2.36	0.53
13:B:289:LEU:HD22	13:B:371:GLU:HB3	1.90	0.53
14:C:39:ALA:HA	14:C:164:ALA:HB3	1.89	0.53
15:D:173:HIS:HB3	15:D:176:GLU:HG3	1.90	0.53
26:R:96:ARG:O	26:R:105:THR:OG1	2.26	0.53
26:R:134:VAL:HB	26:R:215:VAL:HB	1.90	0.53
3:O:71:TYR:HB3	3:O:207:ILE:HG23	1.91	0.53
3:O:275:ARG:HA	3:O:279:SER:HB2	1.89	0.53
3:O:468:MET:O	3:O:472:MET:N	2.35	0.53
3:O:500:GLY:O	3:O:503:GLN:NE2	2.41	0.53
4:6:251:ILE:HG12	4:6:276:LEU:HD13	1.90	0.53
7:7:588:PHE:CZ	7:7:621:LYS:HB3	2.44	0.53
12:A:423:ASP:OD1	12:A:424:ILE:N	2.42	0.53
12:A:503:GLN:OE1	17:F:90:ARG:NH1	2.39	0.53
12:A:884:ASP:OD1	12:A:884:ASP:N	2.41	0.53
13:B:1189:ILE:HG21	18:G:41:LYS:HB2	1.91	0.53
17:F:86:THR:OG1	17:F:89:GLU:OE1	2.16	0.53
18:G:138:THR:HG22	18:G:139:ILE:H	1.74	0.53
1:1:551:ARG:HD3	4:6:340:SER:HA	1.91	0.53
3:O:651:ASN:HA	3:O:654:LEU:HB2	1.90	0.53
5:2:12:GLN:OE1	5:2:12:GLN:N	2.42	0.53
5:2:365:HIS:NE2	5:2:377:GLN:O	2.41	0.53
7:7:302:GLU:HG3	7:7:322:SER:H	1.74	0.53
7:7:343:PHE:HB3	7:7:380:ARG:HA	1.90	0.53
7:7:365:TYR:HB3	7:7:548:HIS:CB	2.39	0.53
10:N:26:DA:H2'	10:N:27:DG:C8	2.44	0.53
12:A:120:GLU:HG2	12:A:123:ARG:HD2	1.91	0.53
16:E:197:LYS:HG3	16:E:211:TYR:CE1	2.40	0.53
21:J:10:CYS:SG	21:J:43:ARG:NH2	2.75	0.53
21:J:46:CYS:O	21:J:49:MET:N	2.41	0.53
23:L:47:ARG:HA	23:L:53:HIS:O	2.09	0.53
29:W:171:LYS:HG2	29:W:174:ARG:HH11	1.73	0.53
3:O:11:LEU:HD21	3:O:97:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:498:THR:HB	3:0:707:ASN:HA	1.90	0.53
7:7:325:VAL:HA	7:7:328:LYS:HB2	1.90	0.53
7:7:625:PRO:HG2	7:7:649:ILE:HG12	1.90	0.53
12:A:793:SER:OG	12:A:795:GLU:OE1	2.22	0.53
1:1:310:UNK:O	1:1:314:UNK:N	2.42	0.53
1:1:370:UNK:O	1:1:372:VAL:N	2.38	0.53
1:1:379:ASN:O	1:1:383:GLU:N	2.37	0.53
2:4:273:ARG:NH2	4:6:372:LEU:HB2	2.23	0.53
4:6:291:LEU:HA	4:6:296:HIS:CE1	2.44	0.53
5:2:20:GLN:O	5:2:24:ARG:N	2.38	0.53
7:7:576:LYS:HZ3	7:7:579:LEU:HB2	1.72	0.53
12:A:41:MET:N	24:M:90:ASN:HD21	2.07	0.53
12:A:565:ILE:HG12	19:H:97:MET:HG2	1.90	0.53
12:A:853:ASP:N	12:A:853:ASP:OD1	2.38	0.53
12:A:1257:ASP:N	12:A:1257:ASP:OD1	2.41	0.53
13:B:86:ARG:NE	13:B:138:GLU:OE2	2.38	0.53
13:B:843:GLN:HB3	13:B:995:ARG:HA	1.91	0.53
16:E:3:GLN:N	16:E:6:GLU:OE1	2.41	0.53
18:G:86:VAL:HG12	18:G:146:LYS:HB2	1.90	0.53
19:H:4:THR:HG21	19:H:7:ASP:HB2	1.91	0.53
1:1:185:LEU:HD13	1:1:210:TRP:HH2	1.74	0.53
3:0:490:LYS:NZ	3:0:700:GLY:O	2.31	0.53
3:0:528:GLU:OE2	3:0:710:THR:OG1	2.26	0.53
3:0:611:ASP:OD1	3:0:612:PHE:N	2.42	0.53
3:0:633:ARG:O	3:0:637:ALA:N	2.31	0.53
5:2:9:SER:O	5:2:12:GLN:N	2.37	0.53
7:7:462:ASN:HA	7:7:500:ARG:NH2	2.24	0.53
12:A:1158:PRO:HB2	12:A:1159:ARG:HH11	1.74	0.53
12:A:1191:TRP:NE1	12:A:1256:GLU:OE1	2.34	0.53
13:B:106:ASP:OD1	13:B:107:GLY:N	2.42	0.53
13:B:241:ARG:NH2	13:B:250:PHE:O	2.41	0.53
14:C:162:GLY:HA3	14:C:170:TRP:CE2	2.44	0.53
24:M:160:GLU:HB2	24:M:163:LEU:HG	1.90	0.53
1:1:380:ARG:HA	1:1:383:GLU:HB2	1.91	0.52
2:4:286:GLY:H	4:6:323:GLY:HA2	1.74	0.52
4:6:175:ARG:N	4:6:178:LEU:O	2.38	0.52
7:7:303:ARG:HH12	7:7:505:ILE:HB	1.73	0.52
7:7:622:MET:HE1	7:7:624:LYS:HB2	1.91	0.52
12:A:392:VAL:HG13	12:A:415:LEU:HD11	1.91	0.52
13:B:654:ARG:H	13:B:657:HIS:CE1	2.26	0.52
18:G:50:ASP:OD2	18:G:75:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:190:ASP:OD1	29:W:193:ARG:NH1	2.41	0.52
2:4:38:THR:O	2:4:42:GLU:N	2.40	0.52
2:4:75:VAL:HB	2:4:87:TYR:H	1.74	0.52
7:7:412:THR:OG1	7:7:413:SER:N	2.42	0.52
12:A:219:PHE:HA	12:A:222:LEU:HD12	1.91	0.52
12:A:850:VAL:O	12:A:1061:GLY:N	2.29	0.52
13:B:597:MET:HG3	13:B:601:ARG:HE	1.74	0.52
16:E:59:SER:HB3	16:E:80:VAL:O	2.09	0.52
17:F:140:ASP:OD1	17:F:142:SER:N	2.40	0.52
21:J:5:VAL:HG12	21:J:6:ARG:H	1.74	0.52
25:Q:380:ASP:OD1	25:Q:380:ASP:N	2.43	0.52
7:7:362:ILE:O	7:7:695:ARG:NH2	2.33	0.52
7:7:365:TYR:HD2	7:7:548:HIS:CG	2.27	0.52
7:7:490:VAL:HB	7:7:519:ARG:HH22	1.74	0.52
12:A:209:ASN:OD1	12:A:213:HIS:NE2	2.42	0.52
12:A:353:ILE:HG13	12:A:482:PHE:HD1	1.74	0.52
13:B:345:LYS:HD3	13:B:348:ARG:HH11	1.75	0.52
13:B:737:THR:OG1	20:I:66:PRO:O	2.23	0.52
15:D:194:LEU:HB3	18:G:86:VAL:HG21	1.91	0.52
16:E:185:ALA:O	16:E:189:GLY:N	2.42	0.52
27:U:282:GLU:HB2	28:V:63:LYS:HG2	1.91	0.52
30:X:189:PRO:HA	30:X:192:LEU:HB3	1.90	0.52
4:6:120:ARG:HH11	4:6:307:PRO:HB2	1.74	0.52
4:6:326:THR:O	4:6:348:PHE:N	2.43	0.52
4:6:424:UNK:O	4:6:426:ARG:N	2.43	0.52
7:7:608:PHE:HB3	7:7:672:GLN:HA	1.91	0.52
12:A:365:GLY:N	12:A:469:ARG:O	2.28	0.52
13:B:798:TYR:O	13:B:821:GLN:NE2	2.43	0.52
23:L:26:THR:HB	23:L:41:SER:HB3	1.91	0.52
23:L:31:CYS:HB2	23:L:48:CYS:SG	2.50	0.52
25:Q:137:VAL:O	26:R:58:ASP:N	2.42	0.52
3:0:28:ILE:HD13	3:0:55:LEU:HB3	1.91	0.52
3:0:512:ILE:HG13	3:0:630:THR:HG23	1.91	0.52
4:6:327:ARG:HA	4:6:347:TYR:HA	1.91	0.52
5:2:108:LEU:HD12	5:2:111:ALA:HB3	1.91	0.52
7:7:153:ALA:O	7:7:157:LEU:N	2.28	0.52
7:7:642:ASN:HB3	7:7:649:ILE:HB	1.91	0.52
12:A:790:ASP:N	12:A:790:ASP:OD1	2.42	0.52
17:F:130:ILE:HB	17:F:148:VAL:HG21	1.91	0.52
26:R:256:ASP:N	26:R:256:ASP:OD1	2.42	0.52
29:W:149:CYS:O	29:W:153:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:342:LEU:O	3:0:346:MET:N	2.42	0.52
3:0:747:HIS:O	3:0:751:ARG:HG2	2.09	0.52
12:A:1053:PHE:O	12:A:1056:SER:OG	2.24	0.52
14:C:214:ASN:O	14:C:214:ASN:ND2	2.38	0.52
30:X:257:GLU:O	30:X:261:LYS:N	2.31	0.52
7:7:395:VAL:O	7:7:398:THR:OG1	2.27	0.52
7:7:545:GLN:HA	7:7:550:ALA:HA	1.91	0.52
9:O:74:VAL:N	9:O:121:MET:O	2.41	0.52
10:N:21:DA:H61	11:T:145:DT:H3	1.57	0.52
12:A:715:GLU:OE1	12:A:774:ARG:NH1	2.33	0.52
18:G:1:MET:N	18:G:80:LYS:O	2.43	0.52
27:U:251:VAL:HG22	27:U:260:CYS:HA	1.91	0.52
2:4:68:ASN:O	5:2:37:ARG:NH2	2.43	0.52
3:0:103:PHE:H	3:0:173:LYS:HE3	1.75	0.52
4:6:334:THR:HA	4:6:343:VAL:O	2.09	0.52
5:2:41:PRO:HA	5:2:44:LYS:HB2	1.92	0.52
6:5:57:LEU:HA	6:5:60:LYS:HD3	1.92	0.52
7:7:417:VAL:HG21	7:7:456:THR:HA	1.92	0.52
13:B:443:ASN:HD21	13:B:445:LYS:HD2	1.75	0.52
14:C:226:ASP:N	14:C:226:ASP:OD1	2.42	0.52
16:E:62:ALA:HB3	16:E:78:LEU:HB3	1.90	0.52
16:E:68:SER:O	16:E:72:PHE:N	2.32	0.52
23:L:38:LEU:HD12	23:L:40:LEU:HD23	1.91	0.52
3:0:507:SER:OG	3:0:685:ARG:NH2	2.34	0.52
12:A:1205:LYS:HB3	12:A:1274:ARG:HH21	1.74	0.52
12:A:1290:LYS:HB3	12:A:1298:TYR:HB3	1.92	0.52
13:B:680:THR:O	13:B:683:SER:OG	2.27	0.52
3:0:11:LEU:HD22	3:0:93:ARG:HG3	1.92	0.52
7:7:491:HIS:CD2	7:7:681:ARG:HH11	2.28	0.52
12:A:408:ASP:H	12:A:430:TRP:CD1	2.28	0.52
15:D:138:ASN:O	15:D:141:LEU:HB3	2.09	0.52
16:E:6:GLU:HA	16:E:9:ILE:HB	1.92	0.52
22:K:29:ASN:ND2	22:K:78:THR:O	2.43	0.52
30:X:262:MET:HA	30:X:265:ASN:HB2	1.92	0.52
4:6:347:TYR:HB2	4:6:356:VAL:HG13	1.91	0.51
5:2:486:ASP:HA	5:2:489:LYS:HD3	1.91	0.51
7:7:349:ASN:OD1	7:7:349:ASN:N	2.24	0.51
9:O:133:LYS:HG3	9:O:152:PHE:HZ	1.76	0.51
12:A:902:LEU:HD22	12:A:926:GLN:HG2	1.90	0.51
15:D:205:ASP:OD1	15:D:206:GLU:N	2.42	0.51
22:K:17:SER:O	22:K:20:LYS:NZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:181:GLN:O	1:1:185:LEU:N	2.34	0.51
3:0:120:VAL:HG13	3:0:132:LYS:HB3	1.92	0.51
5:2:368:ALA:H	5:2:375:LEU:HB3	1.73	0.51
21:J:3:VAL:HG12	21:J:15:GLY:HA2	1.92	0.51
3:0:157:GLU:HA	3:0:160:GLU:HG2	1.92	0.51
4:6:156:PHE:CE2	4:6:160:PHE:HB2	2.45	0.51
5:2:488:LYS:NZ	6:5:36:ASP:OD2	2.43	0.51
7:7:348:ARG:HB3	7:7:405:LYS:HD3	1.92	0.51
12:A:1187:GLN:HG3	12:A:1188:GLN:HG3	1.92	0.51
12:A:1231:ASP:OD1	12:A:1231:ASP:N	2.43	0.51
13:B:438:GLU:OE1	13:B:440:HIS:NE2	2.43	0.51
14:C:66:ARG:NH1	21:J:2:ILE:O	2.44	0.51
2:4:74:ALA:HA	2:4:87:TYR:HD2	1.75	0.51
5:2:223:HIS:O	5:2:227:MET:N	2.42	0.51
5:2:472:SER:O	5:2:476:GLN:NE2	2.39	0.51
7:7:388:CYS:N	7:7:689:ARG:HG2	2.26	0.51
11:T:144:DA:OP2	27:U:255:LYS:NZ	2.35	0.51
12:A:559:VAL:HG13	19:H:78:SER:HB2	1.92	0.51
12:A:563:PRO:HD2	19:H:79:TRP:CD1	2.46	0.51
25:Q:98:TYR:HB2	26:R:95:ILE:O	2.11	0.51
25:Q:110:ASP:OD1	25:Q:111:LEU:N	2.43	0.51
29:W:13:LEU:HB3	29:W:29:LEU:HD11	1.93	0.51
29:W:144:ARG:HH22	29:W:146:GLU:HB2	1.75	0.51
1:1:309:UNK:O	1:1:313:UNK:N	2.44	0.51
2:4:69:SER:HA	5:2:37:ARG:HH12	1.76	0.51
3:0:39:ILE:HG22	3:0:477:THR:HG21	1.91	0.51
3:0:636:LYS:O	3:0:640:GLU:N	2.24	0.51
4:6:219:GLY:HA2	4:6:222:LEU:HD23	1.91	0.51
5:2:72:LEU:HD23	5:2:72:LEU:H	1.75	0.51
9:O:133:LYS:HG3	9:O:152:PHE:CZ	2.46	0.51
12:A:134:ARG:NH1	12:A:221:SER:O	2.43	0.51
12:A:874:ASP:OD1	12:A:875:ALA:N	2.43	0.51
13:B:97:VAL:HG12	26:R:252:ILE:HG21	1.91	0.51
13:B:510:LYS:HD2	13:B:511:PRO:HD2	1.93	0.51
16:E:65:THR:OG1	16:E:68:SER:OG	2.24	0.51
18:G:6:ASP:OD1	18:G:75:ARG:HB2	2.10	0.51
25:Q:343:ARG:NH2	25:Q:346:GLU:O	2.41	0.51
3:0:499:LYS:O	3:0:709:SER:HA	2.11	0.51
7:7:425:LEU:HG	7:7:430:LEU:HD23	1.92	0.51
7:7:590:ALA:O	7:7:594:LEU:HG	2.10	0.51
7:7:622:MET:SD	7:7:623:GLY:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:172:PRO:HB3	12:A:185:TRP:CD2	2.46	0.51
12:A:376:TYR:OH	12:A:495:GLU:OE2	2.28	0.51
12:A:390:GLN:OE1	12:A:393:ARG:NH1	2.35	0.51
12:A:513:SER:HB3	12:A:520:CYS:HB3	1.91	0.51
13:B:340:ALA:O	13:B:348:ARG:NH2	2.43	0.51
20:I:103:CYS:SG	20:I:104:LEU:N	2.83	0.51
24:M:41:GLY:C	24:M:56:LEU:HB3	2.36	0.51
29:W:122:TYR:CZ	29:W:158:GLU:HG2	2.46	0.51
4:6:293:ASP:OD2	4:6:296:HIS:N	2.33	0.51
7:7:475:ASP:OD1	7:7:475:ASP:N	2.44	0.51
12:A:386:ASP:N	12:A:386:ASP:OD1	2.43	0.51
12:A:591:PHE:HA	12:A:595:THR:HG21	1.91	0.51
12:A:698:GLN:CD	20:I:99:LEU:HD11	2.36	0.51
12:A:846:GLU:OE2	12:A:1425:SER:OG	2.29	0.51
2:4:25:LEU:HD23	2:4:160:VAL:HG13	1.93	0.51
3:0:80:GLU:HA	3:0:83:LEU:HB2	1.93	0.51
7:7:610:ASP:N	7:7:610:ASP:OD1	2.43	0.51
9:O:103:ILE:HG23	9:O:112:THR:HG23	1.93	0.51
12:A:95:PHE:HB3	12:A:234:MET:SD	2.51	0.51
12:A:547:LEU:HB3	22:K:60:ALA:HB2	1.93	0.51
13:B:790:ASP:N	13:B:790:ASP:OD1	2.42	0.51
23:L:54:ARG:N	23:L:54:ARG:HD2	2.26	0.51
1:1:208:GLU:OE1	1:1:208:GLU:N	2.37	0.51
1:1:230:PRO:HD3	4:6:244:PRO:HA	1.93	0.51
3:0:493:LEU:H	3:0:678:VAL:HA	1.76	0.51
3:0:528:GLU:HA	3:0:531:LYS:HE3	1.91	0.51
7:7:560:PRO:HA	7:7:711:LYS:HE2	1.93	0.51
12:A:280:GLU:HG2	12:A:289:ILE:HD12	1.92	0.51
13:B:760:ASP:N	13:B:760:ASP:OD1	2.43	0.51
13:B:1187:ASN:HD21	13:B:1190:ASP:C	2.18	0.51
19:H:7:ASP:OD1	19:H:8:ASP:N	2.44	0.51
29:W:109:LEU:HG	29:W:172:LEU:HG	1.92	0.51
6:5:31:VAL:HG11	6:5:40:LEU:HD22	1.92	0.51
7:7:409:VAL:HA	7:7:486:ILE:HB	1.93	0.51
10:N:36:DT:H2''	10:N:37:DC:C5	2.46	0.51
10:N:46:DG:H1'	10:N:47:DG:N7	2.25	0.51
14:C:26:ASP:OD1	14:C:26:ASP:N	2.42	0.51
14:C:111:THR:N	14:C:147:LEU:O	2.39	0.51
16:E:30:ILE:HG23	16:E:34:GLU:CD	2.36	0.51
20:I:80:SER:OG	20:I:105:SER:OG	2.27	0.51
23:L:32:ALA:HB3	23:L:53:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:75:VAL:H	2:4:88:PRO:HD3	1.76	0.50
3:0:628:GLN:N	3:0:628:GLN:OE1	2.44	0.50
3:0:695:LYS:O	3:0:699:GLN:N	2.33	0.50
4:6:349:CYS:HB3	4:6:353:HIS:H	1.76	0.50
7:7:388:CYS:HB2	7:7:392:LYS:HD2	1.91	0.50
7:7:489:GLU:O	7:7:491:HIS:ND1	2.39	0.50
7:7:548:HIS:CD2	7:7:693:ALA:HB1	2.45	0.50
12:A:264:PHE:O	12:A:268:ASP:N	2.34	0.50
13:B:241:ARG:CZ	13:B:243:ALA:HB2	2.41	0.50
13:B:356:LEU:HA	13:B:360:PHE:HB3	1.93	0.50
13:B:789:MET:SD	13:B:951:GLN:NE2	2.69	0.50
13:B:892:LYS:HD3	13:B:905:VAL:HG12	1.92	0.50
25:Q:378:VAL:HG22	25:Q:384:PHE:CE1	2.47	0.50
29:W:183:ILE:O	29:W:187:LYS:HG2	2.11	0.50
3:0:43:PRO:HD3	3:0:483:TYR:HB2	1.92	0.50
3:0:60:GLN:HE22	3:0:204:ASN:HB3	1.75	0.50
3:0:587:ARG:HA	3:0:590:CYS:HB2	1.94	0.50
3:0:639:LEU:HA	3:0:642:MET:HB3	1.93	0.50
4:6:188:ASN:O	4:6:192:HIS:ND1	2.44	0.50
7:7:393:THR:HB	7:7:424:PHE:CE2	2.46	0.50
7:7:670:LEU:O	7:7:706:TYR:N	2.44	0.50
9:O:93:GLU:OE2	9:O:105:ARG:NH1	2.45	0.50
10:N:6:DA:C2	10:N:7:DA:C6	2.99	0.50
12:A:109:HIS:CE1	12:A:185:TRP:HE1	2.29	0.50
12:A:733:ALA:O	12:A:737:LEU:HG	2.11	0.50
12:A:1158:PRO:HB3	12:A:1188:GLN:HB2	1.92	0.50
24:M:188:THR:N	24:M:191:GLU:OE1	2.43	0.50
29:W:62:ARG:HD3	29:W:69:ILE:H	1.75	0.50
1:1:256:ILE:O	1:1:260:PHE:N	2.39	0.50
3:0:39:ILE:HD11	3:0:463:ILE:HG21	1.93	0.50
4:6:144:ASN:HD21	4:6:146:HIS:HB3	1.77	0.50
7:7:680:ARG:HA	7:7:683:GLU:HB2	1.93	0.50
8:3:40:GLU:HA	8:3:43:VAL:HG12	1.92	0.50
10:N:3:DA:H2"	10:N:4:DA:C8	2.46	0.50
12:A:1309:ASP:OD1	12:A:1310:GLY:N	2.44	0.50
13:B:223:VAL:HA	13:B:240:ILE:HB	1.93	0.50
13:B:594:ALA:HA	13:B:617:ARG:HH12	1.76	0.50
13:B:1080:LYS:HG2	14:C:189:THR:OG1	2.11	0.50
24:M:129:ALA:HA	24:M:132:LYS:HE3	1.93	0.50
29:W:97:ALA:HA	30:X:274:LEU:HD21	1.94	0.50
29:W:123:MET:HG3	29:W:130:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:34:PRO:O	2:4:38:THR:N	2.34	0.50
7:7:236:THR:H	7:7:313:VAL:HG21	1.77	0.50
7:7:548:HIS:HD2	7:7:693:ALA:HB1	1.75	0.50
12:A:182:VAL:HA	12:A:201:VAL:HA	1.93	0.50
12:A:1341:ILE:HD11	12:A:1376:THR:HB	1.93	0.50
13:B:400:HIS:NE2	13:B:699:GLU:OE2	2.45	0.50
3:0:103:PHE:HE1	3:0:205:ILE:HG22	1.77	0.50
3:0:350:HIS:HA	3:0:422:PRO:HG3	1.92	0.50
3:0:463:ILE:HG23	3:0:469:TYR:CE1	2.46	0.50
7:7:373:MET:HA	7:7:535:LEU:HG	1.94	0.50
7:7:424:PHE:HD2	7:7:425:LEU:HD22	1.76	0.50
9:O:214:LEU:HD21	9:O:227:PHE:HB2	1.94	0.50
12:A:798:GLY:HA2	12:A:815:PHE:CD2	2.47	0.50
13:B:278:GLN:CD	13:B:337:ARG:HH11	2.20	0.50
13:B:1002:THR:OG1	13:B:1003:ALA:N	2.44	0.50
15:D:145:MET:HA	15:D:148:LEU:HB2	1.93	0.50
18:G:7:LEU:O	18:G:74:TYR:N	2.34	0.50
1:1:284:TRP:O	1:1:288:PHE:N	2.34	0.50
2:4:175:ARG:HA	2:4:208:CYS:SG	2.52	0.50
3:0:103:PHE:N	3:0:173:LYS:HE3	2.27	0.50
4:6:155:ASP:O	4:6:159:GLU:HG2	2.11	0.50
7:7:567:GLN:O	7:7:571:ARG:N	2.45	0.50
7:7:578:MET:HA	7:7:581:TYR:CZ	2.47	0.50
8:3:76:VAL:O	8:3:80:LYS:N	2.34	0.50
10:N:4:DA:C4	10:N:5:DA:C8	3.00	0.50
12:A:754:SER:OG	12:A:755:PHE:N	2.45	0.50
14:C:241:ASP:OD1	14:C:242:GLN:N	2.45	0.50
15:D:40:HIS:CG	18:G:73:LYS:HB3	2.47	0.50
25:Q:337:GLU:HG3	25:Q:340:LYS:HB3	1.94	0.50
2:4:85:TYR:HD2	2:4:88:PRO:HG2	1.76	0.50
3:0:58:ALA:O	3:0:62:HIS:N	2.44	0.50
3:0:256:ALA:HA	3:0:259:ARG:HB2	1.94	0.50
4:6:152:TYR:HB3	4:6:301:PHE:CZ	2.47	0.50
5:2:17:ILE:HG23	5:2:21:VAL:HG23	1.93	0.50
5:2:19:GLN:HG3	5:2:85:HIS:CG	2.47	0.50
7:7:464:ARG:HA	7:7:466:ARG:HG3	1.94	0.50
10:N:9:DA:C6	10:N:10:DA:C6	3.00	0.50
12:A:1187:GLN:HE21	12:A:1188:GLN:HE21	1.60	0.50
13:B:521:LEU:HD22	13:B:633:VAL:HG12	1.92	0.50
24:M:268:GLU:OE2	24:M:319:HIS:NE2	2.44	0.50
29:W:131:TYR:OH	29:W:149:CYS:SG	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:149:CYS:N	29:W:154:GLU:O	2.45	0.50
1:1:551:ARG:O	1:1:555:THR:OG1	2.27	0.50
3:0:354:GLU:OE1	3:0:358:SER:OG	2.28	0.50
3:0:493:LEU:HB2	3:0:678:VAL:HG13	1.92	0.50
3:0:603:ARG:HH21	3:0:626:PRO:HB2	1.77	0.50
5:2:350:TYR:HA	5:2:372:ASN:HD22	1.77	0.50
7:7:365:TYR:CD1	7:7:543:LEU:HB3	2.46	0.50
7:7:636:ARG:HA	7:7:639:ILE:HB	1.93	0.50
13:B:435:THR:HG21	13:B:442:PHE:CD1	2.47	0.50
13:B:651:LEU:O	13:B:654:ARG:NH2	2.45	0.50
16:E:163:GLU:OE2	16:E:167:ARG:NE	2.44	0.50
25:Q:117:HIS:HB2	26:R:135:PHE:CE1	2.46	0.50
1:1:278:PHE:O	1:1:283:PHE:HB2	2.12	0.50
3:0:274:VAL:HG23	3:0:282:LEU:HD11	1.94	0.50
3:0:730:PRO:HG2	3:0:734:GLU:HG3	1.94	0.50
4:6:211:GLN:HA	4:6:214:LEU:HB2	1.94	0.50
7:7:755:GLU:HA	7:7:758:GLU:HG2	1.93	0.50
12:A:326:ARG:NE	12:A:1406:VAL:HG21	2.27	0.50
12:A:1135:ARG:HB3	12:A:1135:ARG:HH11	1.77	0.50
13:B:206:ASN:OD1	13:B:458:LYS:NZ	2.35	0.50
13:B:917:PRO:HG3	13:B:934:LYS:HE3	1.93	0.50
13:B:952:VAL:HG22	13:B:966:VAL:HG22	1.92	0.50
13:B:1074:ASN:HD21	13:B:1076:HIS:HB2	1.77	0.50
21:J:36:LEU:HA	21:J:39:LEU:HB2	1.94	0.50
25:Q:132:ASP:N	25:Q:132:ASP:OD1	2.44	0.50
28:V:85:VAL:HG13	28:V:106:ILE:HB	1.93	0.50
3:0:234:PHE:N	3:0:457:ILE:O	2.45	0.49
3:0:321:ILE:HG13	3:0:323:GLY:H	1.76	0.49
3:0:498:THR:HG23	3:0:684:ARG:HA	1.94	0.49
4:6:124:ARG:NH1	4:6:164:ASN:OD1	2.45	0.49
5:2:336:ASP:O	5:2:351:SER:HB3	2.11	0.49
6:5:24:ASP:HB3	6:5:29:ASP:HA	1.93	0.49
7:7:671:ILE:HG13	7:7:706:TYR:HB2	1.94	0.49
12:A:481:ASP:OD1	12:A:481:ASP:N	2.45	0.49
13:B:435:THR:HG21	13:B:442:PHE:HD1	1.75	0.49
16:E:6:GLU:O	16:E:10:SER:N	2.32	0.49
16:E:62:ALA:N	16:E:78:LEU:O	2.29	0.49
17:F:81:THR:OG1	17:F:136:ARG:NH1	2.45	0.49
18:G:14:HIS:HB3	18:G:17:PHE:CE1	2.47	0.49
24:M:211:LYS:HA	24:M:214:LEU:HD12	1.94	0.49
1:1:540:SER:O	1:1:544:ILE:N	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:628:GLN:NE2	3:0:657:ASP:OD1	2.45	0.49
4:6:363:CYS:SG	4:6:366:CYS:N	2.85	0.49
7:7:370:LEU:HD11	7:7:395:VAL:HA	1.93	0.49
7:7:751:ALA:O	7:7:756:ARG:NE	2.34	0.49
12:A:1153:TYR:CD1	20:I:42:LEU:HA	2.46	0.49
13:B:1004:GLU:HA	14:C:177:GLU:HG2	1.94	0.49
22:K:12:LEU:HD12	22:K:13:GLY:N	2.27	0.49
1:1:188:ASN:HB3	1:1:191:LEU:HB2	1.93	0.49
1:1:337:ILE:HG13	3:0:584:GLU:HB3	1.93	0.49
2:4:50:ILE:O	2:4:54:LEU:N	2.32	0.49
2:4:201:PHE:CZ	4:6:377:ALA:HB3	2.48	0.49
3:0:349:LEU:HD23	3:0:349:LEU:H	1.76	0.49
5:2:87:LEU:HG	5:2:89:PRO:HD3	1.94	0.49
6:5:11:GLN:HE22	6:5:38:THR:HB	1.76	0.49
7:7:228:LYS:N	7:7:231:ARG:O	2.45	0.49
9:O:69:ASN:H	9:O:161:VAL:HB	1.77	0.49
12:A:1030:ARG:NE	12:A:1034:GLU:OE1	2.42	0.49
12:A:1109:LYS:HD3	12:A:1333:ILE:HD13	1.94	0.49
15:D:176:GLU:HB3	15:D:198:LEU:HD11	1.94	0.49
28:V:62:VAL:HG22	28:V:85:VAL:HB	1.94	0.49
30:X:195:LEU:HD23	30:X:210:LEU:HD21	1.95	0.49
3:0:79:ILE:O	3:0:83:LEU:N	2.39	0.49
3:0:244:CYS:O	3:0:247:SER:OG	2.24	0.49
7:7:347:HIS:CE1	7:7:349:ASN:HA	2.48	0.49
7:7:366:GLN:HG3	7:7:548:HIS:CE1	2.48	0.49
7:7:430:LEU:HD11	7:7:435:CYS:HB2	1.94	0.49
9:O:202:ILE:HD11	9:O:222:GLU:HB3	1.94	0.49
12:A:837:ILE:HD11	12:A:1102:LYS:HG2	1.94	0.49
12:A:873:MET:HB2	12:A:1366:ARG:HH21	1.77	0.49
13:B:1084:GLN:HG2	14:C:201:TRP:CH2	2.48	0.49
13:B:1121:GLY:O	13:B:1126:GLY:N	2.45	0.49
25:Q:125:LYS:HB3	25:Q:128:ASN:HB2	1.94	0.49
3:0:234:PHE:HB2	3:0:458:ILE:HA	1.95	0.49
3:0:302:GLN:CD	3:0:302:GLN:H	2.20	0.49
3:0:720:PHE:HD2	3:0:721:LEU:HD12	1.77	0.49
4:6:363:CYS:SG	4:6:367:ASP:N	2.86	0.49
7:7:594:LEU:HD13	7:7:706:TYR:CD2	2.47	0.49
9:O:214:LEU:HB2	9:O:223:ILE:HG23	1.94	0.49
10:N:20:DT:O4	10:N:21:DA:N6	2.46	0.49
12:A:30:ILE:HD13	13:B:1170:THR:HG21	1.94	0.49
12:A:903:ASN:OD1	12:A:904:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:189:ASP:HA	15:D:192:LYS:HG3	1.94	0.49
23:L:32:ALA:HB2	23:L:55:ILE:HB	1.94	0.49
25:Q:363:GLY:HA2	25:Q:395:PHE:HA	1.93	0.49
26:R:108:LEU:HB2	26:R:118:HIS:O	2.12	0.49
27:U:258:TRP:O	27:U:283:ALA:N	2.45	0.49
3:O:615:GLN:OE1	3:O:616:TYR:N	2.46	0.49
3:O:638:ARG:O	3:O:642:MET:N	2.38	0.49
4:6:294:GLU:O	4:6:298:LYS:N	2.45	0.49
5:2:449:ASP:O	5:2:450:ARG:HG3	2.11	0.49
7:7:696:ARG:HH11	7:7:699:GLU:HB2	1.77	0.49
12:A:75:ASN:N	12:A:75:ASN:OD1	2.46	0.49
12:A:365:GLY:HA3	12:A:469:ARG:HB2	1.95	0.49
12:A:557:ASP:OD1	12:A:558:GLY:N	2.46	0.49
12:A:944:ARG:NH2	12:A:1296:GLY:O	2.45	0.49
12:A:1355:VAL:O	12:A:1358:SER:OG	2.16	0.49
14:C:204:SER:N	14:C:207:CYS:SG	2.85	0.49
20:I:16:PRO:HB2	20:I:25:LEU:HD11	1.93	0.49
24:M:108:LYS:HD3	24:M:111:ASN:HB2	1.94	0.49
1:1:190:VAL:HA	1:1:193:LYS:HB2	1.95	0.49
3:O:176:PHE:HB3	3:O:181:LEU:HB2	1.95	0.49
5:2:18:PRO:HB2	5:2:20:GLN:HE22	1.78	0.49
5:2:350:TYR:HA	5:2:372:ASN:ND2	2.28	0.49
5:2:422:LEU:O	5:2:426:CYS:N	2.39	0.49
7:7:421:ARG:HH21	7:7:426:GLN:CD	2.20	0.49
12:A:35:ILE:HG21	12:A:53:LEU:HD12	1.94	0.49
12:A:61:ILE:HA	12:A:74:MET:HG3	1.93	0.49
12:A:993:LEU:HD13	12:A:1046:LEU:HD22	1.94	0.49
12:A:1187:GLN:HE21	12:A:1188:GLN:NE2	2.11	0.49
13:B:120:ARG:NE	13:B:956:THR:O	2.42	0.49
13:B:635:ARG:NH2	13:B:742:GLU:OE2	2.37	0.49
17:F:89:GLU:OE1	17:F:89:GLU:N	2.42	0.49
25:Q:141:ARG:HH22	25:Q:343:ARG:NH1	2.06	0.49
27:U:269:ILE:HD11	28:V:111:LEU:HD11	1.93	0.49
3:O:104:ARG:N	3:O:204:ASN:OD1	2.39	0.49
3:O:233:ILE:HA	3:O:457:ILE:HB	1.95	0.49
4:6:184:GLN:O	4:6:192:HIS:NE2	2.46	0.49
4:6:232:VAL:H	4:6:261:VAL:HG22	1.78	0.49
5:2:75:GLN:NE2	5:2:499:SER:O	2.46	0.49
12:A:1159:ARG:HD2	12:A:1174:PHE:CE2	2.48	0.49
12:A:1258:HIS:O	12:A:1262:LYS:HG2	2.12	0.49
13:B:342:GLY:O	13:B:348:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:824:ILE:N	13:B:1009:ASP:OD2	2.31	0.49
13:B:1032:SER:HB3	13:B:1089:PRO:HG2	1.94	0.49
15:D:35:LEU:HG	15:D:46:GLU:HG3	1.94	0.49
24:M:60:ARG:HB3	24:M:64:ARG:HH21	1.77	0.49
30:X:269:PRO:HG2	30:X:274:LEU:HD22	1.95	0.49
1:1:340:ASP:OD1	3:0:577:GLN:N	2.45	0.49
3:0:138:ASN:HB3	3:0:141:ALA:H	1.77	0.49
3:0:538:VAL:HG22	3:0:598:LEU:HB3	1.94	0.49
3:0:570:LEU:HD13	3:0:586:TYR:HD1	1.77	0.49
4:6:381:HIS:HB2	4:6:449:HIS:CD2	2.48	0.49
7:7:423:GLN:NE2	7:7:662:ILE:HB	2.27	0.49
7:7:423:GLN:HG2	7:7:663:ASP:CG	2.37	0.49
7:7:569:TYR:HA	7:7:577:ARG:CZ	2.43	0.49
7:7:576:LYS:NZ	7:7:579:LEU:HB2	2.28	0.49
7:7:576:LYS:HZ1	7:7:580:LEU:HG	1.78	0.49
9:O:175:LEU:O	9:O:179:HIS:ND1	2.43	0.49
11:T:151:DC:H2'	11:T:152:DG:C8	2.48	0.49
12:A:130:ASP:OD1	12:A:132:LYS:N	2.46	0.49
12:A:358:ASN:OD1	13:B:833:TYR:OH	2.25	0.49
12:A:881:GLN:CD	12:A:959:ASN:HA	2.37	0.49
13:B:322:PHE:CZ	20:I:30:ARG:HB3	2.48	0.49
13:B:806:THR:HB	13:B:809:MET:HG3	1.94	0.49
15:D:56:ARG:HB2	15:D:148:LEU:HD13	1.95	0.49
4:6:215:GLU:OE1	4:6:218:ARG:NE	2.40	0.49
5:2:185:THR:O	5:2:189:PHE:N	2.26	0.49
7:7:754:ARG:O	7:7:758:GLU:N	2.46	0.49
12:A:839:ARG:NH2	12:A:1402:PHE:O	2.46	0.49
12:A:1446:ASP:OD1	12:A:1447:GLU:N	2.44	0.49
14:C:217:ASP:N	14:C:217:ASP:OD1	2.45	0.49
27:U:252:THR:O	27:U:257:ARG:NH1	2.45	0.49
2:4:76:ILE:HG12	2:4:85:TYR:HA	1.95	0.48
7:7:309:ASP:HB3	7:7:337:VAL:HB	1.95	0.48
7:7:334:ASP:O	7:7:336:PRO:HD3	2.13	0.48
8:3:132:LYS:O	8:3:136:TYR:N	2.31	0.48
12:A:737:LEU:HB2	12:A:744:LYS:HD2	1.95	0.48
12:A:1256:GLU:O	12:A:1260:LEU:N	2.32	0.48
13:B:333:PHE:O	13:B:337:ARG:HG2	2.13	0.48
13:B:391:ASP:N	13:B:391:ASP:OD1	2.46	0.48
13:B:486:TYR:HB3	13:B:1096:ARG:HH12	1.78	0.48
15:D:174:PRO:HA	15:D:177:VAL:HG13	1.95	0.48
30:X:271:PHE:O	30:X:273:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:175:ARG:NH1	2:4:252:MET:O	2.45	0.48
3:0:211:HIS:HA	3:0:214:LEU:HB2	1.95	0.48
4:6:335:PHE:N	4:6:343:VAL:H	2.11	0.48
5:2:84:LEU:HD11	5:2:86:LEU:HD23	1.94	0.48
9:O:103:ILE:HA	9:O:113:ALA:O	2.13	0.48
12:A:206:GLU:O	12:A:210:ILE:HG12	2.13	0.48
12:A:1038:THR:OG1	12:A:1039:LYS:N	2.45	0.48
13:B:27:ALA:O	13:B:30:SER:OG	2.29	0.48
15:D:51:ASN:OD1	15:D:53:SER:OG	2.19	0.48
15:D:188:ALA:HA	15:D:207:LEU:HD22	1.94	0.48
1:1:229:GLY:HA3	4:6:242:THR:HG22	1.93	0.48
1:1:257:LEU:HA	1:1:260:PHE:HB2	1.94	0.48
2:4:29:ILE:HD13	2:4:153:MET:HA	1.94	0.48
4:6:271:ALA:O	4:6:275:GLU:N	2.39	0.48
7:7:491:HIS:CD2	7:7:681:ARG:HG2	2.49	0.48
12:A:362:ASP:OD1	12:A:459:ARG:NH2	2.45	0.48
12:A:523:ILE:O	12:A:528:LEU:HB2	2.13	0.48
12:A:871:ASP:OD2	16:E:204:THR:OG1	2.30	0.48
27:U:248:TYR:OH	28:V:74:ASP:OD2	2.30	0.48
1:1:549:SER:O	1:1:553:LEU:N	2.38	0.48
3:0:41:GLU:HB3	3:0:482:SER:HA	1.95	0.48
3:0:254:THR:HA	3:0:257:LEU:HB2	1.94	0.48
3:0:473:LEU:HB2	3:0:475:PHE:CE1	2.49	0.48
5:2:464:THR:OG1	5:2:466:GLN:OE1	2.20	0.48
7:7:365:TYR:HD1	7:7:543:LEU:HD22	1.77	0.48
7:7:719:SER:HA	7:7:722:ARG:HD2	1.96	0.48
12:A:451:HIS:HB2	12:A:454:SER:N	2.27	0.48
12:A:737:LEU:HB3	12:A:741:ASN:HD22	1.78	0.48
13:B:494:HIS:HA	13:B:497:ARG:NH1	2.29	0.48
15:D:50:LEU:HB2	15:D:55:ALA:HB2	1.96	0.48
18:G:81:PRO:HG2	18:G:157:ILE:HG21	1.95	0.48
24:M:143:PRO:HG2	24:M:146:VAL:HG23	1.94	0.48
26:R:72:ARG:O	26:R:223:GLN:HG2	2.13	0.48
3:0:650:GLU:O	3:0:654:LEU:N	2.33	0.48
7:7:368:LYS:HZ1	7:7:543:LEU:HA	1.79	0.48
7:7:541:MET:O	7:7:545:GLN:HB2	2.14	0.48
7:7:604:LYS:HD3	7:7:694:LYS:NZ	2.26	0.48
7:7:604:LYS:O	7:7:669:CYS:N	2.44	0.48
7:7:631:THR:HB	7:7:636:ARG:HH21	1.78	0.48
8:3:139:LEU:O	8:3:143:LEU:N	2.42	0.48
9:O:65:PRO:HG2	9:O:224:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:46:DG:C2	11:T:120:DC:O2	2.66	0.48
12:A:802:ASN:ND2	12:A:812:GLU:OE2	2.46	0.48
13:B:129:PHE:CE2	26:R:266:THR:HG21	2.49	0.48
13:B:586:TRP:NE1	13:B:588:GLY:O	2.43	0.48
16:E:78:LEU:HD11	16:E:109:ILE:HG13	1.94	0.48
24:M:306:GLU:HA	24:M:309:ILE:HB	1.94	0.48
26:R:123:GLU:HG2	26:R:223:GLN:HB3	1.95	0.48
3:O:138:ASN:HD22	3:O:139:GLY:N	2.10	0.48
3:O:144:LYS:HB2	3:O:153:VAL:HG21	1.95	0.48
3:O:194:PHE:HA	3:O:197:ARG:HB3	1.95	0.48
7:7:133:TRP:O	7:7:142:ILE:N	2.40	0.48
7:7:241:ILE:O	7:7:245:LEU:N	2.42	0.48
7:7:423:GLN:HE22	7:7:662:ILE:HB	1.76	0.48
12:A:247:ARG:NH1	12:A:263:THR:OG1	2.46	0.48
12:A:573:SER:N	12:A:576:GLN:OE1	2.24	0.48
13:B:89:GLU:HB3	13:B:135:ARG:HB2	1.95	0.48
13:B:906:SER:O	13:B:941:LEU:HD23	2.14	0.48
13:B:920:PRO:O	13:B:928:ARG:HD2	2.14	0.48
16:E:8:ASN:O	16:E:12:LEU:N	2.37	0.48
16:E:183:PRO:O	16:E:187:TYR:N	2.36	0.48
17:F:147:SER:O	17:F:150:GLU:HG2	2.13	0.48
24:M:187:ARG:HH11	24:M:241:ARG:HD3	1.78	0.48
29:W:30:ASP:HB3	29:W:34:PHE:CZ	2.48	0.48
3:O:123:GLU:HB2	3:O:132:LYS:HZ2	1.79	0.48
3:O:227:SER:HG	3:O:453:PHE:HE1	1.60	0.48
3:O:301:ASP:HB3	3:O:304:GLU:HB2	1.94	0.48
5:2:473:LYS:NZ	5:2:477:ASP:OD1	2.47	0.48
7:7:321:GLU:HG2	7:7:322:SER:HB2	1.95	0.48
7:7:411:CYS:HB3	7:7:417:VAL:HG13	1.94	0.48
12:A:216:VAL:HA	12:A:219:PHE:CZ	2.48	0.48
12:A:535:THR:O	12:A:575:LYS:NZ	2.29	0.48
12:A:847:ASP:OD1	12:A:847:ASP:N	2.47	0.48
12:A:1151:GLU:OE2	20:I:45:ARG:NE	2.31	0.48
15:D:68:ARG:HD2	15:D:72:ARG:HH22	1.78	0.48
27:U:250:LYS:H	27:U:261:SER:HB3	1.77	0.48
29:W:116:ASN:HB3	29:W:164:LYS:HB2	1.95	0.48
7:7:368:LYS:O	7:7:372:LYS:HG3	2.14	0.48
9:O:221:GLU:OE1	9:O:221:GLU:N	2.40	0.48
12:A:243:PRO:HB2	12:A:245:PRO:HD2	1.95	0.48
12:A:251:SER:HA	12:A:257:ARG:HG3	1.96	0.48
13:B:72:GLU:HA	13:B:87:LYS:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:822:ASN:O	21:J:48:ARG:NH1	2.47	0.48
13:B:896:ASP:OD2	23:L:29:TYR:OH	2.32	0.48
16:E:168:TYR:HB3	16:E:170:LEU:HG	1.94	0.48
16:E:201:LYS:HA	16:E:206:GLY:O	2.14	0.48
18:G:26:LEU:HD13	18:G:56:ILE:HD11	1.96	0.48
24:M:173:ALA:HB2	24:M:196:ILE:HD12	1.96	0.48
1:1:504:ILE:O	1:1:508:LYS:N	2.38	0.48
2:4:175:ARG:NH2	2:4:211:ASP:OD2	2.46	0.48
3:0:477:THR:OG1	3:0:478:VAL:N	2.45	0.48
3:0:493:LEU:HB2	3:0:678:VAL:HG22	1.96	0.48
7:7:447:GLN:HG2	7:7:448:THR:HG23	1.95	0.48
12:A:958:VAL:HG21	12:A:1052:GLN:HB3	1.95	0.48
14:C:73:GLN:HG3	14:C:128:ASN:O	2.14	0.48
15:D:166:LEU:O	15:D:169:SER:OG	2.21	0.48
19:H:118:PHE:HB2	19:H:121:LEU:HB2	1.96	0.48
21:J:48:ARG:O	21:J:52:THR:HG22	2.14	0.48
1:1:340:ASP:OD2	3:0:124:ARG:NH2	2.47	0.48
2:4:249:ALA:O	2:4:253:PHE:HB2	2.14	0.48
3:0:642:MET:SD	3:0:646:TYR:HB2	2.53	0.48
7:7:616:GLN:HA	7:7:619:ALA:HB3	1.96	0.48
9:O:69:ASN:OD1	9:O:159:ASN:ND2	2.47	0.48
9:O:191:PRO:HG3	24:M:272:LYS:HD3	1.96	0.48
12:A:957:PRO:HG2	12:A:1018:PHE:CD1	2.49	0.48
13:B:403:LYS:NZ	13:B:696:GLU:OE2	2.46	0.48
13:B:860:MET:HE3	13:B:860:MET:HB3	1.83	0.48
23:L:47:ARG:HG2	23:L:48:CYS:N	2.29	0.48
23:L:48:CYS:HB3	23:L:51:CYS:O	2.14	0.48
1:1:197:GLU:HA	1:1:201:ASN:CG	2.38	0.47
2:4:67:PHE:O	5:2:44:LYS:NZ	2.41	0.47
2:4:239:GLU:OE1	2:4:240:SER:N	2.46	0.47
3:0:158:TYR:HA	3:0:161:ASN:HD21	1.79	0.47
3:0:259:ARG:HA	3:0:262:ARG:HB2	1.95	0.47
3:0:588:LYS:O	3:0:592:ASN:N	2.46	0.47
5:2:350:TYR:HA	5:2:372:ASN:HB2	1.95	0.47
5:2:360:LEU:HD21	5:2:403:HIS:HD1	1.79	0.47
5:2:468:TYR:O	5:2:472:SER:N	2.44	0.47
7:7:619:ALA:HA	7:7:622:MET:HG3	1.96	0.47
10:N:6:DA:H2"	10:N:7:DA:C8	2.49	0.47
12:A:242:PRO:HG2	12:A:247:ARG:HD3	1.95	0.47
12:A:670:ILE:HD13	12:A:805:LEU:HD21	1.96	0.47
13:B:1065:GLN:CD	13:B:1067:ARG:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1096:ARG:O	13:B:1098:MET:N	2.47	0.47
16:E:61:GLN:HG3	16:E:105:PHE:CE1	2.49	0.47
23:L:33:GLU:H	23:L:53:HIS:HD2	1.62	0.47
29:W:108:ARG:HH22	29:W:109:LEU:HD13	1.79	0.47
1:1:561:LEU:O	1:1:565:ALA:N	2.35	0.47
3:0:37:ASN:HB2	3:0:477:THR:HA	1.96	0.47
4:6:142:ARG:HB2	4:6:143:PRO:HD3	1.95	0.47
4:6:391:GLU:HA	4:6:427:TYR:HA	1.95	0.47
5:2:84:LEU:HD21	5:2:86:LEU:HD23	1.96	0.47
7:7:456:THR:O	7:7:460:VAL:HG23	2.14	0.47
7:7:483:GLY:O	7:7:509:ALA:HB3	2.15	0.47
8:3:64:ARG:HG3	8:3:65:LYS:H	1.78	0.47
10:N:7:DA:C4	10:N:8:DA:C8	3.02	0.47
12:A:1226:VAL:HA	12:A:1239:ARG:O	2.13	0.47
17:F:74:ILE:HD11	17:F:142:SER:HB2	1.97	0.47
17:F:100:GLN:HB3	18:G:15:PRO:HB3	1.96	0.47
18:G:119:LEU:HD13	18:G:132:SER:HB3	1.95	0.47
22:K:40:HIS:NE2	22:K:63:VAL:HG21	2.29	0.47
26:R:317:GLY:O	26:R:321:ARG:N	2.42	0.47
27:U:244:MET:HE1	28:V:111:LEU:HB3	1.95	0.47
29:W:147:PHE:O	29:W:156:LEU:N	2.43	0.47
1:1:497:UNK:O	1:1:501:UNK:N	2.48	0.47
3:0:715:SER:O	3:0:719:GLN:NE2	2.40	0.47
5:2:100:LEU:O	5:2:102:PRO:HD3	2.15	0.47
5:2:506:LYS:HG3	5:2:507:ARG:H	1.78	0.47
6:5:48:GLU:HB2	6:5:52:HIS:CE1	2.49	0.47
7:7:303:ARG:HD2	7:7:502:VAL:O	2.13	0.47
9:O:112:THR:HB	9:O:124:THR:HG23	1.96	0.47
10:N:46:DG:N1	11:T:120:DC:C2	2.82	0.47
12:A:202:LEU:HB3	12:A:207:ILE:HD11	1.96	0.47
12:A:717:ASN:N	12:A:717:ASN:OD1	2.45	0.47
13:B:50:SER:OG	13:B:51:PHE:N	2.47	0.47
13:B:129:PHE:CE2	13:B:166:PHE:HB2	2.49	0.47
13:B:583:ASN:HD21	13:B:628:THR:H	1.62	0.47
18:G:15:PRO:HA	18:G:18:PHE:CE1	2.48	0.47
19:H:41:ASP:N	19:H:41:ASP:OD1	2.47	0.47
19:H:109:LYS:HG3	19:H:110:ASP:H	1.79	0.47
29:W:17:VAL:HG11	29:W:29:LEU:HD13	1.96	0.47
2:4:89:GLU:OE2	2:4:92:SER:OG	2.28	0.47
3:0:310:PRO:HG3	3:0:404:THR:HA	1.96	0.47
3:0:618:ARG:NH1	3:0:676:TYR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:681:LEU:HB3	3:0:686:PHE:CE2	2.49	0.47
5:2:19:GLN:O	5:2:23:ASN:N	2.28	0.47
5:2:506:LYS:HG3	5:2:507:ARG:N	2.29	0.47
7:7:370:LEU:HB3	7:7:374:PHE:CE2	2.49	0.47
7:7:447:GLN:HA	7:7:476:PHE:CD1	2.50	0.47
7:7:635:GLU:O	7:7:639:ILE:N	2.44	0.47
8:3:15:ILE:HG23	29:W:176:MET:HG2	1.97	0.47
8:3:36:HIS:NE2	8:3:54:CYS:SG	2.88	0.47
9:O:74:VAL:HG21	9:O:136:SER:HB3	1.97	0.47
12:A:1100:ARG:NH1	12:A:1103:GLU:OE1	2.46	0.47
13:B:40:GLU:OE1	13:B:682:SER:N	2.41	0.47
15:D:140:ASP:O	15:D:144:THR:HG23	2.14	0.47
15:D:147:TYR:CE2	18:G:103:VAL:HA	2.50	0.47
19:H:26:ILE:O	19:H:39:THR:HA	2.14	0.47
20:I:26:LEU:HA	20:I:37:GLU:HA	1.95	0.47
23:L:30:ILE:HG13	23:L:59:ALA:HB2	1.95	0.47
24:M:103:ASP:OD1	24:M:104:MET:N	2.46	0.47
24:M:133:ILE:HG23	24:M:172:MET:HE3	1.97	0.47
27:U:246:CYS:SG	27:U:262:LEU:HB3	2.55	0.47
3:0:267:LEU:HD11	3:0:399:LEU:HD13	1.96	0.47
3:0:418:LEU:HD23	3:0:437:PHE:HB2	1.97	0.47
5:2:174:GLU:H	5:2:185:THR:H	1.61	0.47
5:2:382:SER:HA	5:2:385:ARG:HD3	1.95	0.47
5:2:459:TYR:HD2	5:2:491:PHE:HD1	1.61	0.47
7:7:269:LEU:HD13	7:7:304:GLU:HA	1.96	0.47
7:7:363:ARG:HB2	7:7:548:HIS:ND1	2.29	0.47
7:7:694:LYS:O	7:7:696:ARG:N	2.48	0.47
7:7:726:LEU:HD12	7:7:733:PHE:CD1	2.48	0.47
12:A:416:ARG:O	12:A:417:TYR:HB2	2.15	0.47
15:D:51:ASN:OD1	15:D:54:GLU:N	2.30	0.47
1:1:175:LEU:C	1:1:181:GLN:HE22	2.22	0.47
1:1:474:UNK:O	1:1:478:UNK:N	2.47	0.47
2:4:175:ARG:NH1	2:4:256:PRO:HD3	2.30	0.47
3:0:111:ARG:O	3:0:115:CYS:N	2.35	0.47
4:6:169:MET:C	4:6:185:VAL:HA	2.38	0.47
4:6:177:GLY:C	4:6:209:SER:HB2	2.39	0.47
7:7:304:GLU:HB3	7:7:507:ALA:O	2.14	0.47
7:7:363:ARG:HB2	7:7:548:HIS:CD2	2.50	0.47
12:A:940:ARG:HE	12:A:944:ARG:NH1	2.13	0.47
12:A:1141:THR:HG1	12:A:1274:ARG:H	1.59	0.47
13:B:175:ARG:HE	13:B:199:MET:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:357:GLN:HE21	13:B:357:GLN:HB3	1.49	0.47
15:D:144:THR:HG22	18:G:104:GLY:C	2.39	0.47
20:I:70:ARG:HD3	20:I:84:VAL:HG13	1.96	0.47
1:1:192:MET:HA	1:1:195:PHE:HB3	1.97	0.47
1:1:196:GLN:HA	1:1:200:ILE:HG12	1.97	0.47
1:1:375:LEU:HB3	3:0:571:VAL:HG21	1.96	0.47
1:1:592:LYS:O	1:1:596:LEU:HG	2.14	0.47
1:1:613:THR:O	1:1:617:LYS:N	2.48	0.47
2:4:261:ILE:HG13	5:2:65:TRP:O	2.14	0.47
3:0:308:GLU:CD	3:0:308:GLU:H	2.23	0.47
3:0:568:LEU:N	3:0:595:GLY:O	2.40	0.47
4:6:377:ALA:HA	4:6:380:TYR:CD2	2.49	0.47
5:2:411:LEU:HA	5:2:414:GLU:HG2	1.97	0.47
7:7:320:ASN:OD1	7:7:320:ASN:N	2.48	0.47
7:7:363:ARG:NH1	7:7:693:ALA:HB3	2.29	0.47
