Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:18 PM EST

PDB ID	:	7ML4
EMDB ID	:	EMD-23908
Title	:	RNA polymerase II initially transcribing complex (ITC)
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	:	3.10 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:

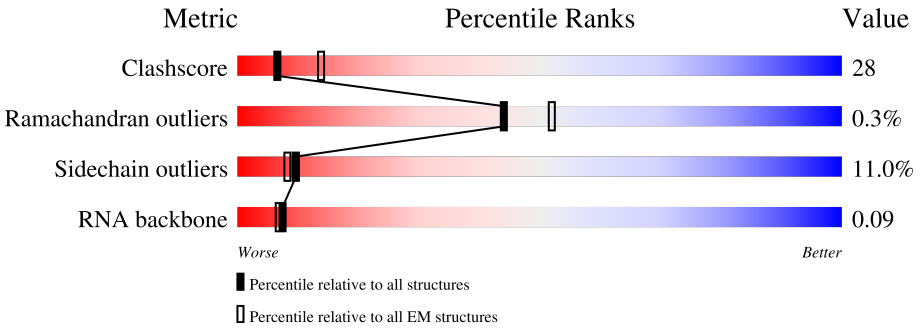
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	Q	735	7% 11% • 80%
2	R	398	5% 18% 18% • 61%
3	D	221	30% 27% 41% • 29%
4	G	171	18% 32% 60% 8%
5	M	345	11% 26% 36% 5% • 32%
6	A	1733	• 36% 38% 7% 19%
7	B	1224	• 45% 38% 8% 9%

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Mol	Chain	Length	Quality of chain
8	C	318	39% 37% 7% 16%
9	E	215	40% 50% 8%
10	F	155	24% 25% 5% 45%
11	H	146	27% 51% 12% 9%
12	I	122	6% 28% 50% 20%
13	J	70	47% 40% 6% 7%
14	K	120	5% 49% 41% 5% 5%
15	L	70	11% 41% 13% 34%
16	3	321	13% 20% 78%
17	0	778	27% 52% 43%
18	4	338	14% 45% 37% 16%
19	6	461	13% 49% 27% 24%
20	1	543	27% 51% 16% 32%
21	7	843	40% 44% 29% 25%
22	5	72	40% 72% 19% 8%
23	2	513	23% 65% 23% 10%
24	X	328	8% 34% 12% 55%
25	U	286	5% 7% 9% 84%
26	V	122	6% 21% 18% 60%
27	N	38	37% 45% 18%
28	T	148	7% 20% 5% 68%
29	O	240	25% 48% 25%
30	W	482	11% 22% 16% 60%
31	P	5	40% 60%

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 crite-

ria:

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

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 62733 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 Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Q	148	1141	731	195	212	3	0	0

- Molecule 2 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	154	1039	652	190	193	4	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 5 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	234	1805	1152	304	333	16	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	1405	11039	6962	1935	2081	61	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	1114	Total	C	N	O	S	0	0
			8861	5610	1549	1647	55		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	85	Total	C	N	O	S	0	0
			688	439	116	130	3		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 13 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	114	Total	C	N	O	S	0	0
			919	590	156	171	2		

- Molecule 15 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 16 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	3	72	Total	C	N	O	0	0
			361	215	72	74		

- Molecule 17 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

- Molecule 18 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	113	UNK	ASP	conflict	UNP A0A7I9C5C2
4	114	UNK	MET	conflict	UNP A0A7I9C5C2

- Molecule 19 is a protein called General transcription and DNA repair factor IIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	412	UNK	ILE	conflict	UNP A0A7I9FQL5
6	413	UNK	LEU	conflict	UNP A0A7I9FQL5
6	414	UNK	LYS	conflict	UNP A0A7I9FQL5
6	415	UNK	ASN	conflict	UNP A0A7I9FQL5
6	416	UNK	HIS	conflict	UNP A0A7I9FQL5
6	417	UNK	LYS	conflict	UNP A0A7I9FQL5
6	418	UNK	ASN	conflict	UNP A0A7I9FQL5
6	419	UNK	ASP	conflict	UNP A0A7I9FQL5
6	420	UNK	LYS	conflict	UNP A0A7I9FQL5
6	421	UNK	LEU	conflict	UNP A0A7I9FQL5
6	422	UNK	LEU	conflict	UNP A0A7I9FQL5
6	423	UNK	THR	conflict	UNP A0A7I9FQL5
6	424	UNK	SER	conflict	UNP A0A7I9FQL5

- Molecule 20 is a protein called Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	367	Total	C	N	O	S	0	0
			2411	1536	438	430	7		

- Molecule 21 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 22 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 23 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 24 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	149	Total	C	N	O	S	0	0
			921	569	168	180	4		

- Molecule 25 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	46	Total	C	N	O	S	0	0
			383	242	67	71	3		

- Molecule 26 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	49	Total	C	N	O	S	0	0
			381	241	63	74	3		

- Molecule 27 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	38	Total	C	N	O	P	0	0
			791	376	161	216	38		

- Molecule 28 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	48	Total	C	N	O	P	0	0
			968	468	150	302	48		

- Molecule 29 is a protein called TATA-box-binding protein.

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

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

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

- Molecule 31 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	5	Total	C	N	O	P	0	0
			110	50	25	31	4		

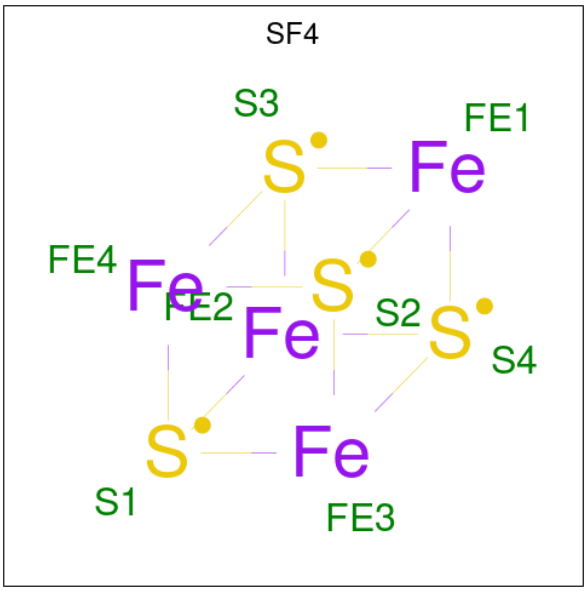
- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	M	1	Total	Zn	0
			1	1	
32	A	2	Total	Zn	0
			2	2	
32	B	1	Total	Zn	0
			1	1	
32	C	1	Total	Zn	0
			1	1	
32	I	2	Total	Zn	0
			2	2	
32	J	1	Total	Zn	0
			1	1	
32	L	1	Total	Zn	0
			1	1	
32	4	1	Total	Zn	0
			1	1	
32	6	4	Total	Zn	0
			4	4	
32	W	1	Total	Zn	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 34 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



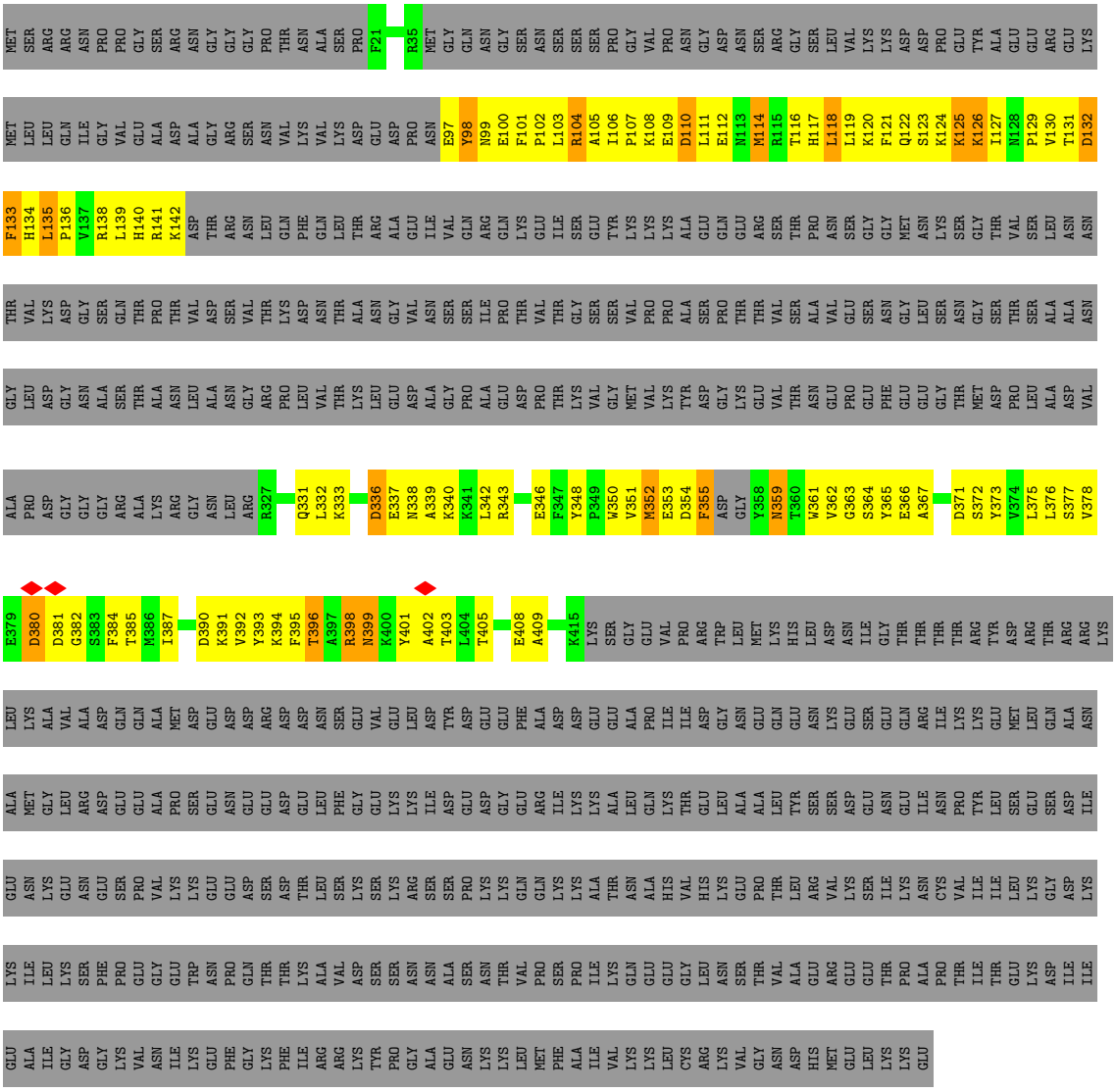
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
34	0	1	8	4	4	0

3 Residue-property plots (i)

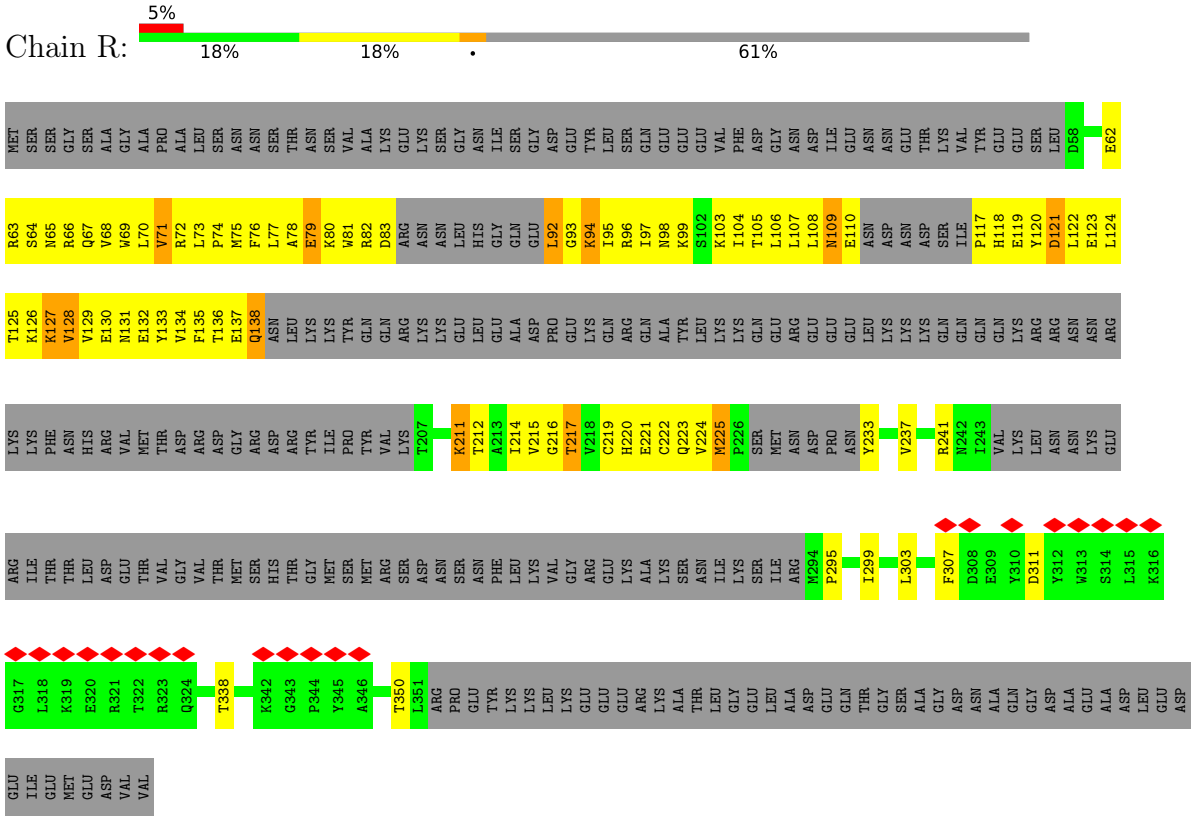
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

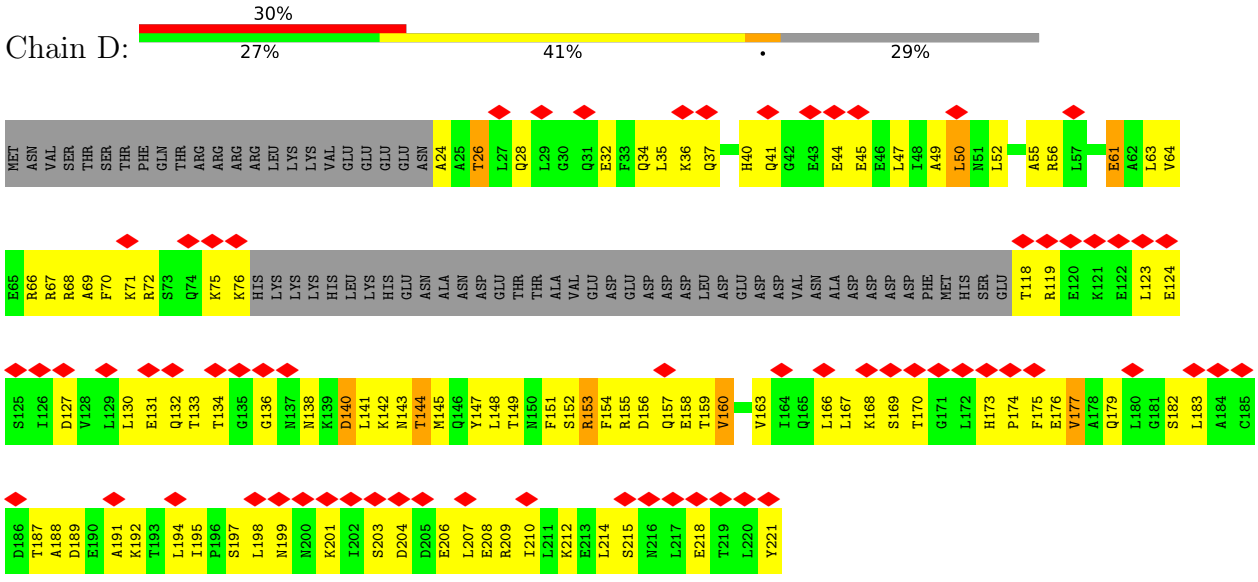
Chain Q: 7% 11% 80%



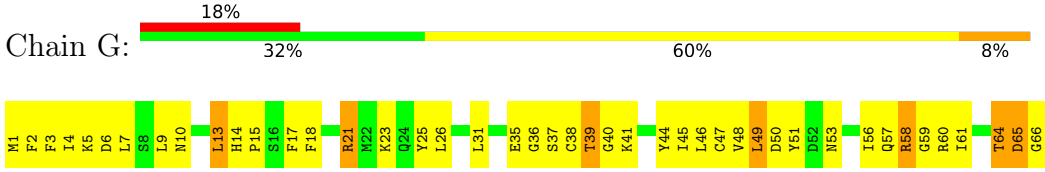
• Molecule 2: Transcription initiation factor IIF subunit beta

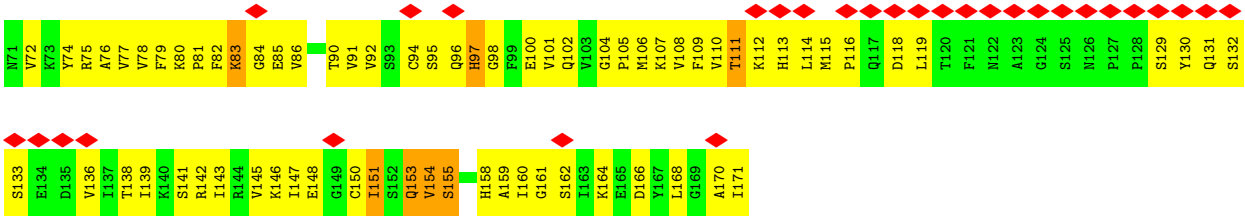


• Molecule 3: DNA-directed RNA polymerase II subunit RPB4



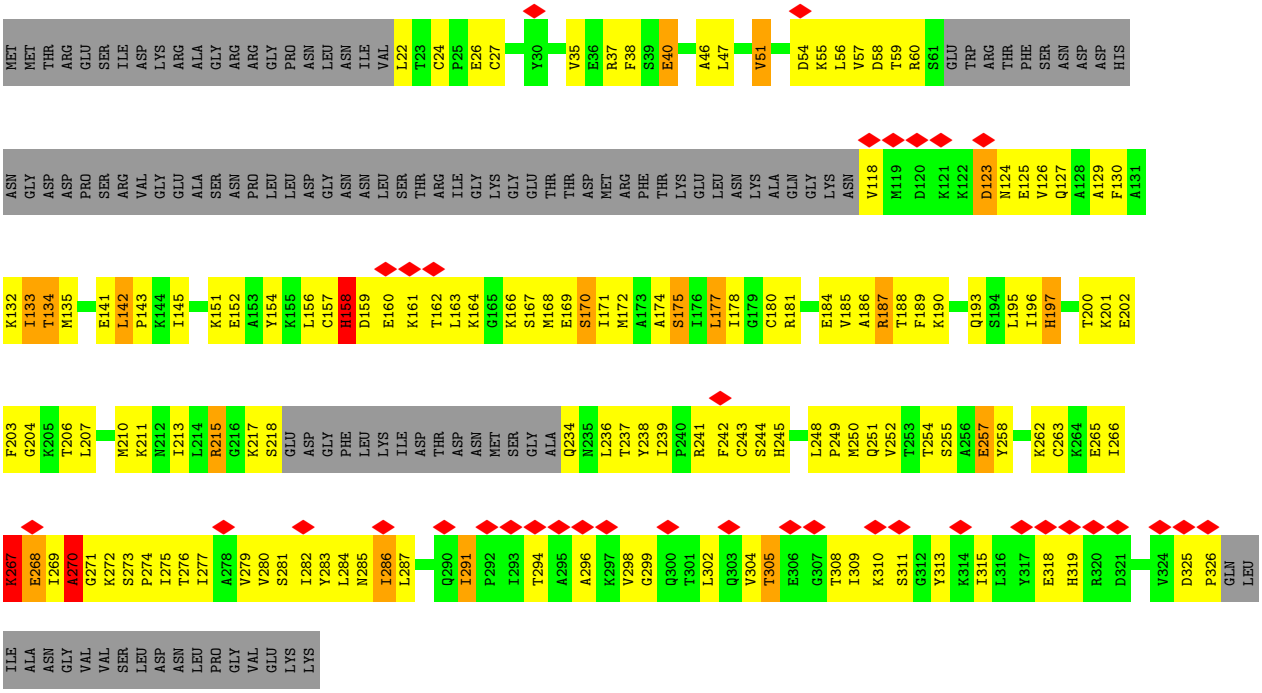
• Molecule 4: DNA-directed RNA polymerase II subunit RPB7





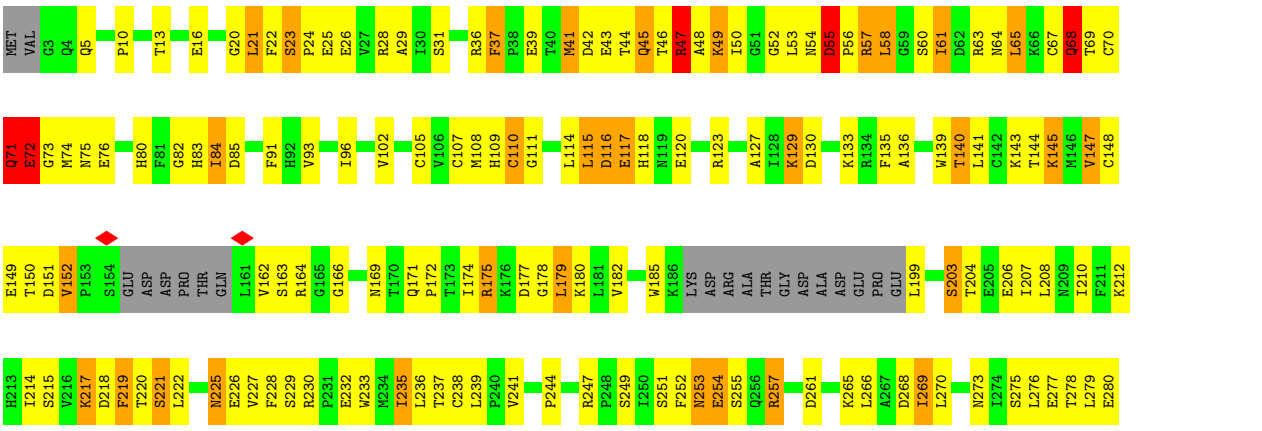
• Molecule 5: Transcription initiation factor IIB