7:7:603:ASP:HB3	7:7:668:THR:HB	1.95	0.47
7:7:608:PHE:HB3	7:7:672:GLN:HG2	1.97	0.47
8:3:29:LEU:HD22	8:3:70:THR:HA	1.96	0.47
9:O:70:ILE:HD13	9:O:127:LYS:HA	1.95	0.47
9:O:106:ILE:O	9:O:110:LYS:HA	2.15	0.47
10:N:45:DC:H2'	10:N:46:DG:C8	2.49	0.47
11:T:144:DA:H2''	11:T:145:DT:H5'	1.97	0.47
13:B:548:GLY:HA3	13:B:630:ALA:HB2	1.97	0.47
13:B:882:THR:OG1	13:B:885:MET:SD	2.69	0.47
14:C:204:SER:OG	14:C:207:CYS:SG	2.58	0.47
16:E:143:ASN:ND2	16:E:145:THR:OG1	2.47	0.47
17:F:97:ARG:HD2	17:F:100:GLN:OE1	2.13	0.47
18:G:35:GLU:HA	18:G:45:ILE:HG22	1.96	0.47
19:H:25:ARG:NH2	19:H:41:ASP:OD1	2.37	0.47
24:M:105:ARG:O	24:M:109:GLU:HB2	2.14	0.47
24:M:125:GLU:O	24:M:129:ALA:N	2.31	0.47
27:U:244:MET:HG2	27:U:267:VAL:HA	1.95	0.47
29:W:65:ARG:HH11	29:W:93:HIS:CE1	2.33	0.47
1:1:196:GLN:O	1:1:201:ASN:N	2.48	0.47
1:1:280:GLU:HB3	1:1:284:TRP:CE2	2.50	0.47
1:1:585:HIS:O	1:1:589:CYS:N	2.33	0.47
2:4:25:LEU:HA	2:4:72:LYS:O	2.14	0.47
2:4:126:VAL:O	2:4:129:ILE:HG23	2.15	0.47
3:0:613:ASP:O	3:0:617:GLY:N	2.24	0.47
4:6:126:LEU:HA	4:6:231:GLU:O	2.15	0.47
6:5:49:PHE:HA	6:5:52:HIS:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:365:TYR:HA	7:7:368:LYS:HE2	1.95	0.47
7:7:467:SER:OG	7:7:468:HIS:N	2.47	0.47
7:7:592:GLN:HB3	7:7:745:ILE:HD13	1.96	0.47
7:7:676:HIS:N	7:7:715:GLU:OE2	2.45	0.47
9:O:91:ASN:ND2	9:O:105:ARG:O	2.48	0.47
9:O:159:ASN:HD21	9:O:161:VAL:HG23	1.79	0.47
12:A:306:ASN:ND2	12:A:313:GLN:OE1	2.48	0.47
13:B:1054:GLY:O	13:B:1058:LEU:HB2	2.15	0.47
15:D:199:ASN:OD1	15:D:199:ASN:N	2.48	0.47
18:G:163:ILE:HA	18:G:168:LEU:HD13	1.95	0.47
30:X:194:LYS:O	30:X:198:SER:N	2.48	0.47
2:4:304:LYS:HE2	2:4:304:LYS:HB2	1.81	0.47
3:0:224:ASN:CG	3:0:228:LYS:HB2	2.39	0.47
3:0:285:GLU:HA	3:0:288:LYS:HB2	1.95	0.47
3:0:504:VAL:HG22	7:7:377:GLY:HA2	1.97	0.47
5:2:401:GLU:HG3	5:2:433:LEU:HD13	1.97	0.47
7:7:409:VAL:HG22	7:7:486:ILE:HD12	1.96	0.47
13:B:1072:MET:HE2	13:B:1072:MET:HB3	1.83	0.47
18:G:112:LYS:HA	18:G:115:MET:HB2	1.97	0.47
4:6:133:SER:O	4:6:204:PRO:HB2	2.15	0.47
4:6:186:SER:HB2	4:6:192:HIS:CE1	2.50	0.47
6:5:5:ARG:HH12	6:5:33:GLU:CD	2.22	0.47
7:7:344:ARG:NE	7:7:378:ARG:HB3	2.29	0.47
7:7:687:LEU:HD13	7:7:726:LEU:HD22	1.97	0.47
12:A:313:GLN:H	24:M:99:GLY:HA3	1.80	0.47
12:A:1121:GLU:HB2	12:A:1321:GLY:O	2.16	0.47
12:A:1426:GLU:OE1	12:A:1426:GLU:N	2.42	0.47
13:B:554:ILE:O	13:B:558:LEU:N	2.41	0.47
17:F:116:ASP:OD2	17:F:119:ARG:N	2.38	0.47
24:M:176:ILE:O	24:M:180:CYS:N	2.26	0.47
3:0:132:LYS:O	3:0:136:MET:N	2.26	0.46
3:0:171:LEU:HD22	3:0:184:TYR:CE2	2.49	0.46
3:0:281:LYS:O	3:0:285:GLU:N	2.39	0.46
5:2:138:TYR:O	5:2:142:LYS:N	2.36	0.46
5:2:380:ARG:HH21	5:2:440:GLN:C	2.21	0.46
7:7:726:LEU:O	7:7:731:TYR:HB2	2.15	0.46
9:O:93:GLU:HG2	28:V:69:TYR:HE2	1.80	0.46
12:A:66:LYS:NZ	12:A:72:GLU:HB3	2.30	0.46
12:A:230:ARG:HB3	12:A:232:GLU:HG3	1.95	0.46
13:B:126:SER:O	13:B:170:LEU:N	2.48	0.46
13:B:599:THR:O	13:B:602:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:7:CYS:SG	21:J:10:CYS:N	2.83	0.46
27:U:243:LEU:HD23	28:V:112:ARG:HB2	1.97	0.46
27:U:262:LEU:HD11	28:V:113:ILE:HG23	1.96	0.46
29:W:67:ILE:HA	29:W:90:LYS:H	1.80	0.46
2:4:27:THR:HG22	2:4:74:ALA:HB3	1.98	0.46
2:4:86:LEU:HD12	2:4:128:GLU:HB3	1.97	0.46
3:0:109:THR:O	3:0:212:TYR:OH	2.23	0.46
4:6:128:LEU:HD11	4:6:233:LEU:HD22	1.97	0.46
7:7:363:ARG:HA	7:7:695:ARG:NE	2.31	0.46
7:7:439:THR:C	7:7:441:ASP:H	2.24	0.46
13:B:39:ARG:NH2	13:B:678:GLU:OE1	2.47	0.46
13:B:327:ARG:HH21	13:B:353:LYS:HE2	1.80	0.46
14:C:112:ASN:OD1	14:C:112:ASN:N	2.48	0.46
16:E:143:ASN:OD1	16:E:146:HIS:N	2.48	0.46
18:G:94:CYS:HA	18:G:99:PHE:HA	1.96	0.46
20:I:74:GLU:HB3	20:I:81:ARG:HG3	1.96	0.46
24:M:126:VAL:O	24:M:130:PHE:N	2.34	0.46
24:M:305:THR:HG22	24:M:307:GLY:H	1.80	0.46
29:W:68:SER:O	29:W:88:TYR:N	2.45	0.46
1:1:318:UNK:HA	1:1:321:PHE:HB3	1.97	0.46
1:1:351:GLY:O	3:0:251:ASP:HB2	2.14	0.46
3:0:214:LEU:HD11	3:0:240:ILE:HG23	1.98	0.46
3:0:241:ASP:OD1	3:0:241:ASP:N	2.46	0.46
3:0:270:ARG:NH2	3:0:388:LEU:O	2.31	0.46
3:0:322:PRO:HB3	3:0:376:PHE:HD2	1.80	0.46
3:0:495:MET:HB2	3:0:680:VAL:HA	1.97	0.46
3:0:514:ASN:HD21	3:0:549:SER:C	2.23	0.46
7:7:438:PHE:C	7:7:459:MET:HG3	2.41	0.46
7:7:694:LYS:NZ	7:7:696:ARG:HH21	2.13	0.46
12:A:270:LEU:O	12:A:274:ILE:N	2.47	0.46
12:A:356:ASP:OD2	22:K:65:HIS:NE2	2.42	0.46
12:A:1444:MET:HE3	17:F:135:ARG:CZ	2.45	0.46
13:B:40:GLU:OE1	13:B:680:THR:OG1	2.30	0.46
18:G:49:LEU:HD11	18:G:75:ARG:HE	1.81	0.46
24:M:103:ASP:O	24:M:107:THR:HG23	2.16	0.46
1:1:212:THR:HB	1:1:213:ARG:HH11	1.80	0.46
1:1:375:LEU:HD13	3:0:571:VAL:HG21	1.97	0.46
1:1:471:UNK:O	1:1:475:UNK:N	2.48	0.46
2:4:26:LEU:HB3	2:4:73:VAL:HG12	1.96	0.46
3:0:94:THR:O	3:0:98:GLY:N	2.39	0.46
3:0:393:VAL:O	3:0:397:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:489:LYS:HE3	3:0:724:MET:HE1	1.97	0.46
5:2:475:ALA:O	5:2:479:GLY:N	2.42	0.46
6:5:24:ASP:HA	6:5:27:MET:SD	2.54	0.46
7:7:489:GLU:HB3	7:7:689:ARG:NH1	2.31	0.46
8:3:85:ARG:O	8:3:89:PHE:N	2.39	0.46
12:A:1140:HIS:NE2	12:A:1272:THR:HB	2.31	0.46
13:B:705:MET:H	13:B:710:LEU:HD12	1.80	0.46
16:E:98:ILE:HA	16:E:101:GLN:HB3	1.96	0.46
16:E:113:GLN:HA	16:E:137:GLU:CD	2.41	0.46
16:E:156:LEU:HB2	16:E:195:VAL:O	2.14	0.46
29:W:174:ARG:HD2	30:X:255:ILE:HD13	1.97	0.46
3:0:63:TYR:HB3	3:0:65:GLU:OE1	2.15	0.46
3:0:238:HIS:HB2	3:0:660:ARG:HD2	1.97	0.46
3:0:304:GLU:OE1	3:0:386:ARG:NH1	2.40	0.46
3:0:327:ARG:HB3	3:0:330:HIS:CD2	2.50	0.46
7:7:492:VAL:HG23	7:7:682:GLN:HE22	1.80	0.46
7:7:588:PHE:O	7:7:592:GLN:N	2.42	0.46
9:O:73:THR:OG1	9:O:158:GLN:OE1	2.22	0.46
12:A:376:TYR:CZ	12:A:498:ARG:HD2	2.51	0.46
12:A:1155:ASP:OD1	12:A:1161:THR:HA	2.16	0.46
12:A:1239:ARG:HH22	12:A:1241:ARG:NH2	2.14	0.46
20:I:27:PHE:N	20:I:36:GLU:O	2.43	0.46
25:Q:120:LYS:HB3	25:Q:120:LYS:HE2	1.73	0.46
27:U:267:VAL:HG23	27:U:276:PHE:CE1	2.50	0.46
1:1:551:ARG:HB2	1:1:616:LEU:HD11	1.97	0.46
3:0:24:TYR:O	3:0:28:ILE:HG22	2.16	0.46
3:0:32:LEU:HD23	3:0:59:TYR:CD1	2.51	0.46
3:0:603:ARG:NH2	3:0:626:PRO:O	2.48	0.46
3:0:709:SER:HB3	3:0:712:MET:HG2	1.98	0.46
4:6:120:ARG:CZ	4:6:309:PRO:HG3	2.46	0.46
5:2:13:TYR:HA	5:2:16:GLU:HB3	1.96	0.46
7:7:547:GLY:H	7:7:550:ALA:HB2	1.80	0.46
12:A:271:LYS:NZ	24:M:92:LEU:O	2.36	0.46
12:A:1341:ILE:HD13	12:A:1380:GLY:H	1.80	0.46
13:B:444:MET:SD	13:B:444:MET:N	2.88	0.46
18:G:5:LYS:HE3	18:G:6:ASP:H	1.79	0.46
1:1:372:VAL:O	1:1:376:LYS:HG3	2.16	0.46
3:0:195:ILE:O	3:0:199:MET:HB2	2.16	0.46
5:2:15:GLU:OE1	5:2:83:SER:HB2	2.16	0.46
6:5:24:ASP:HA	6:5:27:MET:CG	2.45	0.46
12:A:131:SER:OG	12:A:132:LYS:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:306:ASN:ND2	12:A:322:VAL:O	2.48	0.46
12:A:860:LEU:HB2	12:A:862:ASN:OD1	2.14	0.46
12:A:869:GLY:HA3	12:A:1366:ARG:HG2	1.97	0.46
12:A:1263:ILE:O	12:A:1267:MET:N	2.47	0.46
13:B:1152:MET:HE1	13:B:1195:HIS:HB3	1.97	0.46
14:C:16:ASP:OD1	14:C:16:ASP:N	2.47	0.46
24:M:204:GLY:HA2	24:M:207:LEU:HB3	1.98	0.46
1:1:221:ALA:O	1:1:225:SER:N	2.49	0.46
1:1:472:UNK:O	1:1:476:UNK:N	2.49	0.46
2:4:297:SER:O	2:4:300:PRO:HD3	2.15	0.46
3:0:131:GLU:HG3	3:0:393:VAL:HG21	1.97	0.46
3:0:211:HIS:HB3	3:0:215:ASP:HB2	1.98	0.46
7:7:356:LEU:H	7:7:404:LYS:HE2	1.80	0.46
7:7:424:PHE:O	7:7:428:CYS:HB3	2.16	0.46
7:7:659:ASP:HA	7:7:660:THR:HA	1.63	0.46
7:7:668:THR:HG1	7:7:694:LYS:NZ	2.11	0.46
7:7:739:LEU:H	7:7:742:MET:HE2	1.81	0.46
8:3:80:LYS:O	8:3:84:ILE:N	2.38	0.46
12:A:128:ILE:O	12:A:134:ARG:HD3	2.16	0.46
12:A:253:ASN:HB2	12:A:256:GLN:HG2	1.98	0.46
12:A:800:VAL:HG22	12:A:812:GLU:HB3	1.98	0.46
12:A:854:ASN:O	12:A:867:ILE:HA	2.15	0.46
13:B:87:LYS:N	13:B:137:TYR:O	2.38	0.46
23:L:58:LYS:HD2	23:L:58:LYS:HA	1.60	0.46
24:M:108:LYS:HD3	24:M:108:LYS:HA	1.74	0.46
24:M:148:ASP:HA	24:M:151:LYS:HB2	1.98	0.46
25:Q:337:GLU:OE2	25:Q:340:LYS:N	2.49	0.46
29:W:10:LYS:HE3	29:W:33:LEU:HD22	1.98	0.46
1:1:251:LEU:HB2	1:1:255:LYS:HG2	1.97	0.46
1:1:510:ASN:ND2	2:4:265:PRO:O	2.35	0.46
3:0:293:LEU:HD13	3:0:319:GLU:HA	1.98	0.46
3:0:629:TYR:CZ	3:0:636:LYS:HE2	2.50	0.46
7:7:321:GLU:HG3	7:7:504:THR:HA	1.96	0.46
7:7:341:TYR:OH	7:7:509:ALA:HB2	2.16	0.46
7:7:354:ILE:HD11	7:7:405:LYS:O	2.15	0.46
9:O:175:LEU:HD21	9:O:193:LEU:HD22	1.98	0.46
13:B:73:GLN:O	13:B:85:SER:OG	2.28	0.46
13:B:287:ARG:NH1	13:B:324:ILE:O	2.49	0.46
13:B:859:TYR:O	13:B:966:VAL:N	2.39	0.46
26:R:94:LYS:HE2	26:R:107:LEU:HG	1.96	0.46
27:U:257:ARG:HH11	27:U:259:LYS:HG3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:605:LYS:HA	3:0:608:GLU:CD	2.40	0.46
3:0:632:SER:OG	3:0:633:ARG:N	2.49	0.46
3:0:681:LEU:HB3	3:0:686:PHE:CD2	2.51	0.46
7:7:383:ILE:HD11	7:7:531:ILE:HD13	1.98	0.46
7:7:562:THR:OG1	7:7:563:ALA:N	2.49	0.46
7:7:622:MET:HE2	7:7:622:MET:HB2	1.70	0.46
7:7:678:GLY:HA2	7:7:679:SER:HA	1.59	0.46
9:O:191:PRO:CG	24:M:272:LYS:HD3	2.46	0.46
10:N:7:DA:C2	10:N:8:DA:C5	3.04	0.46
12:A:42:ASP:HA	12:A:49:LYS:HB2	1.97	0.46
13:B:901:PRO:HD3	23:L:58:LYS:CG	2.46	0.46
25:Q:103:LEU:HB3	25:Q:386:MET:SD	2.55	0.46
28:V:69:TYR:HA	28:V:77:THR:O	2.16	0.46
1:1:300:UNK:O	1:1:302:UNK:N	2.48	0.45
2:4:312:PHE:HB3	4:6:319:LEU:HD11	1.96	0.45
3:0:70:ILE:HG13	3:0:206:ILE:HG13	1.98	0.45
3:0:123:GLU:OE1	3:0:125:LYS:N	2.49	0.45
3:0:294:HIS:CE1	3:0:297:ASP:HB3	2.52	0.45
3:0:327:ARG:HG3	3:0:330:HIS:H	1.80	0.45
3:0:440:LEU:HB3	3:0:641:PHE:CD2	2.51	0.45
5:2:432:VAL:HA	5:2:433:LEU:HA	1.69	0.45
6:5:53:GLU:CD	6:5:56:ARG:HB2	2.41	0.45
9:O:109:PRO:HG2	9:O:131:ASP:O	2.16	0.45
11:T:137:DA:H2"	11:T:138:DA:C8	2.51	0.45
13:B:1106:ARG:CZ	13:B:1118:PRO:HB3	2.45	0.45
15:D:127:ASP:HB3	15:D:142:LYS:HG3	1.97	0.45
15:D:128:VAL:HA	15:D:131:GLU:HB3	1.97	0.45
24:M:102:THR:HG23	24:M:106:PHE:HB2	1.97	0.45
25:Q:125:LYS:HB2	25:Q:125:LYS:HE3	1.70	0.45
29:W:97:ALA:HB1	30:X:268:LEU:HD13	1.96	0.45
1:1:476:UNK:O	1:1:480:UNK:N	2.49	0.45
2:4:30:ILE:HB	2:4:179:LEU:HD13	1.98	0.45
2:4:314:GLU:O	2:4:318:ALA:N	2.37	0.45
3:0:80:GLU:HB3	3:0:178:PHE:CD2	2.50	0.45
3:0:419:ILE:HD13	3:0:634:ILE:HG12	1.97	0.45
3:0:659:MET:HA	3:0:662:ALA:HB3	1.98	0.45
5:2:51:VAL:HG13	5:2:109:ARG:HE	1.82	0.45
7:7:480:ARG:HG3	7:7:481:GLU:O	2.16	0.45
7:7:636:ARG:O	7:7:640:LEU:N	2.40	0.45
7:7:705:PHE:CZ	7:7:707:SER:HB2	2.51	0.45
12:A:55:ASP:O	12:A:58:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:147:VAL:HA	12:A:170:THR:HA	1.98	0.45
12:A:275:SER:O	12:A:279:LEU:HB2	2.17	0.45
13:B:526:GLU:HG3	13:B:775:LYS:HZ3	1.80	0.45
14:C:27:LEU:HA	14:C:228:PHE:CZ	2.51	0.45
17:F:140:ASP:CG	17:F:142:SER:H	2.25	0.45
4:6:275:GLU:O	4:6:279:ALA:N	2.37	0.45
7:7:539:ASN:HD21	7:7:542:GLU:HB3	1.80	0.45
9:O:197:MET:HE3	9:O:197:MET:HB2	1.88	0.45
10:N:4:DA:H2"	10:N:5:DA:H8	1.80	0.45
10:N:10:DA:N3	10:N:11:DA:C6	2.84	0.45
12:A:315:LEU:HB2	24:M:96:ILE:HA	1.98	0.45
12:A:633:VAL:HG21	12:A:645:LEU:HD22	1.98	0.45
12:A:1359:ASP:OD2	12:A:1361:SER:OG	2.25	0.45
13:B:857:ARG:NH1	13:B:945:GLU:OE2	2.50	0.45
14:C:8:VAL:HG11	22:K:105:PHE:CD1	2.48	0.45
16:E:165:LEU:O	16:E:169:ARG:N	2.47	0.45
19:H:10:PHE:HD2	19:H:57:VAL:HG21	1.81	0.45
19:H:124:ARG:NH1	19:H:126:GLU:OE1	2.49	0.45
1:1:465:UNK:O	1:1:470:UNK:N	2.50	0.45
3:0:134:ARG:HH12	3:0:305:PRO:HD2	1.81	0.45
3:0:587:ARG:O	3:0:591:SER:N	2.35	0.45
5:2:387:LEU:C	5:2:390:GLY:H	2.23	0.45
5:2:466:GLN:CD	5:2:466:GLN:H	2.24	0.45
7:7:223:VAL:H	7:7:337:VAL:HA	1.82	0.45
7:7:593:PHE:O	7:7:597:TYR:N	2.22	0.45
7:7:616:GLN:HE21	7:7:628:TYR:HB2	1.80	0.45
7:7:664:LEU:O	7:7:692:ARG:HG3	2.16	0.45
9:O:157:ILE:HD13	9:O:160:ILE:HD11	1.98	0.45
10:N:7:DA:C2	10:N:8:DA:C4	3.04	0.45
12:A:253:ASN:HA	13:B:935:ARG:HH22	1.80	0.45
12:A:497:THR:HG22	13:B:1146:PHE:HA	1.98	0.45
12:A:698:GLN:HG2	20:I:99:LEU:HD21	1.97	0.45
12:A:1213:GLY:HA3	12:A:1228:TRP:CZ3	2.51	0.45
13:B:414:ALA:O	13:B:418:LYS:N	2.44	0.45
21:J:31:ASP:O	21:J:35:ALA:N	2.48	0.45
25:Q:141:ARG:HB3	25:Q:348:TYR:HB2	1.98	0.45
1:1:477:UNK:O	1:1:481:UNK:N	2.49	0.45
3:0:208:TYR:HD2	3:0:209:SER:O	1.99	0.45
3:0:594:ARG:NE	4:6:241:THR:O	2.34	0.45
5:2:380:ARG:HE	5:2:380:ARG:HB2	1.50	0.45
7:7:302:GLU:CD	7:7:321:GLU:HB3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:397:ILE:HG21	7:7:428:CYS:SG	2.57	0.45
10:N:50:DG:C8	10:N:51:DT:C5	3.04	0.45
12:A:567:LYS:HB3	19:H:96:VAL:HB	1.99	0.45
12:A:828:ALA:O	12:A:831:THR:OG1	2.32	0.45
12:A:916:GLY:HA2	12:A:919:ILE:HB	1.98	0.45
12:A:1209:MET:HE2	12:A:1231:ASP:HA	1.99	0.45
13:B:649:LYS:NZ	13:B:736:THR:HG23	2.31	0.45
13:B:961:LEU:HD23	13:B:961:LEU:HA	1.79	0.45
14:C:260:LEU:O	14:C:263:THR:OG1	2.29	0.45
24:M:126:VAL:HG22	24:M:154:TYR:HE2	1.81	0.45
24:M:289:PHE:HD1	24:M:289:PHE:HA	1.68	0.45
2:4:194:ILE:HA	2:4:197:MET:HE2	1.98	0.45
5:2:352:ASN:ND2	5:2:373:MET:O	2.50	0.45
7:7:370:LEU:O	7:7:373:MET:HG3	2.16	0.45
7:7:564:GLU:CD	7:7:564:GLU:H	2.23	0.45
7:7:621:LYS:HE3	7:7:750:TYR:CD1	2.52	0.45
7:7:699:GLU:HG3	7:7:701:PHE:H	1.82	0.45
9:O:162:GLY:O	9:O:214:LEU:N	2.41	0.45
9:O:194:ILE:HD11	10:N:20:DT:H5''	1.97	0.45
12:A:14:VAL:HB	12:A:1430:LEU:HD13	1.99	0.45
12:A:254:GLU:O	12:A:257:ARG:NH2	2.46	0.45
13:B:399:ASP:OD1	13:B:509:ALA:N	2.49	0.45
13:B:423:LYS:HD3	13:B:423:LYS:HA	1.76	0.45
14:C:183:TRP:CE3	14:C:213:PRO:HD3	2.52	0.45
22:K:12:LEU:HD11	22:K:16:GLU:O	2.16	0.45
26:R:63:ARG:O	26:R:65:ASN:ND2	2.49	0.45
30:X:268:LEU:HA	30:X:268:LEU:HD23	1.74	0.45
2:4:194:ILE:HB	2:4:195:PRO:HD3	1.99	0.45
3:0:13:PRO:HA	3:0:92:TYR:CG	2.50	0.45
3:0:161:ASN:ND2	3:0:189:THR:O	2.49	0.45
5:2:47:ILE:O	5:2:51:VAL:HG23	2.16	0.45
7:7:540:TRP:HB3	7:7:544:SER:OG	2.16	0.45
7:7:565:PHE:CZ	7:7:583:MET:HG3	2.51	0.45
11:T:130:DA:H1'	11:T:131:DC:O4'	2.16	0.45
12:A:88:LYS:HD2	12:A:89:PRO:HD2	1.98	0.45
12:A:1079:MET:HE2	12:A:1097:GLY:HA2	1.99	0.45
12:A:1286:LYS:HB2	12:A:1304:TRP:CE3	2.51	0.45
13:B:91:SER:N	13:B:133:LYS:O	2.44	0.45
13:B:386:LEU:O	13:B:390:LEU:N	2.48	0.45
13:B:1165:ILE:HD13	13:B:1187:ASN:HB2	1.99	0.45
19:H:93:TYR:CG	19:H:143:LEU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:I:103:CYS:HB3	20:I:108:HIS:N	2.32	0.45
24:M:157:CYS:C	24:M:159:ASP:H	2.24	0.45
24:M:157:CYS:HB3	24:M:210:MET:HE1	1.98	0.45
2:4:79:TYR:O	2:4:148:THR:OG1	2.34	0.45
2:4:214:LYS:HG2	2:4:237:HIS:CE1	2.52	0.45
3:0:156:CYS:C	3:0:158:TYR:H	2.25	0.45
3:0:212:TYR:O	3:0:221:ARG:NH2	2.49	0.45
3:0:301:ASP:HB2	3:0:305:PRO:HG3	1.98	0.45
3:0:325:ILE:HG12	3:0:334:PHE:CE2	2.52	0.45
3:0:722:ARG:H	3:0:722:ARG:HG3	1.47	0.45
5:2:47:ILE:HG23	5:2:100:LEU:HD21	1.97	0.45
5:2:371:VAL:HG22	7:7:117:ASP:O	2.17	0.45
7:7:240:ASP:O	7:7:244:MET:N	2.28	0.45
7:7:337:VAL:HG23	7:7:339:GLU:HG3	1.97	0.45
12:A:903:ASN:HD21	12:A:905:ASP:HB3	1.81	0.45
13:B:621:GLU:O	13:B:623:GLU:HG3	2.17	0.45
13:B:728:ARG:HH12	13:B:1048:THR:N	2.15	0.45
13:B:773:MET:HE1	13:B:985:GLY:HA2	1.98	0.45
13:B:1084:GLN:NE2	14:C:191:TYR:HA	2.31	0.45
15:D:40:HIS:NE2	18:G:6:ASP:OD1	2.50	0.45
16:E:48:ASP:OD1	16:E:51:GLY:N	2.48	0.45
19:H:79:TRP:O	19:H:80:ARG:HG3	2.17	0.45
24:M:173:ALA:HB3	24:M:203:PHE:HE1	1.82	0.45
25:Q:343:ARG:HD2	25:Q:343:ARG:HA	1.59	0.45
26:R:270:MET:N	26:R:270:MET:SD	2.89	0.45
29:W:108:ARG:HH12	29:W:109:LEU:HD22	1.82	0.45
3:0:92:TYR:HA	3:0:95:LYS:HB3	1.98	0.45
4:6:139:LYS:NZ	4:6:143:PRO:O	2.32	0.45
4:6:214:LEU:O	4:6:218:ARG:HB2	2.17	0.45
5:2:87:LEU:HD12	5:2:98:ILE:HG23	1.99	0.45
6:5:17:LYS:O	6:5:21:LEU:HG	2.17	0.45
12:A:61:ILE:H	12:A:65:LEU:HD12	1.82	0.45
12:A:708:MET:HB2	12:A:712:GLU:HB3	1.99	0.45
12:A:904:THR:HA	12:A:907:THR:HB	1.99	0.45
13:B:26:THR:OG1	13:B:27:ALA:N	2.49	0.45
13:B:680:THR:OG1	13:B:681:TRP:N	2.50	0.45
16:E:64:PRO:HB2	16:E:69:ILE:HD11	1.97	0.45
16:E:108:GLY:N	16:E:131:THR:O	2.43	0.45
16:E:117:THR:HG1	16:E:120:ALA:H	1.65	0.45
16:E:118:PRO:HA	16:E:121:MET:HB3	1.98	0.45
17:F:99:LEU:O	17:F:102:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:104:ILE:HG21	26:R:122:LEU:HD22	1.97	0.45
1:1:563:HIS:O	1:1:567:HIS:N	2.37	0.45
3:0:22:TYR:O	3:0:26:CYS:N	2.48	0.45
3:0:217:LYS:HE3	3:0:310:PRO:HA	1.98	0.45
3:0:238:HIS:CE1	3:0:462:THR:HB	2.51	0.45
3:0:259:ARG:HA	3:0:262:ARG:HE	1.80	0.45
3:0:425:ILE:HA	3:0:428:ALA:HB2	1.99	0.45
3:0:546:TYR:O	3:0:550:ILE:HG12	2.16	0.45
3:0:618:ARG:HD3	3:0:618:ARG:HA	1.75	0.45
4:6:132:CYS:HA	4:6:204:PRO:HB3	1.99	0.45
4:6:137:LEU:HG	4:6:204:PRO:HG2	1.98	0.45
7:7:485:ILE:O	7:7:511:LEU:N	2.50	0.45
8:3:65:LYS:O	8:3:67:LYS:N	2.50	0.45
10:N:8:DA:N3	10:N:9:DA:C5	2.85	0.45
12:A:414:ASP:OD1	12:A:415:LEU:N	2.50	0.45
12:A:731:ARG:HD3	12:A:731:ARG:HA	1.66	0.45
12:A:1277:GLU:O	12:A:1279:ILE:HG12	2.17	0.45
13:B:59:LEU:HD12	13:B:59:LEU:HA	1.79	0.45
13:B:649:LYS:HE2	13:B:711:GLU:O	2.17	0.45
13:B:791:THR:HG22	13:B:792:MET:HG3	1.98	0.45
13:B:832:GLY:O	13:B:835:GLN:NE2	2.39	0.45
13:B:1009:ASP:OD1	13:B:1009:ASP:N	2.49	0.45
24:M:27:CYS:HB3	24:M:29:VAL:HG13	1.99	0.45
26:R:75:MET:HA	26:R:78:ALA:HB3	1.99	0.45
27:U:269:ILE:HG21	28:V:106:ILE:HG21	1.99	0.45
29:W:183:ILE:HA	29:W:186:LEU:HB2	1.98	0.45
1:1:508:LYS:HG3	1:1:509:ILE:N	2.31	0.44
1:1:629:LYS:O	1:1:633:TYR:N	2.39	0.44
2:4:175:ARG:HH12	2:4:252:MET:C	2.24	0.44
3:0:249:SER:HB2	3:0:436:ARG:NH2	2.32	0.44
3:0:281:LYS:HA	3:0:284:ASP:HB3	1.99	0.44
3:0:553:MET:O	3:0:557:MET:N	2.39	0.44
3:0:568:LEU:O	3:0:597:ILE:N	2.42	0.44
3:0:705:ASP:N	3:0:705:ASP:OD1	2.50	0.44
4:6:322:MET:HE2	4:6:322:MET:HB3	1.73	0.44
5:2:368:ALA:HB3	5:2:370:PHE:HE1	1.81	0.44
7:7:492:VAL:HG12	7:7:493:VAL:HG22	1.99	0.44
9:O:179:HIS:HE1	9:O:237:PHE:CE2	2.35	0.44
10:N:32:DA:H1'	10:N:33:DA:C8	2.52	0.44
12:A:1121:GLU:HB3	12:A:1124:HIS:HB2	1.99	0.44
12:A:1208:THR:OG1	12:A:1231:ASP:OD2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:332:ASP:O	13:B:336:ARG:HG2	2.18	0.44
13:B:704:ALA:HB2	13:B:738:PHE:CD1	2.52	0.44
14:C:61:GLU:HA	14:C:64:ALA:HB3	1.99	0.44
15:D:24:ALA:N	15:D:28:GLN:O	2.49	0.44
16:E:74:ASP:O	16:E:106:GLN:NE2	2.50	0.44
17:F:85:MET:HG3	17:F:89:GLU:HB2	1.99	0.44
18:G:48:VAL:HA	18:G:76:ALA:HA	1.99	0.44
18:G:61:ILE:HG12	18:G:68:ALA:HB2	1.99	0.44
22:K:12:LEU:HD12	22:K:13:GLY:H	1.82	0.44
25:Q:98:TYR:CB	26:R:96:ARG:HA	2.47	0.44
29:W:17:VAL:O	29:W:21:TYR:HB2	2.15	0.44
29:W:66:LEU:HA	29:W:94:ALA:HB2	1.99	0.44
29:W:169:GLN:OE1	29:W:173:ASN:ND2	2.50	0.44
1:1:339:LEU:HD11	3:0:610:ILE:HD11	1.99	0.44
3:0:378:SER:HA	3:0:403:ALA:HB1	1.98	0.44
3:0:539:VAL:HA	3:0:621:LEU:HB2	1.99	0.44
7:7:389:GLY:O	7:7:692:ARG:HA	2.17	0.44
7:7:631:THR:HG22	7:7:632:PRO:O	2.17	0.44
10:N:16:DC:O2	10:N:17:DG:N7	2.50	0.44
12:A:181:LEU:O	12:A:202:LEU:N	2.37	0.44
12:A:336:ILE:HG21	12:A:1401:SER:HA	1.99	0.44
12:A:1390:ASN:HA	12:A:1399:ARG:HD2	1.98	0.44
13:B:102:VAL:HG12	13:B:112:LEU:HB2	1.98	0.44
13:B:890:TYR:CE2	13:B:910:VAL:HG21	2.52	0.44
14:C:84:ARG:HD2	22:K:7:PHE:HB3	1.98	0.44
15:D:143:ASN:O	15:D:147:TYR:N	2.40	0.44
16:E:197:LYS:HE2	16:E:199:ILE:HD11	1.99	0.44
18:G:93:SER:HB3	18:G:100:GLU:HB3	1.98	0.44
25:Q:373:TYR:HB3	26:R:70:LEU:HD11	1.99	0.44
27:U:247:LEU:HD23	28:V:116:CYS:HB3	1.99	0.44
30:X:261:LYS:O	30:X:265:ASN:N	2.38	0.44
1:1:502:ARG:HA	1:1:502:ARG:HD2	1.77	0.44
2:4:50:ILE:HG21	2:4:181:CYS:SG	2.58	0.44
3:0:13:PRO:HA	3:0:92:TYR:CD1	2.53	0.44
3:0:298:ILE:HD12	3:0:298:ILE:HA	1.82	0.44
3:0:471:ARG:HH22	3:0:647:ARG:N	2.15	0.44
3:0:542:PRO:HB3	3:0:626:PRO:HA	1.99	0.44
4:6:403:CYS:HB3	4:6:408:SER:H	1.82	0.44
5:2:406:PRO:O	5:2:409:ARG:NH1	2.51	0.44
7:7:102:ALA:O	7:7:523:LYS:HB3	2.16	0.44
7:7:383:ILE:HG13	7:7:528:ASN:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:443:LYS:HA	7:7:469:ASP:HB3	1.99	0.44
9:O:214:LEU:HB2	9:O:223:ILE:HD12	1.98	0.44
12:A:151:ASP:OD1	12:A:152:VAL:N	2.50	0.44
12:A:1189:SER:N	12:A:1242:VAL:O	2.42	0.44
12:A:1212:VAL:O	12:A:1216:ILE:HG12	2.17	0.44
12:A:1334:ASP:O	12:A:1338:VAL:N	2.44	0.44
12:A:1397:LEU:HD23	12:A:1397:LEU:HA	1.88	0.44
13:B:135:ARG:HA	13:B:135:ARG:HD3	1.79	0.44
13:B:210:LYS:NZ	13:B:462:ALA:O	2.47	0.44
13:B:299:GLU:HG3	13:B:572:HIS:NE2	2.33	0.44
13:B:322:PHE:HZ	20:I:30:ARG:HB3	1.83	0.44
18:G:39:THR:O	18:G:43:GLY:N	2.48	0.44
19:H:101:ALA:HB2	19:H:116:TYR:CZ	2.52	0.44
3:0:143:ARG:HA	3:0:146:GLU:HG2	1.99	0.44
3:0:525:MET:O	3:0:528:GLU:HG2	2.18	0.44
4:6:136:MET:HE3	4:6:237:GLY:HA3	1.98	0.44
4:6:312:LYS:HA	4:6:312:LYS:HD3	1.77	0.44
5:2:118:GLN:O	5:2:122:GLY:N	2.50	0.44
5:2:473:LYS:HD2	5:2:473:LYS:HA	1.80	0.44
6:5:48:GLU:HB2	6:5:52:HIS:HE1	1.82	0.44
7:7:346:ASP:HA	7:7:508:HIS:CG	2.52	0.44
7:7:541:MET:HA	7:7:545:GLN:CD	2.42	0.44
7:7:694:LYS:HZ1	7:7:696:ARG:HH21	1.66	0.44
7:7:752:SER:OG	7:7:754:ARG:HG3	2.16	0.44
8:3:46:ILE:HD12	8:3:63:LEU:HD22	2.00	0.44
10:N:31:DC:H2''	10:N:32:DA:C8	2.52	0.44
12:A:445:ASN:HB2	12:A:455:MET:HG2	1.99	0.44
12:A:474:VAL:HA	12:A:521:MET:HE3	1.98	0.44
12:A:1286:LYS:HB2	12:A:1304:TRP:CZ3	2.53	0.44
13:B:333:PHE:HE1	13:B:337:ARG:HH21	1.65	0.44
19:H:26:ILE:HG13	19:H:42:ILE:HD12	1.99	0.44
26:R:276:ASN:HA	26:R:279:LYS:HE2	1.99	0.44
29:W:15:PHE:O	29:W:19:GLY:N	2.49	0.44
2:4:297:SER:C	2:4:299:ILE:H	2.24	0.44
4:6:231:GLU:HG2	4:6:260:ARG:O	2.17	0.44
7:7:363:ARG:HB3	7:7:548:HIS:HA	1.98	0.44
7:7:439:THR:HB	7:7:441:ASP:H	1.82	0.44
12:A:794:PRO:HB2	12:A:799:PHE:HB3	1.98	0.44
12:A:949:ASP:OD1	12:A:951:GLU:N	2.50	0.44
25:Q:30:ASN:O	25:Q:34:MET:N	2.40	0.44
1:1:373:ASP:HA	1:1:376:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:296:LEU:HD22	2:4:300:PRO:HG3	2.00	0.44
3:0:68:LYS:HZ2	3:0:204:ASN:HA	1.81	0.44
3:0:162:LEU:O	3:0:167:VAL:HG23	2.17	0.44
3:0:259:ARG:HB3	3:0:259:ARG:NH1	2.33	0.44
3:0:422:PRO:HG2	3:0:423:TYR:CD2	2.53	0.44
3:0:591:SER:O	4:6:272:ILE:HB	2.17	0.44
4:6:403:CYS:SG	4:6:437:CYS:HB3	2.57	0.44
5:2:29:PRO:O	5:2:33:LEU:N	2.45	0.44
5:2:69:ASN:OD1	5:2:69:ASN:N	2.50	0.44
6:5:48:GLU:O	6:5:52:HIS:ND1	2.51	0.44
7:7:411:CYS:CB	7:7:417:VAL:HG22	2.48	0.44
12:A:16:GLU:OE2	12:A:1418:LEU:HD21	2.18	0.44
12:A:339:ASN:ND2	13:B:1117:GLN:OE1	2.51	0.44
12:A:1115:SER:OG	12:A:1116:LEU:N	2.51	0.44
12:A:1342:GLU:HG3	16:E:198:ILE:HD13	2.00	0.44
12:A:1412:ALA:HA	12:A:1417:GLU:HG3	1.99	0.44
17:F:92:ARG:O	17:F:96:THR:OG1	2.31	0.44
18:G:26:LEU:HD23	18:G:26:LEU:HA	1.88	0.44
22:K:49:GLU:OE2	22:K:52:ASN:ND2	2.44	0.44
24:M:123:ASP:O	24:M:127:GLN:N	2.33	0.44
24:M:157:CYS:SG	24:M:158:HIS:N	2.88	0.44
28:V:81:LYS:HA	28:V:81:LYS:HD3	1.76	0.44
1:1:230:PRO:O	1:1:232:UNK:N	2.51	0.44
2:4:225:GLN:O	2:4:229:ASP:HB3	2.18	0.44
7:7:403:ILE:HG13	7:7:405:LYS:N	2.23	0.44
7:7:538:ALA:HB1	7:7:729:GLN:HB3	2.00	0.44
9:O:158:GLN:HB3	10:N:23:DA:C4'	2.42	0.44
12:A:224:PHE:CD2	12:A:231:PRO:HG3	2.53	0.44
12:A:376:TYR:CE1	12:A:498:ARG:HD2	2.53	0.44
12:A:563:PRO:HB3	12:A:572:TRP:CE2	2.53	0.44
12:A:1262:LYS:O	12:A:1266:THR:OG1	2.31	0.44
13:B:61:ASP:N	13:B:61:ASP:OD1	2.48	0.44
13:B:997:GLU:OE1	13:B:997:GLU:N	2.28	0.44
13:B:1065:GLN:OE1	13:B:1067:ARG:N	2.49	0.44
15:D:144:THR:O	15:D:148:LEU:HG	2.18	0.44
26:R:71:VAL:HA	26:R:222:CYS:O	2.17	0.44
29:W:116:ASN:O	29:W:165:ASN:HB2	2.16	0.44
30:X:274:LEU:HA	30:X:277:LYS:HB2	2.00	0.44
1:1:234:UNK:O	1:1:262:ASN:ND2	2.51	0.44
3:0:7:ASP:O	3:0:62:HIS:NE2	2.50	0.44
3:0:199:MET:HA	3:0:202:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:128:LEU:HD23	4:6:129:THR:N	2.33	0.44
4:6:141:LEU:HB2	4:6:144:ASN:O	2.16	0.44
4:6:165:PRO:HG2	4:6:375:HIS:HB3	2.00	0.44
5:2:273:LYS:HE2	5:2:277:MET:SD	2.57	0.44
5:2:367:LYS:HB2	5:2:375:LEU:HD23	2.00	0.44
7:7:579:LEU:HD13	7:7:766:LYS:HE3	1.99	0.44
9:O:169:PRO:HA	9:O:208:VAL:O	2.17	0.44
12:A:231:PRO:O	12:A:234:MET:HB3	2.18	0.44
12:A:590:ARG:HH21	12:A:621:THR:HG1	1.62	0.44
13:B:451:LYS:HG3	24:M:138:ASP:HB3	1.99	0.44
13:B:542:MET:HG2	13:B:747:MET:HB3	2.00	0.44
13:B:1006:ILE:HG23	21:J:45:CYS:HB3	1.99	0.44
22:K:77:THR:OG1	22:K:81:TYR:HB3	2.18	0.44
26:R:95:ILE:HG22	26:R:97:ILE:HG23	1.99	0.44
27:U:244:MET:HG2	27:U:267:VAL:HG22	2.00	0.44
3:0:338:LEU:O	3:0:342:LEU:HG	2.17	0.44
3:0:669:VAL:HG13	3:0:670:LEU:HG	2.00	0.44
7:7:354:ILE:HG12	7:7:452:LEU:HD21	2.00	0.44
7:7:383:ILE:HD13	7:7:383:ILE:HA	1.80	0.44
7:7:568:GLU:CD	7:7:580:LEU:HD13	2.43	0.44
7:7:642:ASN:CG	7:7:649:ILE:HD13	2.43	0.44
12:A:335:ARG:HA	12:A:335:ARG:HD3	1.75	0.44
12:A:1153:TYR:HB2	12:A:1192:LEU:HB3	2.00	0.44
12:A:1258:HIS:HA	12:A:1261:LYS:HD3	2.00	0.44
12:A:1329:THR:HG22	12:A:1331:SER:H	1.82	0.44
12:A:1409:LEU:O	12:A:1413:GLY:N	2.38	0.44
12:A:1428:VAL:HG13	13:B:1151:LEU:HD21	1.99	0.44
13:B:583:ASN:ND2	13:B:628:THR:H	2.15	0.44
15:D:55:ALA:O	15:D:59:ILE:HG12	2.18	0.44
18:G:25:TYR:O	18:G:29:LYS:HG2	2.18	0.44
20:I:8:ARG:NH1	20:I:8:ARG:HB2	2.33	0.44
24:M:87:LEU:HD13	24:M:130:PHE:CE2	2.52	0.44
29:W:34:PHE:CE1	30:X:201:THR:HA	2.52	0.44
3:0:486:THR:O	3:0:673:LYS:NZ	2.51	0.43
3:0:732:ASP:OD1	3:0:733:GLN:N	2.46	0.43
4:6:190:GLN:HA	4:6:193:ILE:HB	2.01	0.43
4:6:211:GLN:HB3	4:6:244:PRO:CD	2.42	0.43
7:7:594:LEU:HD22	7:7:706:TYR:CZ	2.53	0.43
7:7:715:GLU:HA	7:7:718:TYR:CD1	2.53	0.43
8:3:135:THR:O	8:3:139:LEU:N	2.37	0.43
9:O:105:ARG:HG2	9:O:112:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:390:GLN:NE2	12:A:394:ASN:OD1	2.42	0.43
12:A:535:THR:HG21	12:A:617:VAL:HB	2.00	0.43
12:A:940:ARG:HH21	12:A:944:ARG:HH12	1.65	0.43
13:B:48:LEU:HD23	13:B:173:MET:SD	2.58	0.43
13:B:848:ARG:NH1	21:J:8:PHE:O	2.51	0.43
14:C:88:CYS:HB2	14:C:91:HIS:O	2.18	0.43
14:C:153:LEU:HD12	14:C:153:LEU:HA	1.81	0.43
16:E:29:PHE:C	16:E:30:ILE:HD12	2.42	0.43
16:E:180:ARG:NH2	16:E:192:ARG:H	2.16	0.43
18:G:21:ARG:HG3	18:G:25:TYR:CZ	2.53	0.43
24:M:163:LEU:HA	24:M:166:LYS:HG2	2.00	0.43
25:Q:126:LYS:H	25:Q:126:LYS:HE2	1.82	0.43
25:Q:138:ARG:O	25:Q:352:MET:HA	2.18	0.43
26:R:120:TYR:CG	26:R:226:PRO:HA	2.53	0.43
1:1:588:ASP:O	1:1:592:LYS:N	2.34	0.43
2:4:35:LYS:O	2:4:39:THR:N	2.34	0.43
3:0:243:VAL:O	3:0:247:SER:N	2.43	0.43
3:0:745:ILE:H	3:0:745:ILE:HG13	1.64	0.43
4:6:294:GLU:HA	4:6:297:LEU:HB3	2.00	0.43
5:2:148:HIS:O	5:2:153:THR:N	2.51	0.43
5:2:396:ILE:HG12	5:2:400:LEU:HG	1.99	0.43
9:O:94:TYR:O	28:V:71:PHE:HB3	2.17	0.43
12:A:41:MET:HG2	12:A:42:ASP:H	1.83	0.43
12:A:269:ILE:O	12:A:273:ASN:N	2.44	0.43
13:B:216:GLU:OE1	13:B:500:THR:OG1	2.35	0.43
13:B:989:THR:OG1	13:B:990:ILE:N	2.51	0.43
16:E:57:MET:HE2	16:E:57:MET:HB2	1.92	0.43
18:G:64:THR:C	18:G:66:GLY:H	2.26	0.43
26:R:64:SER:C	26:R:216:GLY:HA2	2.43	0.43
29:W:18:ARG:NH2	30:X:247:ASN:HA	2.33	0.43
29:W:149:CYS:HB2	29:W:156:LEU:HD21	2.00	0.43
30:X:274:LEU:HD12	30:X:277:LYS:HB2	2.00	0.43
1:1:189:LYS:HE3	1:1:189:LYS:HB3	1.78	0.43
4:6:234:ILE:HB	4:6:263:VAL:HB	1.99	0.43
5:2:31:THR:HG22	5:2:226:PHE:HD2	1.82	0.43
5:2:273:LYS:HG2	5:2:277:MET:HG2	2.00	0.43
5:2:346:LYS:NZ	5:2:376:GLY:O	2.39	0.43
6:5:23:ILE:O	6:5:27:MET:HG3	2.18	0.43
7:7:457:TYR:OH	7:7:488:ASP:N	2.31	0.43
7:7:550:ALA:O	7:7:702:ASN:HB2	2.18	0.43
7:7:608:PHE:N	7:7:671:ILE:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:471:ASN:ND2	12:A:650:GLN:OE1	2.39	0.43
12:A:664:THR:HG22	13:B:1014:PRO:HB3	2.00	0.43
12:A:752:LYS:HD3	12:A:752:LYS:HA	1.73	0.43
13:B:209:GLU:CD	13:B:485:ARG:HE	2.26	0.43
13:B:227:LYS:H	13:B:395:GLN:NE2	2.15	0.43
13:B:515:HIS:HB3	13:B:518:HIS:CD2	2.54	0.43
13:B:1155:SER:OG	13:B:1156:ASP:OD1	2.31	0.43
15:D:29:LEU:HD13	18:G:82:PHE:CZ	2.53	0.43
16:E:165:LEU:HD11	16:E:172:GLU:HG2	2.00	0.43
18:G:38:CYS:SG	18:G:39:THR:N	2.91	0.43
24:M:276:THR:HB	24:M:308:THR:HG21	2.00	0.43
25:Q:117:HIS:CG	25:Q:391:LYS:HB2	2.53	0.43
2:4:153:MET:HE3	2:4:153:MET:HB2	1.82	0.43
3:0:16:LYS:H	3:0:16:LYS:HG2	1.60	0.43
3:0:53:LEU:O	3:0:57:ILE:HG12	2.19	0.43
3:0:278:ASP:O	3:0:281:LYS:NZ	2.51	0.43
3:0:377:CYS:SG	3:0:407:THR:OG1	2.57	0.43
3:0:492:PHE:CZ	3:0:700:GLY:HA3	2.53	0.43
5:2:350:TYR:H	5:2:407:GLN:NE2	2.16	0.43
5:2:384:ARG:HG2	5:2:387:LEU:HD22	2.00	0.43
7:7:354:ILE:O	7:7:404:LYS:NZ	2.39	0.43
7:7:699:GLU:HB3	7:7:702:ASN:HD22	1.83	0.43
9:O:205:LEU:HD23	9:O:207:PHE:CZ	2.53	0.43
11:T:133:DT:H2'	11:T:134:DT:C6	2.53	0.43
11:T:150:DG:C2	11:T:151:DC:C2	3.06	0.43
12:A:91:PHE:HA	12:A:235:ILE:HA	1.99	0.43
12:A:465:TYR:CD1	13:B:976:ILE:HG13	2.53	0.43
12:A:1136:SER:HB2	12:A:1274:ARG:CZ	2.49	0.43
12:A:1199:ARG:O	12:A:1203:ASN:N	2.43	0.43
12:A:1224:LEU:O	12:A:1226:VAL:HG23	2.17	0.43
13:B:664:THR:HG23	13:B:678:GLU:HA	2.00	0.43
13:B:857:ARG:HH12	13:B:942:ARG:NH1	2.17	0.43
13:B:918:ILE:HD11	13:B:935:ARG:HB3	2.00	0.43
16:E:20:LYS:HB2	16:E:35:VAL:HG22	2.00	0.43
18:G:47:CYS:N	18:G:77:VAL:HG22	2.31	0.43
19:H:101:ALA:HB2	19:H:116:TYR:CE2	2.54	0.43
20:I:17:ARG:HA	20:I:17:ARG:HD2	1.61	0.43
25:Q:128:ASN:O	25:Q:128:ASN:ND2	2.51	0.43
26:R:126:LYS:O	26:R:220:HIS:ND1	2.46	0.43
27:U:258:TRP:HE1	27:U:285:TRP:HB2	1.83	0.43
1:1:212:THR:HB	1:1:213:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:487:UNK:N	2:4:55:GLU:OE2	2.51	0.43
3:0:71:TYR:HD1	3:0:72:CYS:N	2.16	0.43
4:6:136:MET:HA	4:6:145:ARG:HD2	1.99	0.43
4:6:262:LYS:HB2	4:6:287:PHE:CD2	2.49	0.43
4:6:363:CYS:HB3	4:6:368:LEU:H	1.83	0.43
4:6:377:ALA:HA	4:6:380:TYR:CG	2.54	0.43
7:7:324:GLU:O	7:7:328:LYS:N	2.52	0.43
12:A:332:LYS:HE2	12:A:332:LYS:HB2	1.85	0.43
12:A:913:LEU:HA	12:A:979:SER:N	2.33	0.43
12:A:951:GLU:O	12:A:954:TRP:NE1	2.52	0.43
13:B:285:ILE:HA	13:B:288:ALA:HB3	2.01	0.43
13:B:825:VAL:HA	13:B:1010:LEU:O	2.18	0.43
13:B:828:ALA:HB2	13:B:1085:ILE:HD12	2.00	0.43
22:K:107:THR:O	22:K:111:LEU:HG	2.18	0.43
26:R:63:ARG:NH1	26:R:66:ARG:HE	2.16	0.43
27:U:262:LEU:N	27:U:279:ALA:O	2.46	0.43
3:0:60:GLN:O	3:0:67:ARG:NH1	2.41	0.43
3:0:173:LYS:HE2	3:0:173:LYS:O	2.18	0.43
3:0:383:LEU:O	3:0:387:THR:HG23	2.18	0.43
3:0:540:PHE:HD1	3:0:602:ALA:HA	1.84	0.43
3:0:694:PRO:HG2	3:0:697:ILE:HB	2.01	0.43
4:6:272:ILE:HA	4:6:275:GLU:HB3	2.00	0.43
4:6:349:CYS:HB3	4:6:352:CYS:SG	2.58	0.43
4:6:403:CYS:SG	4:6:404:PHE:N	2.91	0.43
5:2:11:THR:HA	5:2:14:LEU:HB2	1.99	0.43
7:7:302:GLU:CG	7:7:322:SER:H	2.32	0.43
7:7:326:VAL:HA	7:7:329:ARG:HH21	1.83	0.43
7:7:348:ARG:O	7:7:405:LYS:HD3	2.18	0.43
10:N:7:DA:C4	10:N:8:DA:N7	2.86	0.43
10:N:35:DG:H2''	10:N:36:DT:H71	1.99	0.43
12:A:23:SER:O	12:A:27:VAL:HG23	2.18	0.43
12:A:140:THR:O	12:A:143:LYS:HG2	2.19	0.43
12:A:415:LEU:HD13	12:A:415:LEU:HA	1.83	0.43
13:B:856:PHE:HE1	13:B:969:ARG:HG3	1.83	0.43
13:B:879:ARG:HA	13:B:885:MET:SD	2.59	0.43
14:C:147:LEU:HD23	14:C:147:LEU:HA	1.80	0.43
15:D:162:ALA:O	15:D:166:LEU:N	2.47	0.43
23:L:53:HIS:C	23:L:54:ARG:HD2	2.43	0.43
29:W:97:ALA:HB1	30:X:268:LEU:HD22	2.00	0.43
1:1:229:GLY:HA2	1:1:230:PRO:HD3	1.83	0.43
3:0:304:GLU:N	3:0:305:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:349:CYS:CB	4:6:352:CYS:SG	3.07	0.43
5:2:25:LEU:HD13	5:2:25:LEU:HA	1.80	0.43
7:7:416:SER:O	7:7:661:SER:OG	2.36	0.43
7:7:670:LEU:HD23	7:7:691:LEU:HD23	1.99	0.43
8:3:51:PRO:HB3	8:3:64:ARG:HD2	2.00	0.43
8:3:137:GLU:O	8:3:141:LYS:N	2.38	0.43
9:O:113:ALA:HB2	9:O:139:TYR:CE2	2.54	0.43
12:A:1171:GLN:HA	12:A:1174:PHE:HB2	2.01	0.43
13:B:486:TYR:CA	13:B:1096:ARG:HH22	2.30	0.43
13:B:883:LEU:HD13	13:B:931:TYR:CE1	2.54	0.43
13:B:910:VAL:HG13	13:B:938:SER:HB2	2.00	0.43
14:C:37:MET:HE3	14:C:176:ILE:HD12	2.00	0.43
16:E:115:ASN:N	16:E:115:ASN:OD1	2.50	0.43
20:I:28:GLU:HA	20:I:35:VAL:HG22	2.00	0.43
21:J:28:ASP:N	21:J:28:ASP:OD1	2.51	0.43
23:L:47:ARG:HH22	23:L:49:LYS:HA	1.83	0.43
24:M:92:LEU:HD23	24:M:92:LEU:HA	1.87	0.43
24:M:270:ALA:O	24:M:277:ILE:HG12	2.18	0.43
26:R:299:ILE:O	26:R:303:LEU:N	2.39	0.43
29:W:9:VAL:O	29:W:13:LEU:HG	2.19	0.43
29:W:9:VAL:HG22	29:W:189:ILE:HD13	2.00	0.43
1:1:185:LEU:HD13	1:1:210:TRP:CH2	2.53	0.43
1:1:370:UNK:C	1:1:372:VAL:H	2.30	0.43
3:0:114:LEU:HD22	3:0:192:PRO:HB2	2.00	0.43
3:0:119:GLU:HA	3:0:122:LYS:NZ	2.34	0.43
4:6:233:LEU:HD23	4:6:234:ILE:N	2.34	0.43
7:7:386:LEU:HB3	7:7:513:LEU:HB3	2.00	0.43
7:7:407:VAL:HG22	7:7:484:PHE:HB2	2.01	0.43
7:7:411:CYS:SG	7:7:420:TRP:HD1	2.41	0.43
7:7:539:ASN:ND2	7:7:542:GLU:HB3	2.34	0.43
7:7:679:SER:H	7:7:682:GLN:HG3	1.83	0.43
9:O:193:LEU:HB3	9:O:206:ILE:HB	2.00	0.43
10:N:35:DG:C2'	10:N:36:DT:H71	2.49	0.43
12:A:455:MET:HE1	13:B:1138:MET:HG2	2.01	0.43
12:A:1161:THR:H	12:A:1167:GLU:CD	2.26	0.43
12:A:1230:GLU:HB2	12:A:1233:ASP:OD1	2.18	0.43
13:B:499:ASN:OD1	13:B:500:THR:N	2.51	0.43
13:B:894:ASP:N	13:B:898:LEU:O	2.39	0.43
13:B:1138:MET:SD	13:B:1143:ALA:HB3	2.59	0.43
14:C:22:LEU:HD12	14:C:22:LEU:HA	1.87	0.43
16:E:78:LEU:HD21	16:E:109:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:37:LYS:N	22:K:69:ALA:O	2.52	0.43
27:U:255:LYS:N	27:U:255:LYS:HD2	2.34	0.43
1:1:255:LYS:O	1:1:259:ILE:HG12	2.19	0.43
2:4:85:TYR:HB3	2:4:88:PRO:HD2	2.00	0.43
2:4:192:GLN:O	2:4:196:ILE:HG13	2.19	0.43
3:0:49:THR:HA	3:0:52:LEU:HD12	2.01	0.43
3:0:245:ILE:HG13	3:0:638:ARG:CZ	2.49	0.43
3:0:436:ARG:HD2	3:0:437:PHE:H	1.83	0.43
3:0:502:ASP:OD1	3:0:502:ASP:N	2.51	0.43
4:6:138:GLU:OE2	4:6:140:ASP:HB2	2.18	0.43
4:6:159:GLU:HA	4:6:162:ASP:HB3	2.00	0.43
4:6:336:CYS:SG	4:6:337:SER:N	2.92	0.43
6:5:25:ALA:HA	6:5:29:ASP:HB2	2.01	0.43
6:5:44:PRO:HA	6:5:47:VAL:HG23	2.01	0.43
7:7:363:ARG:HB2	7:7:548:HIS:CE1	2.54	0.43
7:7:464:ARG:NH2	7:7:466:ARG:HH12	2.15	0.43
8:3:43:VAL:HG22	8:3:47:PHE:HD2	1.84	0.43
9:O:106:ILE:HG13	9:O:109:PRO:O	2.19	0.43
9:O:185:TYR:HB2	9:O:193:LEU:HD12	2.00	0.43
12:A:549:MET:HE3	12:A:656:TRP:HB2	2.01	0.43
12:A:1127:ASP:HB2	12:A:1130:GLN:HB3	2.00	0.43
13:B:259:TYR:HD1	13:B:259:TYR:HA	1.72	0.43
13:B:1037:LEU:HB3	13:B:1062:HIS:HD2	1.84	0.43
13:B:1201:LYS:HZ2	13:B:1205:GLN:CD	2.27	0.43
16:E:124:VAL:O	16:E:126:SER:N	2.51	0.43
19:H:33:GLN:HB3	19:H:35:GLN:OE1	2.18	0.43
24:M:267:LYS:HG3	24:M:268:GLU:H	1.84	0.43
26:R:104:ILE:HG13	26:R:124:LEU:HD21	2.01	0.43
30:X:133:GLU:O	30:X:137:LYS:N	2.42	0.43
2:4:276:CYS:O	2:4:280:GLY:N	2.31	0.43
3:0:169:ASP:CG	3:0:170:TYR:H	2.27	0.43
3:0:314:GLN:HB2	3:0:317:LEU:HD22	2.01	0.43
3:0:327:ARG:HB3	3:0:330:HIS:CG	2.53	0.43
3:0:441:ASP:HB3	3:0:444:ILE:HG12	2.00	0.43
3:0:446:ILE:O	3:0:449:VAL:HG22	2.19	0.43
3:0:473:LEU:HB2	3:0:475:PHE:CD1	2.54	0.43
3:0:535:ASP:OD1	3:0:535:ASP:N	2.52	0.43
4:6:128:LEU:HD21	4:6:235:VAL:HG23	2.01	0.43
4:6:178:LEU:O	4:6:180:GLN:NE2	2.52	0.43
5:2:438:VAL:O	5:2:442:ARG:N	2.35	0.43
5:2:492:PHE:CG	6:5:9:LEU:HD23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:397:ILE:HG13	7:7:424:PHE:HE2	1.84	0.43
7:7:510:LYS:HB2	7:7:531:ILE:HG13	2.00	0.43
9:O:195:TYR:HD1	9:O:204:LEU:HD13	1.84	0.43
11:T:134:DT:H2"	11:T:135:DG:C8	2.54	0.43
12:A:143:LYS:HG3	12:A:144:THR:HG23	2.01	0.43
12:A:226:GLU:CD	12:A:226:GLU:H	2.26	0.43
12:A:579:SER:HB3	12:A:611:GLN:HA	2.01	0.43
12:A:592:ASP:N	12:A:595:THR:OG1	2.52	0.43
12:A:737:LEU:HD13	12:A:741:ASN:ND2	2.34	0.43
12:A:1155:ASP:OD2	12:A:1241:ARG:NH1	2.52	0.43
13:B:289:LEU:HA	13:B:289:LEU:HD23	1.79	0.43
15:D:47:LEU:HD21	18:G:3:PHE:CD2	2.54	0.43
16:E:50:MET:HE2	16:E:50:MET:HB2	1.86	0.43
18:G:83:LYS:HG3	18:G:150:CYS:SG	2.59	0.43
24:M:128:ALA:O	24:M:132:LYS:N	2.46	0.43
24:M:144:LYS:O	24:M:147:LYS:HB3	2.19	0.43
24:M:279:VAL:HG21	24:M:304:VAL:HG21	2.01	0.43
1:1:580:LYS:HA	1:1:583:TYR:HD2	1.84	0.42
2:4:123:GLU:HA	2:4:126:VAL:HB	2.01	0.42
3:0:318:THR:HG23	3:0:376:PHE:CE1	2.54	0.42
3:0:396:PHE:O	3:0:400:LYS:NZ	2.52	0.42
3:0:643:ARG:HG2	3:0:649:ARG:HA	2.01	0.42
4:6:138:GLU:CD	4:6:140:ASP:HB2	2.44	0.42
4:6:233:LEU:HA	4:6:262:LYS:O	2.18	0.42
5:2:154:PRO:HD2	5:2:355:LEU:HD23	2.01	0.42
5:2:370:PHE:HB2	5:2:373:MET:N	2.25	0.42
7:7:558:TRP:O	7:7:737:THR:OG1	2.29	0.42
12:A:707:GLY:HA2	12:A:1281:ARG:HD2	2.01	0.42
12:A:1452:LYS:H	12:A:1452:LYS:HG2	1.63	0.42
13:B:86:ARG:HG3	13:B:138:GLU:HG2	2.00	0.42
13:B:1076:HIS:O	14:C:31:ASN:ND2	2.50	0.42
16:E:64:PRO:HB3	16:E:75:MET:HE2	2.01	0.42
20:I:72:ASP:OD1	20:I:72:ASP:N	2.51	0.42
24:M:157:CYS:O	24:M:159:ASP:N	2.52	0.42
26:R:108:LEU:HD11	26:R:120:TYR:HB2	2.01	0.42
26:R:277:PHE:N	26:R:279:LYS:HE2	2.23	0.42
3:0:11:LEU:HG	3:0:96:GLU:OE1	2.19	0.42
3:0:135:ARG:HH21	3:0:393:VAL:HG23	1.85	0.42
4:6:350:PRO:HD2	4:6:370:LEU:HD22	2.01	0.42
7:7:625:PRO:HD2	7:7:649:ILE:HG23	2.00	0.42
9:O:95:ASN:HB3	9:O:98:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:88:LYS:HZ2	12:A:205:GLU:H	1.68	0.42
12:A:815:PHE:HA	12:A:818:MET:HE2	2.01	0.42
12:A:956:LEU:HD23	12:A:956:LEU:HA	1.88	0.42
12:A:1435:PRO:HA	12:A:1439:GLY:O	2.19	0.42
13:B:209:GLU:OE1	13:B:485:ARG:NE	2.52	0.42
15:D:144:THR:HG21	18:G:46:LEU:HD21	2.01	0.42
18:G:116:PRO:HD2	18:G:163:ILE:HG13	2.01	0.42
24:M:258:TYR:O	24:M:262:LYS:HG2	2.19	0.42
25:Q:98:TYR:HB2	26:R:96:ARG:HA	2.01	0.42
29:W:148:LEU:HD23	29:W:148:LEU:HA	1.89	0.42
1:1:195:PHE:CZ	1:1:199:VAL:HG21	2.54	0.42
3:0:69:ILE:C	3:0:70:ILE:HD12	2.44	0.42
3:0:162:LEU:O	3:0:167:VAL:N	2.46	0.42
3:0:280:GLN:CD	3:0:280:GLN:H	2.27	0.42
3:0:336:LYS:O	3:0:340:GLU:HG2	2.20	0.42
3:0:539:VAL:HG22	3:0:599:LEU:HA	2.01	0.42
4:6:148:MET:HE2	4:6:148:MET:HB3	1.88	0.42
4:6:211:GLN:HE22	4:6:246:ASP:C	2.28	0.42
4:6:404:PHE:HB3	4:6:435:GLU:O	2.20	0.42
5:2:56:GLU:CD	5:2:97:MET:HB3	2.45	0.42
5:2:247:ARG:O	5:2:251:GLN:N	2.36	0.42
5:2:433:LEU:HA	5:2:433:LEU:HD23	1.82	0.42
5:2:499:SER:HA	5:2:502:LEU:HD12	2.01	0.42
7:7:488:ASP:O	7:7:489:GLU:HG3	2.20	0.42
7:7:569:TYR:HA	7:7:577:ARG:NE	2.34	0.42
7:7:577:ARG:HG2	7:7:580:LEU:CB	2.49	0.42
10:N:9:DA:C1'	10:N:10:DA:H5'	2.46	0.42
10:N:28:DT:H1'	10:N:29:DT:H5'	2.01	0.42
12:A:29:ALA:HB1	13:B:1184:GLY:HA2	2.02	0.42
12:A:317:LYS:HB2	12:A:317:LYS:HE3	1.76	0.42
12:A:573:SER:O	12:A:576:GLN:HG3	2.18	0.42
13:B:639:ILE:HG12	13:B:691:GLU:HB2	2.01	0.42
13:B:773:MET:HB2	13:B:773:MET:HE3	1.82	0.42
13:B:1046:PRO:HB2	13:B:1047:PHE:CD1	2.54	0.42
14:C:6:PRO:HB3	14:C:25:VAL:HB	2.01	0.42
14:C:148:ARG:N	14:C:151:GLN:OE1	2.33	0.42
15:D:125:SER:O	15:D:129:LEU:N	2.44	0.42
18:G:2:PHE:CE1	18:G:79:PHE:HB2	2.54	0.42
18:G:38:CYS:C	18:G:155:SER:HA	2.44	0.42
19:H:91:ASP:OD1	19:H:91:ASP:N	2.52	0.42
21:J:17:LYS:HG3	21:J:39:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:129:ALA:O	24:M:133:ILE:HG12	2.19	0.42
25:Q:120:LYS:HE3	26:R:132:GLU:HB3	1.99	0.42
26:R:73:LEU:HD23	26:R:77:LEU:HD13	2.01	0.42
27:U:247:LEU:HD13	28:V:118:SER:HB3	2.01	0.42
27:U:269:ILE:HD13	28:V:108:VAL:HG11	2.01	0.42
1:1:221:ALA:O	1:1:225:SER:OG	2.36	0.42
3:0:74:ARG:NH2	3:0:236:GLU:HB3	2.31	0.42
3:0:83:LEU:HD21	3:0:107:GLY:N	2.35	0.42
3:0:516:PRO:HA	3:0:520:ARG:H	1.84	0.42
7:7:364:PRO:HD3	7:7:695:ARG:HD3	2.01	0.42
7:7:369:SER:O	7:7:372:LYS:HB2	2.19	0.42
7:7:723:GLN:HB2	7:7:733:PHE:CZ	2.54	0.42
10:N:6:DA:H2"	10:N:7:DA:H8	1.83	0.42
12:A:150:THR:HA	12:A:166:GLY:HA2	2.01	0.42
12:A:208:LEU:O	12:A:212:LYS:HG3	2.19	0.42
13:B:190:TYR:HD1	21:J:63:TYR:HE1	1.67	0.42
13:B:195:CYS:SG	13:B:197:PHE:HB2	2.59	0.42
13:B:703:ILE:HA	13:B:740:HIS:O	2.20	0.42
13:B:864:LYS:HG3	13:B:872:GLU:OE1	2.20	0.42
13:B:1204:PHE:CE2	13:B:1216:LEU:HD11	2.55	0.42
14:C:61:GLU:O	14:C:65:HIS:N	2.37	0.42
15:D:163:VAL:O	15:D:167:LEU:N	2.38	0.42
15:D:189:ASP:OD1	18:G:167:TYR:OH	2.28	0.42
20:I:78:CYS:SG	20:I:80:SER:OG	2.59	0.42
28:V:61:THR:HB	28:V:86:THR:HB	2.00	0.42
28:V:81:LYS:HA	28:V:109:ASP:O	2.19	0.42
29:W:144:ARG:HH12	29:W:146:GLU:HB2	1.84	0.42
29:W:183:ILE:O	29:W:187:LYS:N	2.37	0.42
1:1:205:PRO:HA	1:1:206:PRO:HD3	1.93	0.42
2:4:138:LYS:O	2:4:142:GLN:N	2.52	0.42
3:0:226:VAL:O	3:0:230:SER:OG	2.19	0.42
3:0:374:LEU:HB3	3:0:410:SER:HG	1.84	0.42
4:6:143:PRO:HB2	4:6:147:ALA:HB3	2.01	0.42
5:2:416:LEU:HA	5:2:432:VAL:HG21	2.00	0.42
9:O:70:ILE:O	9:O:124:THR:HA	2.19	0.42
12:A:290:GLU:O	12:A:294:SER:N	2.39	0.42
13:B:128:LEU:N	13:B:168:GLY:O	2.43	0.42
17:F:79:ARG:HB3	17:F:146:TRP:CZ2	2.55	0.42
17:F:113:GLY:O	17:F:115:THR:HG23	2.19	0.42
18:G:57:GLN:HG2	18:G:58:ARG:N	2.34	0.42
24:M:187:ARG:NH1	24:M:241:ARG:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:129:PRO:HG2	25:Q:132:ASP:CG	2.45	0.42
26:R:314:SER:O	26:R:318:LEU:N	2.42	0.42
29:W:95:ILE:HD12	29:W:193:ARG:HH11	1.84	0.42
3:0:117:HIS:HE1	3:0:119:GLU:HB3	1.83	0.42
3:0:541:PHE:HA	3:0:623:ILE:HB	2.02	0.42
3:0:722:ARG:O	3:0:726:GLN:N	2.50	0.42
5:2:370:PHE:CE1	5:2:375:LEU:HB2	2.54	0.42
7:7:325:VAL:HG13	7:7:328:LYS:HD2	2.01	0.42
7:7:757:ARG:NH1	7:7:758:GLU:HA	2.33	0.42
9:O:161:VAL:HG13	9:O:215:THR:HB	2.02	0.42
12:A:1208:THR:HG22	12:A:1211:GLN:CD	2.44	0.42
12:A:1445:ILE:HG22	18:G:59:GLY:O	2.19	0.42
13:B:46:GLN:NE2	13:B:47:GLN:HG2	2.34	0.42
13:B:247:GLY:C	13:B:249:ARG:H	2.28	0.42
13:B:564:GLU:N	13:B:589:VAL:O	2.53	0.42
13:B:766:ARG:HD3	13:B:766:ARG:HA	1.73	0.42
13:B:1000:PRO:HB2	13:B:1072:MET:HE2	2.01	0.42
19:H:96:VAL:HG22	19:H:143:LEU:HG	2.00	0.42
22:K:6:ARG:O	22:K:9:LEU:HB2	2.19	0.42
30:X:272:ALA:C	30:X:275:PRO:HD2	2.44	0.42
1:1:546:LEU:O	1:1:550:CYS:N	2.40	0.42
2:4:30:ILE:HD13	2:4:179:LEU:HB2	2.02	0.42
3:0:133:CYS:HA	3:0:136:MET:HB3	2.00	0.42
3:0:245:ILE:HD11	3:0:441:ASP:C	2.45	0.42
3:0:402:ILE:O	3:0:406:ALA:N	2.36	0.42
3:0:442:ALA:O	3:0:446:ILE:HG12	2.20	0.42
3:0:671:ARG:N	3:0:675:ASP:OD2	2.53	0.42
5:2:36:TYR:HD2	5:2:37:ARG:HD3	1.85	0.42
5:2:71:LYS:HD2	5:2:72:LEU:N	2.35	0.42
5:2:75:GLN:HA	5:2:78:ILE:HG12	2.01	0.42
7:7:635:GLU:O	7:7:639:ILE:HG13	2.19	0.42
8:3:69:LYS:HB2	8:3:71:GLN:HE22	1.84	0.42
9:O:70:ILE:N	9:O:126:ALA:O	2.51	0.42
12:A:1139:GLU:O	12:A:1275:GLY:HA3	2.19	0.42
13:B:102:VAL:HG13	13:B:110:HIS:CD2	2.55	0.42
13:B:541:LEU:HD23	13:B:541:LEU:HA	1.83	0.42
13:B:649:LYS:HZ2	13:B:736:THR:HA	1.85	0.42
13:B:901:PRO:HD2	23:L:60:ARG:HA	2.02	0.42
14:C:59:ALA:HB3	14:C:62:PHE:HB2	2.01	0.42
16:E:124:VAL:HG13	16:E:132:ILE:HB	2.02	0.42
19:H:10:PHE:CG	19:H:28:ALA:HB1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:103:LEU:HB2	26:R:92:LEU:HD22	2.01	0.42
25:Q:118:LEU:HB3	25:Q:392:VAL:HG23	2.02	0.42
1:1:192:MET:HE2	1:1:192:MET:HB2	1.93	0.42
1:1:344:UNK:C	1:1:347:PRO:HD2	2.49	0.42
1:1:511:ALA:HB2	2:4:264:LYS:HD2	2.02	0.42
2:4:71:ASN:OD1	2:4:71:ASN:N	2.41	0.42
2:4:273:ARG:HB2	4:6:324:PHE:CE1	2.55	0.42
3:0:134:ARG:HH22	3:0:304:GLU:C	2.28	0.42
5:2:276:LEU:HG	5:2:280:SER:OG	2.20	0.42
5:2:350:TYR:O	5:2:372:ASN:HB2	2.20	0.42
5:2:350:TYR:N	5:2:407:GLN:OE1	2.47	0.42
7:7:399:ALA:O	7:7:402:THR:HB	2.20	0.42
7:7:612:VAL:HG13	7:7:613:TYR:H	1.84	0.42
10:N:15:DG:H2"	10:N:16:DC:H6	1.85	0.42
12:A:492:PRO:O	12:A:493:GLN:NE2	2.53	0.42
12:A:519:PRO:O	12:A:624:SER:HB2	2.20	0.42
12:A:565:ILE:O	12:A:570:PRO:HA	2.19	0.42
12:A:601:LYS:HB3	12:A:603:ASN:OD1	2.20	0.42
12:A:851:HIS:C	12:A:853:ASP:H	2.28	0.42
13:B:71:LEU:HD12	13:B:71:LEU:HA	1.85	0.42
13:B:329:THR:O	13:B:333:PHE:HB3	2.20	0.42
13:B:365:THR:HG23	13:B:374:LYS:HE2	2.00	0.42
13:B:685:LEU:HD23	13:B:690:VAL:HG13	2.00	0.42
13:B:840:ILE:HB	13:B:1011:ILE:HB	2.02	0.42
13:B:876:LYS:O	13:B:878:GLN:NE2	2.52	0.42
19:H:35:GLN:NE2	19:H:128:ASN:HD22	2.18	0.42
19:H:77:ARG:HD3	19:H:77:ARG:HA	1.88	0.42
25:Q:342:LEU:O	25:Q:346:GLU:HG3	2.20	0.42
29:W:12:LEU:HB2	29:W:185:SER:HB2	2.02	0.42
29:W:23:GLY:O	29:W:26:VAL:HG12	2.19	0.42
2:4:123:GLU:O	2:4:127:GLU:HG2	2.20	0.42
2:4:218:SER:HA	2:4:237:HIS:CD2	2.54	0.42
3:0:79:ILE:HG23	3:0:207:ILE:HB	2.02	0.42
3:0:408:LEU:HD22	3:0:412:TYR:HE2	1.85	0.42
3:0:495:MET:HE1	3:0:717:THR:HB	2.01	0.42
3:0:510:PHE:CG	3:0:511:GLU:N	2.88	0.42
4:6:269:GLN:HG3	4:6:288:TYR:HE2	1.85	0.42
5:2:414:GLU:OE2	7:7:169:HIS:N	2.52	0.42
7:7:715:GLU:O	7:7:719:SER:OG	2.37	0.42
8:3:134:ARG:O	8:3:138:GLU:N	2.38	0.42
12:A:983:ILE:H	12:A:983:ILE:HG12	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1195:LEU:HD11	12:A:1238:ILE:HD12	2.01	0.42
12:A:1390:ASN:O	12:A:1399:ARG:HD2	2.19	0.42
13:B:190:TYR:HD1	21:J:63:TYR:CE1	2.38	0.42
16:E:23:VAL:HG22	16:E:28:TYR:HB2	2.01	0.42
16:E:39:LEU:O	16:E:43:LYS:HG3	2.20	0.42
24:M:252:VAL:O	24:M:255:SER:OG	2.31	0.42
26:R:134:VAL:O	26:R:215:VAL:N	2.42	0.42
1:1:184:LEU:HD13	1:1:220:PHE:CD1	2.55	0.42
3:0:28:ILE:HD11	3:0:56:THR:HG23	2.02	0.42
3:0:244:CYS:SG	3:0:446:ILE:HD11	2.59	0.42
3:0:257:LEU:O	3:0:261:THR:HG23	2.20	0.42
4:6:155:ASP:HA	4:6:158:HIS:CE1	2.54	0.42
4:6:209:SER:OG	4:6:242:THR:O	2.38	0.42
5:2:450:ARG:NH2	6:5:58:LEU:HB2	2.35	0.42
5:2:481:LEU:HD23	5:2:481:LEU:HA	1.89	0.42
6:5:6:LYS:H	6:5:6:LYS:HG3	1.52	0.42
7:7:437:VAL:HG13	7:7:454:VAL:HG13	2.02	0.42
7:7:646:ASN:ND2	7:7:648:GLN:OE1	2.48	0.42
9:O:109:PRO:HB2	9:O:111:THR:HG23	2.02	0.42
12:A:16:GLU:HG2	12:A:1418:LEU:HD11	2.02	0.42
12:A:1364:ASN:HD21	12:A:1366:ARG:HD2	1.85	0.42
13:B:304:ASP:OD1	13:B:306:ASN:N	2.53	0.42
14:C:183:TRP:CD2	14:C:213:PRO:HD3	2.55	0.42
24:M:124:ASN:O	24:M:127:GLN:HG2	2.20	0.42
24:M:206:THR:O	24:M:209:ILE:HG12	2.19	0.42
25:Q:134:HIS:CD2	25:Q:135:LEU:H	2.38	0.42
27:U:257:ARG:HE	27:U:257:ARG:HB3	1.58	0.42
2:4:210:ILE:O	2:4:233:GLY:HA3	2.20	0.41
3:0:467:ASP:C	3:0:470:PRO:HD2	2.45	0.41
3:0:586:TYR:CE1	3:0:598:LEU:HB2	2.55	0.41
5:2:243:SER:O	5:2:247:ARG:N	2.42	0.41
5:2:249:MET:O	5:2:253:MET:N	2.33	0.41
5:2:347:ILE:HG22	5:2:373:MET:HE1	2.01	0.41
5:2:370:PHE:N	5:2:370:PHE:CD1	2.88	0.41
7:7:310:ILE:HG12	7:7:338:LEU:HB3	2.02	0.41
7:7:383:ILE:HG13	7:7:528:ASN:CA	2.50	0.41
7:7:410:LEU:HD13	7:7:485:ILE:HG23	2.02	0.41
7:7:493:VAL:HG12	7:7:494:PRO:HD2	2.02	0.41
9:O:73:THR:HG23	9:O:158:GLN:HG3	2.01	0.41
12:A:66:LYS:HG3	12:A:72:GLU:HA	2.02	0.41
12:A:150:THR:O	12:A:164:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:914:GLU:OE1	12:A:978:PRO:HB2	2.20	0.41
12:A:1116:LEU:N	12:A:1308:THR:O	2.53	0.41
14:C:35:ARG:HH21	22:K:41:THR:H	1.66	0.41
14:C:112:ASN:ND2	21:J:19:GLU:OE2	2.53	0.41
16:E:177:ARG:O	16:E:212:ARG:NH1	2.53	0.41
19:H:111:LEU:HD22	19:H:111:LEU:H	1.85	0.41
19:H:134:ASN:OD1	19:H:134:ASN:N	2.36	0.41
19:H:142:LEU:C	19:H:143:LEU:HD12	2.44	0.41
25:Q:103:LEU:HD12	26:R:92:LEU:HA	2.01	0.41
26:R:124:LEU:HD13	26:R:127:LYS:HE3	2.00	0.41
27:U:244:MET:HB2	28:V:113:ILE:HA	2.02	0.41
27:U:263:LYS:HG3	27:U:277:GLN:O	2.20	0.41
29:W:65:ARG:HH11	29:W:93:HIS:CG	2.37	0.41
2:4:161:ASN:HA	2:4:164:SER:HB3	2.01	0.41
3:0:312:LEU:O	3:0:314:GLN:N	2.52	0.41
3:0:347:LYS:HE2	3:0:347:LYS:HB2	1.86	0.41
3:0:372:LYS:HE2	3:0:376:PHE:CZ	2.55	0.41
4:6:264:LEU:HD22	4:6:300:LEU:HD13	2.01	0.41
5:2:141:ASN:O	5:2:145:THR:N	2.36	0.41
5:2:408:MET:HG3	5:2:411:LEU:HB3	2.02	0.41
7:7:467:SER:O	7:7:471:GLN:NE2	2.52	0.41
7:7:472:LYS:O	7:7:476:PHE:N	2.44	0.41
7:7:476:PHE:CE1	7:7:480:ARG:HB2	2.55	0.41
7:7:526:ASP:HB2	7:7:529:PHE:CD2	2.56	0.41
7:7:723:GLN:O	7:7:726:LEU:HB2	2.20	0.41
8:3:43:VAL:HG22	8:3:47:PHE:CD2	2.54	0.41
12:A:412:ARG:O	24:M:51:VAL:HG12	2.20	0.41
12:A:417:TYR:CE2	24:M:35:VAL:HG21	2.52	0.41
12:A:445:ASN:OD1	12:A:446:ARG:N	2.53	0.41
12:A:1157:ASP:CG	12:A:1160:SER:H	2.28	0.41
12:A:1364:ASN:ND2	12:A:1366:ARG:HD2	2.35	0.41
13:B:199:MET:HE2	13:B:492:LEU:HD21	2.00	0.41
13:B:269:ILE:O	13:B:282:ILE:HG23	2.20	0.41
13:B:451:LYS:HA	13:B:451:LYS:HD2	1.85	0.41
13:B:637:LEU:HD23	13:B:637:LEU:HA	1.78	0.41
13:B:1167:GLY:O	13:B:1215:ARG:HA	2.20	0.41
15:D:47:LEU:HD21	18:G:3:PHE:CE2	2.55	0.41
16:E:108:GLY:O	16:E:132:ILE:HA	2.20	0.41
19:H:130:ARG:H	19:H:130:ARG:HD2	1.85	0.41
20:I:93:LYS:HE2	20:I:93:LYS:HB3	1.86	0.41
22:K:77:THR:HG23	22:K:83:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:126:ILE:H	29:W:126:ILE:HD12	1.85	0.41
30:X:259:PHE:O	30:X:262:MET:HG2	2.20	0.41
1:1:263:TYR:HB2	1:1:266:VAL:HG12	2.01	0.41
3:0:48:LYS:HE3	3:0:48:LYS:HB3	1.95	0.41
3:0:77:SER:HA	3:0:80:GLU:CD	2.45	0.41
3:0:421:GLU:HB2	3:0:434:ILE:HG12	2.02	0.41
4:6:362:VAL:HG13	4:6:368:LEU:C	2.45	0.41
5:2:346:LYS:HE2	5:2:377:GLN:HB2	2.01	0.41
5:2:431:GLN:CD	5:2:435:PRO:HD2	2.45	0.41
7:7:363:ARG:HD3	7:7:548:HIS:CD2	2.54	0.41
7:7:374:PHE:HA	7:7:379:ALA:HA	2.01	0.41
10:N:13:DG:C4	10:N:14:DC:C4	3.08	0.41
12:A:170:THR:HG23	12:A:185:TRP:HD1	1.85	0.41
12:A:353:ILE:HG21	12:A:487:MET:SD	2.61	0.41
12:A:592:ASP:C	12:A:595:THR:HG1	2.27	0.41
12:A:1020:CYS:N	12:A:1023:ARG:HH21	2.19	0.41
13:B:60:GLN:OE1	13:B:95:ILE:HG22	2.21	0.41
13:B:345:LYS:HD3	13:B:348:ARG:NH1	2.36	0.41
13:B:837:ASP:N	13:B:837:ASP:OD1	2.53	0.41
20:I:17:ARG:O	20:I:25:LEU:HD12	2.20	0.41
24:M:185:VAL:HG12	24:M:186:ALA:H	1.85	0.41
26:R:63:ARG:HE	26:R:63:ARG:HB2	1.52	0.41
1:1:270:TYR:HE2	1:1:284:TRP:HE1	1.69	0.41
2:4:259:ARG:N	2:4:260:PRO:HD3	2.36	0.41
2:4:287:PHE:CE1	4:6:321:LYS:HB2	2.54	0.41
3:0:117:HIS:ND1	3:0:120:VAL:HG23	2.35	0.41
3:0:156:CYS:O	3:0:157:GLU:HB3	2.19	0.41
3:0:555:GLN:HA	3:0:560:LEU:HD22	2.02	0.41
3:0:651:ASN:OD1	3:0:651:ASN:N	2.52	0.41
5:2:450:ARG:HH21	6:5:58:LEU:HB2	1.84	0.41
7:7:389:GLY:HA3	7:7:689:ARG:O	2.20	0.41
7:7:676:HIS:HD2	7:7:714:GLN:HE22	1.67	0.41
10:N:40:DG:H2"	10:N:41:DA:N7	2.35	0.41
12:A:434:ARG:NH1	12:A:440:ASP:OD2	2.42	0.41
12:A:1027:ALA:O	12:A:1031:VAL:HG23	2.20	0.41
12:A:1194:ARG:HE	12:A:1237:ILE:HD12	1.84	0.41
13:B:106:ASP:OD1	13:B:108:VAL:HG12	2.20	0.41
13:B:343:ILE:C	13:B:348:ARG:HH12	2.28	0.41
13:B:614:SER:OG	13:B:697:GLU:OE1	2.20	0.41
13:B:649:LYS:HZ3	13:B:736:THR:HG23	1.85	0.41
18:G:116:PRO:HD3	18:G:164:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:89:LEU:HB3	19:H:143:LEU:HD21	2.02	0.41
20:I:61:ASP:O	20:I:64:SER:OG	2.37	0.41
1:1:235:UNK:O	1:1:239:PRO:HD2	2.20	0.41
2:4:65:LEU:O	5:2:37:ARG:NH2	2.53	0.41
2:4:275:SER:HB2	2:4:281:ARG:C	2.45	0.41
3:0:48:LYS:O	3:0:52:LEU:N	2.42	0.41
3:0:140:GLN:O	3:0:144:LYS:HG3	2.20	0.41
4:6:374:THR:O	4:6:378:ARG:HG2	2.20	0.41
12:A:149:GLU:O	12:A:166:GLY:HA2	2.20	0.41
12:A:450:LEU:HD12	12:A:451:HIS:HD2	1.85	0.41
12:A:576:GLN:HG3	12:A:576:GLN:H	1.57	0.41
12:A:687:LYS:HE2	12:A:794:PRO:HG2	2.03	0.41
13:B:570:VAL:HB	13:B:573:GLN:OE1	2.20	0.41
13:B:1038:SER:O	21:J:33:GLY:HA3	2.20	0.41
16:E:41:ASP:HA	16:E:44:ALA:HB3	2.02	0.41
19:H:83:GLN:HA	22:K:54:ARG:NH1	2.34	0.41
25:Q:121:PHE:HB2	26:R:131:ASN:HB3	2.02	0.41
25:Q:378:VAL:HA	25:Q:384:PHE:HD1	1.85	0.41
29:W:147:PHE:HB2	29:W:156:LEU:HB2	2.02	0.41
1:1:596:LEU:O	1:1:600:VAL:N	2.38	0.41
2:4:177:LEU:HD12	2:4:211:ASP:O	2.20	0.41
3:0:77:SER:O	3:0:80:GLU:HG2	2.21	0.41
3:0:117:HIS:CD2	3:0:156:CYS:HA	2.55	0.41
3:0:307:VAL:H	3:0:382:SER:HB3	1.86	0.41
3:0:609:GLY:N	3:0:668:ARG:HH12	2.19	0.41
3:0:633:ARG:HB2	3:0:636:LYS:HB2	2.02	0.41
4:6:138:GLU:OE2	4:6:145:ARG:NH2	2.51	0.41
4:6:362:VAL:HA	4:6:369:MET:HA	2.02	0.41
5:2:276:LEU:O	5:2:280:SER:N	2.53	0.41
7:7:302:GLU:HG3	7:7:322:SER:N	2.36	0.41
7:7:440:SER:HA	7:7:470:SER:H	1.85	0.41
7:7:489:GLU:OE1	7:7:491:HIS:HE1	2.04	0.41
7:7:519:ARG:CG	7:7:522:ASP:HB2	2.51	0.41
8:3:131:GLU:O	8:3:135:THR:N	2.37	0.41
12:A:134:ARG:HH12	12:A:221:SER:HA	1.85	0.41
12:A:230:ARG:HB2	12:A:233:TRP:CE2	2.56	0.41
12:A:412:ARG:HB3	24:M:51:VAL:HG11	2.03	0.41
13:B:357:GLN:NE2	13:B:358:LYS:HG3	2.35	0.41
24:M:294:THR:O	24:M:296:ALA:N	2.54	0.41
25:Q:123:SER:HB3	25:Q:361:TRP:CH2	2.54	0.41
26:R:261:VAL:O	26:R:264:SER:OG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:244:MET:HE2	28:V:111:LEU:HD22	2.03	0.41
1:1:375:LEU:HD21	3:0:551:VAL:HG11	2.03	0.41
2:4:32:ILE:HG12	2:4:77:ALA:HB1	2.02	0.41
2:4:160:VAL:O	2:4:164:SER:N	2.34	0.41
3:0:537:MET:N	3:0:586:TYR:OH	2.52	0.41
4:6:196:LEU:HA	4:6:199:ILE:HB	2.02	0.41
4:6:274:LYS:HD2	4:6:285:GLU:HG2	2.02	0.41
5:2:10:VAL:O	5:2:14:LEU:HD13	2.20	0.41
7:7:373:MET:HE2	7:7:382:GLY:H	1.86	0.41
9:O:139:TYR:O	9:O:143:ILE:HG12	2.20	0.41
12:A:943:LEU:HD23	12:A:943:LEU:HA	1.85	0.41
12:A:1111:MET:HE2	12:A:1111:MET:HB3	1.86	0.41
12:A:1373:ASP:O	12:A:1377:THR:HG23	2.21	0.41
13:B:737:THR:OG1	13:B:737:THR:O	2.38	0.41
13:B:830:TYR:CZ	13:B:1000:PRO:HD3	2.56	0.41
21:J:44:TYR:HA	21:J:47:ARG:CB	2.51	0.41
24:M:30:TYR:CG	24:M:31:PRO:HD2	2.56	0.41
24:M:185:VAL:HA	24:M:237:THR:HG21	2.02	0.41
25:Q:138:ARG:HG2	26:R:58:ASP:N	2.36	0.41
29:W:74:GLU:H	29:W:83:GLU:HA	1.86	0.41
29:W:134:LEU:HD23	29:W:134:LEU:HA	1.86	0.41
2:4:212:VAL:O	2:4:235:TYR:HA	2.21	0.41
3:0:140:GLN:HG2	3:0:143:ARG:HE	1.86	0.41
3:0:498:THR:O	3:0:506:ILE:HG12	2.20	0.41
3:0:704:ALA:O	3:0:708:LEU:HD21	2.21	0.41
4:6:198:SER:O	4:6:202:GLN:N	2.53	0.41
4:6:281:ASN:O	4:6:284:ASP:N	2.42	0.41
4:6:451:CYS:HB3	4:6:454:CYS:HB2	2.02	0.41
5:2:87:LEU:HD23	5:2:87:LEU:H	1.85	0.41
7:7:439:THR:HB	7:7:442:ASN:H	1.86	0.41
7:7:576:LYS:HE2	7:7:766:LYS:C	2.46	0.41
12:A:532:ARG:HD3	12:A:749:ALA:HB2	2.02	0.41
13:B:799:PRO:CB	13:B:818:PRO:HG2	2.51	0.41
14:C:241:ASP:HB3	22:K:109:TRP:CE2	2.55	0.41
16:E:39:LEU:O	16:E:42:PHE:HB3	2.21	0.41
16:E:46:TYR:CE2	16:E:58:MET:HA	2.56	0.41
16:E:46:TYR:CD2	16:E:58:MET:HG2	2.56	0.41
16:E:178:ILE:HG23	16:E:214:CYS:HA	2.03	0.41
21:J:43:ARG:NE	21:J:45:CYS:SG	2.89	0.41
22:K:13:GLY:H	22:K:37:LYS:NZ	2.19	0.41
24:M:126:VAL:HG22	24:M:154:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:94:LYS:HE2	26:R:94:LYS:HB2	1.95	0.41
1:1:171:LYS:HA	1:1:214:ILE:HD12	2.02	0.41
2:4:293:LEU:HG	4:6:380:TYR:HE1	1.85	0.41
2:4:303:ASN:HB2	2:4:311:GLN:HG2	2.02	0.41
3:0:101:GLU:HG3	3:0:173:LYS:HZ1	1.86	0.41
3:0:106:LEU:HD22	3:0:176:PHE:HB2	2.02	0.41
3:0:111:ARG:HG3	3:0:193:TYR:CG	2.55	0.41
3:0:158:TYR:HA	3:0:161:ASN:ND2	2.36	0.41
3:0:210:TYR:HE1	3:0:234:PHE:CD1	2.39	0.41
3:0:239:ASN:HA	3:0:242:ASN:HD21	1.86	0.41
3:0:264:ALA:HB1	3:0:336:LYS:HE2	2.03	0.41
4:6:116:THR:N	4:6:117:PRO:HD3	2.35	0.41
4:6:120:ARG:HB3	4:6:309:PRO:HD3	2.03	0.41
4:6:211:GLN:HB2	4:6:243:ASP:CG	2.46	0.41
5:2:349:SER:OG	5:2:374:VAL:HG23	2.21	0.41
5:2:366:LEU:HD13	5:2:374:VAL:HG12	2.01	0.41
6:5:5:ARG:NH1	6:5:33:GLU:OE2	2.44	0.41
6:5:14:PRO:HA	6:5:17:LYS:HD2	2.02	0.41
7:7:230:ASN:O	7:7:345:ASN:HB3	2.21	0.41
7:7:366:GLN:CG	7:7:548:HIS:HE1	2.32	0.41
7:7:421:ARG:NH2	7:7:432:PRO:HG3	2.34	0.41
7:7:497:MET:HE2	7:7:497:MET:HB2	1.87	0.41
7:7:530:LEU:HD13	7:7:530:LEU:HA	1.97	0.41
7:7:668:THR:HG23	7:7:702:ASN:C	2.46	0.41
7:7:679:SER:H	7:7:682:GLN:CG	2.34	0.41
9:O:73:THR:HG22	9:O:122:VAL:HG22	2.02	0.41
10:N:11:DA:C4	10:N:12:DG:C5	3.09	0.41
12:A:416:ARG:HG3	12:A:417:TYR:CD1	2.56	0.41
12:A:1340:GLY:HA2	16:E:183:PRO:HD2	2.03	0.41
12:A:1363:VAL:HB	12:A:1368:MET:HE2	2.03	0.41
12:A:1408:ILE:HD13	12:A:1408:ILE:HA	1.88	0.41
13:B:276:ILE:HA	13:B:338:GLY:HA3	2.02	0.41
13:B:328:GLU:OE1	13:B:328:GLU:N	2.33	0.41
13:B:435:THR:O	13:B:439:ALA:N	2.53	0.41
13:B:603:LEU:O	13:B:608:ASP:N	2.54	0.41
13:B:773:MET:SD	13:B:987:LYS:HB3	2.60	0.41
13:B:1174:LYS:HB2	13:B:1179:GLN:HB2	2.02	0.41
13:B:1175:LEU:HA	13:B:1178:ASN:HA	2.03	0.41
15:D:209:ARG:HE	15:D:210:ILE:HG12	1.86	0.41
18:G:22:MET:O	18:G:26:LEU:N	2.42	0.41
18:G:38:CYS:HA	18:G:44:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:115:MET:HE3	18:G:119:LEU:HD23	2.03	0.41
18:G:151:ILE:HD13	18:G:151:ILE:HA	1.95	0.41
20:I:10:CYS:SG	20:I:32:CYS:HB3	2.61	0.41
21:J:20:SER:O	21:J:24:LEU:HG	2.21	0.41
22:K:10:PHE:HA	22:K:37:LYS:HB3	2.01	0.41
22:K:60:ALA:O	22:K:73:LEU:HD12	2.21	0.41
25:Q:110:ASP:HB2	25:Q:114:MET:HE3	2.02	0.41
27:U:252:THR:HG23	27:U:257:ARG:HH12	1.86	0.41
27:U:254:THR:O	27:U:256:ALA:N	2.54	0.41
27:U:257:ARG:HG2	27:U:283:ALA:O	2.21	0.41
29:W:56:PRO:HA	29:W:59:ALA:HB3	2.03	0.41
29:W:67:ILE:HA	29:W:89:VAL:HA	2.03	0.41
1:1:280:GLU:HB3	1:1:284:TRP:CD2	2.56	0.41
3:0:2:LYS:HA	3:0:10:VAL:O	2.19	0.41
3:0:69:ILE:HG23	3:0:231:ILE:HG23	2.03	0.41
3:0:584:GLU:O	3:0:588:LYS:N	2.39	0.41
4:6:278:LYS:N	4:6:285:GLU:OE1	2.54	0.41
4:6:299:GLU:HA	4:6:302:ASN:OD1	2.20	0.41
4:6:326:THR:HG23	4:6:348:PHE:HB2	2.03	0.41
4:6:338:CYS:HB3	4:6:364:PRO:HG3	2.02	0.41
5:2:39:LEU:HB3	5:2:43:ALA:HB3	2.02	0.41
6:5:30:ILE:H	6:5:30:ILE:HG12	1.60	0.41
7:7:401:CYS:O	7:7:404:LYS:HD3	2.20	0.41
7:7:596:GLN:HG3	7:7:600:ARG:NH2	2.35	0.41
8:3:39:CYS:O	8:3:43:VAL:HG12	2.21	0.41
9:O:91:ASN:O	9:O:104:MET:HG3	2.20	0.41
12:A:456:MET:HG2	12:A:510:GLN:HG3	2.02	0.41
12:A:567:LYS:O	19:H:95:TYR:HA	2.21	0.41
12:A:768:GLN:OE1	12:A:816:HIS:HA	2.21	0.41
12:A:872:GLY:O	12:A:1058:VAL:HG12	2.21	0.41
12:A:1191:TRP:CE3	12:A:1191:TRP:HA	2.56	0.41
13:B:293:PRO:HG2	13:B:296:GLU:HB2	2.02	0.41
13:B:599:THR:O	13:B:603:LEU:HG	2.21	0.41
15:D:67:ARG:HA	15:D:70:PHE:HB3	2.03	0.41
16:E:67:GLU:OE1	16:E:68:SER:OG	2.38	0.41
18:G:65:ASP:O	18:G:67:SER:N	2.54	0.41
20:I:59:VAL:O	20:I:62:ILE:HG22	2.21	0.41
20:I:75:CYS:SG	20:I:108:HIS:HB3	2.61	0.41
21:J:44:TYR:HA	21:J:47:ARG:HB2	2.03	0.41
21:J:52:THR:OG1	21:J:52:THR:O	2.39	0.41
22:K:61:TYR:HB3	22:K:73:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:101:PHE:HB3	25:Q:383:SER:HA	2.03	0.41
29:W:159:ASP:OD1	29:W:160:ASP:N	2.53	0.41
2:4:175:ARG:HD3	2:4:255:ASP:HB2	2.02	0.40
2:4:176:LEU:HD23	2:4:176:LEU:H	1.86	0.40
3:0:4:TYR:OH	3:0:9:PRO:HG3	2.21	0.40
3:0:589:ALA:HB3	3:0:596:ALA:HB2	2.02	0.40
5:2:19:GLN:HG3	5:2:85:HIS:CD2	2.57	0.40
6:5:16:ILE:O	6:5:19:LEU:HB2	2.19	0.40
7:7:234:VAL:O	7:7:315:SER:HA	2.21	0.40
7:7:310:ILE:HD11	7:7:338:LEU:HD23	2.03	0.40
7:7:409:VAL:HG13	7:7:486:ILE:HD12	2.03	0.40
9:O:101:ALA:HB2	9:O:116:PHE:CE2	2.56	0.40
12:A:761:MET:HA	12:A:804:TYR:HB2	2.03	0.40
12:A:870:GLU:OE1	16:E:202:SER:HB2	2.21	0.40
12:A:1124:HIS:HB3	12:A:1130:GLN:HG2	2.03	0.40
12:A:1132:LYS:HD3	12:A:1132:LYS:HA	1.90	0.40
13:B:555:ILE:H	13:B:555:ILE:HG13	1.37	0.40
13:B:865:LYS:NZ	13:B:871:THR:HG23	2.36	0.40
14:C:78:GLU:H	14:C:78:GLU:CD	2.21	0.40
18:G:115:MET:HG2	18:G:163:ILE:HG12	2.04	0.40
19:H:10:PHE:CD1	19:H:28:ALA:HB1	2.56	0.40
19:H:104:PHE:CE2	19:H:137:GLN:HG2	2.56	0.40
20:I:111:THR:HG23	20:I:113:ASP:H	1.86	0.40
1:1:517:UNK:O	1:1:519:UNK:N	2.54	0.40
2:4:192:GLN:O	2:4:195:PRO:HD2	2.21	0.40
2:4:205:LYS:HA	2:4:205:LYS:HD2	1.95	0.40
3:0:57:ILE:O	3:0:61:MET:HG2	2.21	0.40
3:0:192:PRO:HA	3:0:195:ILE:HB	2.03	0.40
3:0:703:ASP:HA	3:0:706:LEU:HD23	2.03	0.40
3:0:735:GLY:O	3:0:739:TRP:N	2.49	0.40
4:6:232:VAL:O	4:6:261:VAL:HG13	2.21	0.40
4:6:261:VAL:HB	4:6:280:THR:HG21	2.02	0.40
4:6:266:LEU:O	4:6:268:ALA:N	2.50	0.40
4:6:270:VAL:HB	4:6:273:CYS:HB2	2.02	0.40
4:6:280:THR:OG1	4:6:281:ASN:ND2	2.54	0.40
5:2:349:SER:HA	5:2:407:GLN:NE2	2.37	0.40
5:2:370:PHE:HA	7:7:116:HIS:C	2.47	0.40
12:A:811:GLN:H	12:A:811:GLN:CD	2.25	0.40
13:B:87:LYS:O	13:B:137:TYR:N	2.33	0.40
13:B:249:ARG:N	13:B:249:ARG:HD2	2.36	0.40
13:B:628:THR:C	13:B:632:ARG:HH21	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:925:LEU:HD12	13:B:928:ARG:HH22	1.86	0.40
13:B:1074:ASN:CG	13:B:1076:HIS:H	2.29	0.40
18:G:37:SER:O	18:G:45:ILE:N	2.48	0.40
27:U:262:LEU:HB2	27:U:279:ALA:HB3	2.04	0.40
29:W:52:THR:HG23	29:W:53:GLU:HG3	2.03	0.40
1:1:387:MET:C	1:1:389:LEU:H	2.30	0.40
3:0:224:ASN:HA	3:0:227:SER:OG	2.21	0.40
3:0:337:ARG:HD2	8:3:82:VAL:HA	2.04	0.40
3:0:341:TYR:CD1	3:0:366:LEU:HD12	2.56	0.40
3:0:351:VAL:N	3:0:422:PRO:HD3	2.37	0.40
3:0:661:HIS:HA	3:0:664:GLN:HE21	1.85	0.40
4:6:193:ILE:HD13	4:6:193:ILE:HA	1.93	0.40
5:2:217:ASP:O	5:2:221:VAL:HG23	2.22	0.40
6:5:53:GLU:HA	6:5:56:ARG:CB	2.50	0.40
7:7:370:LEU:HD23	7:7:370:LEU:HA	1.95	0.40
10:N:41:DA:H2"	10:N:42:DA:C8	2.56	0.40
12:A:1235:LYS:O	12:A:1237:ILE:HG12	2.22	0.40
13:B:280:ILE:HG23	13:B:284:ILE:HD12	2.03	0.40
13:B:483:LEU:HD12	13:B:484:ASN:H	1.86	0.40
13:B:579:ARG:NH2	13:B:623:GLU:OE2	2.34	0.40
18:G:14:HIS:HD1	18:G:16:SER:H	1.68	0.40
20:I:58:VAL:HA	20:I:62:ILE:HG21	2.02	0.40
24:M:132:LYS:O	24:M:136:LEU:N	2.53	0.40
24:M:179:GLY:O	24:M:183:ALA:N	2.50	0.40
29:W:124:CYS:SG	29:W:154:GLU:HB2	2.62	0.40
29:W:190:ASP:HA	29:W:193:ARG:CZ	2.52	0.40
1:1:473:UNK:O	1:1:477:UNK:N	2.54	0.40
2:4:176:LEU:HG	2:4:210:ILE:HG13	2.04	0.40
2:4:273:ARG:HG2	4:6:373:SER:HB3	2.03	0.40
3:0:159:HIS:O	3:0:162:LEU:HB3	2.21	0.40
3:0:374:LEU:HD23	3:0:410:SER:HB2	2.03	0.40
3:0:419:ILE:O	3:0:436:ARG:N	2.55	0.40
4:6:127:ILE:HG13	4:6:170:GLY:N	2.28	0.40
5:2:31:THR:HA	5:2:226:PHE:CD2	2.56	0.40
5:2:81:MET:HB3	5:2:81:MET:HE2	1.77	0.40
5:2:408:MET:HE2	5:2:408:MET:HB2	1.95	0.40
7:7:342:ASP:HB2	7:7:345:ASN:CG	2.47	0.40
7:7:634:GLN:OE1	7:7:635:GLU:N	2.54	0.40
12:A:411:ASP:OD1	12:A:412:ARG:N	2.54	0.40
12:A:596:THR:HG22	12:A:598:LEU:H	1.86	0.40
12:A:857:ARG:HD3	12:A:861:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1135:ARG:NH2	12:A:1139:GLU:OE1	2.54	0.40
12:A:1383:SER:O	12:A:1388:GLY:HA3	2.21	0.40
15:D:188:ALA:HA	15:D:207:LEU:HD13	2.03	0.40
17:F:93:ILE:HD13	17:F:93:ILE:HA	1.81	0.40
19:H:16:ASP:HB3	19:H:25:ARG:HB2	2.04	0.40
23:L:53:HIS:C	23:L:54:ARG:HH11	2.29	0.40
24:M:30:TYR:CD1	24:M:31:PRO:HD2	2.57	0.40
24:M:214:LEU:O	24:M:218:SER:OG	2.28	0.40
2:4:272:PHE:HD1	2:4:272:PHE:HA	1.74	0.40
3:0:216:PRO:HA	3:0:219:ALA:HB3	2.04	0.40
3:0:377:CYS:SG	3:0:406:ALA:HB3	2.62	0.40
3:0:539:VAL:O	3:0:600:SER:N	2.51	0.40
3:0:629:TYR:HE1	3:0:633:ARG:HA	1.87	0.40
3:0:747:HIS:HD2	3:0:751:ARG:HH11	1.70	0.40
4:6:133:SER:HB2	4:6:206:GLY:O	2.22	0.40
4:6:319:LEU:H	4:6:319:LEU:HD12	1.86	0.40
7:7:102:ALA:N	7:7:332:GLU:OE2	2.55	0.40
7:7:165:SER:C	7:7:172:GLU:H	2.28	0.40
7:7:303:ARG:HG2	7:7:506:ALA:HA	2.03	0.40
7:7:561:MET:HG2	7:7:566:TYR:CE1	2.56	0.40
7:7:593:PHE:HA	7:7:745:ILE:HG21	2.03	0.40
12:A:601:LYS:HE2	12:A:603:ASN:HD21	1.87	0.40
12:A:726:ARG:HD3	12:A:766:GLY:HA3	2.02	0.40
13:B:313:MET:HE2	13:B:313:MET:HB3	1.98	0.40
13:B:566:LEU:HB2	13:B:588:GLY:HA2	2.03	0.40
13:B:648:HIS:HD2	13:B:712:PRO:HA	1.87	0.40
13:B:1177:HIS:HB2	13:B:1179:GLN:HG3	2.03	0.40
15:D:47:LEU:HD22	15:D:49:ALA:HB2	2.03	0.40
16:E:37:LEU:HA	16:E:38:PRO:HD3	1.95	0.40
22:K:94:ILE:HA	22:K:94:ILE:HD13	1.87	0.40
24:M:315:ILE:HG13	24:M:316:LEU:HD22	2.03	0.40
26:R:135:PHE:HA	26:R:214:ILE:HA	2.03	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	1	256/542 (47%)	236 (92%)	18 (7%)	2 (1%)	16	52
2	4	279/338 (82%)	237 (85%)	42 (15%)	0	100	100
3	0	752/778 (97%)	677 (90%)	75 (10%)	0	100	100
4	6	336/461 (73%)	297 (88%)	37 (11%)	2 (1%)	21	57
5	2	456/513 (89%)	406 (89%)	50 (11%)	0	100	100
6	5	64/72 (89%)	54 (84%)	10 (16%)	0	100	100
7	7	630/843 (75%)	541 (86%)	89 (14%)	0	100	100
8	3	136/321 (42%)	122 (90%)	14 (10%)	0	100	100
9	O	178/240 (74%)	173 (97%)	5 (3%)	0	100	100
12	A	1386/1733 (80%)	1269 (92%)	115 (8%)	2 (0%)	48	81
13	B	1133/1224 (93%)	1057 (93%)	74 (6%)	2 (0%)	43	75
14	C	260/318 (82%)	243 (94%)	17 (6%)	0	100	100
15	D	153/221 (69%)	142 (93%)	11 (7%)	0	100	100
16	E	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
17	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
18	G	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
19	H	132/146 (90%)	118 (89%)	13 (10%)	1 (1%)	16	52
20	I	114/122 (93%)	101 (89%)	13 (11%)	0	100	100
21	J	63/70 (90%)	54 (86%)	9 (14%)	0	100	100
22	K	110/120 (92%)	105 (96%)	5 (4%)	0	100	100
23	L	43/70 (61%)	33 (77%)	10 (23%)	0	100	100
24	M	273/345 (79%)	243 (89%)	30 (11%)	0	100	100
25	Q	140/735 (19%)	130 (93%)	10 (7%)	0	100	100
26	R	176/400 (44%)	167 (95%)	9 (5%)	0	100	100
27	U	42/286 (15%)	38 (90%)	4 (10%)	0	100	100
28	V	46/122 (38%)	44 (96%)	2 (4%)	0	100	100
29	W	189/482 (39%)	183 (97%)	6 (3%)	0	100	100
30	X	152/328 (46%)	139 (91%)	12 (8%)	1 (1%)	18	54
All	All	7960/11371 (70%)	7248 (91%)	702 (9%)	10 (0%)	49	81