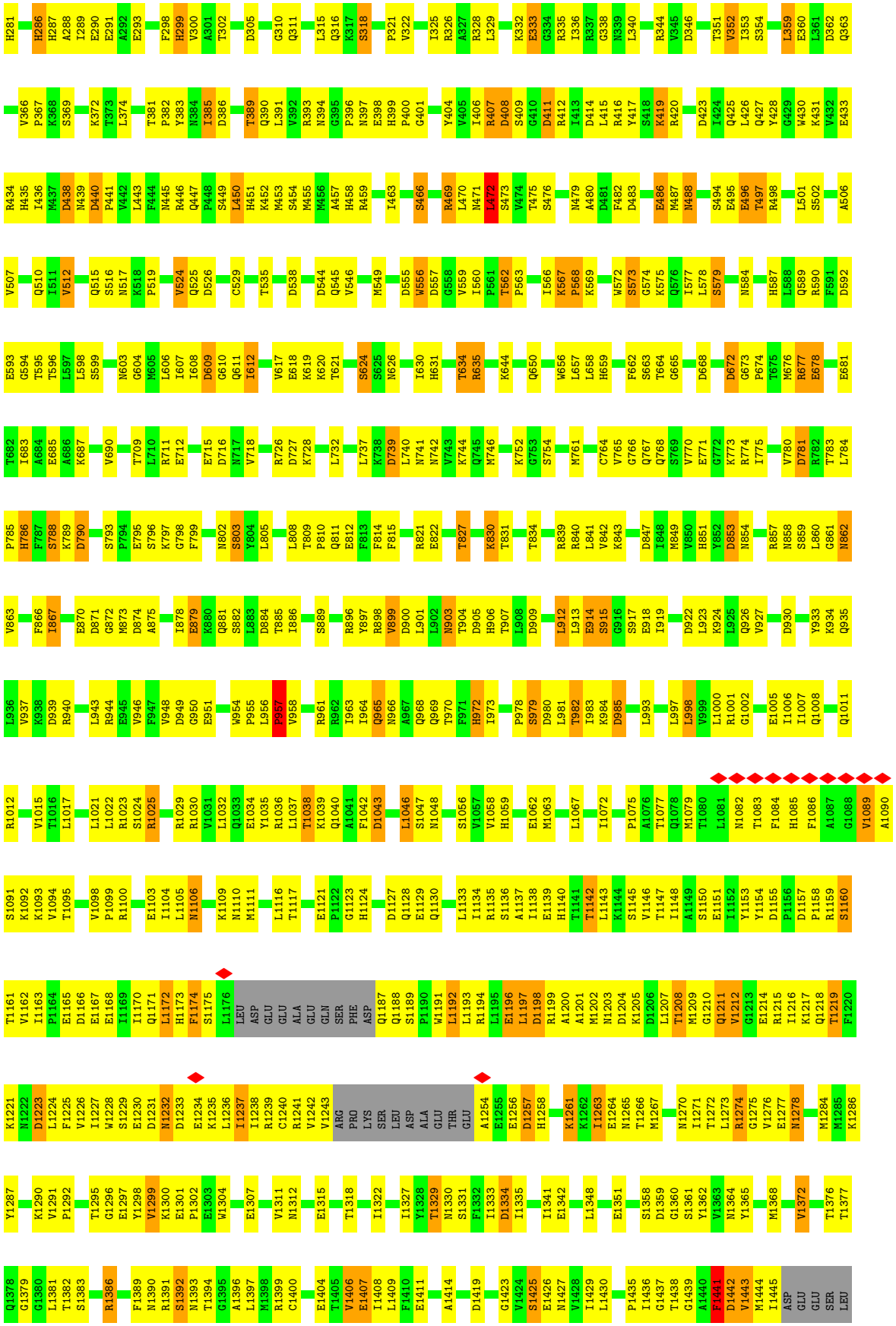
Chain M:



• Molecule 6: DNA-directed RNA polymerase subunit

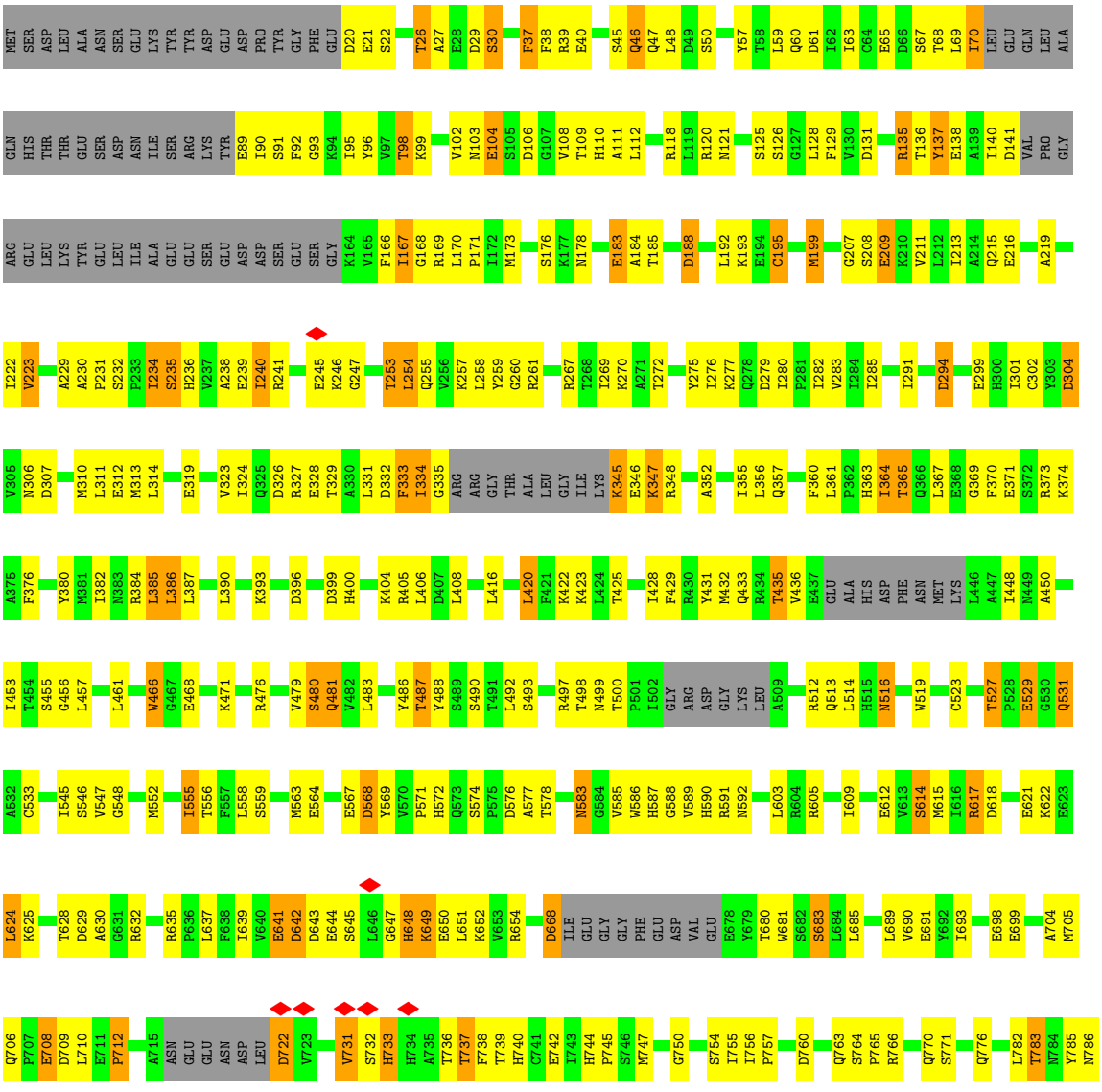
Chain A:

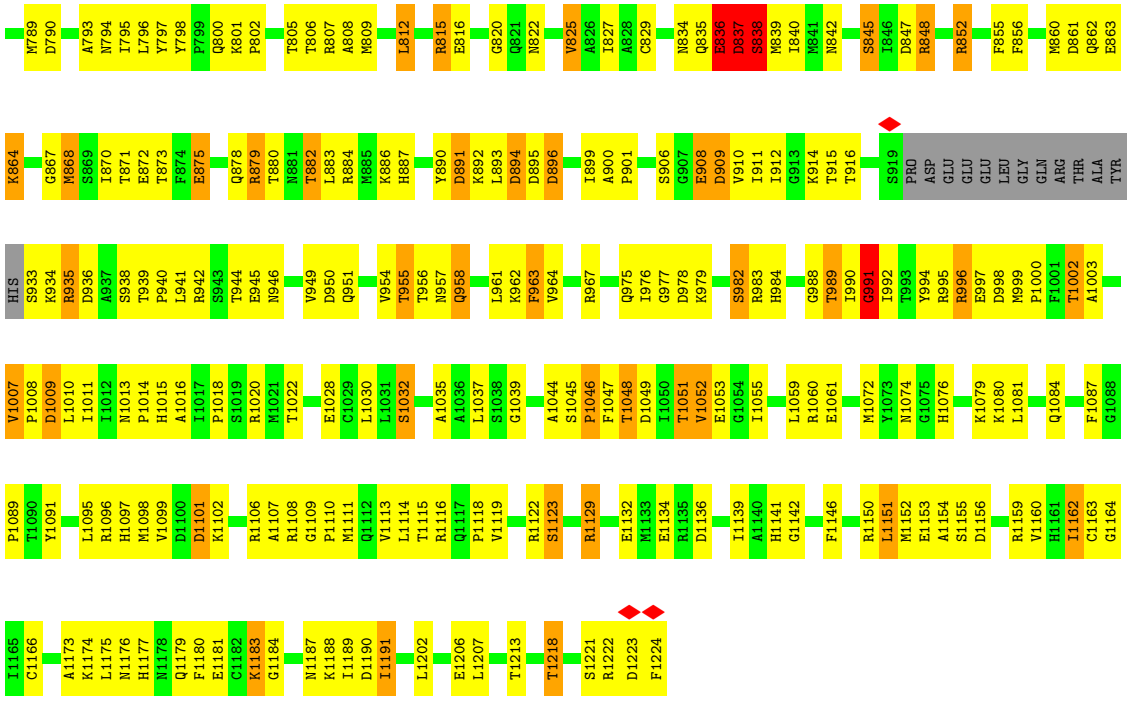




• Molecule 7: DNA-directed RNA polymerase subunit beta

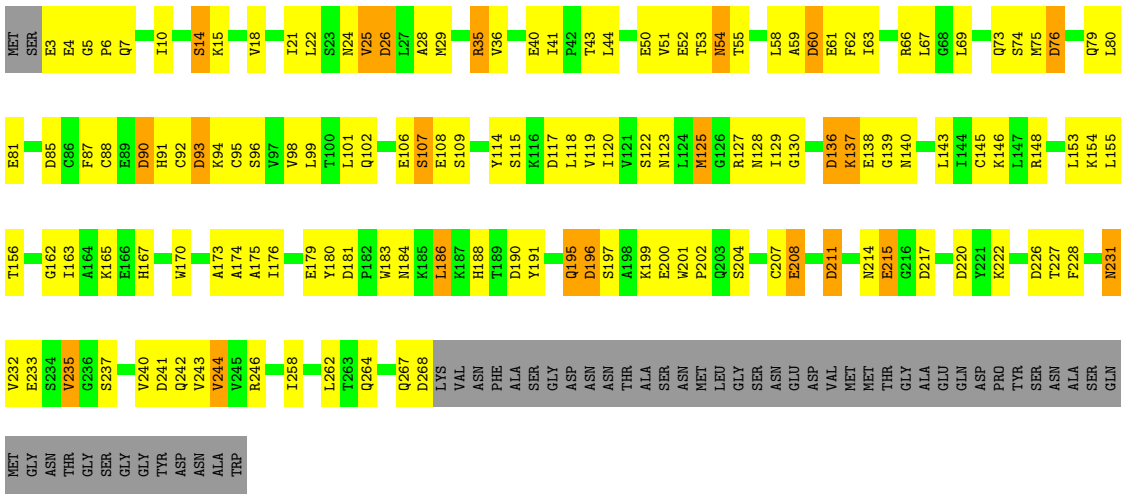
Chain B:





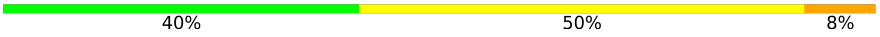
• Molecule 8: DNA-directed RNA polymerase II subunit RPB3

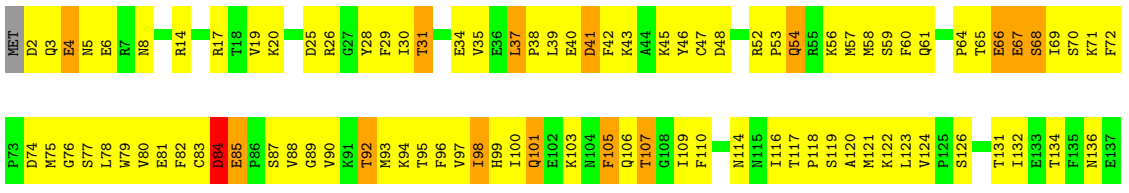
Chain C:

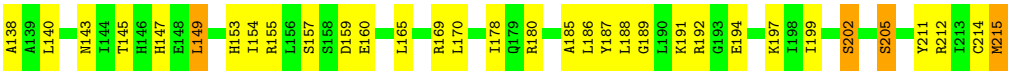


• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

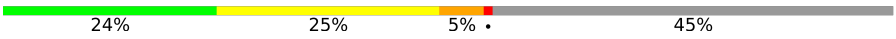


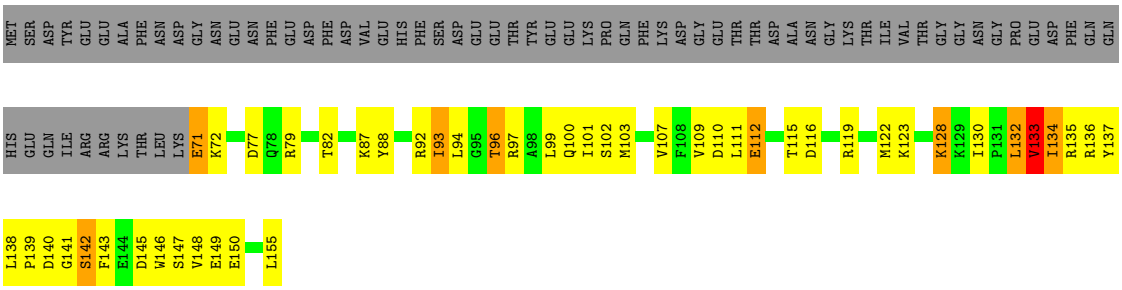




• Molecule 10: DNA-directed RNA polymerases I,II,and III subunit RPABC2

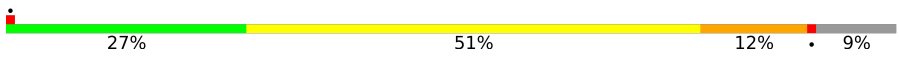
Chain F:

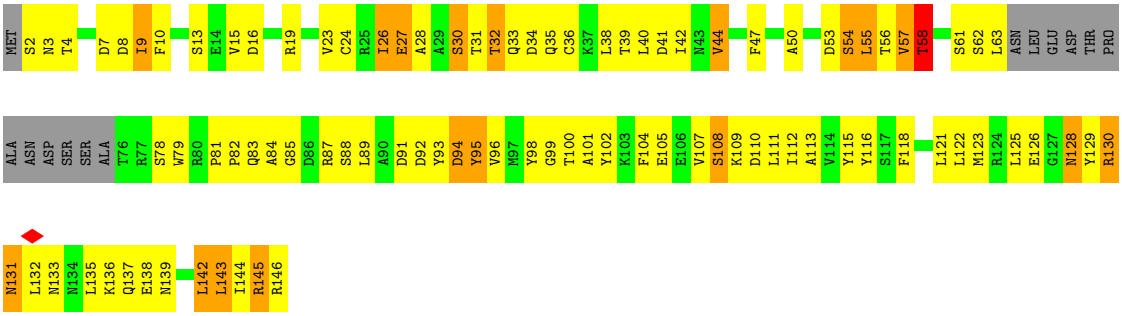




• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

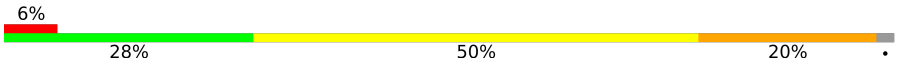
Chain H:

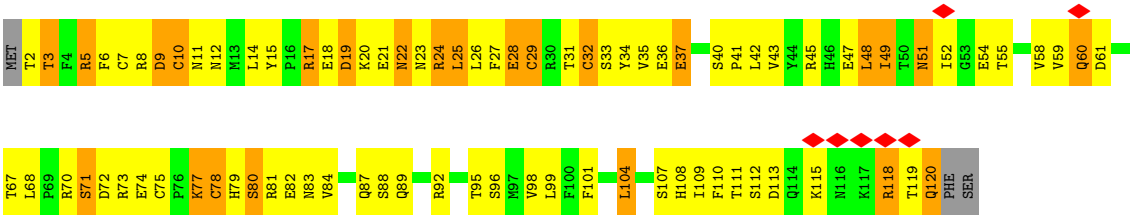




• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

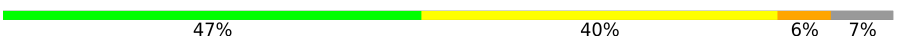
Chain I:

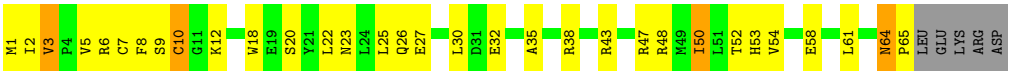




• Molecule 13: DNA-directed RNA polymerases II subunit RPABC5

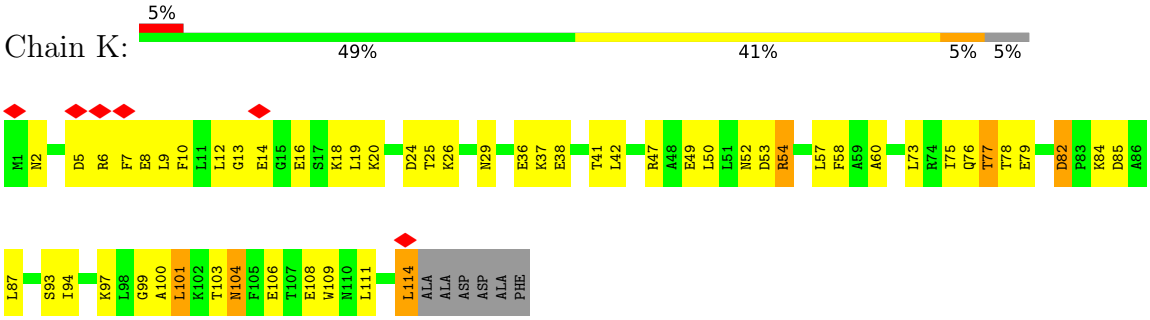
Chain J:





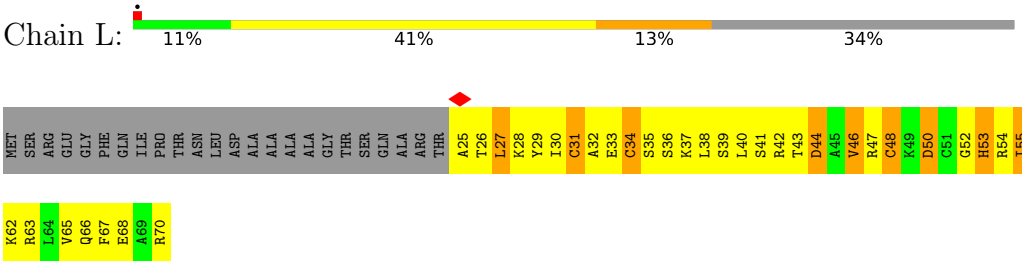
• Molecule 14: DNA-directed RNA polymerase II subunit RPB11

Chain K:



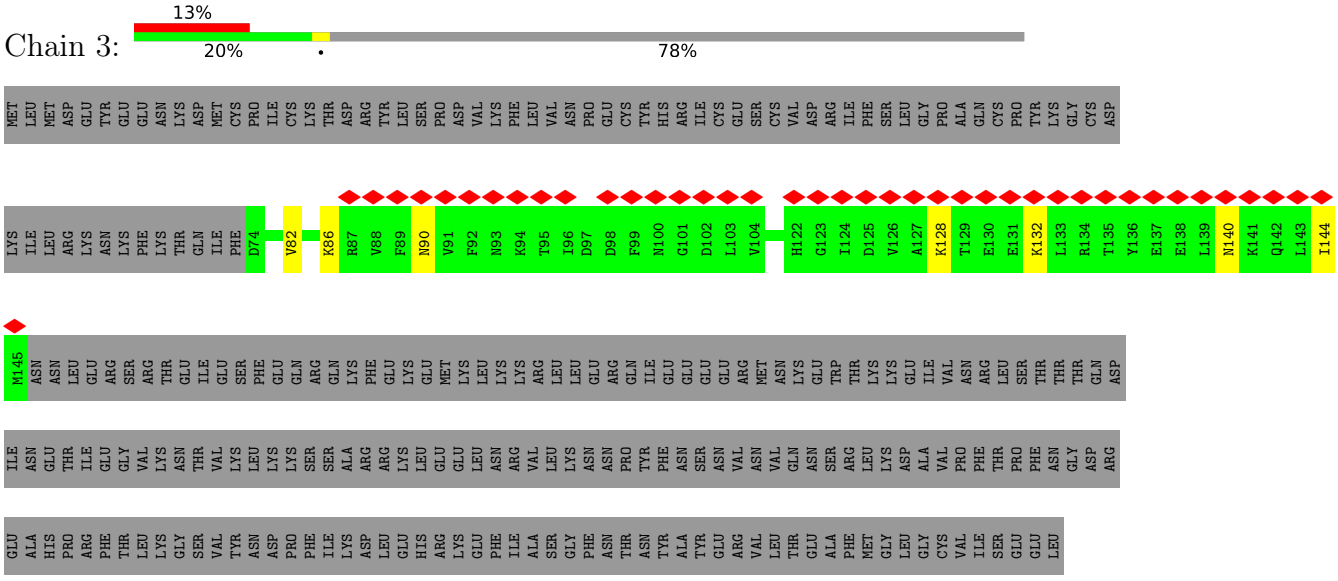
• Molecule 15: DNA-directed RNA polymerases II subunit RPABC4

Chain L:



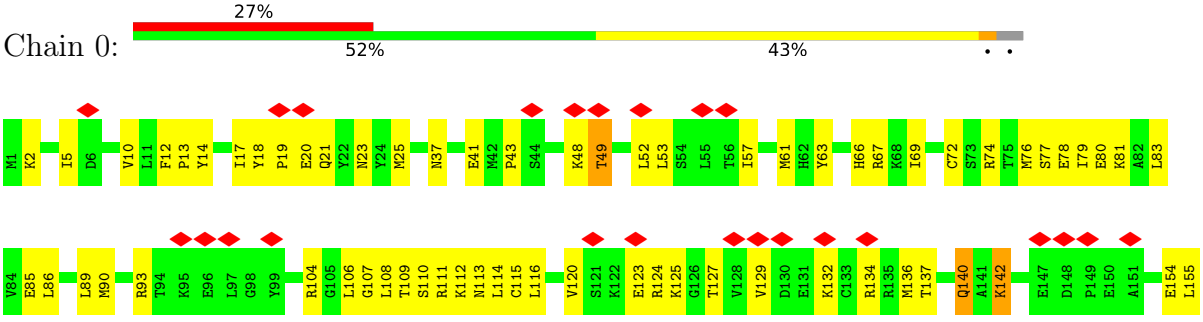
• Molecule 16: BJ4_G0050160.mRNA.1.CDS.1