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	6	411	PRO
13	B	364	ILE
1	1	230	PRO
4	6	425	SER
13	B	363	HIS
12	A	464	PRO
19	H	110	ASP
12	A	465	TYR
30	X	272	ALA
1	1	239	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1	169/395 (43%)	151 (89%)	18 (11%)	6	24
2	4	154/298 (52%)	130 (84%)	24 (16%)	2	15
3	0	686/707 (97%)	601 (88%)	85 (12%)	4	20
4	6	247/406 (61%)	201 (81%)	46 (19%)	1	11
5	2	258/468 (55%)	212 (82%)	46 (18%)	2	12
6	5	53/66 (80%)	40 (76%)	13 (24%)	1	5
7	7	372/737 (50%)	283 (76%)	89 (24%)	1	5
8	3	53/303 (18%)	49 (92%)	4 (8%)	12	36
9	O	152/205 (74%)	145 (95%)	7 (5%)	24	47
12	A	1221/1520 (80%)	1085 (89%)	136 (11%)	6	23
13	B	995/1061 (94%)	890 (89%)	105 (11%)	6	24
14	C	230/274 (84%)	208 (90%)	22 (10%)	8	28
15	D	139/200 (70%)	120 (86%)	19 (14%)	3	17
16	E	195/197 (99%)	174 (89%)	21 (11%)	6	24
17	F	73/137 (53%)	67 (92%)	6 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	G	152/152 (100%)	140 (92%)	12 (8%)	11	35
19	H	119/128 (93%)	102 (86%)	17 (14%)	3	17
20	I	110/116 (95%)	101 (92%)	9 (8%)	10	34
21	J	60/65 (92%)	52 (87%)	8 (13%)	4	18
22	K	97/102 (95%)	87 (90%)	10 (10%)	7	25
23	L	40/57 (70%)	31 (78%)	9 (22%)	1	6
24	M	245/299 (82%)	216 (88%)	29 (12%)	5	21
25	Q	109/641 (17%)	101 (93%)	8 (7%)	13	37
26	R	107/363 (30%)	97 (91%)	10 (9%)	8	29
27	U	40/260 (15%)	39 (98%)	1 (2%)	42	62
28	V	47/108 (44%)	43 (92%)	4 (8%)	10	33
29	W	155/429 (36%)	148 (96%)	7 (4%)	24	47
30	X	62/295 (21%)	61 (98%)	1 (2%)	55	70
All	All	6340/9989 (64%)	5574 (88%)	766 (12%)	7	21