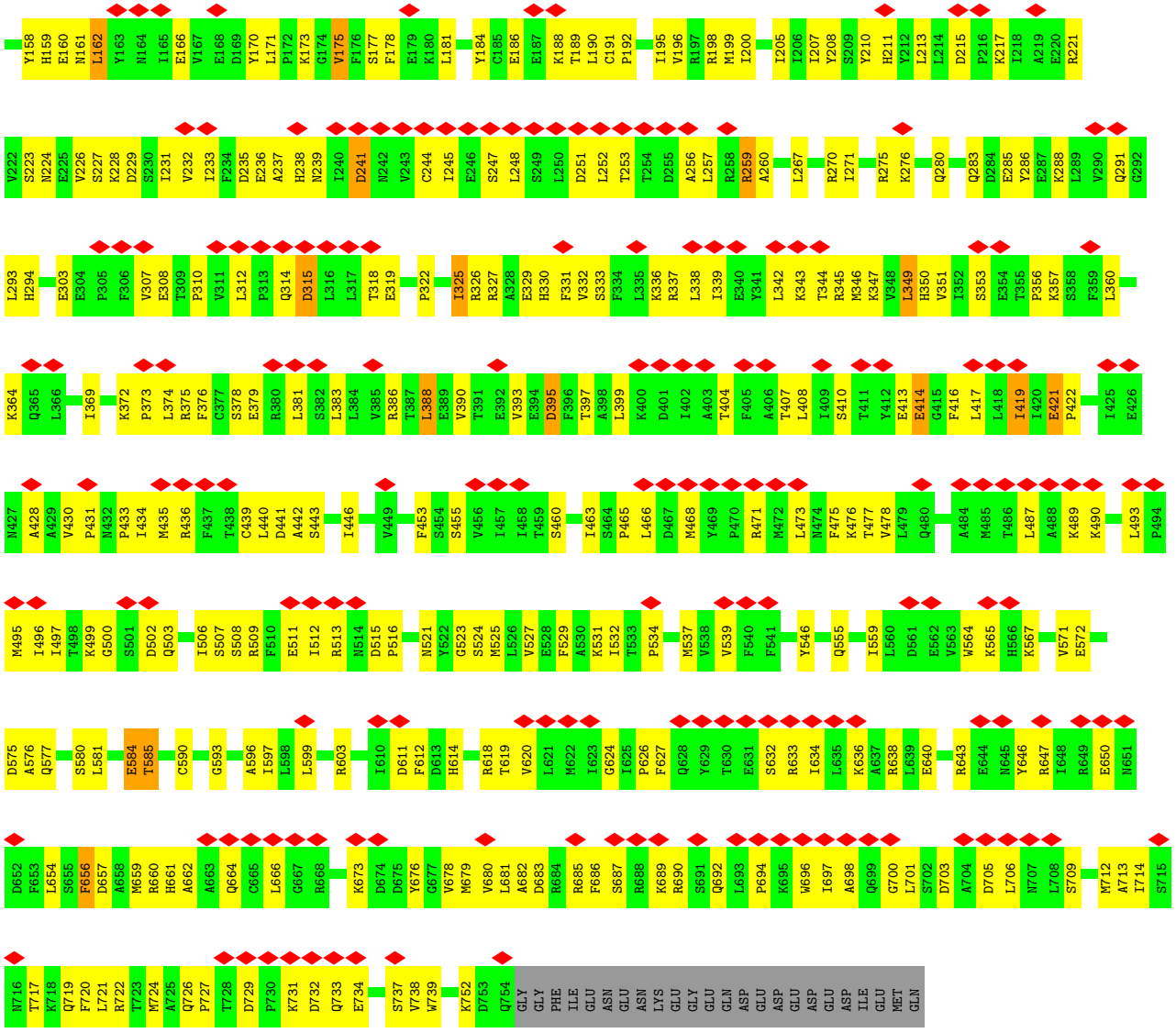
Chain 3:



• Molecule 17: General transcription and DNA repair factor IIH helicase subunit XPD

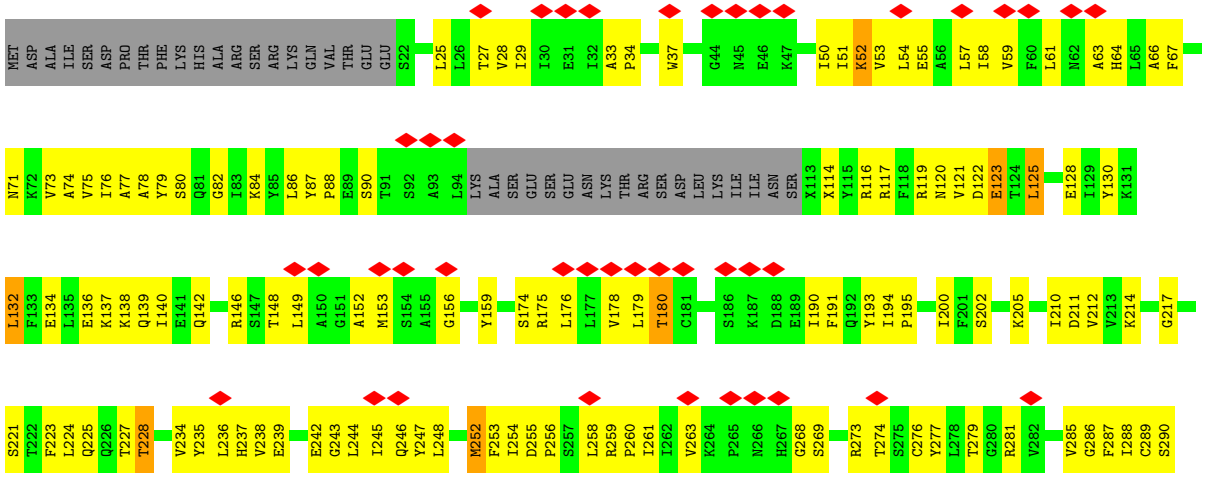
Chain 0:

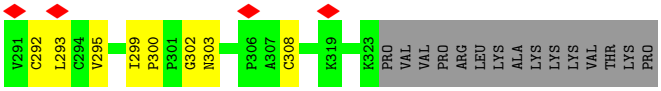




• Molecule 18: General transcription and DNA repair factor IIH subunit TFB4

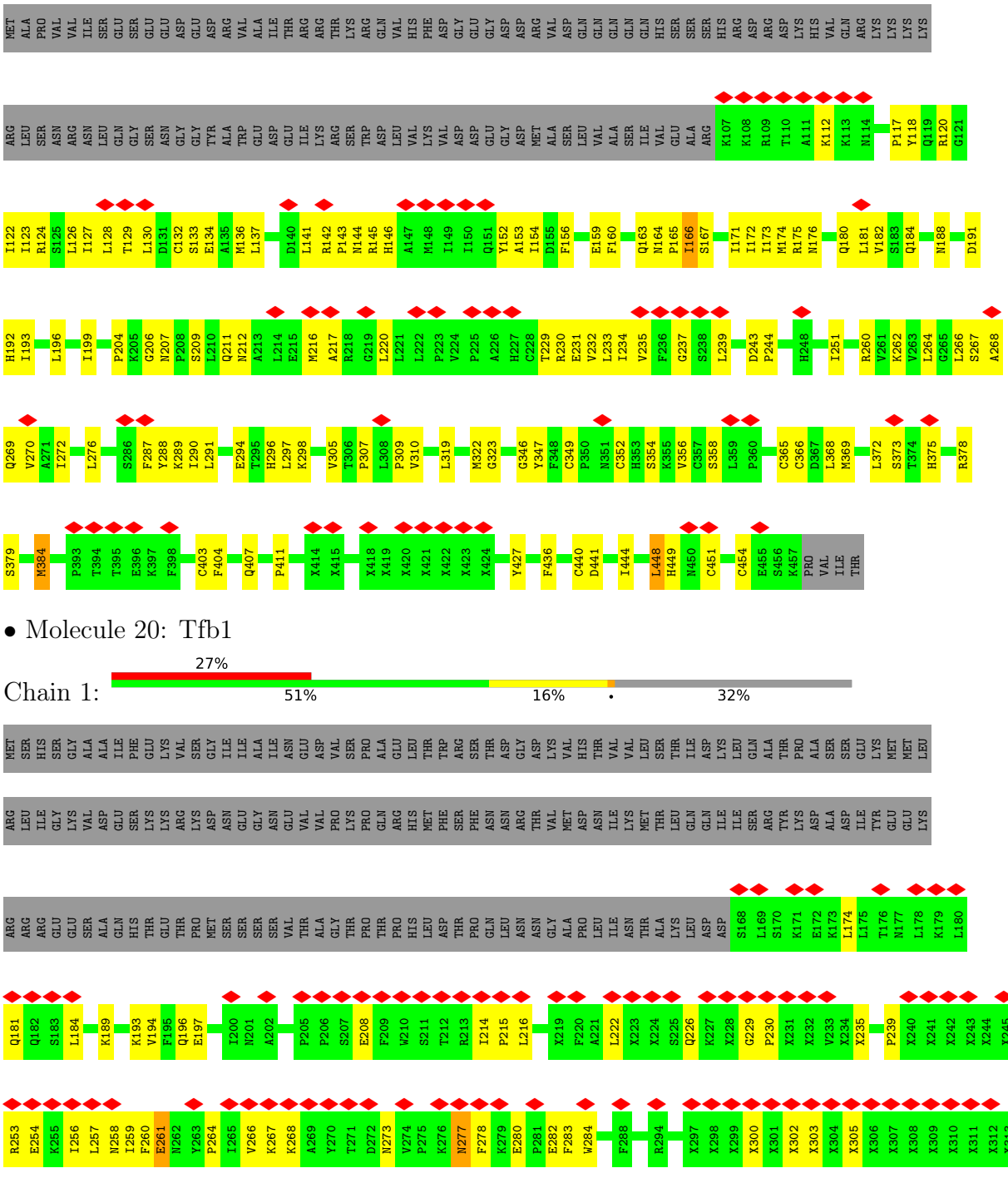
Chain 4:





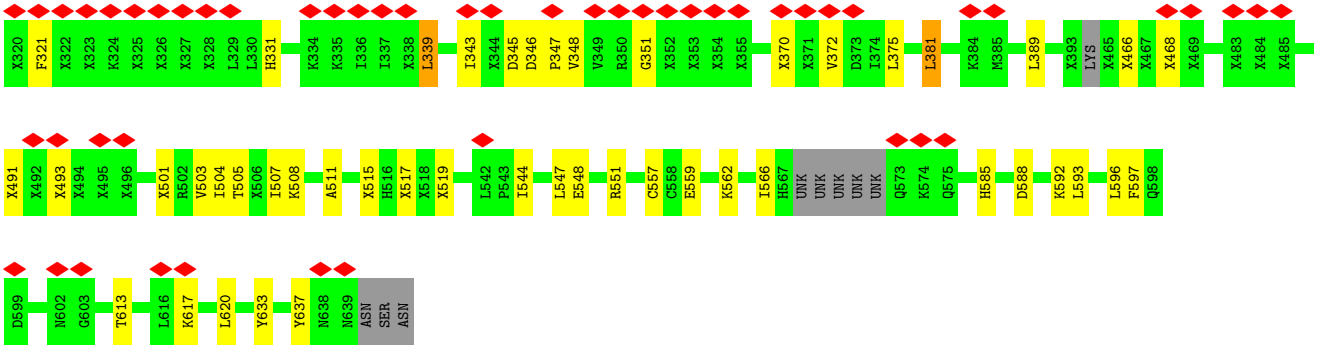
• Molecule 19: General transcription and DNA repair factor IIH

Chain 6:



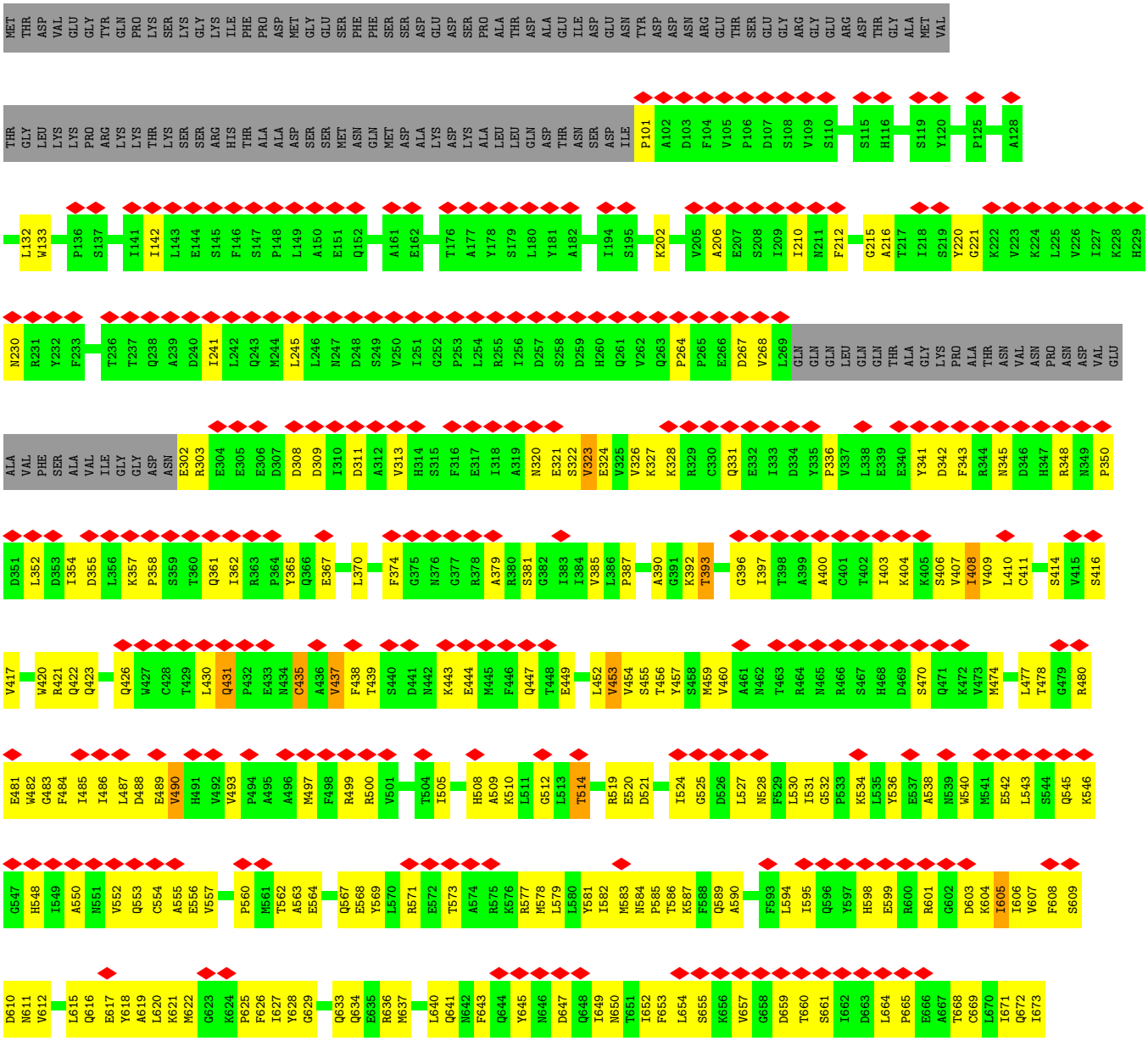
• Molecule 20: Tfb1

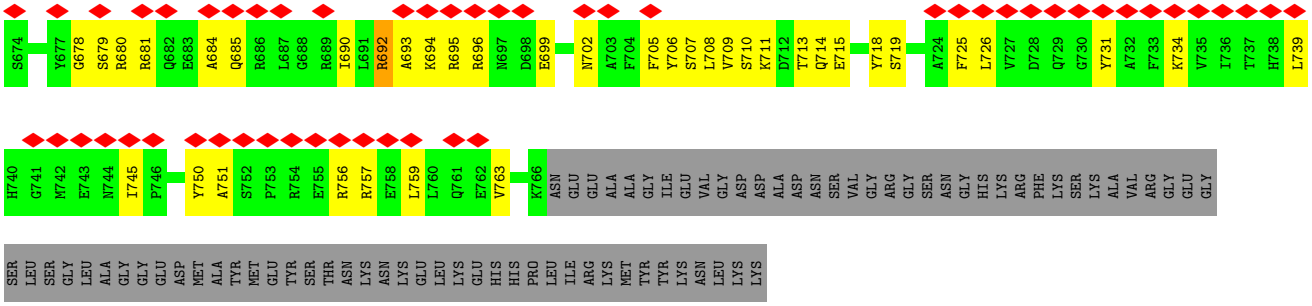
Chain 1:



• Molecule 21: General transcription and DNA repair factor IIH helicase subunit XPB

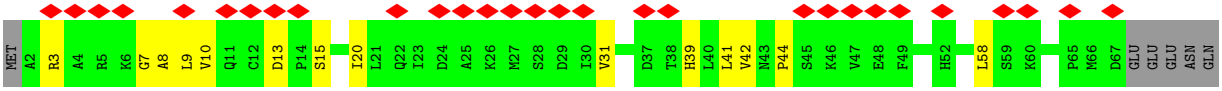
Chain 7:





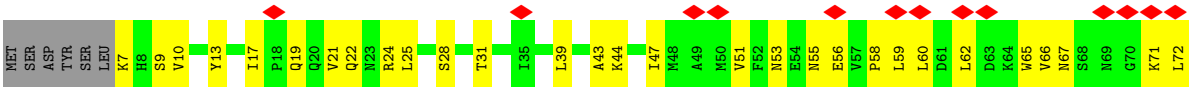
• Molecule 22: General transcription and DNA repair factor IIH subunit TFB5

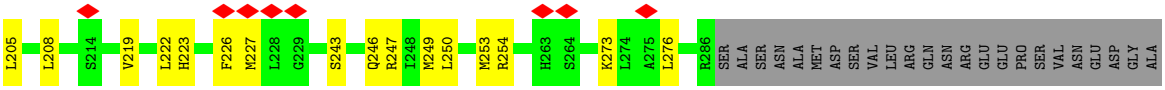
Chain 5:

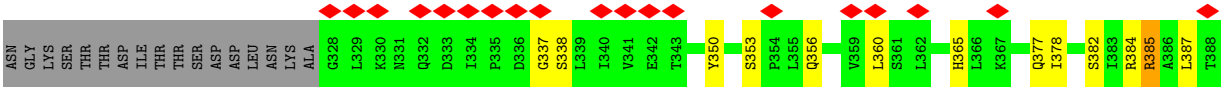


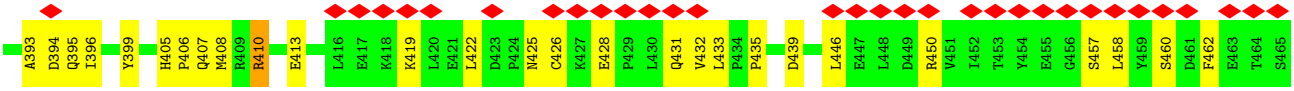
• Molecule 23: RNA polymerase II transcription factor B subunit 2

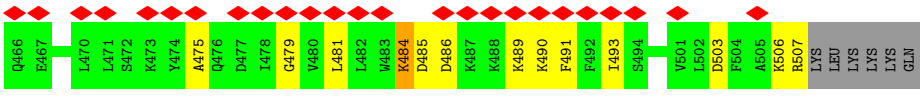
Chain 2:





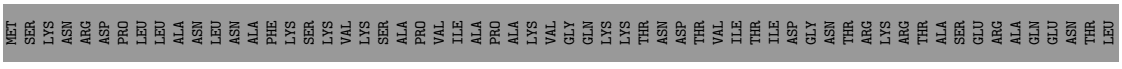


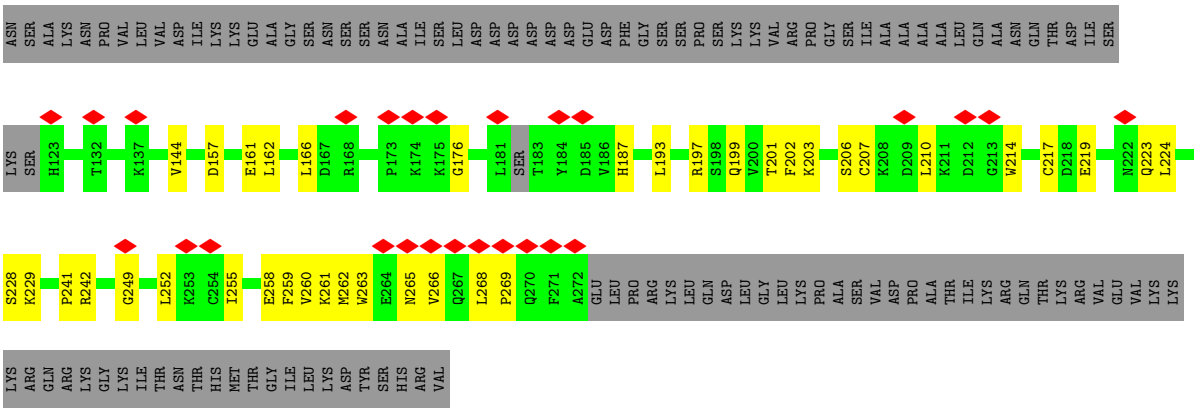




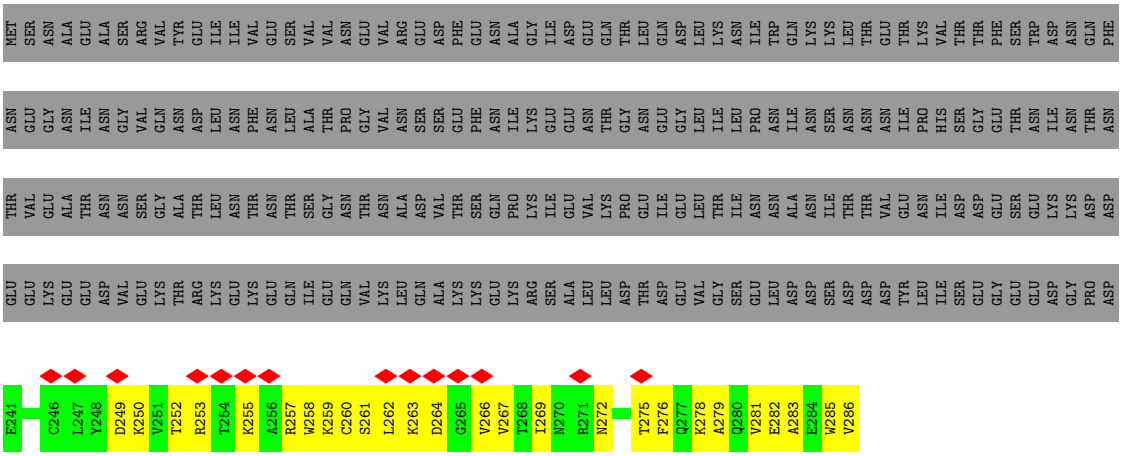
• Molecule 24: Transcription initiation factor IIE subunit beta

Chain X:

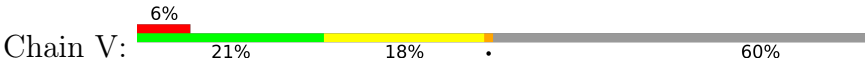


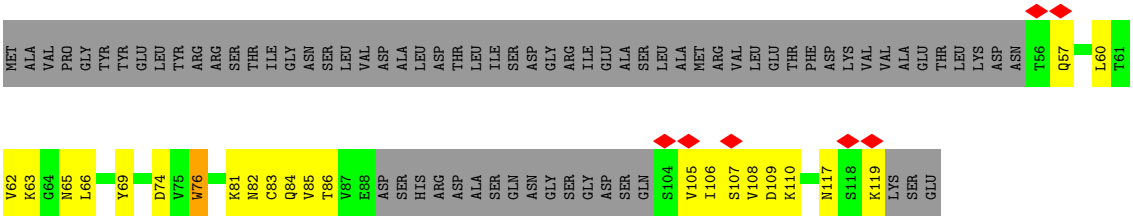


• Molecule 25: Transcription initiation factor IIA large subunit

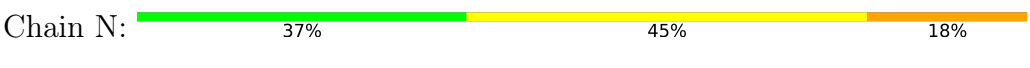


• Molecule 26: Transcription initiation factor IIA subunit 2



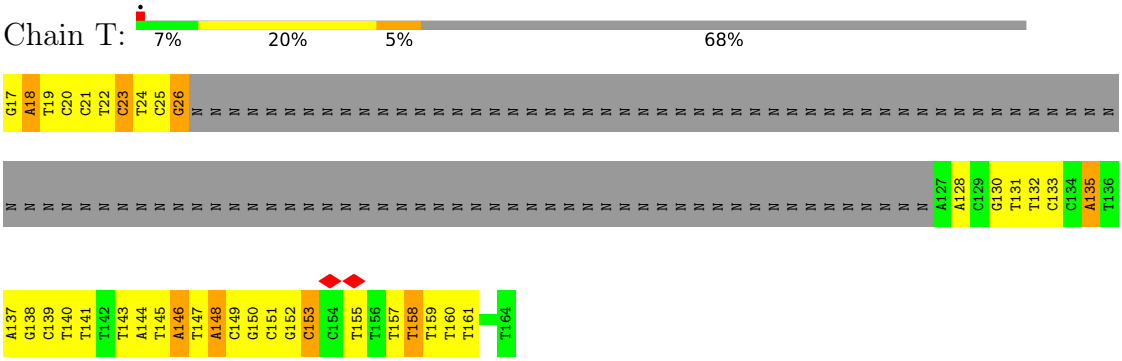


• Molecule 27: non-template strand DNA



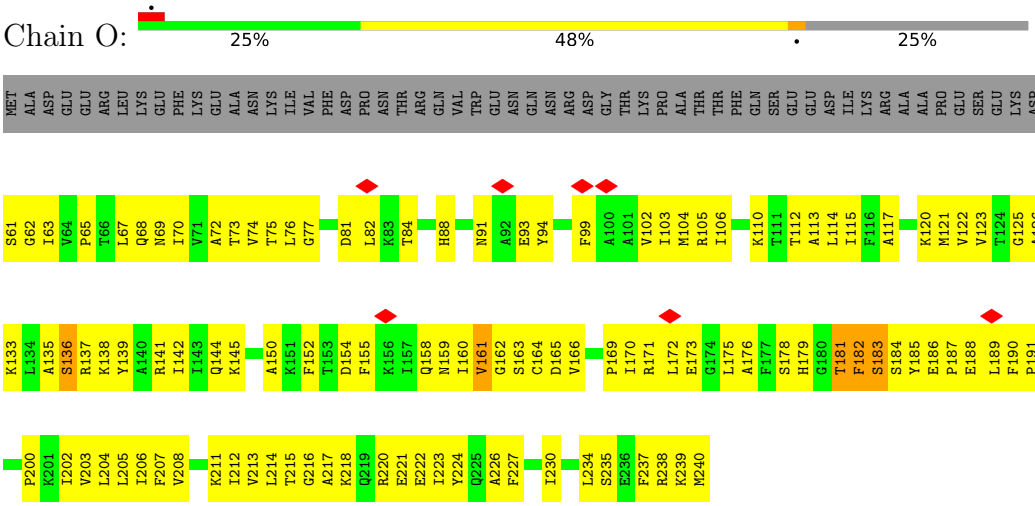
• Molecule 28: template strand DNA

Chain T:



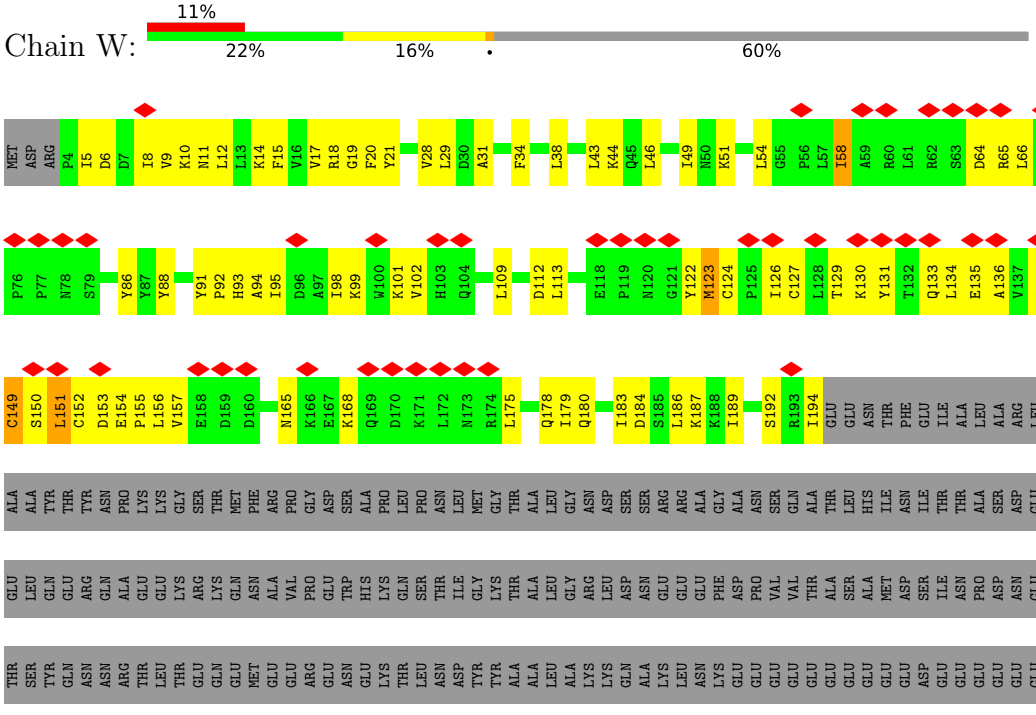
• Molecule 29: TATA-box-binding protein

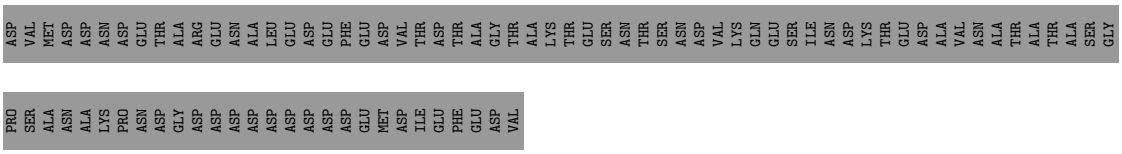
Chain O:



• Molecule 30: Transcription initiation factor IIE subunit alpha

Chain W:





• Molecule 31: RNA

Chain P:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254448	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	444.13998, 503.49997, 508.8	wwPDB
Map dimensions	419, 475, 480	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: MG, ZN, SF4

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	Q	0.49	0/1165	0.55	0/1576
2	R	0.35	0/1047	0.50	0/1422
3	D	0.32	0/1262	0.52	0/1693
4	G	0.53	0/1368	0.57	0/1844
5	M	0.40	0/1828	0.54	0/2459
6	A	1.01	5/11237 (0.0%)	0.74	4/15195 (0.0%)
7	B	1.08	0/9033	0.73	1/12181 (0.0%)
8	C	0.98	0/2133	0.71	0/2891
9	E	0.94	0/1788	0.65	1/2406 (0.0%)
10	F	1.17	0/700	0.76	1/945 (0.1%)
11	H	0.95	0/1086	0.74	0/1470
12	I	0.76	0/989	0.63	0/1331
13	J	1.19	0/541	0.79	0/727
14	K	0.94	0/937	0.66	0/1265
15	L	0.82	0/365	0.77	0/485
16	3	0.23	0/360	0.35	0/501
17	0	0.25	0/6226	0.43	0/8407
18	4	0.26	0/2062	0.46	0/2805
19	6	0.25	0/2506	0.44	0/3402
20	1	0.24	0/1896	0.39	0/2543
21	7	0.25	0/4521	0.43	0/6036
22	5	0.23	0/502	0.42	0/677
23	2	0.24	0/3057	0.42	0/4071
24	X	0.25	0/929	0.43	0/1272
25	U	0.25	0/389	0.48	0/523
26	V	0.26	0/384	0.44	0/518
27	N	0.53	0/893	1.35	16/1377 (1.2%)
28	T	0.51	0/1076	1.45	24/1654 (1.5%)
29	O	0.29	0/1443	0.47	0/1942
30	W	0.27	0/1490	0.44	0/2014
31	P	0.69	0/124	1.59	3/193 (1.6%)
All	All	0.73	5/63337 (0.0%)	0.65	50/85825 (0.1%)

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
1	Q	0	1
4	G	0	1
5	M	0	3
6	A	0	9
7	B	0	5
10	F	0	1
11	H	0	3
All	All	0	23

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	786	HIS	CA-C	-5.82	1.37	1.52
6	A	656	TRP	CB-CG	-5.68	1.40	1.50
6	A	55	ASP	C-N	-5.65	1.23	1.34
6	A	512	VAL	C-N	-5.34	1.21	1.34
6	A	556	TRP	CB-CG	-5.17	1.41	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N	23	DA	O4'-C4'-C3'	-12.58	98.45	106.00
28	T	20	DC	O4'-C4'-C3'	-8.81	100.72	106.00
27	N	23	DA	C4'-C3'-C2'	-8.56	95.39	103.10
27	N	16	DC	O4'-C1'-N1	8.37	113.86	108.00
28	T	19	DT	O4'-C4'-C3'	-8.21	101.07	106.00
28	T	23	DC	N1-C2-O2	-8.12	114.03	118.90
28	T	23	DC	N3-C2-O2	7.81	127.37	121.90
28	T	19	DT	C4'-C3'-C2'	-7.66	96.21	103.10
28	T	146	DA	O4'-C4'-C3'	-7.23	101.61	104.50
31	P	9	G	O4'-C1'-N9	-7.13	102.49	108.20
28	T	153	DC	O4'-C1'-N1	7.11	112.97	108.00
27	N	16	DC	C3'-C2'-C1'	-6.93	94.19	102.50
27	N	16	DC	O4'-C1'-C2'	-6.74	100.50	105.90
27	N	25	DA	C4'-C3'-C2'	-6.70	97.07	103.10
27	N	20	DT	O4'-C4'-C3'	-6.39	101.94	104.50
27	N	30	DA	O4'-C1'-N9	6.33	112.43	108.00
27	N	16	DC	C4'-C3'-C2'	-6.29	97.44	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	T	153	DC	C1'-O4'-C4'	-6.17	103.92	110.10
10	F	133	VAL	CG1-CB-CG2	-6.12	101.12	110.90
28	T	133	DC	C1'-O4'-C4'	-6.05	104.05	110.10
31	P	6	G	O4'-C1'-N9	6.02	113.02	108.20
28	T	23	DC	C3'-C2'-C1'	-6.02	95.28	102.50
9	E	84	ASP	C-N-CA	-5.95	106.82	121.70
6	A	472	LEU	CA-CB-CG	-5.95	101.62	115.30
28	T	18	DA	O4'-C4'-C3'	-5.91	102.14	104.50
28	T	23	DC	O4'-C1'-N1	5.90	112.13	108.00
27	N	23	DA	C1'-O4'-C4'	-5.85	104.25	110.10
27	N	14	DC	C3'-C2'-C1'	-5.80	95.53	102.50
31	P	9	G	N9-C1'-C2'	5.80	121.54	114.00
28	T	148	DA	O4'-C1'-N9	5.76	112.03	108.00
28	T	148	DA	C4'-C3'-C2'	-5.73	97.94	103.10
27	N	23	DA	O4'-C1'-N9	5.67	111.97	108.00
28	T	139	DC	C3'-C2'-C1'	-5.59	95.79	102.50
27	N	25	DA	O4'-C4'-C3'	-5.53	102.29	104.50
28	T	133	DC	O4'-C1'-N1	5.47	111.83	108.00
28	T	135	DA	C3'-C2'-C1'	-5.42	96.00	102.50
28	T	26	DG	O4'-C4'-C3'	-5.39	102.34	104.50
6	A	761	MET	C-N-CA	-5.34	108.34	121.70
28	T	19	DT	O4'-C1'-N1	5.26	111.68	108.00
6	A	1442	ASP	CB-CA-C	-5.25	99.90	110.40
27	N	37	DG	C3'-C2'-C1'	-5.18	96.28	102.50
28	T	158	DT	O4'-C1'-N1	5.15	111.60	108.00
28	T	18	DA	C4'-C3'-C2'	-5.14	98.47	103.10
28	T	26	DG	C4'-C3'-C2'	-5.09	98.52	103.10
27	N	12	DG	C1'-O4'-C4'	-5.06	105.04	110.10
7	B	624	LEU	CA-CB-CG	5.04	126.90	115.30
6	A	21	LEU	CA-CB-CG	-5.03	103.73	115.30
28	T	23	DC	C6-N1-C2	5.03	122.31	120.30
27	N	14	DC	C4'-C3'-C2'	-5.02	98.58	103.10
28	T	139	DC	C4'-C3'-C2'	-5.02	98.58	103.10

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1441	PHE	Peptide
6	A	1443	VAL	Peptide
6	A	47	ARG	Peptide
6	A	524	VAL	Peptide

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Mol	Chain	Res	Type	Group
6	A	55	ASP	Peptide
6	A	568	PRO	Peptide
6	A	65	LEU	Peptide
6	A	71	GLN	Peptide
6	A	957	PRO	Peptide
7	B	648	HIS	Peptide
7	B	836	GLU	Peptide
7	B	837	ASP	Peptide
7	B	838	SER	Peptide
7	B	991	GLY	Peptide
10	F	133	VAL	Peptide
4	G	56	ILE	Peptide
11	H	131	ASN	Peptide
11	H	54	SER	Peptide
11	H	57	VAL	Peptide
5	M	267	LYS	Peptide
5	M	268	GLU	Peptide
5	M	270	ALA	Peptide
1	Q	125	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1141	0	1027	130	0
2	R	1039	0	857	124	0
3	D	1253	0	1275	102	0
4	G	1340	0	1357	118	0
5	M	1805	0	1895	115	0
6	A	11039	0	11122	727	0
7	B	8861	0	8884	494	0
8	C	2095	0	2051	112	0
9	E	1752	0	1776	112	0
10	F	688	0	707	73	0
11	H	1068	0	1040	123	0
12	I	971	0	927	96	0
13	J	532	0	542	27	0
14	K	919	0	929	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	363	0	389	50	0
16	3	361	0	150	4	0
17	0	6108	0	6167	270	0
18	4	2041	0	1954	108	0
19	6	2527	0	2321	96	0
20	1	2411	0	1879	57	0
21	7	4447	0	3905	197	0
22	5	498	0	506	11	0
23	2	3011	0	2600	82	0
24	X	921	0	650	33	0
25	U	383	0	384	26	0
26	V	381	0	388	22	0
27	N	791	0	426	40	0
28	T	968	0	552	55	0
29	O	1416	0	1493	151	0
30	W	1469	0	1433	88	0
31	P	110	0	56	13	0
32	4	1	0	0	0	0
32	6	4	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	W	1	0	0	0	0
33	A	1	0	0	0	0
34	0	8	0	0	2	0
All	All	62733	0	59642	3374	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 28.