All (766) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	180	LEU
1	1	214	ILE
1	1	257	LEU
1	1	263	TYR
1	1	276	LYS
1	1	280	GLU
1	1	287	PHE
1	1	340	ASP
1	1	348	VAL
1	1	381	LEU
1	1	508	LYS
1	1	553	LEU
1	1	556	THR
1	1	563	HIS
1	1	564	PHE
1	1	583	TYR
1	1	585	HIS
1	1	593	LEU
2	4	30	ILE

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Mol	Chain	Res	Type
2	4	43	GLU
2	4	132	LEU
2	4	134	GLU
2	4	137	LYS
2	4	149	LEU
2	4	161	ASN
2	4	162	ARG
2	4	175	ARG
2	4	180	THR
2	4	229	ASP
2	4	236	LEU
2	4	239	GLU
2	4	244	LEU
2	4	245	ILE
2	4	246	GLN
2	4	253	PHE
2	4	254	ILE
2	4	258	LEU
2	4	259	ARG
2	4	262	ILE
2	4	273	ARG
2	4	287	PHE
2	4	288	ILE
3	0	14	TYR
3	0	28	ILE
3	0	32	LEU
3	0	34	VAL
3	0	39	ILE
3	0	48	LYS
3	0	54	SER
3	0	66	HIS
3	0	80	GLU
3	0	85	GLU
3	0	109	THR
3	0	111	ARG
3	0	113	ASN
3	0	115	CYS
3	0	116	LEU
3	0	131	GLU
3	0	133	CYS
3	0	138	ASN
3	0	148	ASP