All (3374) 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)
6:A:68:GLN:NE2	6:A:80:HIS:ND1	1.92	1.16
11:H:55:LEU:H	11:H:146:ARG:HA	1.12	1.10
6:A:1444:MET:HA	10:F:133:VAL:HA	1.19	1.09
6:A:68:GLN:NE2	6:A:80:HIS:CE1	2.23	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:68:GLN:HE22	6:A:80:HIS:CG	1.74	1.05
6:A:68:GLN:NE2	6:A:80:HIS:CG	2.27	1.01
17:0:191:CYS:HB3	34:0:801:SF4:S3	2.00	1.00
15:L:31:CYS:SG	15:L:34:CYS:N	2.34	0.99
6:A:1423:GLY:O	6:A:1427:ASN:ND2	1.99	0.95
5:M:271:GLY:HA2	5:M:277:ILE:HG13	1.48	0.95
7:B:757:PRO:HD3	7:B:983:ARG:HE	1.32	0.94
18:4:228:THR:HG21	18:4:235:TYR:HB2	1.48	0.93
9:E:99:HIS:O	9:E:103:LYS:NZ	2.02	0.93
11:H:128:ASN:O	11:H:131:ASN:ND2	2.02	0.93
1:Q:98:TYR:HA	2:R:98:ASN:HA	1.49	0.92
11:H:55:LEU:N	11:H:146:ARG:HA	1.83	0.92
21:7:411:CYS:H	21:7:456:THR:HA	1.33	0.92
8:C:66:ARG:NH2	13:J:3:VAL:O	2.02	0.91
7:B:188:ASP:OD1	7:B:188:ASP:N	2.00	0.91
1:Q:377:SER:HB3	1:Q:385:THR:H	1.35	0.91
6:A:43:GLU:O	6:A:45:GLN:NE2	2.03	0.90
9:E:41:ASP:OD1	9:E:41:ASP:N	2.01	0.89
6:A:57:ARG:O	6:A:68:GLN:HG2	1.69	0.89
6:A:68:GLN:HE22	6:A:80:HIS:CD2	1.89	0.89
12:I:19:ASP:HB3	12:I:24:ARG:H	1.37	0.89
6:A:985:ASP:OD1	6:A:985:ASP:N	2.04	0.89
7:B:838:SER:OG	7:B:989:THR:N	2.05	0.89
6:A:68:GLN:HE21	6:A:80:HIS:CE1	1.88	0.88
12:I:78:CYS:SG	12:I:79:HIS:N	2.46	0.88
7:B:195:CYS:HG	7:B:783:THR:HG1	1.21	0.88
5:M:141:GLU:OE1	7:B:103:ASN:ND2	2.07	0.86
6:A:49:LYS:NZ	6:A:55:ASP:O	2.08	0.86
9:E:56:LYS:HE2	9:E:84:ASP:HB2	1.57	0.86
8:C:211:ASP:OD1	8:C:211:ASP:N	2.07	0.86
7:B:668:ASP:N	7:B:668:ASP:OD1	2.05	0.86
6:A:746:MET:HE3	7:B:1015:HIS:HA	1.58	0.86
8:C:3:GLU:O	8:C:7:GLN:NE2	2.08	0.86
11:H:54:SER:HB3	11:H:146:ARG:HB3	1.56	0.86
30:W:43:LEU:HG	30:W:54:LEU:HD11	1.56	0.85
6:A:1232:ASN:ND2	6:A:1233:ASP:OD1	2.09	0.85
7:B:229:ALA:O	7:B:261:ARG:NH2	2.09	0.85
15:L:50:ASP:OD1	15:L:50:ASP:N	2.08	0.85
3:D:206:GLU:HG2	3:D:209:ARG:HE	1.41	0.85
8:C:76:ASP:N	8:C:76:ASP:OD1	2.08	0.85
6:A:1334:ASP:N	6:A:1334:ASP:OD1	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:148:ARG:NH1	13:J:64:ASN:O	2.11	0.84
6:A:767:GLN:NE2	6:A:768:GLN:O	2.10	0.84
12:I:32:CYS:SG	12:I:33:SER:N	2.50	0.84
6:A:290:GLU:OE1	6:A:290:GLU:N	2.09	0.84
6:A:383:TYR:HB3	10:F:115:THR:HG23	1.58	0.84
6:A:71:GLN:O	6:A:73:GLY:N	2.10	0.83
6:A:853:ASP:OD1	6:A:853:ASP:N	2.11	0.83
6:A:362:ASP:OD2	6:A:459:ARG:NH1	2.11	0.83
6:A:1197:LEU:HD11	6:A:1238:ILE:HD11	1.60	0.83
11:H:131:ASN:O	11:H:133:ASN:N	2.12	0.83
30:W:149:CYS:SG	30:W:150:SER:N	2.52	0.83
6:A:567:LYS:HB2	11:H:96:VAL:H	1.44	0.82
7:B:837:ASP:OD1	7:B:837:ASP:N	2.09	0.82
7:B:167:ILE:HD11	7:B:453:ILE:HD12	1.60	0.82
5:M:215:ARG:HB3	29:O:181:THR:HG23	1.61	0.82
29:O:68:GLN:H	29:O:162:GLY:HA2	1.45	0.82
6:A:1151:GLU:OE2	12:I:45:ARG:NH1	2.13	0.82
2:R:63:ARG:HE	2:R:65:ASN:HB3	1.43	0.82
6:A:1158:PRO:HB3	6:A:1188:GLN:HE22	1.45	0.81
9:E:40:GLU:OE1	9:E:40:GLU:N	2.13	0.81
6:A:674:PRO:O	6:A:677:ARG:NH1	2.14	0.81
29:O:206:ILE:HG12	29:O:212:ILE:HG23	1.62	0.81
21:7:490:VAL:HB	21:7:519:ARG:HH22	1.43	0.81
23:2:71:LYS:NZ	23:2:75:GLN:OE1	2.14	0.81
27:N:23:DA:H2"	29:O:158:GLN:HB3	1.62	0.81
6:A:49:LYS:NZ	6:A:55:ASP:OD2	2.12	0.81
6:A:120:GLU:OE2	6:A:123:ARG:NH1	2.13	0.81
6:A:1443:VAL:HG21	10:F:93:ILE:HD11	1.62	0.81
7:B:979:LYS:NZ	31:P:9:G:O3'	2.14	0.81
6:A:25:GLU:OE1	6:A:25:GLU:N	2.10	0.81
12:I:7:CYS:O	12:I:11:ASN:N	2.12	0.81
3:D:55:ALA:HB3	3:D:148:LEU:HD21	1.61	0.81
4:G:95:SER:O	4:G:130:TYR:OH	1.99	0.81
6:A:1173:HIS:CE1	6:A:1228:TRP:H	1.99	0.80
7:B:647:GLY:HA3	7:B:648:HIS:HB3	1.62	0.80
6:A:46:THR:O	6:A:48:ALA:N	2.14	0.80
6:A:127:ALA:O	6:A:129:LYS:NZ	2.14	0.80
6:A:567:LYS:O	6:A:569:LYS:N	2.14	0.80
9:E:54:GLN:OE1	9:E:57:MET:N	2.15	0.80
13:J:10:CYS:SG	13:J:43:ARG:NH2	2.52	0.80
6:A:37:PHE:HB2	6:A:39:GLU:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:848:ARG:NH1	13:J:8:PHE:O	2.15	0.80
7:B:891:ASP:N	7:B:891:ASP:OD1	2.10	0.80
2:R:138:GLN:NE2	2:R:138:GLN:H	1.79	0.80
18:4:285:VAL:HA	19:6:323:GLY:HA2	1.64	0.80
29:O:192:GLY:HA2	29:O:207:PHE:HA	1.64	0.80
9:E:67:GLU:OE1	9:E:67:GLU:N	2.15	0.79
11:H:135:LEU:O	11:H:137:GLN:NE2	2.13	0.79
3:D:192:LYS:HG2	3:D:199:ASN:HA	1.64	0.79
12:I:8:ARG:NH1	12:I:9:ASP:OD1	2.14	0.79
7:B:641:GLU:O	7:B:650:GLU:N	2.15	0.79
6:A:147:VAL:HG23	6:A:149:GLU:H	1.45	0.79
7:B:763:GLN:HG2	7:B:765:PRO:HD2	1.64	0.79
7:B:708:GLU:OE1	7:B:708:GLU:N	2.15	0.79
7:B:706:GLN:H	7:B:710:LEU:HD23	1.48	0.79
23:2:7:LYS:HG2	23:2:9:SER:H	1.48	0.79
1:Q:339:ALA:O	1:Q:343:ARG:N	2.14	0.79
6:A:590:ARG:NH1	6:A:592:ASP:OD1	2.16	0.79
6:A:1008:GLN:HB3	6:A:1012:ARG:HH22	1.47	0.79
7:B:199:MET:N	7:B:199:MET:SD	2.52	0.79
5:M:188:THR:HG22	5:M:190:LYS:H	1.48	0.78
6:A:1215:ARG:NH2	6:A:1272:THR:O	2.15	0.78
7:B:1218:THR:O	7:B:1218:THR:OG1	2.01	0.78
6:A:5:GLN:O	7:B:1159:ARG:NH2	2.16	0.78
6:A:1442:ASP:HB2	10:F:136:ARG:N	1.99	0.78
19:6:126:LEU:HD11	19:6:233:LEU:HB2	1.66	0.78
6:A:438:ASP:OD1	6:A:438:ASP:N	2.15	0.78
7:B:270:LYS:HB3	7:B:279:ASP:HB3	1.66	0.78
5:M:157:CYS:SG	5:M:158:HIS:N	2.54	0.78
7:B:1163:CYS:HB3	7:B:1166:CYS:SG	2.24	0.78
6:A:1162:VAL:HG11	12:I:41:PRO:HG3	1.65	0.78
6:A:926:GLN:NE2	6:A:930:ASP:OD1	2.17	0.78
6:A:219:PHE:HD1	6:A:220:THR:H	1.32	0.78
30:W:92:PRO:HA	30:W:95:ILE:HD12	1.66	0.78
6:A:152:VAL:O	6:A:162:VAL:N	2.15	0.77
3:D:123:LEU:HD11	3:D:145:MET:HB3	1.66	0.77
18:4:79:TYR:HB3	18:4:140:ILE:HG23	1.65	0.77
29:O:102:VAL:HB	29:O:115:ILE:HB	1.66	0.77
6:A:67:CYS:SG	6:A:80:HIS:CE1	2.78	0.77
7:B:997:GLU:OE2	7:B:997:GLU:N	2.12	0.77
17:0:356:PRO:HG2	17:0:413:GLU:HA	1.66	0.77
6:A:746:MET:HE1	7:B:1018:PRO:HG2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1084:GLN:NE2	8:C:190:ASP:O	2.17	0.77
7:B:957:ASN:OD1	7:B:958:GLN:N	2.17	0.77
20:1:557:CYS:SG	20:1:585:HIS:NE2	2.57	0.77
18:4:175:ARG:HE	18:4:256:PRO:HG3	1.47	0.77
6:A:278:THR:HA	6:A:281:HIS:NE2	1.99	0.77
8:C:14:SER:OG	8:C:15:LYS:N	2.14	0.77
3:D:151:PHE:O	3:D:153:ARG:NH1	2.18	0.77
2:R:99:LYS:O	2:R:103:LYS:N	2.18	0.76
5:M:281:SER:O	5:M:285:ASN:ND2	2.18	0.76
11:H:56:THR:O	11:H:144:ILE:N	2.18	0.76
27:N:23:DA:N6	28:T:143:DT:O4	2.18	0.76
4:G:64:THR:OG1	4:G:65:ASP:OD1	2.04	0.76
7:B:135:ARG:NH1	7:B:136:THR:O	2.19	0.76
1:Q:337:GLU:OE2	1:Q:340:LYS:N	2.18	0.76
7:B:235:SER:OG	7:B:236:HIS:ND1	2.16	0.76
12:I:22:ASN:OD1	12:I:22:ASN:N	2.19	0.76
7:B:1187:ASN:HD21	7:B:1190:ASP:HB3	1.49	0.76
25:U:253:ARG:NH1	28:T:144:DA:OP1	2.19	0.76
6:A:1062:GLU:OE1	10:F:88:TYR:OH	2.04	0.76
7:B:1175:LEU:O	7:B:1176:ASN:ND2	2.18	0.76
6:A:118:HIS:HA	6:A:123:ARG:HH22	1.49	0.76
6:A:982:THR:N	6:A:985:ASP:OD2	2.18	0.76
13:J:1:MET:O	13:J:53:HIS:NE2	2.18	0.76
7:B:89:GLU:N	7:B:135:ARG:O	2.18	0.76
7:B:567:GLU:OE1	7:B:567:GLU:N	2.18	0.76
6:A:1215:ARG:O	6:A:1218:GLN:NE2	2.17	0.75
6:A:1215:ARG:O	6:A:1219:THR:OG1	2.04	0.75
9:E:3:GLN:O	9:E:6:GLU:N	2.19	0.75
17:0:134:ARG:NH2	17:0:303:GLU:O	2.19	0.75
29:O:191:PRO:HG2	29:O:207:PHE:HE1	1.51	0.75
5:M:24:CYS:SG	5:M:27:CYS:N	2.57	0.75
6:A:107:CYS:SG	6:A:110:CYS:N	2.59	0.75
12:I:17:ARG:O	12:I:26:LEU:N	2.18	0.75
25:U:262:LEU:HB2	25:U:279:ALA:HB3	1.68	0.75
7:B:996:ARG:HH22	8:C:173:ALA:HB1	1.51	0.75
8:C:60:ASP:OD1	8:C:60:ASP:N	2.15	0.75
3:D:140:ASP:N	3:D:140:ASP:OD1	2.16	0.75
5:M:193:GLN:HE22	5:M:197:HIS:HA	1.51	0.75
18:4:136:GLU:HA	18:4:140:ILE:HG13	1.68	0.75
18:4:84:LYS:HB3	18:4:132:LEU:HD12	1.67	0.75
3:D:119:ARG:HD2	3:D:155:ARG:HH22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:185:TRP:H	6:A:199:LEU:HD12	1.53	0.74
7:B:864:LYS:HB3	7:B:872:GLU:H	1.51	0.74
1:Q:132:ASP:N	1:Q:132:ASP:OD1	2.21	0.74
4:G:46:LEU:HD12	4:G:77:VAL:HG12	1.70	0.74
15:L:48:CYS:O	15:L:52:GLY:N	2.17	0.74
6:A:1005:GLU:N	6:A:1005:GLU:OE1	2.19	0.74
7:B:529:GLU:HA	7:B:533:CYS:HB2	1.69	0.74
8:C:61:GLU:OE1	8:C:61:GLU:N	2.18	0.74
2:R:75:MET:N	2:R:75:MET:SD	2.60	0.74
17:0:618:ARG:NH1	17:0:676:TYR:O	2.20	0.74
1:Q:120:LYS:O	1:Q:395:PHE:N	2.15	0.74
19:6:132:CYS:HB2	19:6:175:ARG:HG2	1.68	0.74
28:T:144:DA:N3	29:O:69:ASN:ND2	2.35	0.74
17:0:74:ARG:NH1	17:0:239:ASN:OD1	2.21	0.74
20:1:214:ILE:HG13	20:1:215:PRO:HD3	1.70	0.74
29:O:73:THR:HG22	29:O:122:VAL:HG22	1.70	0.74
7:B:867:GLY:HA3	7:B:870:ILE:HB	1.70	0.74
6:A:795:GLU:N	6:A:795:GLU:OE1	2.20	0.73
7:B:642:ASP:OD1	7:B:642:ASP:N	2.18	0.73
7:B:982:SER:OG	7:B:983:ARG:N	2.20	0.73
10:F:149:GLU:N	10:F:149:GLU:OE2	2.20	0.73
30:W:123:MET:HA	30:W:130:LYS:HA	1.70	0.73
2:R:74:PRO:HD2	2:R:224:VAL:HB	1.70	0.73
7:B:326:ASP:O	7:B:329:THR:OG1	2.06	0.73
6:A:711:ARG:NH1	12:I:95:THR:O	2.21	0.73
6:A:821:ARG:HH12	7:B:527:THR:HG21	1.53	0.73
12:I:27:PHE:N	12:I:36:GLU:O	2.21	0.73
6:A:1147:THR:HA	6:A:1197:LEU:HA	1.71	0.73
7:B:195:CYS:SG	7:B:783:THR:OG1	2.43	0.73
9:E:48:ASP:OD1	9:E:52:ARG:N	2.22	0.73
17:0:37:ASN:HB2	17:0:477:THR:HG22	1.70	0.73
6:A:951:GLU:O	6:A:954:TRP:NE1	2.20	0.73
7:B:739:THR:OG1	7:B:740:HIS:ND1	2.20	0.73
9:E:52:ARG:HD3	9:E:53:PRO:HD2	1.70	0.73
6:A:232:GLU:OE1	6:A:232:GLU:N	2.21	0.73
29:O:183:SER:HB3	29:O:193:LEU:HD11	1.69	0.73
6:A:939:ASP:OD2	6:A:1023:ARG:NH1	2.22	0.73
6:A:1157:ASP:OD1	6:A:1160:SER:N	2.21	0.73
3:D:32:GLU:O	4:G:5:LYS:NZ	2.17	0.73
7:B:886:LYS:HE3	7:B:940:PRO:HD3	1.70	0.73
6:A:1426:GLU:OE1	6:A:1426:GLU:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:411:CYS:HA	21:7:488:ASP:HB2	1.71	0.73
4:G:57:GLN:OE1	4:G:57:GLN:N	2.22	0.72
6:A:1278:ASN:HD22	6:A:1312:ASN:HB2	1.54	0.72
10:F:130:ILE:HG22	10:F:132:LEU:HD23	1.71	0.72
12:I:87:GLN:O	12:I:89:GLN:NE2	2.22	0.72
21:7:381:SER:HB3	21:7:509:ALA:HB1	1.70	0.72
6:A:1197:LEU:HD12	6:A:1236:LEU:HB3	1.71	0.72
9:E:66:GLU:O	9:E:69:ILE:N	2.22	0.72
15:L:47:ARG:NH2	15:L:52:GLY:O	2.22	0.72
17:0:140:GLN:NE2	17:0:386:ARG:O	2.21	0.72
6:A:1167:GLU:O	6:A:1171:GLN:NE2	2.17	0.72
3:D:119:ARG:NH1	3:D:152:SER:O	2.21	0.72
11:H:83:GLN:O	11:H:87:ARG:NH1	2.21	0.72
6:A:399:HIS:O	6:A:401:GLY:N	2.22	0.72
11:H:56:THR:HA	11:H:145:ARG:NH1	2.04	0.72
11:H:94:ASP:OD1	11:H:94:ASP:N	2.21	0.72
1:Q:375:LEU:HB3	1:Q:387:ILE:HB	1.71	0.72
17:0:41:GLU:HB2	17:0:466:LEU:HD21	1.71	0.72
17:0:350:HIS:HA	17:0:422:PRO:HD3	1.72	0.72
21:7:601:ARG:O	21:7:696:ARG:NH2	2.22	0.72
2:R:127:LYS:HD3	2:R:220:HIS:CE1	2.25	0.72
6:A:47:ARG:HG2	6:A:257:ARG:HH12	1.54	0.72
6:A:359:LEU:O	6:A:471:ASN:ND2	2.22	0.72
12:I:19:ASP:OD2	12:I:22:ASN:N	2.22	0.72
19:6:262:LYS:HG3	19:6:287:PHE:HB3	1.70	0.72
23:2:82:LYS:HE2	23:2:89:PRO:HG3	1.72	0.72
7:B:816:GLU:OE1	7:B:816:GLU:N	2.23	0.72
11:H:57:VAL:HA	11:H:144:ILE:CA	2.19	0.72
29:O:195:TYR:HB3	29:O:204:LEU:HB2	1.71	0.72
5:M:244:SER:HB3	7:B:108:VAL:HG13	1.71	0.72
14:K:108:GLU:O	14:K:111:LEU:HB2	1.90	0.71
29:O:196:ARG:HG2	29:O:203:VAL:HG13	1.71	0.71
6:A:434:ARG:NH2	6:A:440:ASP:OD2	2.23	0.71
6:A:1208:THR:H	6:A:1211:GLN:CD	1.93	0.71
7:B:486:TYR:OH	7:B:794:ASN:ND2	2.23	0.71
10:F:92:ARG:O	10:F:96:THR:OG1	2.07	0.71
19:6:141:LEU:HD23	19:6:145:ARG:HA	1.70	0.71
6:A:152:VAL:N	6:A:162:VAL:O	2.20	0.71
7:B:67:SER:HB2	7:B:92:PHE:HD2	1.56	0.71
17:0:446:ILE:HG21	17:0:473:LEU:HB3	1.72	0.71
29:O:193:LEU:O	29:O:206:ILE:N	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:38:LEU:HD21	30:W:43:LEU:HD22	1.72	0.71
6:A:488:ASN:OD1	6:A:488:ASN:N	2.18	0.71
7:B:1028:GLU:O	7:B:1032:SER:OG	2.08	0.71
6:A:1128:GLN:HG3	6:A:1284:MET:HE1	1.73	0.71
7:B:310:MET:HG3	7:B:386:LEU:HD12	1.73	0.71
21:7:603:ASP:OD1	21:7:696:ARG:NH1	2.24	0.71
6:A:918:GLU:OE1	6:A:918:GLU:N	2.17	0.71
9:E:66:GLU:OE1	9:E:66:GLU:N	2.23	0.71
17:0:66:HIS:ND1	17:0:229:ASP:O	2.23	0.71
30:W:127:CYS:HB2	30:W:151:LEU:HD12	1.71	0.71
2:R:106:LEU:N	2:R:120:TYR:O	2.22	0.71
12:I:6:PHE:HA	12:I:12:ASN:O	1.91	0.71
29:O:104:MET:HB3	29:O:113:ALA:HB3	1.71	0.71
29:O:65:PRO:HA	29:O:164:CYS:HB3	1.73	0.71
6:A:385:ILE:O	6:A:389:THR:OG1	2.08	0.70
27:N:34:DA:H2	28:T:132:DT:H3	1.36	0.70
29:O:133:LYS:HD2	29:O:137:ARG:HH21	1.55	0.70
8:C:5:GLY:O	8:C:24:ASN:ND2	2.25	0.70
11:H:2:SER:N	11:H:61:SER:HG	1.89	0.70
6:A:107:CYS:HA	6:A:171:GLN:HE22	1.57	0.70
6:A:788:SER:OG	6:A:789:LYS:N	2.22	0.70
7:B:499:ASN:OD1	7:B:500:THR:N	2.23	0.70
11:H:2:SER:OG	11:H:3:ASN:N	2.21	0.70
4:G:84:GLY:N	4:G:147:ILE:O	2.24	0.70
7:B:957:ASN:N	7:B:961:LEU:O	2.21	0.70
6:A:273:ASN:ND2	6:A:277:GLU:OE2	2.25	0.70
6:A:560:ILE:N	11:H:78:SER:OG	2.17	0.70
7:B:641:GLU:N	7:B:650:GLU:O	2.25	0.70
3:D:56:ARG:HH21	3:D:152:SER:HB3	1.55	0.70
6:A:1121:GLU:OE2	6:A:1124:HIS:ND1	2.24	0.70
9:E:59:SER:OG	9:E:82:PHE:N	2.23	0.70
9:E:159:ASP:N	9:E:159:ASP:OD1	2.19	0.70
19:6:117:PRO:HB3	19:6:384:MET:HA	1.74	0.70
5:M:130:PHE:O	5:M:134:THR:OG1	2.09	0.70
6:A:496:GLU:OE1	6:A:496:GLU:N	2.22	0.70
30:W:149:CYS:SG	30:W:151:LEU:N	2.65	0.70
4:G:45:ILE:HA	4:G:78:VAL:HG12	1.71	0.70
8:C:53:THR:HG22	8:C:154:LYS:HB3	1.74	0.70
11:H:126:GLU:O	11:H:130:ARG:NH2	2.25	0.70
12:I:74:GLU:OE2	12:I:79:HIS:ND1	2.25	0.70
14:K:108:GLU:HA	14:K:111:LEU:HD13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1199:ARG:O	6:A:1203:ASN:ND2	2.23	0.70
8:C:123:ASN:ND2	8:C:125:MET:SD	2.65	0.70
19:6:165:PRO:HG2	19:6:375:HIS:HA	1.72	0.70
21:7:355:ASP:H	21:7:431:GLN:HE22	1.40	0.70
3:D:214:LEU:O	3:D:218:GLU:N	2.25	0.69
3:D:56:ARG:HB2	3:D:148:LEU:HD22	1.74	0.69
3:D:167:LEU:O	3:D:170:THR:OG1	2.08	0.69
6:A:41:MET:SD	6:A:42:ASP:N	2.65	0.69
6:A:268:ASP:HB3	6:A:299:HIS:NE2	2.08	0.69
6:A:775:ILE:O	6:A:797:LYS:NZ	2.25	0.69
23:2:462:PHE:HB2	23:2:489:LYS:HB3	1.74	0.69
1:Q:375:LEU:N	1:Q:387:ILE:O	2.21	0.69
6:A:618:GLU:OE1	6:A:619:LYS:N	2.25	0.69
7:B:896:ASP:N	7:B:896:ASP:OD1	2.23	0.69
9:E:40:GLU:HA	9:E:43:LYS:HE2	1.72	0.69
10:F:147:SER:N	10:F:150:GLU:OE2	2.23	0.69
6:A:935:GLN:NE2	6:A:939:ASP:OD1	2.25	0.69
17:0:259:ARG:NH2	17:0:397:THR:OG1	2.25	0.69
2:R:94:LYS:NZ	2:R:107:LEU:O	2.24	0.69
3:D:148:LEU:O	3:D:152:SER:N	2.25	0.69
9:E:92:THR:O	9:E:95:THR:OG1	2.10	0.69
21:7:557:VAL:HB	21:7:708:LEU:HA	1.75	0.69
26:V:84:GLN:HA	26:V:107:SER:HA	1.74	0.69
6:A:1174:PHE:H	6:A:1174:PHE:HD1	1.40	0.69
3:D:127:ASP:HB3	3:D:142:LYS:HD2	1.74	0.69
6:A:1030:ARG:NH2	6:A:1035:TYR:OH	2.25	0.69
6:A:1173:HIS:CG	6:A:1227:ILE:HG23	2.28	0.69
19:6:136:MET:HA	19:6:145:ARG:HD2	1.75	0.69
7:B:245:GLU:HG2	7:B:246:LYS:HG2	1.73	0.69
9:E:136:ASN:OD1	9:E:138:ALA:N	2.26	0.69
10:F:133:VAL:O	10:F:134:ILE:HG13	1.92	0.69
12:I:9:ASP:OD1	12:I:9:ASP:N	2.24	0.69
17:0:727:PRO:HG3	19:6:289:LYS:HA	1.75	0.69
19:6:269:GLN:HG3	19:6:288:TYR:HE2	1.57	0.69
8:C:75:MET:O	8:C:246:ARG:NH2	2.20	0.69
11:H:98:TYR:OH	11:H:138:GLU:OE2	2.07	0.69
21:7:587:LYS:HD3	21:7:673:ILE:HD12	1.74	0.69
6:A:23:SER:OG	6:A:26:GLU:N	2.22	0.69
6:A:219:PHE:HD1	6:A:220:THR:N	1.91	0.69
7:B:63:ILE:O	7:B:65:GLU:N	2.25	0.69
6:A:56:PRO:HB2	6:A:57:ARG:NH1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1376:THR:O	9:E:212:ARG:NH2	2.26	0.68
7:B:585:VAL:O	7:B:587:HIS:ND1	2.26	0.68
29:O:186:GLU:O	29:O:190:PHE:N	2.26	0.68
5:M:263:CYS:HA	5:M:266:ILE:HG22	1.75	0.68
6:A:1161:THR:HG21	6:A:1166:ASP:HB2	1.74	0.68
7:B:223:VAL:HG22	7:B:384:ARG:HH21	1.58	0.68
17:0:571:VAL:HG11	20:1:375:LEU:HD22	1.75	0.68
21:7:582:ILE:HG21	21:7:611:ASN:HD21	1.58	0.68
7:B:311:LEU:HA	7:B:314:LEU:HD12	1.74	0.68
9:E:197:LYS:HE2	9:E:199:ILE:HD11	1.74	0.68
1:Q:99:ASN:HB3	2:R:97:ILE:HB	1.73	0.68
1:Q:121:PHE:HB2	2:R:131:ASN:HD21	1.58	0.68
6:A:1134:ILE:O	6:A:1137:ALA:N	2.26	0.68
7:B:185:THR:N	7:B:188:ASP:OD2	2.24	0.68
7:B:326:ASP:OD1	7:B:327:ARG:N	2.26	0.68
7:B:975:GLN:N	7:B:978:ASP:OD2	2.24	0.68
2:R:69:TRP:CD1	2:R:219:CYS:HB3	2.29	0.68
5:M:59:THR:H	5:M:60:ARG:HH11	1.41	0.68
6:A:55:ASP:OD1	6:A:58:LEU:N	2.26	0.68
6:A:1386:ARG:NE	6:A:1404:GLU:OE2	2.24	0.68
7:B:800:GLN:OE1	7:B:822:ASN:ND2	2.22	0.68
21:7:489:GLU:OE1	21:7:685:GLN:NE2	2.26	0.68
7:B:1097:HIS:NE2	31:P:9:G:H4'	2.09	0.68
15:L:66:GLN:OE1	15:L:67:PHE:N	2.26	0.68
15:L:68:GLU:OE2	15:L:70:ARG:NH1	2.26	0.68
6:A:871:ASP:OD1	6:A:873:MET:N	2.17	0.68
7:B:516:ASN:N	7:B:516:ASN:OD1	2.21	0.68
9:E:26:ARG:NH1	9:E:188:LEU:O	2.27	0.68
11:H:110:ASP:O	11:H:128:ASN:HB2	1.94	0.68
7:B:990:ILE:HG22	7:B:991:GLY:H	1.59	0.68
8:C:136:ASP:OD2	8:C:139:GLY:N	2.26	0.68
9:E:67:GLU:CD	9:E:67:GLU:H	1.97	0.68
12:I:7:CYS:HB2	12:I:29:CYS:HB2	1.75	0.68
12:I:73:ARG:O	12:I:83:ASN:ND2	2.26	0.68
4:G:90:THR:O	4:G:102:GLN:N	2.24	0.68
6:A:150:THR:HA	6:A:166:GLY:O	1.94	0.68
7:B:1000:PRO:HB2	7:B:1072:MET:HE2	1.74	0.68
8:C:196:ASP:OD2	8:C:199:LYS:N	2.22	0.68
11:H:35:GLN:OE1	11:H:35:GLN:N	2.20	0.68
6:A:526:ASP:HB2	7:B:835:GLN:OE1	1.93	0.68
7:B:1122:ARG:N	28:T:23:DC:OP1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:THR:OG1	3:D:119:ARG:N	2.27	0.67
6:A:1396:ALA:N	6:A:1419:ASP:OD2	2.26	0.67
18:4:53:VAL:HG13	18:4:179:LEU:HD23	1.76	0.67
12:I:5:ARG:HB2	12:I:14:LEU:HB2	1.75	0.67
21:7:487:LEU:HB2	21:7:512:GLY:HA2	1.74	0.67
1:Q:99:ASN:N	2:R:97:ILE:O	2.26	0.67
5:M:170:SER:HB3	5:M:206:THR:HG21	1.75	0.67
8:C:3:GLU:N	8:C:6:PRO:O	2.27	0.67
21:7:615:LEU:HD11	21:7:653:PHE:HB3	1.76	0.67
3:D:67:ARG:HA	3:D:70:PHE:HB3	1.76	0.67
4:G:129:SER:OG	4:G:131:GLN:NE2	2.26	0.67
8:C:92:CYS:SG	8:C:94:LYS:N	2.62	0.67
6:A:898:ARG:O	6:A:1029:ARG:NH1	2.27	0.67
7:B:466:TRP:N	7:B:476:ARG:O	2.27	0.67
6:A:287:HIS:ND1	6:A:290:GLU:OE2	2.28	0.67
6:A:624:SER:O	6:A:624:SER:OG	2.08	0.67
6:A:881:GLN:NE2	6:A:957:PRO:O	2.28	0.67
6:A:1148:ILE:HB	6:A:1196:GLU:HG2	1.74	0.67
17:0:500:GLY:HA3	17:0:521:ASN:HD21	1.60	0.67
21:7:553:GLN:HB3	21:7:734:LYS:HE2	1.76	0.67
7:B:760:ASP:N	7:B:760:ASP:OD1	2.26	0.67
23:2:458:LEU:HD11	23:2:490:LYS:HB3	1.77	0.67
6:A:1445:ILE:H	10:F:133:VAL:HG23	1.60	0.67
18:4:289:CYS:SG	18:4:290:SER:N	2.68	0.67
4:G:146:LYS:NZ	4:G:148:GLU:OE1	2.25	0.66
8:C:26:ASP:OD2	8:C:29:MET:N	2.22	0.66
8:C:92:CYS:O	8:C:96:SER:OG	2.13	0.66
21:7:499:ARG:NH2	21:7:525:GLY:O	2.27	0.66
6:A:874:ASP:OD1	6:A:875:ALA:N	2.28	0.66
7:B:328:GLU:OE1	7:B:328:GLU:N	2.24	0.66
29:O:93:GLU:O	29:O:103:ILE:N	2.18	0.66
2:R:68:VAL:O	2:R:219:CYS:N	2.27	0.66
3:D:154:PHE:CE2	3:D:163:VAL:HG21	2.31	0.66
4:G:96:GLN:H	30:W:145:THR:HB	1.60	0.66
18:4:175:ARG:NH1	18:4:252:MET:O	2.28	0.66
29:O:162:GLY:O	29:O:214:LEU:N	2.23	0.66
4:G:101:VAL:N	4:G:108:VAL:O	2.28	0.66
5:M:186:ALA:HB3	5:M:241:ARG:HD2	1.76	0.66
5:M:201:LYS:HE3	27:N:19:DA:H3'	1.76	0.66
6:A:56:PRO:O	6:A:57:ARG:NH1	2.28	0.66
6:A:1329:THR:OG1	6:A:1330:ASN:N	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:178:ASN:O	7:B:178:ASN:ND2	2.29	0.66
11:H:142:LEU:HG	11:H:143:LEU:N	2.10	0.66
15:L:30:ILE:HG23	15:L:36:SER:O	1.95	0.66
17:0:288:LYS:O	17:0:291:GLN:NE2	2.28	0.66
17:0:496:ILE:HD12	17:0:686:PHE:HB3	1.78	0.66
21:7:606:ILE:O	21:7:671:ILE:N	2.26	0.66
2:R:98:ASN:OD1	2:R:99:LYS:N	2.23	0.66
4:G:110:VAL:HG13	4:G:162:SER:HA	1.76	0.66
6:A:76:GLU:OE2	7:B:1159:ARG:NH1	2.28	0.66
17:0:112:LYS:NZ	17:0:123:GLU:O	2.28	0.66
19:6:209:SER:OG	19:6:212:ASN:ND2	2.22	0.66
20:1:174:LEU:O	20:1:181:GLN:NE2	2.26	0.66
7:B:708:GLU:CD	7:B:709:ASP:H	1.98	0.66
1:Q:343:ARG:NH2	1:Q:346:GLU:OE2	2.21	0.66
29:O:206:ILE:HD13	29:O:234:LEU:HD21	1.78	0.66
9:E:74:ASP:OD1	9:E:74:ASP:N	2.24	0.66
11:H:57:VAL:HA	11:H:144:ILE:HA	1.77	0.66
14:K:24:ASP:OD1	14:K:25:THR:N	2.29	0.66
17:0:69:ILE:HG23	17:0:231:ILE:HG23	1.77	0.66
21:7:579:LEU:HD22	21:7:611:ASN:HD22	1.60	0.66
24:X:187:HIS:HA	24:X:214:TRP:HB2	1.77	0.66
1:Q:104:ARG:HD2	2:R:92:LEU:HB3	1.77	0.66
6:A:215:SER:OG	6:A:217:LYS:N	2.28	0.66
6:A:1063:MET:SD	6:A:1436:ILE:HD12	2.36	0.66
6:A:1229:SER:N	6:A:1237:ILE:O	2.21	0.66
7:B:1139:ILE:O	7:B:1142:GLY:N	2.28	0.66
11:H:57:VAL:HG23	11:H:144:ILE:HA	1.78	0.66
21:7:560:PRO:HA	21:7:711:LYS:HE2	1.77	0.66
21:7:607:VAL:O	21:7:654:LEU:N	2.29	0.66
28:T:147:DT:O4	28:T:148:DA:N6	2.29	0.66
4:G:97:HIS:O	4:G:112:LYS:N	2.29	0.65
6:A:900:ASP:OD1	6:A:903:ASN:N	2.29	0.65
6:A:1287:TYR:OH	6:A:1307:GLU:OE2	2.10	0.65
7:B:137:TYR:HD1	7:B:137:TYR:H	1.44	0.65
7:B:737:THR:O	7:B:737:THR:OG1	2.10	0.65
12:I:34:TYR:OH	12:I:36:GLU:OE2	2.13	0.65
27:N:37:DG:O6	28:T:128:DA:N6	2.29	0.65
5:M:234:GLN:NE2	29:O:173:GLU:OE2	2.27	0.65
7:B:1008:PRO:HB3	7:B:1087:PHE:HE1	1.60	0.65
2:R:73:LEU:HD12	2:R:74:PRO:HD2	1.78	0.65
2:R:98:ASN:HB3	2:R:103:LYS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:36:GLY:N	4:G:45:ILE:O	2.30	0.65
29:O:163:SER:HA	29:O:213:VAL:HA	1.78	0.65
6:A:739:ASP:OD1	6:A:739:ASP:N	2.27	0.65
7:B:213:ILE:O	7:B:215:GLN:NE2	2.27	0.65
7:B:862:GLN:HB3	7:B:963:PHE:HB2	1.79	0.65
6:A:1436:ILE:O	6:A:1439:GLY:N	2.20	0.65
7:B:216:GLU:OE2	7:B:404:LYS:HG2	1.96	0.65
17:0:446:ILE:HG13	17:0:473:LEU:HD22	1.78	0.65
29:O:193:LEU:N	29:O:206:ILE:O	2.29	0.65
1:Q:352:MET:N	1:Q:352:MET:SD	2.70	0.65
9:E:29:PHE:HB2	9:E:65:THR:HG22	1.78	0.65
19:6:124:ARG:NH2	19:6:231:GLU:OE1	2.29	0.65
21:7:456:THR:HG23	21:7:459:MET:H	1.61	0.65
29:O:136:SER:HB2	29:O:152:PHE:HE1	1.61	0.65
4:G:83:LYS:HD2	4:G:83:LYS:H	1.62	0.65
6:A:16:GLU:OE2	7:B:1221:SER:N	2.23	0.65
6:A:821:ARG:NH1	7:B:527:THR:HG21	2.12	0.65
7:B:253:THR:OG1	7:B:253:THR:O	2.12	0.65
7:B:802:PRO:HG2	7:B:805:THR:HG22	1.78	0.65
27:N:19:DA:H2"	27:N:20:DT:H5'	1.79	0.65
6:A:362:ASP:OD1	6:A:362:ASP:N	2.22	0.65
18:4:255:ASP:O	18:4:259:ARG:NH1	2.29	0.65
1:Q:380:ASP:OD1	1:Q:380:ASP:N	2.27	0.65
7:B:825:VAL:HG23	7:B:1010:LEU:HB3	1.78	0.65
9:E:20:LYS:NZ	9:E:34:GLU:O	2.15	0.65
9:E:191:LYS:N	9:E:194:GLU:OE1	2.25	0.65
23:2:350:TYR:N	23:2:407:GLN:OE1	2.25	0.65
30:W:149:CYS:HB3	30:W:154:GLU:H	1.62	0.65
6:A:1442:ASP:HA	10:F:134:ILE:C	2.17	0.64
7:B:104:GLU:OE2	15:L:54:ARG:NE	2.30	0.64
7:B:280:ILE:HB	7:B:285:ILE:HD11	1.77	0.64
17:0:534:PRO:HD3	17:0:721:LEU:HD21	1.78	0.64
6:A:82:GLY:O	6:A:241:VAL:N	2.28	0.64
6:A:1443:VAL:N	10:F:134:ILE:O	2.29	0.64
8:C:36:VAL:HG23	8:C:40:GLU:HB2	1.79	0.64
12:I:45:ARG:NH2	12:I:47:GLU:OE2	2.29	0.64
23:2:87:LEU:HD12	23:2:98:ILE:HG23	1.80	0.64
23:2:387:LEU:HD11	23:2:393:ALA:HB2	1.79	0.64
29:O:76:LEU:HD22	29:O:150:ALA:HB1	1.79	0.64
2:R:62:GLU:OE1	2:R:62:GLU:N	2.28	0.64
6:A:43:GLU:O	6:A:44:THR:OG1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:609:ASP:OD1	6:A:610:GLY:N	2.31	0.64
17:0:580:SER:HB3	20:1:339:LEU:H	1.62	0.64
21:7:520:GLU:H	21:7:681:ARG:HH12	1.45	0.64
29:O:179:HIS:HB3	29:O:182:PHE:HD2	1.63	0.64
1:Q:104:ARG:CZ	1:Q:105:ALA:H	2.10	0.64
1:Q:116:THR:O	1:Q:117:HIS:ND1	2.31	0.64
6:A:1142:THR:O	6:A:1145:SER:OG	2.15	0.64
1:Q:373:TYR:H	2:R:82:ARG:NH2	1.96	0.64
5:M:60:ARG:H	5:M:60:ARG:HD2	1.62	0.64
6:A:401:GLY:O	6:A:435:HIS:ND1	2.31	0.64
7:B:69:LEU:HD13	7:B:429:PHE:HB2	1.80	0.64
8:C:5:GLY:O	8:C:7:GLN:NE2	2.31	0.64
17:0:293:LEU:HD13	17:0:319:GLU:HA	1.79	0.64
18:4:51:ILE:O	18:4:55:GLU:N	2.20	0.64
19:6:130:LEU:N	19:6:172:ILE:O	2.30	0.64
19:6:322:MET:HB2	19:6:369:MET:HB2	1.79	0.64
1:Q:363:GLY:HA2	1:Q:395:PHE:HA	1.80	0.64
6:A:471:ASN:OD1	6:A:472:LEU:N	2.31	0.64
6:A:1297:GLU:OE1	6:A:1297:GLU:N	2.23	0.64
7:B:20:ASP:OD2	7:B:22:SER:N	2.31	0.64
7:B:618:ASP:OD1	7:B:621:GLU:N	2.29	0.64
8:C:90:ASP:OD1	8:C:91:HIS:ND1	2.31	0.64
18:4:59:VAL:HB	18:4:245:ILE:HD11	1.78	0.64
24:X:214:TRP:HD1	24:X:217:CYS:HG	1.44	0.64
25:U:281:VAL:HG22	26:V:62:VAL:HB	1.79	0.64
9:E:157:SER:OG	9:E:159:ASP:OD1	2.13	0.64
1:Q:140:HIS:NE2	1:Q:353:GLU:OE2	2.30	0.64
12:I:82:GLU:OE1	12:I:82:GLU:N	2.30	0.64
18:4:239:GLU:HG2	18:4:242:GLU:HB2	1.79	0.64
30:W:144:ARG:HH12	30:W:146:GLU:HB3	1.63	0.64
1:Q:117:HIS:HB2	2:R:135:PHE:CE1	2.33	0.64
6:A:225:ASN:OD1	6:A:228:PHE:N	2.21	0.64
6:A:556:TRP:O	14:K:26:LYS:NZ	2.22	0.64
6:A:780:VAL:N	7:B:699:GLU:OE1	2.29	0.64
7:B:979:LYS:NZ	31:P:9:G:O2'	2.31	0.64
9:E:4:GLU:O	9:E:8:ASN:HB2	1.98	0.64
17:0:124:ARG:HH22	17:0:577:GLN:H	1.46	0.64
18:4:82:GLY:H	18:4:148:THR:HG21	1.63	0.64
30:W:65:ARG:HE	30:W:93:HIS:HB3	1.62	0.64
8:C:3:GLU:OE2	14:K:104:ASN:HB2	1.97	0.64
17:0:113:ASN:ND2	20:1:346:ASP:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:571:VAL:HG22	17:0:599:LEU:HD21	1.80	0.64
7:B:1136:ASP:N	7:B:1136:ASP:OD1	2.27	0.63
7:B:1187:ASN:OD1	7:B:1188:LYS:N	2.31	0.63
11:H:32:THR:OG1	11:H:33:GLN:N	2.29	0.63
18:4:29:ILE:HD11	18:4:156:GLY:HA3	1.80	0.63
21:7:303:ARG:HA	21:7:320:ASN:HA	1.78	0.63
30:W:21:TYR:OH	30:W:64:ASP:OD2	2.16	0.63
6:A:316:GLN:O	6:A:318:SER:OG	2.14	0.63
6:A:1438:THR:O	10:F:92:ARG:NH1	2.30	0.63
7:B:882:THR:HA	7:B:934:LYS:O	1.98	0.63
19:6:142:ARG:HB2	19:6:143:PRO:HD3	1.79	0.63
24:X:255:ILE:HD13	30:W:178:GLN:HB3	1.79	0.63
1:Q:101:PHE:CZ	1:Q:382:GLY:HA3	2.32	0.63
1:Q:109:GLU:OE1	1:Q:109:GLU:N	2.28	0.63
8:C:74:SER:OG	8:C:237:SER:OG	2.13	0.63
17:0:80:GLU:HA	17:0:83:LEU:HB2	1.80	0.63
19:6:173:ILE:HD12	19:6:175:ARG:HD2	1.79	0.63
20:1:593:LEU:O	20:1:597:PHE:N	2.30	0.63
1:Q:332:LEU:HB2	7:B:429:PHE:CZ	2.34	0.63
6:A:1234:GLU:OE1	6:A:1234:GLU:N	2.32	0.63
7:B:65:GLU:O	7:B:67:SER:N	2.31	0.63
7:B:864:LYS:HG2	7:B:871:THR:HA	1.79	0.63
9:E:46:TYR:CD1	9:E:58:MET:HG2	2.33	0.63
11:H:55:LEU:O	11:H:146:ARG:NE	2.31	0.63
17:0:722:ARG:HA	19:6:267:SER:HB2	1.80	0.63
23:2:59:LEU:HD22	23:2:96:LEU:HD12	1.80	0.63
2:R:69:TRP:HD1	2:R:219:CYS:HB3	1.61	0.63
4:G:47:CYS:SG	4:G:48:VAL:N	2.72	0.63
4:G:49:LEU:HD21	4:G:77:VAL:HG23	1.81	0.63
6:A:21:LEU:HD12	6:A:229:SER:HB2	1.80	0.63
6:A:567:LYS:HB2	11:H:95:TYR:HA	1.80	0.63
9:E:79:TRP:NE1	9:E:81:GLU:OE1	2.30	0.63
17:0:419:ILE:HG12	17:0:436:ARG:HB3	1.80	0.63
21:7:303:ARG:HB3	21:7:323:VAL:HG13	1.80	0.63
6:A:535:THR:HG21	6:A:617:VAL:H	1.64	0.63
7:B:135:ARG:HH12	7:B:138:GLU:HB2	1.62	0.63
7:B:332:ASP:O	7:B:348:ARG:NH1	2.32	0.63
7:B:977:GLY:HA3	7:B:1099:VAL:HG11	1.80	0.63
3:D:63:LEU:HB3	3:D:130:LEU:HD22	1.79	0.63
3:D:173:HIS:N	3:D:176:GLU:OE2	2.32	0.63
21:7:365:TYR:OH	21:7:390:ALA:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1445:ILE:N	10:F:133:VAL:HG23	2.13	0.63
7:B:1002:THR:OG1	7:B:1003:ALA:N	2.32	0.63
9:E:101:GLN:H	9:E:101:GLN:CD	1.99	0.63
17:0:436:ARG:HE	17:0:634:ILE:HG21	1.62	0.63
19:6:291:LEU:HA	19:6:296:HIS:CD2	2.33	0.63
21:7:302:GLU:HG3	21:7:321:GLU:HB3	1.80	0.63
21:7:483:GLY:HA2	21:7:508:HIS:HB2	1.80	0.63
7:B:46:GLN:OE1	7:B:47:GLN:N	2.32	0.63
7:B:282:ILE:O	7:B:285:ILE:N	2.31	0.63
21:7:599:GLU:HG2	21:7:650:ASN:HB2	1.80	0.63
23:2:246:GLN:O	23:2:250:LEU:N	2.26	0.63
29:O:129:GLU:OE1	29:O:220:ARG:NH2	2.32	0.63
29:O:171:ARG:N	29:O:237:PHE:O	2.26	0.63
1:Q:366:GLU:HB3	1:Q:392:VAL:HG13	1.80	0.62
6:A:65:LEU:O	6:A:67:CYS:N	2.30	0.62
6:A:136:ALA:O	6:A:140:THR:OG1	2.16	0.62
6:A:420:ARG:HB3	6:A:423:ASP:HB3	1.81	0.62
7:B:895:ASP:N	7:B:895:ASP:OD1	2.32	0.62
7:B:1098:MET:N	7:B:1098:MET:SD	2.72	0.62
7:B:1153:GLU:OE1	7:B:1153:GLU:N	2.31	0.62
19:6:217:ALA:HB1	19:6:232:VAL:HG21	1.80	0.62
4:G:148:GLU:HB2	4:G:160:ILE:HG22	1.81	0.62
7:B:37:PHE:HD2	7:B:38:PHE:N	1.97	0.62
4:G:60:ARG:O	4:G:69:GLU:N	2.31	0.62
5:M:255:SER:OG	5:M:285:ASN:OD1	2.14	0.62
6:A:1082:ASN:OD1	6:A:1083:THR:N	2.32	0.62
6:A:1123:GLY:HA3	6:A:1124:HIS:CG	2.34	0.62
17:0:116:LEU:HD21	17:0:186:GLU:HA	1.81	0.62
17:0:666:LEU:HD22	17:0:679:MET:HB3	1.81	0.62
19:6:188:ASN:O	19:6:192:HIS:ND1	2.32	0.62
29:O:193:LEU:HB3	29:O:206:ILE:HB	1.80	0.62
1:Q:103:LEU:HD21	2:R:95:ILE:HG22	1.81	0.62
2:R:106:LEU:HB2	2:R:120:TYR:HB2	1.82	0.62
6:A:903:ASN:OD1	6:A:904:THR:N	2.32	0.62
11:H:55:LEU:O	11:H:145:ARG:HD2	1.98	0.62
11:H:142:LEU:O	11:H:143:LEU:HG	1.98	0.62
12:I:19:ASP:N	12:I:24:ARG:O	2.32	0.62
17:0:79:ILE:HG23	17:0:207:ILE:HG22	1.79	0.62
17:0:378:SER:OG	17:0:407:THR:OG1	2.17	0.62