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Mol	Chain	Res	Type
3	0	155	LEU
3	0	162	LEU
3	0	163	TYR
3	0	165	ILE
3	0	175	VAL
3	0	190	LEU
3	0	206	ILE
3	0	207	ILE
3	0	213	LEU
3	0	222	VAL
3	0	226	VAL
3	0	231	ILE
3	0	232	VAL
3	0	248	LEU
3	0	250	LEU
3	0	251	ASP
3	0	253	THR
3	0	255	ASP
3	0	284	ASP
3	0	290	VAL
3	0	298	ILE
3	0	312	LEU
3	0	318	THR
3	0	338	LEU
3	0	344	THR
3	0	350	HIS
3	0	351	VAL
3	0	352	ILE
3	0	355	THR
3	0	383	LEU
3	0	401	ASP
3	0	411	THR
3	0	430	VAL
3	0	435	MET
3	0	447	LYS
3	0	449	VAL
3	0	453	PHE
3	0	456	VAL
3	0	458	ILE
3	0	477	THR
3	0	487	LEU
3	0	506	ILE

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Mol	Chain	Res	Type
3	0	520	ARG
3	0	531	LYS
3	0	535	ASP
3	0	539	VAL
3	0	545	LEU
3	0	560	LEU
3	0	572	GLU
3	0	599	LEU
3	0	614	HIS
3	0	615	GLN
3	0	627	PHE
3	0	639	LEU
3	0	649	ARG
3	0	651	ASN
3	0	654	LEU
3	0	657	ASP
3	0	674	ASP
3	0	705	ASP
3	0	710	THR
3	0	711	ASP
3	0	722	ARG
3	0	742	GLU
3	0	745	ILE
3	0	754	GLN
4	6	115	ILE
4	6	119	GLN
4	6	120	ARG
4	6	134	GLU
4	6	136	MET
4	6	138	GLU
4	6	146	HIS
4	6	148	MET
4	6	149	ILE
4	6	150	ILE
4	6	154	ILE
4	6	155	ASP
4	6	158	HIS
4	6	164	ASN
4	6	166	ILE
4	6	185	VAL
4	6	194	ASP
4	6	202	GLN