5:M:37:ARG:HG3	6:A:416:ARG:HH21	1.64	0.62
6:A:67:CYS:H	6:A:71:GLN:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:982:THR:OG1	6:A:985:ASP:OD1	2.07	0.62
7:B:432:MET:O	7:B:435:THR:OG1	2.14	0.62
7:B:757:PRO:HD3	7:B:983:ARG:NE	2.10	0.62
11:H:82:PRO:HA	11:H:87:ARG:HD2	1.81	0.62
7:B:705:MET:HE1	7:B:745:PRO:HB3	1.82	0.62
18:4:27:THR:HG22	18:4:74:ALA:HB3	1.80	0.62
21:7:308:ASP:OD1	21:7:309:ASP:N	2.33	0.62
2:R:73:LEU:HD21	2:R:77:LEU:HG	1.81	0.62
2:R:138:GLN:H	2:R:138:GLN:HE21	1.45	0.62
8:C:214:ASN:ND2	8:C:217:ASP:OD1	2.32	0.62
12:I:19:ASP:HB3	12:I:24:ARG:N	2.12	0.62
15:L:61:THR:OG1	15:L:62:LYS:N	2.29	0.62
5:M:51:VAL:HG11	6:A:412:ARG:HB2	1.82	0.62
6:A:41:MET:O	6:A:49:LYS:HA	1.99	0.62
6:A:1442:ASP:OD2	10:F:135:ARG:HA	1.99	0.62
12:I:92:ARG:O	12:I:95:THR:OG1	2.13	0.62
18:4:200:ILE:HG12	18:4:227:THR:HG23	1.80	0.62
18:4:212:VAL:HG21	18:4:224:LEU:HB3	1.80	0.62
1:Q:120:LYS:HB2	1:Q:394:LYS:HD2	1.82	0.62
1:Q:131:THR:OG1	1:Q:132:ASP:OD1	2.13	0.62
5:M:35:VAL:HG23	5:M:46:ALA:HB2	1.81	0.62
17:0:339:ILE:HD12	17:0:342:LEU:HD21	1.82	0.62
21:7:365:TYR:HB3	21:7:543:LEU:HD21	1.81	0.62
2:R:69:TRP:NE1	2:R:220:HIS:HB3	2.15	0.62
5:M:158:HIS:ND1	5:M:158:HIS:O	2.33	0.62
7:B:883:LEU:O	7:B:884:ARG:NE	2.33	0.62
18:4:29:ILE:HD13	18:4:153:MET:HA	1.82	0.62
20:1:547:LEU:O	20:1:551:ARG:N	2.33	0.62
3:D:63:LEU:HD22	3:D:130:LEU:HB3	1.82	0.61
5:M:267:LYS:HE2	29:O:240:MET:HB2	1.81	0.61
6:A:310:GLY:O	6:A:311:GLN:NE2	2.33	0.61
6:A:886:ILE:HD11	6:A:950:GLY:HA2	1.81	0.61
10:F:110:ASP:O	10:F:123:LYS:NZ	2.33	0.61
1:Q:119:LEU:HD12	2:R:133:TYR:HB2	1.82	0.61
6:A:1392:SER:OG	6:A:1393:ASN:N	2.32	0.61
8:C:262:LEU:HD11	14:K:87:LEU:HD23	1.80	0.61
18:4:273:ARG:HH11	19:6:373:SER:HB3	1.65	0.61
2:R:123:GLU:O	2:R:222:CYS:HB3	2.00	0.61
3:D:41:GLN:OE1	3:D:41:GLN:N	2.33	0.61
9:E:72:PHE:HB2	9:E:75:MET:HE2	1.82	0.61
11:H:110:ASP:OD1	11:H:110:ASP:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:289:CYS:HA	19:6:319:LEU:HD12	1.82	0.61
23:2:84:LEU:HD11	23:2:86:LEU:HD23	1.81	0.61
29:O:93:GLU:HB3	29:O:103:ILE:HB	1.82	0.61
29:O:235:SER:OG	29:O:238:ARG:NH2	2.33	0.61
2:R:73:LEU:HD23	2:R:78:ALA:HA	1.81	0.61
8:C:14:SER:HA	14:K:114:LEU:HD13	1.81	0.61
10:F:133:VAL:O	10:F:133:VAL:HG12	2.00	0.61
27:N:19:DA:H4'	29:O:189:LEU:HG	1.81	0.61
6:A:268:ASP:HB3	6:A:299:HIS:CD2	2.35	0.61
6:A:842:VAL:HG11	7:B:1136:ASP:OD2	2.01	0.61
7:B:838:SER:OG	7:B:989:THR:O	2.10	0.61
7:B:1180:PHE:HB3	7:B:1191:ILE:HD13	1.82	0.61
7:B:1187:ASN:OD1	7:B:1189:ILE:N	2.28	0.61
8:C:76:ASP:OD2	8:C:128:ASN:N	2.30	0.61
8:C:114:TYR:N	8:C:117:ASP:OD2	2.32	0.61
21:7:608:PHE:HB3	21:7:672:GLN:HA	1.83	0.61
6:A:68:GLN:HE22	6:A:80:HIS:CE1	2.06	0.61
29:O:207:PHE:HB2	29:O:211:LYS:HB2	1.82	0.61
1:Q:127:ILE:O	2:R:133:TYR:OH	2.18	0.61
1:Q:398:ARG:NH1	7:B:328:GLU:OE2	2.33	0.61
2:R:225:MET:N	2:R:225:MET:SD	2.74	0.61
6:A:130:ASP:O	6:A:133:LYS:N	2.33	0.61
7:B:385:LEU:HD23	7:B:386:LEU:HD23	1.82	0.61
11:H:57:VAL:HB	11:H:145:ARG:CB	2.30	0.61
18:4:202:SER:HA	18:4:205:LYS:HB3	1.82	0.61
1:Q:102:PRO:HA	2:R:93:GLY:O	2.01	0.61
2:R:105:THR:HA	2:R:121:ASP:HA	1.83	0.61
5:M:251:GLN:OE1	5:M:251:GLN:N	2.33	0.61
6:A:177:ASP:OD1	6:A:180:LYS:HB2	2.00	0.61
6:A:225:ASN:OD1	6:A:227:VAL:N	2.34	0.61
6:A:626:ASN:O	6:A:631:HIS:ND1	2.26	0.61
7:B:173:MET:O	7:B:176:SER:OG	2.12	0.61
7:B:911:ILE:HG13	7:B:912:ILE:HG13	1.81	0.61
17:0:315:ASP:OD1	17:0:315:ASP:N	2.29	0.61
17:0:372:LYS:HA	17:0:375:ARG:HD3	1.83	0.61
21:7:699:GLU:O	21:7:702:ASN:ND2	2.34	0.61
29:O:68:GLN:N	29:O:161:VAL:O	2.34	0.61
6:A:57:ARG:HB2	6:A:68:GLN:HB3	1.83	0.61
6:A:665:GLY:N	6:A:668:ASP:OD2	2.21	0.61
6:A:870:GLU:OE1	9:E:202:SER:HB2	2.01	0.61
6:A:1189:SER:OG	6:A:1256:GLU:OE1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1445:ILE:HB	10:F:133:VAL:HG23	1.83	0.61
7:B:722:ASP:OD1	7:B:722:ASP:N	2.34	0.61
21:7:607:VAL:HB	21:7:653:PHE:HA	1.82	0.61
30:W:122:TYR:N	30:W:131:TYR:O	2.33	0.61
2:R:69:TRP:CE2	2:R:220:HIS:HB3	2.36	0.61
7:B:37:PHE:HD2	7:B:38:PHE:H	1.49	0.61
7:B:786:ASN:N	7:B:786:ASN:OD1	2.24	0.61
17:0:159:HIS:NE2	17:0:303:GLU:OE2	2.34	0.61
17:0:673:LYS:NZ	17:0:737:SER:OG	2.34	0.61
29:O:179:HIS:O	29:O:183:SER:N	2.34	0.61
7:B:512:ARG:NH1	7:B:533:CYS:O	2.33	0.60
7:B:901:PRO:HG2	15:L:60:ARG:HA	1.82	0.60
12:I:71:SER:OG	12:I:72:ASP:N	2.32	0.60
17:0:507:SER:HG	17:0:685:ARG:HH22	1.46	0.60
17:0:593:GLY:HA2	19:6:272:ILE:HG21	1.83	0.60
18:4:29:ILE:HB	18:4:178:VAL:HG22	1.82	0.60
27:N:24:DA:N6	28:T:141:DT:O4	2.34	0.60
1:Q:401:TYR:CZ	12:I:32:CYS:HB2	2.36	0.60
4:G:97:HIS:HA	4:G:112:LYS:HD3	1.82	0.60
6:A:739:ASP:OD2	11:H:19:ARG:NE	2.34	0.60
7:B:365:THR:HG21	7:B:370:PHE:CD2	2.37	0.60
8:C:73:GLN:O	8:C:130:GLY:N	2.24	0.60
9:E:98:ILE:HA	9:E:101:GLN:HE22	1.66	0.60
12:I:59:VAL:HG23	12:I:61:ASP:H	1.66	0.60
17:0:114:LEU:HB3	17:0:192:PRO:HG2	1.83	0.60
3:D:189:ASP:HA	3:D:192:LYS:HE3	1.82	0.60
6:A:344:ARG:NH2	7:B:1118:PRO:O	2.33	0.60
7:B:241:ARG:HG2	7:B:253:THR:HB	1.83	0.60
8:C:43:THR:OG1	8:C:44:LEU:N	2.30	0.60
11:H:107:VAL:N	11:H:111:LEU:O	2.34	0.60
23:2:384:ARG:HA	23:2:387:LEU:HB2	1.82	0.60
5:M:243:CYS:HA	5:M:248:LEU:HD12	1.84	0.60
6:A:230:ARG:HD2	6:A:233:TRP:CH2	2.36	0.60
6:A:1199:ARG:NH2	6:A:1233:ASP:O	2.35	0.60
7:B:568:ASP:N	7:B:568:ASP:OD1	2.33	0.60
7:B:936:ASP:OD1	7:B:938:SER:N	2.34	0.60
18:4:119:ARG:O	18:4:123:GLU:N	2.27	0.60
19:6:349:CYS:HB3	19:6:352:CYS:SG	2.40	0.60
21:7:671:ILE:HG23	21:7:708:LEU:HD13	1.83	0.60
6:A:386:ASP:N	6:A:386:ASP:OD2	2.33	0.60
6:A:411:ASP:N	6:A:411:ASP:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:771:GLU:N	6:A:822:GLU:OE2	2.32	0.60
6:A:998:LEU:HA	6:A:1011:GLN:HE22	1.67	0.60
6:A:1140:HIS:HB2	6:A:1276:VAL:O	2.02	0.60
7:B:121:ASN:HA	7:B:207:GLY:HA3	1.82	0.60
17:0:77:SER:OG	17:0:81:LYS:NZ	2.31	0.60
18:4:79:TYR:O	18:4:148:THR:OG1	2.15	0.60
25:U:263:LYS:HZ3	25:U:278:LYS:HG2	1.66	0.60
1:Q:121:PHE:HB2	2:R:131:ASN:ND2	2.17	0.60
1:Q:129:PRO:HG2	1:Q:132:ASP:HB2	1.84	0.60
6:A:208:LEU:O	6:A:212:LYS:HG3	2.02	0.60
7:B:680:THR:O	7:B:683:SER:OG	2.11	0.60
7:B:878:GLN:OE1	7:B:878:GLN:N	2.35	0.60
14:K:58:PHE:HB3	14:K:76:GLN:HB3	1.83	0.60
18:4:114:UNK:C	18:4:116:ARG:H	2.15	0.60
21:7:421:ARG:HH11	21:7:437:VAL:HG11	1.67	0.60
4:G:15:PRO:HA	4:G:18:PHE:CE1	2.37	0.60
6:A:148:CYS:H	6:A:169:ASN:H	1.49	0.60
6:A:175:ARG:N	6:A:182:VAL:O	2.33	0.60
6:A:206:GLU:O	6:A:210:ILE:HG12	2.00	0.60
6:A:517:ASN:O	6:A:517:ASN:ND2	2.35	0.60
6:A:587:HIS:NE2	6:A:969:GLN:HG3	2.17	0.60
7:B:1150:ARG:O	7:B:1154:ALA:HB3	2.01	0.60
8:C:241:ASP:OD1	8:C:242:GLN:N	2.33	0.60
18:4:190:ILE:HD12	18:4:277:TYR:HE1	1.66	0.60
20:1:259:ILE:HG22	20:1:266:VAL:HG11	1.82	0.60
21:7:664:LEU:HD12	21:7:690:ILE:HD13	1.84	0.60
1:Q:375:LEU:O	1:Q:387:ILE:N	2.23	0.60
4:G:97:HIS:HE1	30:W:146:GLU:HG3	1.66	0.60
7:B:277:LYS:NZ	7:B:333:PHE:O	2.27	0.60
19:6:130:LEU:HD23	19:6:235:VAL:HG21	1.84	0.60
6:A:475:THR:OG1	6:A:480:ALA:O	2.19	0.60
6:A:1092:LYS:O	6:A:1094:VAL:N	2.34	0.60
6:A:1342:GLU:OE2	9:E:212:ARG:NH1	2.34	0.60
7:B:61:ASP:N	7:B:61:ASP:OD1	2.34	0.60
7:B:365:THR:HG1	7:B:367:LEU:H	1.50	0.60
7:B:801:LYS:O	13:J:52:THR:OG1	2.20	0.60
11:H:56:THR:HB	11:H:93:TYR:HB3	1.84	0.60
11:H:94:ASP:OD2	11:H:146:ARG:NH2	2.35	0.60
20:1:504:ILE:O	20:1:508:LYS:N	2.34	0.60
21:7:608:PHE:N	21:7:671:ILE:O	2.35	0.60
22:5:9:LEU:HD11	22:5:39:HIS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:93:GLY:HA2	2:R:109:ASN:HB2	1.83	0.60
6:A:544:ASP:N	6:A:544:ASP:OD1	2.30	0.60
6:A:1035:TYR:HB3	6:A:1037:LEU:HD21	1.84	0.60
17:0:112:LYS:HG2	20:1:345:ASP:HB3	1.83	0.60
17:0:241:ASP:OD1	17:0:241:ASP:N	2.29	0.60
3:D:52:LEU:HD12	3:D:148:LEU:HD23	1.84	0.59
7:B:635:ARG:NH1	7:B:742:GLU:OE2	2.30	0.59
9:E:26:ARG:HH12	9:E:189:GLY:HA3	1.67	0.59
21:7:459:MET:O	21:7:470:SER:OG	2.14	0.59
6:A:575:LYS:O	6:A:579:SER:OG	2.19	0.59
6:A:830:LYS:HG3	6:A:1082:ASN:HB3	1.84	0.59
7:B:213:ILE:HG13	7:B:481:GLN:HE21	1.67	0.59
7:B:776:GLN:HB2	7:B:1095:LEU:HD22	1.82	0.59
17:0:346:MET:HG2	17:0:435:MET:HG2	1.84	0.59
1:Q:338:ASN:O	1:Q:342:LEU:N	2.28	0.59
3:D:195:ILE:HG22	3:D:198:LEU:H	1.66	0.59
6:A:56:PRO:HB2	6:A:57:ARG:HH12	1.67	0.59
7:B:1129:ARG:HD3	28:T:21:DC:OP1	2.01	0.59
8:C:215:GLU:OE1	8:C:215:GLU:N	2.33	0.59
17:0:20:GLU:HG2	17:0:43:PRO:HG2	1.84	0.59
17:0:61:MET:SD	17:0:93:ARG:NH1	2.75	0.59
24:X:259:PHE:HE1	30:W:109:LEU:HD11	1.66	0.59
26:V:66:LEU:HD21	26:V:69:TYR:HB3	1.83	0.59
1:Q:120:LYS:HB3	1:Q:394:LYS:HZ2	1.67	0.59
2:R:63:ARG:HG2	2:R:65:ASN:H	1.67	0.59
5:M:177:LEU:O	5:M:181:ARG:HG2	2.02	0.59
5:M:187:ARG:O	5:M:238:TYR:OH	2.21	0.59
6:A:1214:GLU:O	6:A:1218:GLN:HG3	2.03	0.59
11:H:58:THR:H	11:H:143:LEU:C	2.04	0.59
12:I:32:CYS:SG	12:I:34:TYR:N	2.62	0.59
30:W:144:ARG:NH1	30:W:146:GLU:O	2.36	0.59
6:A:715:GLU:OE2	6:A:774:ARG:NE	2.32	0.59
6:A:1442:ASP:OD1	6:A:1443:VAL:N	2.35	0.59
11:H:8:ASP:OD1	11:H:9:ILE:N	2.34	0.59
13:J:32:GLU:OE1	13:J:32:GLU:N	2.22	0.59
21:7:714:GLN:HG2	21:7:718:TYR:HE2	1.67	0.59
29:O:206:ILE:HG23	29:O:212:ILE:HD12	1.85	0.59
6:A:219:PHE:O	6:A:222:LEU:HG	2.03	0.59
6:A:446:ARG:HG3	6:A:487:MET:HG2	1.83	0.59
7:B:486:TYR:CZ	7:B:1096:ARG:HD2	2.37	0.59
17:0:155:LEU:HD12	17:0:160:GLU:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:457:TYR:HB2	21:7:493:VAL:HG21	1.83	0.59
28:T:147:DT:H2'	28:T:148:DA:H5"	1.85	0.59
6:A:609:ASP:O	6:A:611:GLN:N	2.36	0.59
6:A:790:ASP:N	6:A:790:ASP:OD1	2.33	0.59
6:A:914:GLU:OE1	6:A:978:PRO:HB2	2.02	0.59
6:A:1151:GLU:HG2	12:I:45:ARG:HB2	1.84	0.59
6:A:1159:ARG:NH2	6:A:1175:SER:OG	2.26	0.59
7:B:345:LYS:HB3	7:B:347:LYS:HG2	1.83	0.59
20:1:208:GLU:OE1	20:1:208:GLU:N	2.33	0.59
21:7:101:PRO:O	21:7:331:GLN:NE2	2.35	0.59
21:7:324:GLU:HA	21:7:327:LYS:HE2	1.83	0.59
21:7:709:VAL:HG21	21:7:719:SER:HB3	1.83	0.59
24:X:261:LYS:O	24:X:265:ASN:ND2	2.35	0.59
6:A:42:ASP:OD2	6:A:47:ARG:NE	2.36	0.59
6:A:203:SER:N	6:A:206:GLU:OE2	2.35	0.59
7:B:118:ARG:NH1	7:B:209:GLU:OE2	2.33	0.59
7:B:304:ASP:OD1	7:B:306:ASN:ND2	2.32	0.59
7:B:480:SER:O	7:B:480:SER:OG	2.20	0.59
17:0:69:ILE:HD12	17:0:205:ILE:HB	1.85	0.59
17:0:440:LEU:HD22	17:0:638:ARG:HA	1.84	0.59
21:7:328:LYS:O	21:7:331:GLN:NE2	2.36	0.59
21:7:411:CYS:N	21:7:456:THR:HA	2.12	0.59
29:O:202:ILE:HD11	29:O:222:GLU:HB3	1.84	0.59
6:A:690:VAL:HG22	6:A:718:VAL:HG22	1.83	0.59
6:A:1153:TYR:CE1	6:A:1163:ILE:HD11	2.38	0.59
13:J:3:VAL:HG11	13:J:18:TRP:HB2	1.84	0.59
17:0:443:SER:HA	17:0:446:ILE:HB	1.85	0.59
18:4:261:ILE:HG13	23:2:66:VAL:HA	1.84	0.59
6:A:1106:ASN:N	6:A:1106:ASN:OD1	2.36	0.59
7:B:487:THR:O	7:B:490:SER:N	2.35	0.59
7:B:643:ASP:C	7:B:645:SER:H	2.07	0.59
9:E:87:SER:H	9:E:114:ASN:HB2	1.67	0.59
14:K:77:THR:OG1	14:K:78:THR:O	2.20	0.59
17:0:170:TYR:HA	17:0:199:MET:HE1	1.84	0.59
17:0:353:SER:HB2	17:0:417:LEU:HD11	1.84	0.59
6:A:217:LYS:HG3	6:A:218:ASP:N	2.18	0.58
6:A:793:SER:O	6:A:796:SER:OG	2.18	0.58
6:A:966:ASN:O	6:A:970:THR:OG1	2.15	0.58
6:A:1407:GLU:CD	6:A:1407:GLU:H	2.06	0.58
7:B:909:ASP:OD1	7:B:909:ASP:N	2.34	0.58
11:H:57:VAL:HB	11:H:145:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:441:ASP:OD1	17:0:646:TYR:OH	2.21	0.58
21:7:556:GLU:HG2	21:7:707:SER:HB3	1.84	0.58
6:A:1386:ARG:O	6:A:1390:ASN:HB3	2.03	0.58
7:B:1037:LEU:O	13:J:47:ARG:NH2	2.33	0.58
26:V:86:THR:HG23	26:V:105:VAL:HG22	1.85	0.58
29:O:105:ARG:NE	29:O:112:THR:OG1	2.35	0.58
6:A:949:ASP:OD1	6:A:950:GLY:N	2.36	0.58
11:H:50:ALA:N	11:H:53:ASP:OD2	2.21	0.58
17:0:468:MET:SD	17:0:471:ARG:NH1	2.77	0.58
4:G:60:ARG:HA	10:F:133:VAL:HG11	1.85	0.58
4:G:111:THR:HB	4:G:114:LEU:HD13	1.85	0.58
7:B:583:ASN:N	7:B:583:ASN:OD1	2.34	0.58
7:B:706:GLN:O	7:B:710:LEU:HB2	2.02	0.58
9:E:100:ILE:HG23	9:E:105:PHE:HB2	1.85	0.58
2:R:66:ARG:N	2:R:216:GLY:HA3	2.18	0.58
5:M:244:SER:HB3	7:B:108:VAL:HA	1.85	0.58
6:A:1229:SER:OG	6:A:1237:ILE:N	2.19	0.58
7:B:371:GLU:OE2	7:B:371:GLU:N	2.22	0.58
14:K:53:ASP:OD1	14:K:54:ARG:N	2.36	0.58
17:0:238:HIS:HB2	17:0:660:ARG:HD2	1.85	0.58
17:0:280:GLN:OE1	17:0:283:GLN:NE2	2.37	0.58
18:4:28:VAL:HB	18:4:75:VAL:HA	1.86	0.58
20:1:343:ILE:O	20:1:345:ASP:N	2.33	0.58
6:A:351:THR:HG22	6:A:352:VAL:H	1.69	0.58
6:A:1002:GLY:H	6:A:1007:ILE:HG21	1.69	0.58
7:B:216:GLU:OE1	7:B:500:THR:OG1	2.21	0.58
9:E:165:LEU:HD13	9:E:170:LEU:HB2	1.84	0.58
11:H:27:GLU:OE1	11:H:28:ALA:N	2.36	0.58
17:0:286:TYR:O	17:0:326:ARG:NH1	2.37	0.58
21:7:417:VAL:HG12	21:7:437:VAL:HG12	1.85	0.58
21:7:595:ILE:HA	21:7:605:ILE:HD13	1.85	0.58
21:7:640:LEU:HA	21:7:643:PHE:HB3	1.85	0.58
4:G:6:ASP:OD1	4:G:75:ARG:NH1	2.37	0.58
5:M:171:ILE:O	5:M:175:SER:OG	2.22	0.58
6:A:406:ILE:HB	6:A:431:LYS:HB2	1.86	0.58
6:A:811:GLN:OE1	6:A:811:GLN:N	2.28	0.58
6:A:1438:THR:HG23	10:F:92:ARG:HB2	1.85	0.58
7:B:590:HIS:NE2	7:B:592:ASN:O	2.32	0.58
1:Q:405:THR:O	1:Q:409:ALA:N	2.25	0.58
2:R:62:GLU:OE1	2:R:214:ILE:N	2.36	0.58
6:A:203:SER:OG	6:A:204:THR:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:880:THR:O	7:B:933:SER:OG	2.18	0.58
11:H:118:PHE:HB2	11:H:121:LEU:HB2	1.84	0.58
17:0:78:GLU:HA	17:0:81:LYS:HD2	1.86	0.58
6:A:329:LEU:HD21	7:B:1206:GLU:OE1	2.04	0.58
6:A:452:LYS:HB2	7:B:1141:HIS:CE1	2.39	0.58
6:A:1095:THR:HG22	6:A:1100:ARG:HB2	1.84	0.58
6:A:1133:LEU:O	6:A:1136:SER:OG	2.16	0.58
7:B:639:ILE:HD11	7:B:691:GLU:HB2	1.84	0.58
9:E:169:ARG:HD3	10:F:140:ASP:OD2	2.03	0.58
4:G:111:THR:H	4:G:114:LEU:HD22	1.69	0.58
6:A:269:ILE:HG13	6:A:299:HIS:HB3	1.83	0.58
6:A:399:HIS:O	6:A:435:HIS:ND1	2.36	0.58
6:A:1148:ILE:O	12:I:48:LEU:HG	2.04	0.58
17:0:624:GLY:HA2	17:0:683:ASP:HB2	1.85	0.58
22:5:10:VAL:HG11	22:5:20:ILE:HG21	1.85	0.58
28:T:147:DT:H1'	29:O:207:PHE:CZ	2.38	0.58
1:Q:99:ASN:OD1	1:Q:100:GLU:N	2.37	0.57