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Mol	Chain	Res	Type
4	6	210	LEU
4	6	214	LEU
4	6	222	LEU
4	6	227	HIS
4	6	241	THR
4	6	247	ILE
4	6	262	LYS
4	6	263	VAL
4	6	274	LYS
4	6	284	ASP
4	6	291	LEU
4	6	293	ASP
4	6	297	LEU
4	6	303	GLU
4	6	305	VAL
4	6	308	LEU
4	6	310	VAL
4	6	320	VAL
4	6	326	THR
4	6	363	CYS
4	6	368	LEU
4	6	372	LEU
4	6	375	HIS
4	6	384	MET
4	6	386	LEU
4	6	406	CYS
4	6	448	LEU
4	6	449	HIS
5	2	11	THR
5	2	14	LEU
5	2	16	GLU
5	2	17	ILE
5	2	22	GLN
5	2	25	LEU
5	2	28	SER
5	2	42	LEU
5	2	48	MET
5	2	55	ASN
5	2	56	GLU
5	2	59	LEU
5	2	60	LEU
5	2	61	ASP

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Mol	Chain	Res	Type
5	2	63	ASP
5	2	71	LYS
5	2	74	PHE
5	2	99	ASN
5	2	112	LEU
5	2	208	LEU
5	2	222	LEU
5	2	278	LEU
5	2	286	ARG
5	2	348	TYR
5	2	349	SER
5	2	352	ASN
5	2	371	VAL
5	2	374	VAL
5	2	380	ARG
5	2	396	ILE
5	2	413	GLU
5	2	414	GLU
5	2	425	ASN
5	2	432	VAL
5	2	450	ARG
5	2	457	SER
5	2	464	THR
5	2	470	LEU
5	2	474	TYR
5	2	476	GLN
5	2	481	LEU
5	2	484	LYS
5	2	486	ASP
5	2	487	LYS
5	2	491	PHE
5	2	493	ILE
6	5	5	ARG
6	5	6	LYS
6	5	20	ILE
6	5	24	ASP
6	5	26	LYS
6	5	30	ILE
6	5	36	ASP
6	5	42	VAL
6	5	46	LYS
6	5	48	GLU

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Mol	Chain	Res	Type
6	5	50	VAL
6	5	54	LEU
6	5	58	LEU
7	7	348	ARG
7	7	349	ASN
7	7	351	ASP
7	7	355	ASP
7	7	356	LEU
7	7	357	LYS
7	7	361	GLN
7	7	362	ILE
7	7	363	ARG
7	7	365	TYR
7	7	380	ARG
7	7	383	ILE
7	7	384	ILE
7	7	385	VAL
7	7	386	LEU
7	7	393	THR
7	7	395	VAL
7	7	403	ILE
7	7	411	CYS
7	7	419	GLN
7	7	420	TRP
7	7	421	ARG
7	7	427	TRP
7	7	428	CYS
7	7	431	GLN
7	7	433	GLU
7	7	435	CYS
7	7	437	VAL
7	7	440	SER
7	7	444	GLU
7	7	445	MET
7	7	447	GLN
7	7	452	LEU
7	7	453	VAL
7	7	456	THR
7	7	464	ARG
7	7	469	ASP
7	7	472	LYS
7	7	475	ASP

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Mol	Chain	Res	Type
7	7	484	PHE
7	7	489	GLU
7	7	491	HIS
7	7	492	VAL
7	7	493	VAL
7	7	497	MET
7	7	501	VAL
7	7	508	HIS
7	7	510	LYS
7	7	514	THR
7	7	518	VAL
7	7	524	ILE
7	7	530	LEU
7	7	534	LYS
7	7	535	LEU
7	7	545	GLN
7	7	552	VAL
7	7	564	GLU
7	7	566	TYR
7	7	571	ARG
7	7	576	LYS
7	7	578	MET
7	7	579	LEU
7	7	587	LYS
7	7	601	ARG
7	7	605	ILE
7	7	612	VAL
7	7	620	LEU
7	7	626	PHE
7	7	634	GLN
7	7	637	MET
7	7	638	ASN
7	7	641	GLN
7	7	645	TYR
7	7	663	ASP
7	7	664	LEU
7	7	666	GLU
7	7	669	CYS
7	7	671	ILE
7	7	691	LEU
7	7	692	ARG
7	7	698	ASP

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Mol	Chain	Res	Type
7	7	712	ASP
7	7	716	MET
7	7	719	SER
7	7	722	ARG
7	7	723	GLN
7	7	726	LEU
7	7	729	GLN
7	7	760	LEU
8	3	34	CYS
8	3	36	HIS
8	3	53	GLN
8	3	63	LEU
9	O	153	THR
9	O	159	ASN
9	O	173	GLU
9	O	188	GLU
9	O	214	LEU
9	O	215	THR
9	O	234	LEU
12	A	23	SER
12	A	25	GLU
12	A	47	ARG
12	A	53	LEU
12	A	54	ASN
12	A	55	ASP
12	A	61	ILE
12	A	62	ASP
12	A	69	THR
12	A	75	ASN
12	A	76	GLU
12	A	77	CYS
12	A	81	PHE
12	A	84	ILE
12	A	91	PHE
12	A	106	VAL
12	A	124	GLN
12	A	141	LEU
12	A	147	VAL
12	A	167	CYS
12	A	174	ILE
12	A	175	ARG
12	A	177	ASP

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Mol	Chain	Res	Type
12	A	182	VAL
12	A	199	LEU
12	A	201	VAL
12	A	203	SER
12	A	232	GLU
12	A	235	ILE
12	A	239	LEU
12	A	256	GLN
12	A	268	ASP
12	A	279	LEU
12	A	289	ILE
12	A	299	HIS
12	A	308	ILE
12	A	346	ASP
12	A	351	THR
12	A	379	VAL
12	A	420	ARG
12	A	438	ASP
12	A	450	LEU
12	A	465	TYR
12	A	470	LEU
12	A	474	VAL
12	A	486	GLU
12	A	489	LEU
12	A	501	LEU
12	A	505	CYS
12	A	523	ILE
12	A	524	VAL
12	A	525	GLN
12	A	526	ASP
12	A	529	CYS
12	A	538	ASP
12	A	544	ASP
12	A	546	VAL
12	A	566	ILE
12	A	576	GLN
12	A	577	ILE
12	A	592	ASP
12	A	598	LEU
12	A	603	ASN
12	A	622	VAL
12	A	640	GLN

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Mol	Chain	Res	Type
12	A	666	ILE
12	A	672	ASP
12	A	690	VAL
12	A	691	LEU
12	A	694	THR
12	A	709	THR
12	A	712	GLU
12	A	717	ASN
12	A	758	ILE
12	A	765	VAL
12	A	770	VAL
12	A	790	ASP
12	A	795	GLU
12	A	801	GLU
12	A	848	ILE
12	A	862	ASN
12	A	867	ILE
12	A	884	ASP
12	A	889	SER
12	A	890	ASP
12	A	900	ASP
12	A	909	ASP
12	A	919	ILE
12	A	931	GLU
12	A	949	ASP
12	A	953	ASN
12	A	961	ARG
12	A	979	SER
12	A	982	THR
12	A	983	ILE
12	A	1038	THR
12	A	1107	VAL
12	A	1113	THR
12	A	1128	GLN
12	A	1130	GLN
12	A	1135	ARG
12	A	1138	ILE
12	A	1144	LYS
12	A	1163	ILE
12	A	1165	GLU
12	A	1171	GLN
12	A	1174	PHE

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Mol	Chain	Res	Type
12	A	1195	LEU
12	A	1197	LEU
12	A	1206	ASP
12	A	1209	MET
12	A	1211	GLN
12	A	1220	PHE
12	A	1231	ASP
12	A	1242	VAL
12	A	1243	VAL
12	A	1256	GLU
12	A	1266	THR
12	A	1272	THR
12	A	1295	THR
12	A	1305	VAL
12	A	1327	ILE
12	A	1330	ASN
12	A	1334	ASP
12	A	1350	LYS
12	A	1359	ASP
12	A	1377	THR
12	A	1382	THR
12	A	1393	ASN
12	A	1400	CYS
12	A	1404	GLU
12	A	1406	VAL
12	A	1407	GLU
12	A	1424	VAL
12	A	1448	GLU
12	A	1450	LEU
13	B	25	ILE
13	B	26	THR
13	B	35	SER
13	B	58	THR
13	B	61	ASP
13	B	86	ARG
13	B	91	SER
13	B	101	MET
13	B	102	VAL
13	B	183	GLU
13	B	185	THR
13	B	222	ILE
13	B	223	VAL

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Mol	Chain	Res	Type
13	B	240	ILE
13	B	244	LEU
13	B	245	GLU
13	B	253	THR
13	B	259	TYR
13	B	269	ILE
13	B	272	THR
13	B	282	ILE
13	B	294	ASP
13	B	317	CYS
13	B	333	PHE
13	B	357	GLN
13	B	363	HIS
13	B	364	ILE
13	B	391	ASP
13	B	399	ASP
13	B	420	LEU
13	B	428	ILE
13	B	461	LEU
13	B	476	ARG
13	B	479	VAL
13	B	487	THR
13	B	502	ILE
13	B	513	GLN
13	B	527	THR
13	B	555	ILE
13	B	570	VAL
13	B	591	ARG
13	B	595	ARG
13	B	598	GLU
13	B	610	ASN
13	B	612	GLU
13	B	624	LEU
13	B	644	GLU
13	B	650	GLU
13	B	654	ARG
13	B	657	HIS
13	B	680	THR
13	B	690	VAL
13	B	691	GLU
13	B	697	GLU
13	B	734	HIS

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Mol	Chain	Res	Type
13	B	755	ILE
13	B	786	ASN
13	B	790	ASP
13	B	795	ILE
13	B	805	THR
13	B	806	THR
13	B	861	ASP
13	B	864	LYS
13	B	880	THR
13	B	889	THR
13	B	898	LEU
13	B	916	THR
13	B	918	ILE
13	B	955	THR
13	B	956	THR
13	B	959	ASP
13	B	964	VAL
13	B	967	ARG
13	B	971	THR
13	B	982	SER
13	B	986	GLN
13	B	989	THR
13	B	993	THR
13	B	996	ARG
13	B	1002	THR
13	B	1009	ASP
13	B	1022	THR
13	B	1049	ASP
13	B	1051	THR
13	B	1058	LEU
13	B	1074	ASN
13	B	1080	LYS
13	B	1081	LEU
13	B	1093	GLN
13	B	1098	MET
13	B	1103	ILE
13	B	1115	THR
13	B	1119	VAL
13	B	1133	MET
13	B	1138	MET
13	B	1145	SER
13	B	1149	GLU

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Mol	Chain	Res	Type
13	B	1152	MET
13	B	1153	GLU
13	B	1163	CYS
13	B	1166	CYS
13	B	1177	HIS
13	B	1192	TYR
13	B	1215	ARG
13	B	1222	ARG
14	C	8	VAL
14	C	10	ILE
14	C	12	GLU
14	C	50	GLU
14	C	72	LEU
14	C	82	TYR
14	C	91	HIS
14	C	95	CYS
14	C	99	LEU
14	C	106	GLU
14	C	110	THR
14	C	112	ASN
14	C	115	SER
14	C	163	ILE
14	C	165	LYS
14	C	176	ILE
14	C	196	ASP
14	C	211	ASP
14	C	214	ASN
14	C	215	GLU
14	C	219	PHE
14	C	240	VAL
15	D	38	ILE
15	D	52	LEU
15	D	58	VAL
15	D	61	GLU
15	D	68	ARG
15	D	122	GLU
15	D	124	GLU
15	D	131	GLU
15	D	137	ASN
15	D	142	LYS
15	D	160	VAL
15	D	172	LEU

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Mol	Chain	Res	Type
15	D	173	HIS
15	D	175	PHE
15	D	177	VAL
15	D	187	THR
15	D	207	LEU
15	D	209	ARG
15	D	220	LEU
16	E	8	ASN
16	E	11	ARG
16	E	30	ILE
16	E	31	THR
16	E	33	GLU
16	E	34	GLU
16	E	39	LEU
16	E	50	MET
16	E	67	GLU
16	E	81	GLU
16	E	84	ASP
16	E	92	THR
16	E	93	MET
16	E	107	THR
16	E	117	THR
16	E	131	THR
16	E	134	THR
16	E	145	THR
16	E	182	ASP
16	E	207	ARG
16	E	213	ILE
17	F	82	THR
17	F	86	THR
17	F	100	GLN
17	F	110	ASP
17	F	111	LEU
17	F	133	VAL
18	G	5	LYS
18	G	6	ASP
18	G	17	PHE
18	G	33	GLU
18	G	39	THR
18	G	49	LEU
18	G	58	ARG
18	G	77	VAL

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Mol	Chain	Res	Type
18	G	101	VAL
18	G	134	GLU
18	G	138	THR
18	G	148	GLU
19	H	10	PHE
19	H	13	SER
19	H	14	GLU
19	H	16	ASP
19	H	23	VAL
19	H	25	ARG
19	H	41	ASP
19	H	42	ILE
19	H	44	VAL
19	H	46	LEU
19	H	58	THR
19	H	110	ASP
19	H	112	ILE
19	H	131	ASN
19	H	133	ASN
19	H	134	ASN
19	H	135	LEU
20	I	4	PHE
20	I	5	ARG
20	I	8	ARG
20	I	37	GLU
20	I	60	GLN
20	I	67	THR
20	I	89	GLN
20	I	108	HIS
20	I	115	LYS
21	J	2	ILE
21	J	5	VAL
21	J	7	CYS
21	J	10	CYS
21	J	28	ASP
21	J	31	ASP
21	J	39	LEU
21	J	57	ILE
22	K	5	ASP
22	K	10	PHE
22	K	11	LEU
22	K	16	GLU

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Mol	Chain	Res	Type
22	K	19	LEU
22	K	32	VAL
22	K	38	GLU
22	K	75	ILE
22	K	77	THR
22	K	92	ASN
23	L	26	THR
23	L	31	CYS
23	L	37	LYS
23	L	46	VAL
23	L	53	HIS
23	L	54	ARG
23	L	58	LYS
23	L	60	ARG
23	L	65	VAL
24	M	23	THR
24	M	48	CYS
24	M	51	VAL
24	M	52	LEU
24	M	54	ASP
24	M	87	LEU
24	M	101	THR
24	M	102	THR
24	M	104	MET
24	M	105	ARG
24	M	125	GLU
24	M	152	GLU
24	M	156	LEU
24	M	166	LYS
24	M	168	MET
24	M	185	VAL
24	M	197	HIS
24	M	198	VAL
24	M	200	THR
24	M	234	GLN
24	M	236	LEU
24	M	242	PHE
24	M	243	CYS
24	M	264	LYS
24	M	277	ILE
24	M	287	LEU
24	M	289	PHE

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Mol	Chain	Res	Type
24	M	319	HIS
24	M	321	ASP
25	Q	114	MET
25	Q	116	THR
25	Q	120	LYS
25	Q	126	LYS
25	Q	132	ASP
25	Q	140	HIS
25	Q	346	GLU
25	Q	359	ASN
26	R	63	ARG
26	R	76	PHE
26	R	118	HIS
26	R	123	GLU
26	R	128	VAL
26	R	129	VAL
26	R	132	GLU
26	R	225	MET
26	R	256	ASP
26	R	280	VAL
27	U	255	LYS
28	V	74	ASP
28	V	85	VAL
28	V	108	VAL
28	V	112	ARG
29	W	12	LEU
29	W	17	VAL
29	W	133	GLN
29	W	139	LEU
29	W	141	ASN
29	W	143	ASP
29	W	152	CYS
30	X	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	379	ASN
1	1	621	ASN
3	0	23	ASN
3	0	37	ASN
3	0	60	GLN

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Mol	Chain	Res	Type
3	0	88	ASN
3	0	291	GLN
3	0	294	HIS
3	0	664	GLN
4	6	151	GLN
4	6	188	ASN
4	6	211	GLN
4	6	449	HIS
5	2	85	HIS
5	2	372	ASN
5	2	395	GLN
5	2	498	ASN
6	5	52	HIS
7	7	347	HIS
7	7	366	GLN
7	7	592	GLN
7	7	676	HIS
7	7	682	GLN
7	7	697	ASN
7	7	761	GLN
12	A	4	GLN
12	A	109	HIS
12	A	256	GLN
12	A	451	HIS
12	A	700	ASN
12	A	741	ASN
12	A	935	GLN
12	A	953	ASN
12	A	965	GLN
12	A	996	ASN
12	A	1040	GLN
12	A	1124	HIS
12	A	1187	GLN
12	A	1218	GLN
12	A	1330	ASN
12	A	1364	ASN
12	A	1427	ASN
13	B	60	GLN
13	B	73	GLN
13	B	110	HIS
13	B	350	GLN
13	B	363	HIS

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Mol	Chain	Res	Type
13	B	395	GLN
13	B	443	ASN
13	B	449	ASN
13	B	518	HIS
13	B	794	ASN
13	B	1040	ASN
13	B	1062	HIS
14	C	65	HIS
14	C	135	GLN
14	C	252	GLN
15	D	34	GLN
16	E	5	ASN
16	E	63	ASN
16	E	114	ASN
19	H	11	GLN
19	H	83	GLN
19	H	128	ASN
20	I	89	GLN
20	I	90	GLN
22	K	29	ASN
22	K	40	HIS
22	K	110	ASN
23	L	53	HIS
24	M	114	GLN
24	M	127	GLN
24	M	212	ASN
24	M	303	GLN
26	R	65	ASN
30	X	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 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	$\# Z > 2$
32	SF4	0	801	3	0,12,12	-	-	-		

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
32	SF4	0	801	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	801	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	84.64
1	1	355:UNK	C	368:UNK	N	13.08
1	1	519:UNK	C	537:GLU	N	12.00

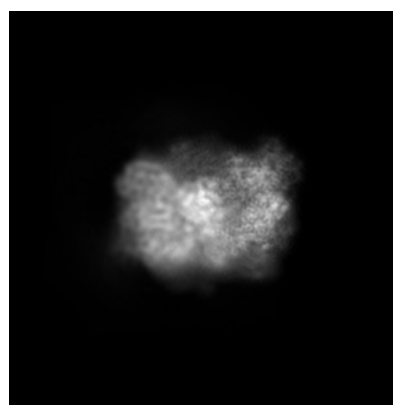
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23905. These allow visual inspection of the internal detail of the map and identification of artifacts.

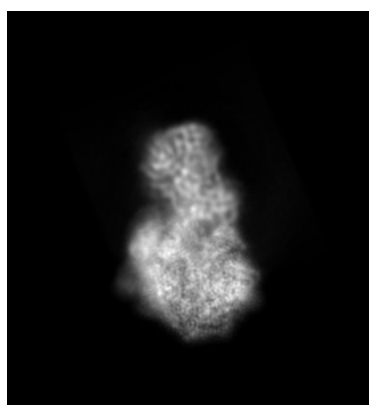
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

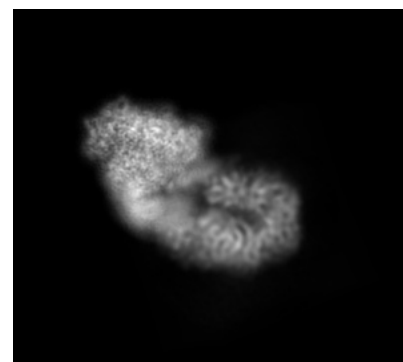
6.1.1 Primary map



X



Y

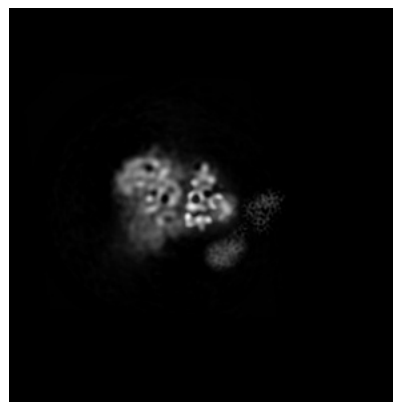


Z

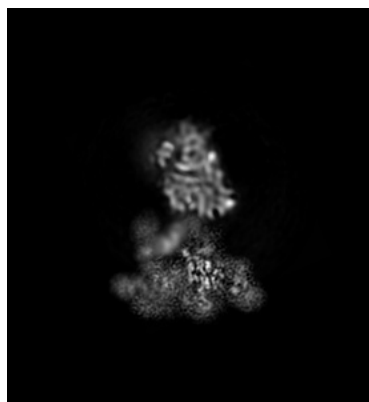
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

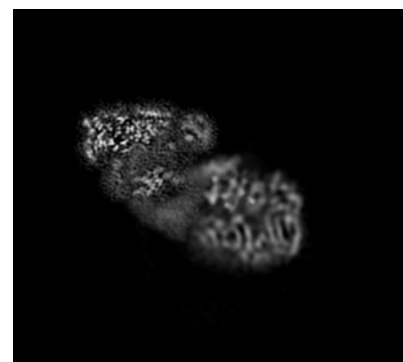
6.2.1 Primary map



X Index: 214



Y Index: 191

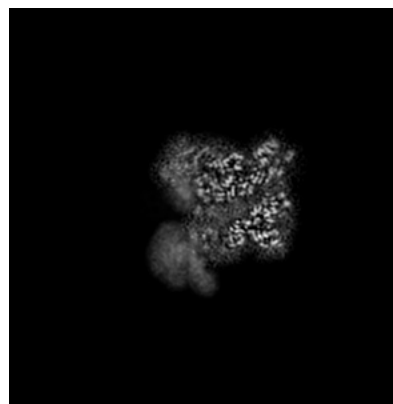


Z Index: 198

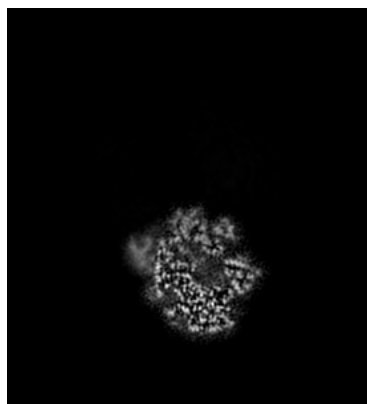
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

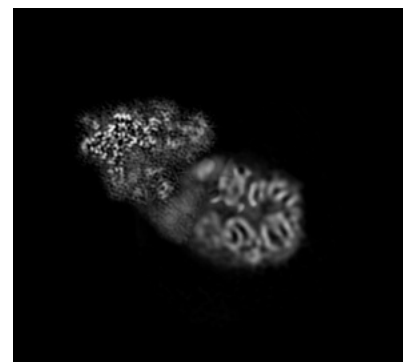
6.3.1 Primary map



X Index: 131



Y Index: 252

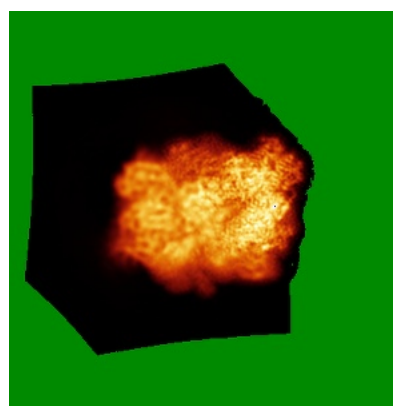


Z Index: 192

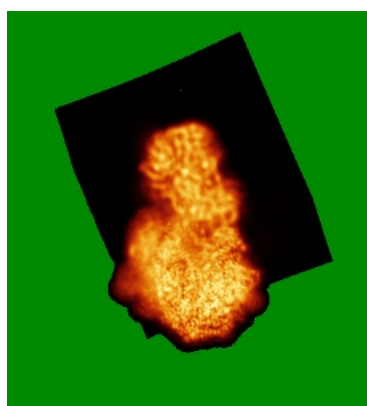
The images above show the largest variance slices of the map in three orthogonal directions.

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

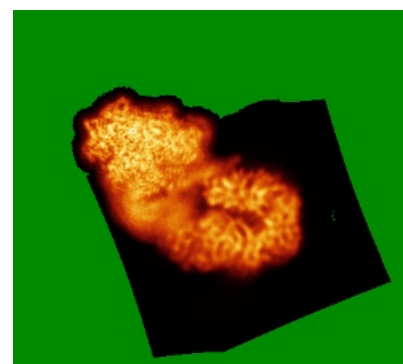
6.4.1 Primary map



X



Y

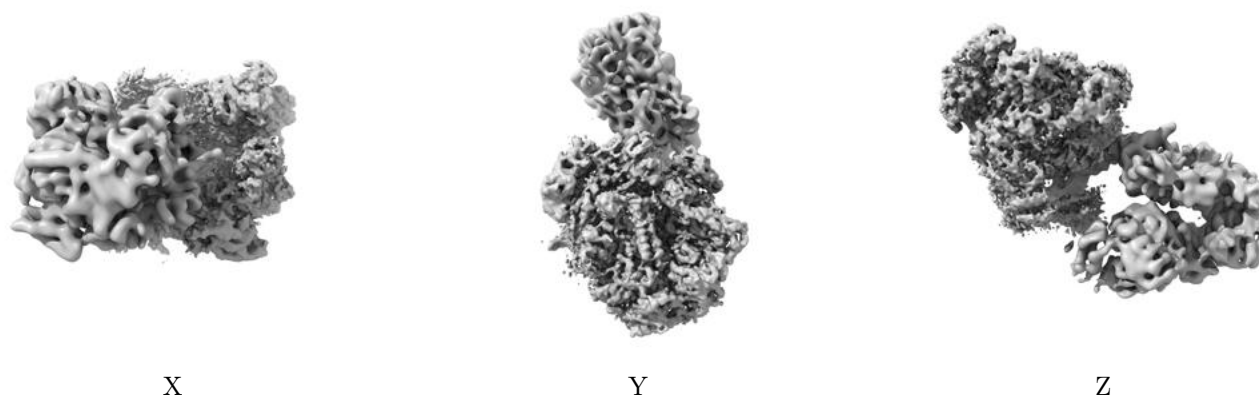


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

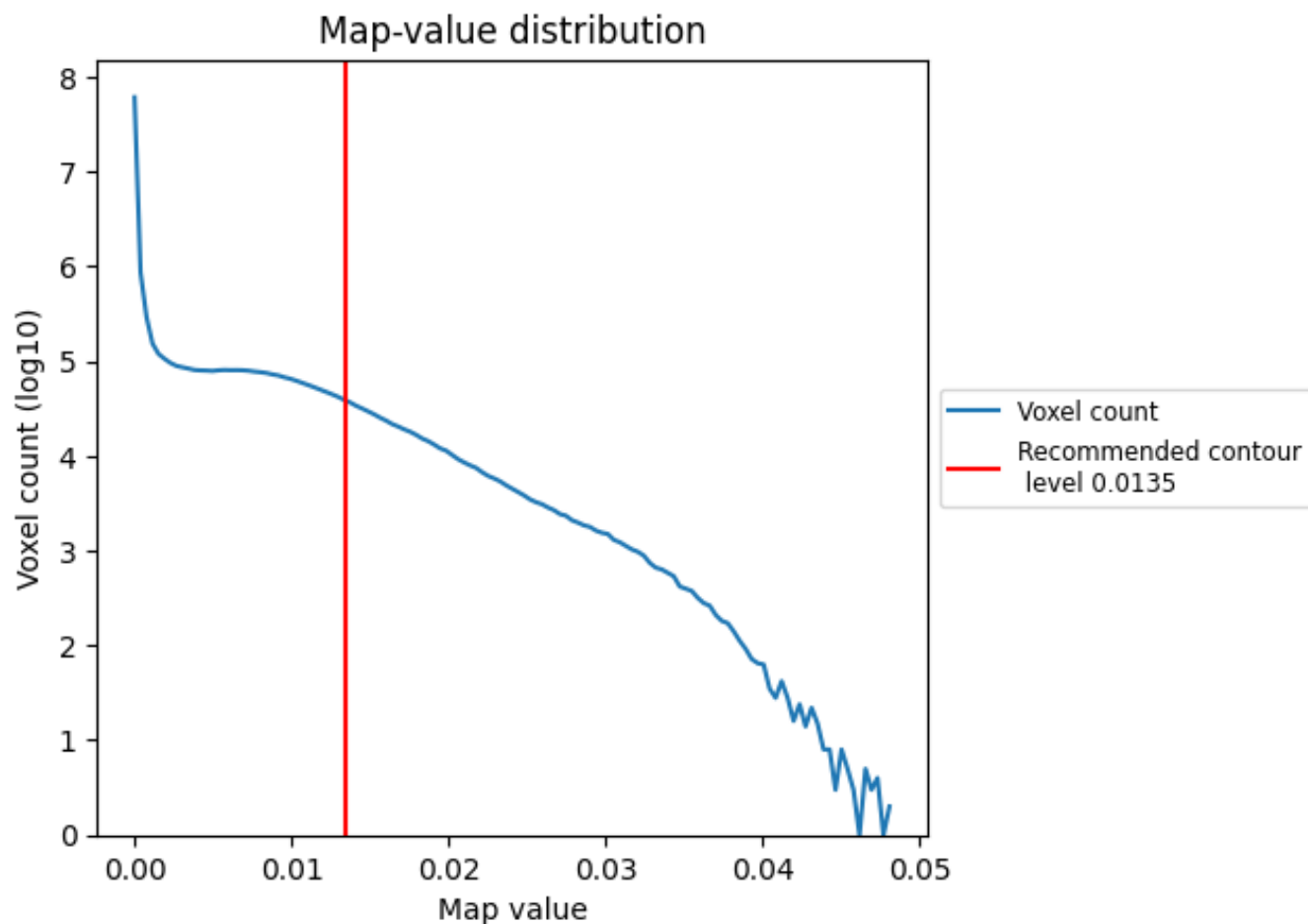
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

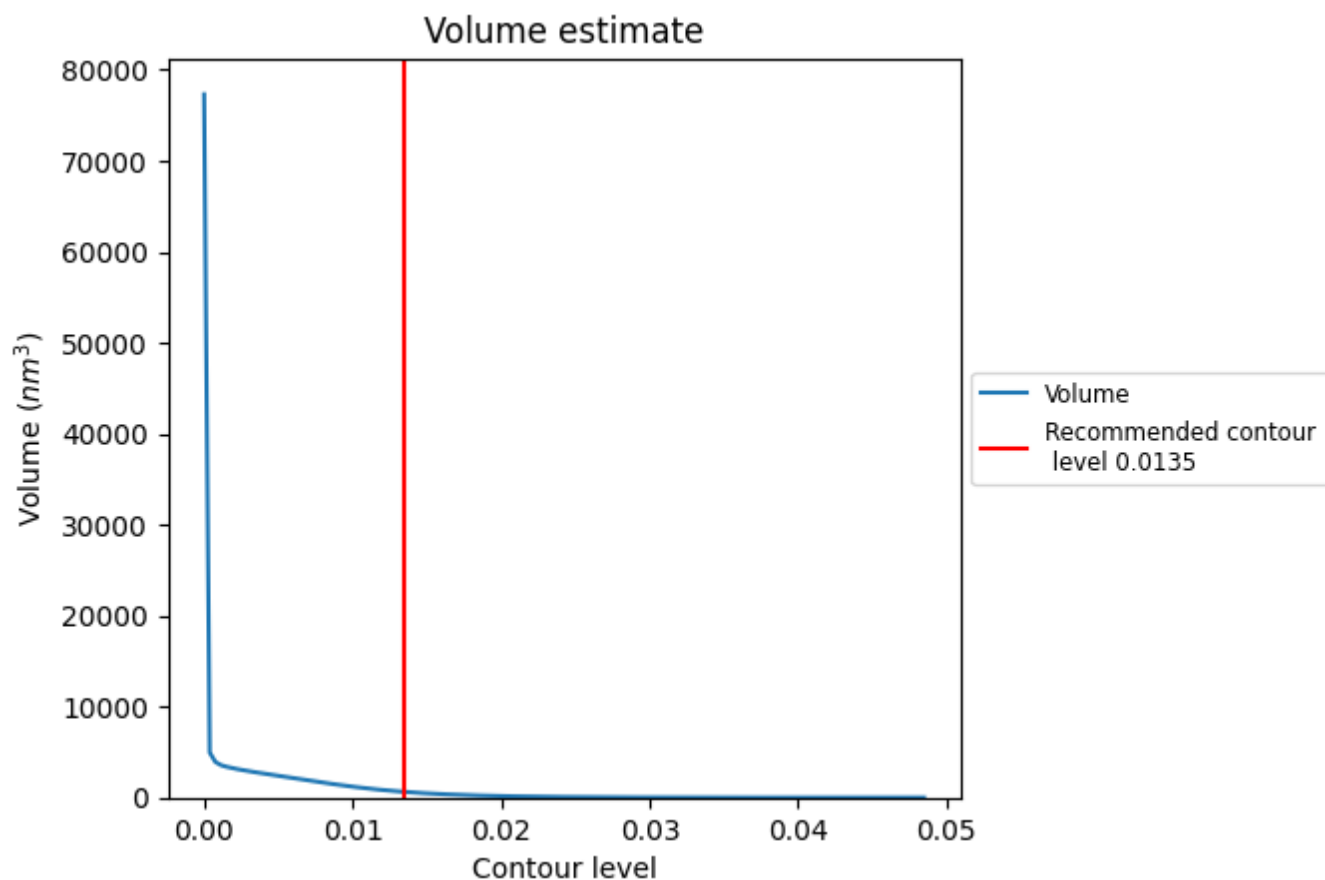
This section contains the results of statistical analysis of the map.

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 626 nm³; this corresponds to an approximate mass of 565 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.

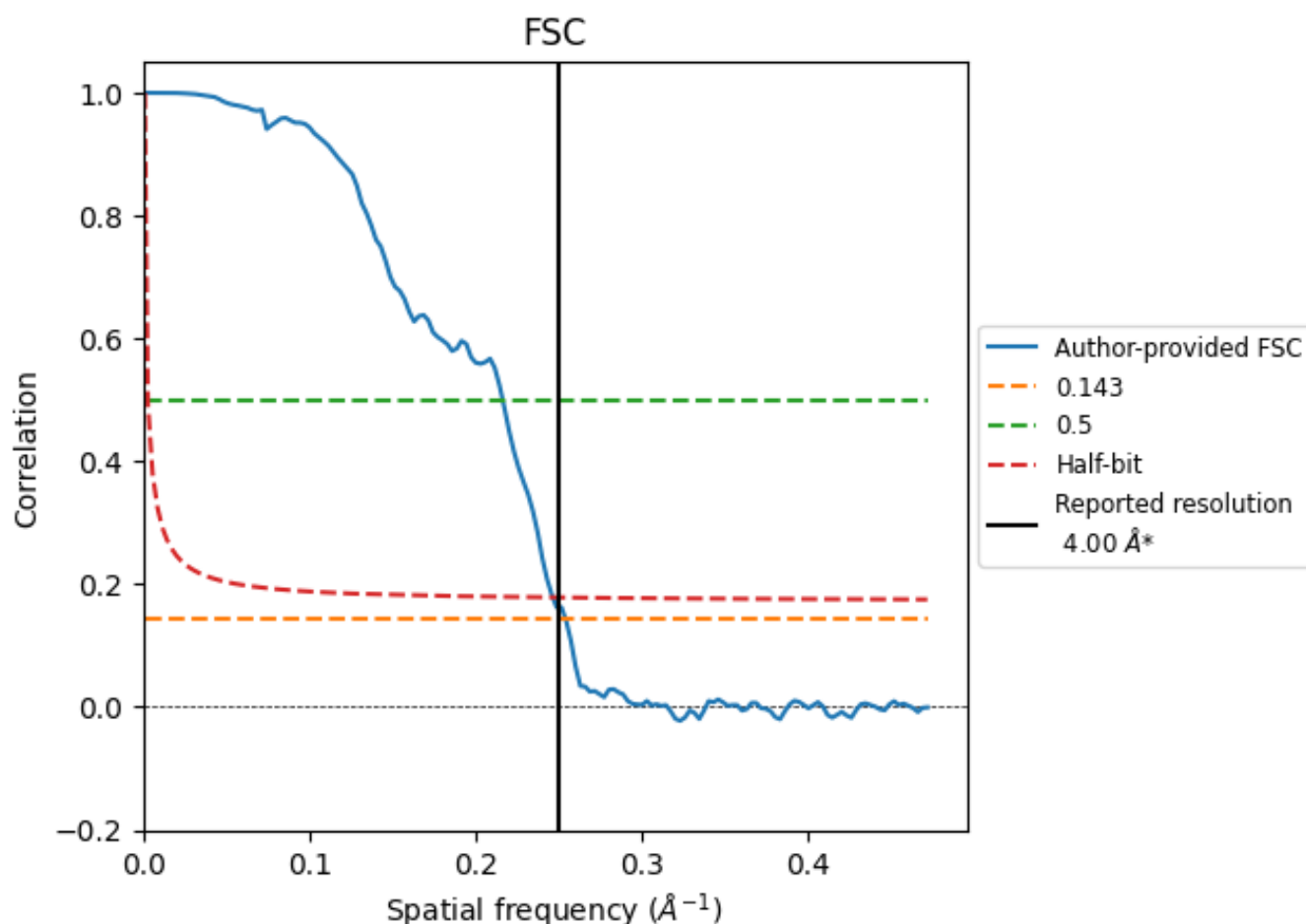
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	4.63	4.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23905 and PDB model 7ML1. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

This section was not generated.

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

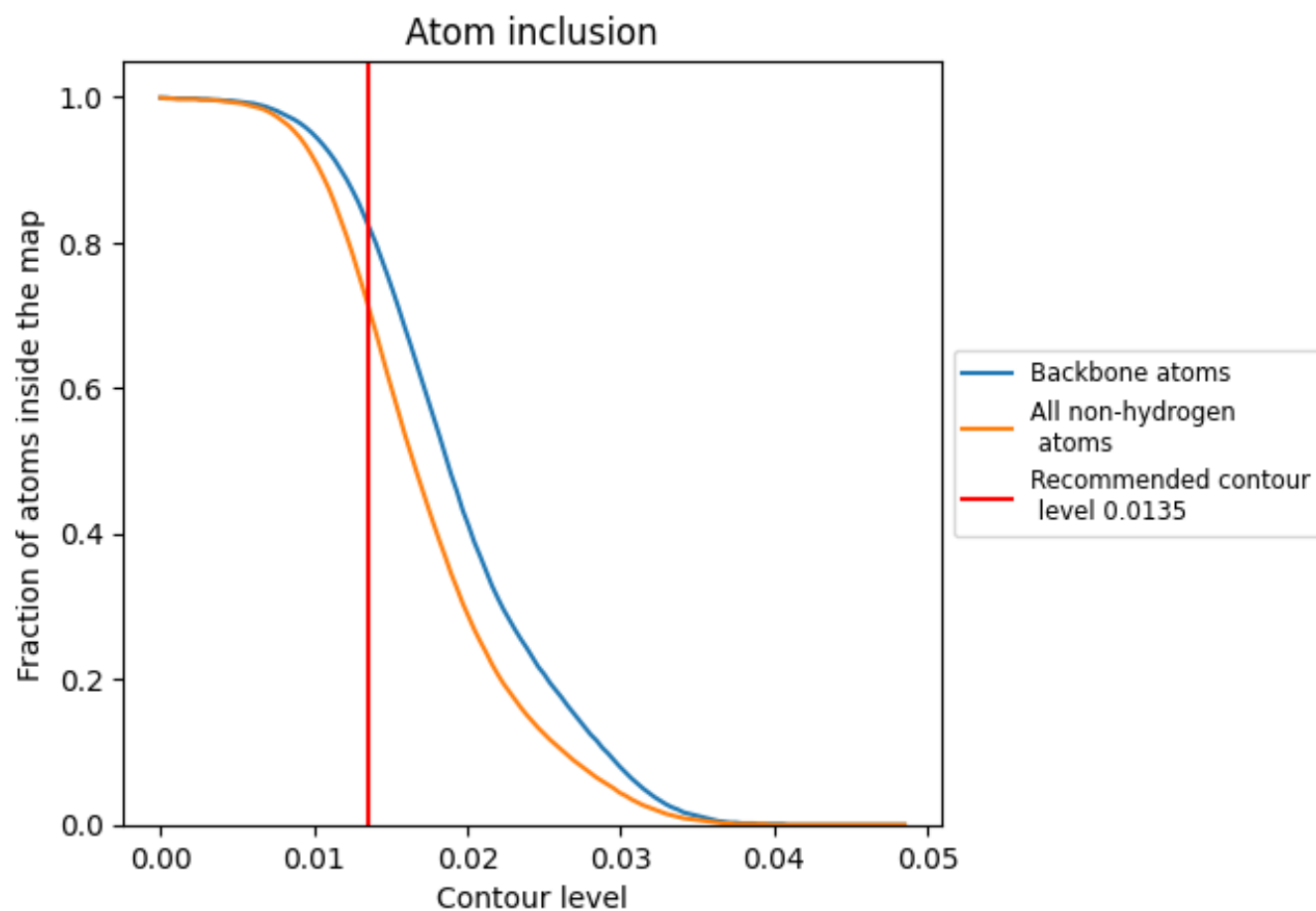


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



At the recommended contour level, 83% of all backbone atoms, 72% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.2910
0	 0.6340	 0.1760
1	 0.6450	 0.2160
2	 0.8020	 0.1990
3	 0.0820	 0.1450
4	 0.7700	 0.1940
5	 0.7150	 0.1830
6	 0.7740	 0.2030
7	 0.7140	 0.1470
A	 0.8460	 0.4220
B	 0.8510	 0.4330
C	 0.8900	 0.4570
D	 0.5210	 0.2800
E	 0.8380	 0.4000
F	 0.8800	 0.4500
G	 0.7240	 0.3180
H	 0.8460	 0.4070
I	 0.7490	 0.3410
J	 0.8670	 0.4430
K	 0.7820	 0.3930
L	 0.8010	 0.3570
M	 0.3860	 0.2450
N	 0.6130	 0.1410
O	 0.3700	 0.0900
Q	 0.7420	 0.2460
R	 0.6120	 0.2190
T	 0.6550	 0.1430
U	 0.0060	 0.0650
V	 0.0180	 0.0760
W	 0.4290	 0.1480
X	 0.4160	 0.1520