6:A:949:ASP:OD1	6:A:951:GLU:N	2.37	0.57
7:B:861:ASP:OD1	7:B:862:GLN:N	2.36	0.57
17:0:395:ASP:OD1	17:0:395:ASP:N	2.30	0.57
18:4:273:ARG:NH1	19:6:373:SER:HB3	2.18	0.57
21:7:715:GLU:HA	21:7:718:TYR:HD2	1.68	0.57
28:T:21:DC:H2'	28:T:22:DT:C6	2.39	0.57
3:D:154:PHE:HE2	3:D:163:VAL:HG21	1.68	0.57
6:A:118:HIS:HA	6:A:123:ARG:NH2	2.19	0.57
12:I:60:GLN:OE1	12:I:60:GLN:N	2.20	0.57
12:I:101:PHE:HE1	12:I:112:SER:HB3	1.69	0.57
21:7:481:GLU:HB3	21:7:508:HIS:NE2	2.19	0.57
2:R:338:THR:N	2:R:350:THR:O	2.37	0.57
4:G:158:HIS:CE1	30:W:138:GLN:HE22	2.22	0.57
5:M:262:LYS:HA	5:M:265:GLU:OE1	2.05	0.57
6:A:840:ARG:NH2	6:A:1106:ASN:OD1	2.37	0.57
7:B:861:ASP:OD1	7:B:914:LYS:NZ	2.28	0.57
21:7:554:CYS:HB3	21:7:726:LEU:HD13	1.86	0.57
25:U:269:ILE:HG21	26:V:106:ILE:HG21	1.85	0.57
30:W:68:SER:O	30:W:88:TYR:N	2.33	0.57
6:A:107:CYS:SG	6:A:109:HIS:N	2.68	0.57
6:A:1147:THR:OG1	6:A:1196:GLU:O	2.16	0.57
8:C:102:GLN:HG3	8:C:154:LYS:HG3	1.86	0.57
11:H:55:LEU:H	11:H:146:ARG:CA	2.01	0.57
15:L:44:ASP:OD2	15:L:46:VAL:N	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:343:LYS:HG2	17:0:347:LYS:HZ2	1.69	0.57
18:4:221:SER:O	18:4:225:GLN:N	2.31	0.57
23:2:396:ILE:HD12	23:2:399:TYR:HB3	1.86	0.57
25:U:266:VAL:HG13	25:U:275:THR:HG22	1.86	0.57
7:B:756:ILE:HG12	7:B:770:GLN:HG2	1.86	0.57
7:B:1177:HIS:HB3	7:B:1179:GLN:NE2	2.18	0.57
18:4:245:ILE:HA	18:4:248:LEU:HB2	1.86	0.57
19:6:196:LEU:HA	19:6:199:ILE:HD12	1.87	0.57
3:D:154:PHE:HZ	3:D:214:LEU:HD22	1.70	0.57
4:G:91:VAL:HB	4:G:139:ILE:HA	1.86	0.57
6:A:1148:ILE:HA	12:I:49:ILE:HD11	1.86	0.57
9:E:123:LEU:O	9:E:126:SER:OG	2.20	0.57
20:1:503:VAL:O	20:1:507:ILE:N	2.37	0.57
21:7:604:LYS:H	21:7:668:THR:HB	1.70	0.57
22:5:31:VAL:HA	22:5:42:VAL:HG13	1.86	0.57
25:U:260:CYS:N	25:U:281:VAL:O	2.28	0.57
4:G:4:ILE:HA	4:G:77:VAL:HG22	1.87	0.57
5:M:188:THR:HG22	5:M:190:LYS:N	2.18	0.57
6:A:781:ASP:OD1	6:A:781:ASP:N	2.34	0.57
6:A:1210:GLY:O	6:A:1214:GLU:HG2	2.05	0.57
7:B:1048:THR:OG1	7:B:1049:ASP:N	2.30	0.57
11:H:7:ASP:OD1	11:H:8:ASP:N	2.37	0.57
21:7:267:ASP:O	21:7:348:ARG:NE	2.36	0.57
21:7:311:ASP:OD1	21:7:311:ASP:N	2.31	0.57
24:X:249:GLY:H	30:W:18:ARG:NH2	2.02	0.57
2:R:95:ILE:HD13	2:R:106:LEU:HG	1.85	0.57
3:D:175:PHE:O	3:D:179:GLN:HG2	2.04	0.57
4:G:142:ARG:HB3	4:G:171:ILE:HD12	1.87	0.57
6:A:567:LYS:HB2	11:H:96:VAL:N	2.18	0.57
6:A:635:ARG:HH11	6:A:635:ARG:HA	1.69	0.57
6:A:786:HIS:N	6:A:786:HIS:CD2	2.72	0.57
6:A:922:ASP:OD1	6:A:923:LEU:N	2.37	0.57
10:F:79:ARG:NH1	10:F:145:ASP:O	2.37	0.57
12:I:2:THR:OG1	12:I:3:THR:N	2.38	0.57
15:L:61:THR:HG1	15:L:63:ARG:HH11	1.52	0.57
6:A:147:VAL:HG22	6:A:149:GLU:OE2	2.04	0.57
6:A:741:ASN:ND2	6:A:744:LYS:H	2.03	0.57
7:B:60:GLN:OE1	7:B:95:ILE:HG22	2.05	0.57
7:B:324:ILE:HD11	7:B:333:PHE:HD2	1.69	0.57
7:B:650:GLU:OE2	7:B:651:LEU:N	2.36	0.57
7:B:942:ARG:HB2	7:B:945:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:83:GLN:HA	14:K:54:ARG:NH2	2.20	0.57
21:7:636:ARG:HH22	21:7:657:VAL:HG21	1.70	0.57
28:T:22:DT:O4	28:T:23:DC:N4	2.38	0.57
28:T:146:DA:OP1	29:O:68:GLN:NE2	2.37	0.57
30:W:109:LEU:HD12	30:W:175:LEU:HD22	1.87	0.57
6:A:997:LEU:O	6:A:1011:GLN:NE2	2.38	0.57
7:B:807:ARG:HG2	7:B:1045:SER:OG	2.05	0.57
8:C:92:CYS:SG	8:C:93:ASP:N	2.78	0.57
17:0:104:ARG:HH22	17:0:171:LEU:HB2	1.68	0.57
17:0:224:ASN:HA	17:0:227:SER:HB3	1.87	0.57
17:0:539:VAL:HG22	17:0:599:LEU:HA	1.86	0.57
18:4:52:LYS:HD3	18:4:243:GLY:HA2	1.86	0.57
25:U:276:PHE:HB3	26:V:60:LEU:HG	1.87	0.57
3:D:119:ARG:HD3	3:D:221:TYR:HB2	1.87	0.56
9:E:4:GLU:O	9:E:8:ASN:CB	2.53	0.56
12:I:11:ASN:O	12:I:12:ASN:ND2	2.38	0.56
17:0:351:VAL:HG21	17:0:633:ARG:HD2	1.86	0.56
20:1:501:UNK:HA	20:1:504:ILE:HB	1.87	0.56
29:O:204:LEU:HD13	29:O:230:ILE:HG12	1.87	0.56
31:P:7:A:H3'	31:P:8:G:O4'	2.05	0.56
5:M:187:ARG:HA	5:M:187:ARG:HE	1.69	0.56
6:A:28:ARG:NH2	6:A:85:ASP:OD1	2.26	0.56
6:A:1157:ASP:OD1	6:A:1159:ARG:N	2.37	0.56
8:C:51:VAL:HA	8:C:155:LEU:HB3	1.87	0.56
17:0:104:ARG:NH1	17:0:171:LEU:O	2.39	0.56
21:7:499:ARG:HH12	21:7:525:GLY:H	1.52	0.56
24:X:263:TRP:HZ3	30:W:179:ILE:HD11	1.70	0.56
3:D:191:ALA:O	3:D:195:ILE:N	2.25	0.56
3:D:197:SER:O	3:D:201:LYS:NZ	2.29	0.56
4:G:94:CYS:SG	4:G:95:SER:N	2.78	0.56
5:M:249:PRO:HB2	5:M:251:GLN:HE22	1.70	0.56
6:A:1239:ARG:HH12	6:A:1241:ARG:HH12	1.50	0.56
7:B:955:THR:OG1	7:B:956:THR:N	2.37	0.56
7:B:1099:VAL:O	7:B:1102:LYS:N	2.20	0.56
9:E:54:GLN:HE22	9:E:56:LYS:H	1.53	0.56
12:I:7:CYS:SG	12:I:10:CYS:N	2.71	0.56
13:J:48:ARG:O	13:J:52:THR:HG22	2.04	0.56
17:0:196:VAL:HA	17:0:199:MET:HB2	1.87	0.56
21:7:585:PRO:HG2	21:7:756:ARG:HG2	1.87	0.56
28:T:145:DT:H4'	29:O:68:GLN:HE21	1.69	0.56
2:R:63:ARG:HD3	2:R:66:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:69:TRP:HA	2:R:220:HIS:O	2.05	0.56
2:R:124:LEU:HD13	2:R:127:LYS:HD2	1.87	0.56
4:G:6:ASP:HA	4:G:75:ARG:HA	1.86	0.56
6:A:767:GLN:NE2	6:A:798:GLY:O	2.38	0.56
6:A:884:ASP:OD1	6:A:884:ASP:N	2.37	0.56
7:B:259:TYR:HE2	7:B:270:LYS:HB2	1.69	0.56
7:B:590:HIS:NE2	7:B:591:ARG:O	2.38	0.56
9:E:47:CYS:HA	9:E:53:PRO:HA	1.86	0.56
11:H:113:ALA:HA	11:H:125:LEU:O	2.05	0.56
28:T:25:DC:H2'	28:T:26:DG:C8	2.41	0.56
1:Q:371:ASP:OD1	1:Q:372:SER:N	2.35	0.56
6:A:915:SER:O	6:A:919:ILE:HG12	2.05	0.56
7:B:335:GLY:HA3	7:B:348:ARG:HH21	1.69	0.56
7:B:577:ALA:HB1	7:B:589:VAL:HB	1.88	0.56
10:F:140:ASP:OD1	10:F:141:GLY:N	2.39	0.56
17:0:257:LEU:HD22	17:0:346:MET:HE2	1.88	0.56
17:0:430:VAL:HG12	30:W:18:ARG:HH12	1.70	0.56
21:7:554:CYS:HA	21:7:705:PHE:HB3	1.88	0.56
23:2:377:GLN:O	23:2:382:SER:OG	2.24	0.56
29:O:202:ILE:HG21	29:O:214:LEU:HD23	1.86	0.56
30:W:28:VAL:HG13	30:W:43:LEU:HD21	1.86	0.56
3:D:26:THR:OG1	3:D:28:GLN:NE2	2.39	0.56
6:A:253:ASN:ND2	6:A:255:SER:H	2.03	0.56
7:B:629:ASP:OD1	7:B:630:ALA:N	2.39	0.56
12:I:10:CYS:SG	12:I:31:THR:OG1	2.63	0.56
17:0:310:PRO:HG3	17:0:404:THR:HG23	1.86	0.56
17:0:576:ALA:HB2	20:1:343:ILE:HD11	1.88	0.56
23:2:43:ALA:HB2	23:2:77:ALA:HB1	1.86	0.56
29:O:105:ARG:HG2	29:O:112:THR:HA	1.87	0.56
7:B:272:THR:OG1	7:B:279:ASP:OD1	2.19	0.56
8:C:174:ALA:HB1	8:C:233:GLU:HG2	1.87	0.56
9:E:25:ASP:OD2	9:E:187:TYR:OH	2.16	0.56
9:E:124:VAL:HA	9:E:132:ILE:HD11	1.86	0.56
19:6:163:GLN:OE1	19:6:378:ARG:NH1	2.38	0.56
2:R:66:ARG:HD2	2:R:215:VAL:HG13	1.87	0.56
4:G:84:GLY:HA2	4:G:146:LYS:HZ3	1.70	0.56
4:G:113:HIS:O	4:G:164:LYS:NZ	2.22	0.56
6:A:42:ASP:OD1	6:A:47:ARG:NH2	2.39	0.56
7:B:98:THR:OG1	7:B:99:LYS:N	2.38	0.56
7:B:739:THR:HG1	7:B:740:HIS:CE1	2.21	0.56
7:B:834:ASN:HB2	7:B:839:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:58:THR:N	11:H:143:LEU:O	2.38	0.56
12:I:51:ASN:N	12:I:51:ASN:OD1	2.35	0.56
23:2:338:SER:O	23:2:356:GLN:NE2	2.39	0.56
3:D:131:GLU:HG3	3:D:136:GLY:HA2	1.88	0.56
7:B:839:MET:HB2	7:B:1011:ILE:O	2.06	0.56
18:4:254:ILE:HG22	18:4:259:ARG:HA	1.88	0.56
30:W:140:LEU:HB2	30:W:147:PHE:CD1	2.41	0.56
2:R:67:GLN:C	2:R:219:CYS:HB2	2.27	0.56
10:F:135:ARG:HD2	10:F:143:PHE:CE1	2.41	0.56
18:4:225:GLN:NE2	18:4:268:GLY:O	2.39	0.56
26:V:81:LYS:HE2	26:V:110:LYS:HG3	1.87	0.56
29:O:171:ARG:HB2	29:O:237:PHE:HB3	1.87	0.56
29:O:178:SER:HB3	29:O:237:PHE:HZ	1.70	0.56
1:Q:373:TYR:OH	2:R:72:ARG:NH1	2.39	0.55
5:M:157:CYS:O	5:M:159:ASP:N	2.39	0.55
6:A:91:PHE:HA	6:A:235:ILE:HG22	1.88	0.55
6:A:1166:ASP:HB3	6:A:1239:ARG:HD2	1.87	0.55
6:A:1443:VAL:HG12	10:F:132:LEU:O	2.07	0.55
7:B:996:ARG:HD2	7:B:1007:VAL:HG11	1.87	0.55
17:0:198:ARG:NH1	17:0:199:MET:SD	2.80	0.55
17:0:251:ASP:OD1	17:0:436:ARG:NH1	2.35	0.55
17:0:537:MET:SD	17:0:567:LYS:NZ	2.77	0.55
18:4:82:GLY:N	18:4:148:THR:HG21	2.21	0.55
22:5:31:VAL:HG22	22:5:42:VAL:HG22	1.87	0.55
1:Q:99:ASN:O	2:R:97:ILE:N	2.38	0.55
1:Q:336:ASP:OD1	1:Q:337:GLU:N	2.39	0.55
2:R:74:PRO:HB2	2:R:76:PHE:CD1	2.41	0.55
3:D:215:SER:HA	3:D:218:GLU:HB2	1.87	0.55
5:M:213:ILE:O	5:M:217:LYS:HG2	2.06	0.55
6:A:351:THR:HG22	6:A:352:VAL:N	2.21	0.55
6:A:1199:ARG:HE	6:A:1236:LEU:HD21	1.70	0.55
7:B:232:SER:O	7:B:261:ARG:NH1	2.39	0.55
11:H:87:ARG:NE	11:H:87:ARG:HA	2.20	0.55
29:O:205:LEU:HB2	29:O:213:VAL:HB	1.87	0.55
1:Q:138:ARG:HH22	1:Q:355:PHE:HB3	1.70	0.55
6:A:47:ARG:HG2	6:A:257:ARG:NH1	2.21	0.55
7:B:1134:GLU:N	7:B:1134:GLU:OE1	2.33	0.55
17:0:162:LEU:HD12	17:0:166:GLU:HG2	1.88	0.55
17:0:499:LYS:HB3	17:0:503:GLN:HA	1.87	0.55
18:4:59:VAL:O	18:4:63:ALA:N	2.30	0.55
18:4:75:VAL:HG12	18:4:86:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:221:GLY:H	21:7:336:PRO:HG2	1.72	0.55
21:7:407:VAL:HB	21:7:452:LEU:HD22	1.87	0.55
4:G:96:GLN:N	30:W:145:THR:HB	2.21	0.55
6:A:445:ASN:N	6:A:445:ASN:OD1	2.38	0.55
6:A:1168:GLU:HA	6:A:1171:GLN:HG2	1.89	0.55
6:A:1295:THR:OG1	6:A:1297:GLU:OE2	2.21	0.55
6:A:1318:THR:O	9:E:14:ARG:NH2	2.38	0.55
6:A:1442:ASP:HA	10:F:135:ARG:N	2.22	0.55
7:B:512:ARG:NH2	7:B:531:GLN:O	2.39	0.55
21:7:457:TYR:HE1	21:7:487:LEU:HD22	1.71	0.55
2:R:66:ARG:NH1	2:R:215:VAL:O	2.37	0.55
5:M:161:LYS:O	5:M:164:LYS:HB2	2.06	0.55
6:A:803:SER:OG	6:A:805:LEU:N	2.36	0.55
7:B:423:LYS:NZ	7:B:468:GLU:OE2	2.29	0.55
12:I:77:LYS:HZ3	12:I:108:HIS:HB2	1.71	0.55
1:Q:124:LYS:HG2	1:Q:126:LYS:NZ	2.21	0.55
1:Q:372:SER:OG	2:R:73:LEU:N	2.38	0.55
2:R:94:LYS:NZ	2:R:94:LYS:O	2.35	0.55
6:A:567:LYS:HZ2	6:A:568:PRO:N	2.05	0.55
6:A:1329:THR:OG1	6:A:1331:SER:N	2.32	0.55
11:H:54:SER:HB3	11:H:146:ARG:CB	2.33	0.55
16:3:86:LYS:O	16:3:90:ASN:N	2.39	0.55
20:1:251:LEU:HB3	20:1:254:GLU:HB2	1.89	0.55
3:D:179:GLN:HB3	3:D:195:ILE:HD13	1.89	0.55
6:A:1154:TYR:HB2	6:A:1191:TRP:CZ3	2.41	0.55
6:A:1202:MET:HG3	6:A:1236:LEU:HD13	1.87	0.55
12:I:15:TYR:O	12:I:27:PHE:HA	2.07	0.55
12:I:29:CYS:SG	12:I:31:THR:OG1	2.59	0.55
23:2:140:ALA:O	23:2:144:GLU:N	2.37	0.55
25:U:259:LYS:HA	25:U:282:GLU:HG2	1.88	0.55
1:Q:362:VAL:O	1:Q:396:THR:N	2.35	0.55
2:R:211:LYS:H	2:R:211:LYS:HD2	1.71	0.55
4:G:13:LEU:HD11	4:G:17:PHE:HB2	1.89	0.55
6:A:107:CYS:HA	6:A:171:GLN:NE2	2.21	0.55
6:A:579:SER:HB3	6:A:611:GLN:HA	1.88	0.55
18:4:88:PRO:HB2	19:6:407:GLN:NE2	2.22	0.55
18:4:137:LYS:HG3	18:4:139:GLN:HG3	1.89	0.55
19:6:122:ILE:HG21	19:6:379:SER:HB3	1.88	0.55
21:7:323:VAL:HA	21:7:326:VAL:HB	1.87	0.55
21:7:564:GLU:HA	21:7:567:GLN:HB2	1.89	0.55
30:W:31:ALA:HA	30:W:34:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1:MET:HB3	4:G:82:PHE:HE2	1.71	0.55
6:A:980:ASP:OD2	6:A:1039:LYS:HB3	2.06	0.55
7:B:946:ASN:OD1	7:B:946:ASN:N	2.39	0.55
9:E:89:GLY:O	9:E:92:THR:OG1	2.22	0.55
17:0:248:LEU:HB2	17:0:439:CYS:HB2	1.89	0.55
18:4:28:VAL:N	18:4:74:ALA:O	2.32	0.55
21:7:215:GLY:O	21:7:220:TYR:N	2.28	0.55
21:7:385:VAL:HG23	21:7:538:ALA:H	1.72	0.55
1:Q:121:PHE:N	2:R:131:ASN:OD1	2.39	0.55
4:G:115:MET:HE3	4:G:119:LEU:HD23	1.88	0.55
6:A:878:ILE:HG21	6:A:955:PRO:HB2	1.90	0.55
8:C:93:ASP:N	8:C:93:ASP:OD1	2.40	0.55
11:H:47:PHE:HE1	11:H:94:ASP:HB2	1.72	0.55
26:V:69:TYR:HB2	26:V:76:TRP:CZ3	2.41	0.55
2:R:73:LEU:HD11	2:R:77:LEU:HD23	1.89	0.54
6:A:1116:LEU:HB2	6:A:1311:VAL:HG22	1.89	0.54
7:B:979:LYS:HZ3	31:P:10:A:P	2.29	0.54
8:C:88:CYS:SG	8:C:92:CYS:HB3	2.47	0.54
17:0:496:ILE:HG13	17:0:706:LEU:HD13	1.90	0.54
1:Q:127:ILE:HG23	1:Q:129:PRO:HD3	1.88	0.54
3:D:40:HIS:HE1	4:G:74:TYR:O	1.91	0.54
6:A:596:THR:C	6:A:598:LEU:H	2.11	0.54
7:B:331:LEU:HD23	7:B:352:ALA:HB3	1.90	0.54
7:B:334:ILE:O	7:B:348:ARG:NE	2.41	0.54
18:4:75:VAL:H	18:4:88:PRO:HD3	1.71	0.54
18:4:292:CYS:HB2	18:4:308:CYS:SG	2.47	0.54
19:6:267:SER:HA	19:6:290:ILE:HD12	1.89	0.54
21:7:435:CYS:HA	21:7:453:VAL:HA	1.89	0.54
6:A:419:LYS:NZ	6:A:419:LYS:H	2.04	0.54
6:A:798:GLY:HA2	6:A:815:PHE:CD2	2.43	0.54
6:A:1090:ALA:HA	6:A:1093:LYS:HG3	1.89	0.54
6:A:1299:VAL:HG23	6:A:1300:LYS:O	2.07	0.54
10:F:110:ASP:OD1	10:F:110:ASP:N	2.38	0.54
17:0:280:GLN:HA	17:0:283:GLN:HG2	1.89	0.54
18:4:77:ALA:HB3	18:4:132:LEU:HD11	1.87	0.54
21:7:569:TYR:HA	21:7:577:ARG:HH11	1.71	0.54
21:7:617:GLU:O	21:7:621:LYS:NZ	2.40	0.54
4:G:85:GLU:HB3	4:G:147:ILE:HD12	1.88	0.54
8:C:98:VAL:H	8:C:122:SER:HB3	1.73	0.54
11:H:58:THR:N	11:H:143:LEU:HB2	2.22	0.54
17:0:493:LEU:HB2	17:0:678:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:516:PRO:HB2	21:7:358:PRO:HD2	1.89	0.54
23:2:486:ASP:O	23:2:489:LYS:NZ	2.27	0.54
30:W:9:VAL:HG11	30:W:91:TYR:HB3	1.90	0.54
30:W:149:CYS:SG	30:W:152:CYS:N	2.70	0.54
2:R:106:LEU:HD11	2:R:122:LEU:HB2	1.89	0.54
5:M:202:GLU:O	5:M:206:THR:OG1	2.22	0.54
6:A:57:ARG:HG3	6:A:68:GLN:HB3	1.88	0.54
6:A:108:MET:HE2	6:A:171:GLN:HB3	1.90	0.54
6:A:298:PHE:O	6:A:302:THR:HG22	2.07	0.54
6:A:1197:LEU:HB2	6:A:1236:LEU:HD12	1.89	0.54
7:B:862:GLN:CB	7:B:963:PHE:HB2	2.36	0.54
11:H:128:ASN:O	11:H:128:ASN:ND2	2.41	0.54
19:6:128:LEU:HA	19:6:233:LEU:HB3	1.88	0.54
21:7:637:MET:HA	21:7:640:LEU:HB2	1.88	0.54
23:2:62:LEU:HA	23:2:65:TRP:HD1	1.72	0.54
26:V:83:CYS:O	26:V:108:VAL:N	2.34	0.54
29:O:215:THR:OG1	29:O:216:GLY:N	2.40	0.54
30:W:123:MET:HG2	30:W:157:VAL:HB	1.88	0.54
2:R:118:HIS:ND1	2:R:120:TYR:OH	2.39	0.54
6:A:923:LEU:O	6:A:927:VAL:HG12	2.08	0.54
7:B:355:ILE:HG22	7:B:356:LEU:HD23	1.90	0.54
7:B:954:VAL:HG22	7:B:964:VAL:HG22	1.89	0.54
13:J:6:ARG:HA	13:J:12:LYS:O	2.08	0.54
14:K:82:ASP:OD2	14:K:85:ASP:N	2.36	0.54
18:4:234:VAL:HG11	18:4:252:MET:HG3	1.89	0.54
19:6:182:VAL:HG21	19:6:199:ILE:HD11	1.88	0.54
23:2:432:VAL:HG23	23:2:433:LEU:HD23	1.90	0.54
24:X:201:THR:HG22	30:W:34:PHE:HA	1.88	0.54
30:W:66:LEU:HA	30:W:94:ALA:HB2	1.89	0.54
2:R:237:VAL:O	2:R:241:ARG:N	2.39	0.54
5:M:143:PRO:HB2	5:M:145:ILE:HG22	1.90	0.54
6:A:215:SER:OG	6:A:218:ASP:OD1	2.23	0.54
6:A:590:ARG:NH2	6:A:621:THR:OG1	2.40	0.54
6:A:606:LEU:HD21	6:A:608:ILE:HD11	1.88	0.54
6:A:1110:ASN:OD1	6:A:1110:ASN:N	2.36	0.54
20:1:544:ILE:O	20:1:548:GLU:N	2.33	0.54
21:7:710:SER:O	21:7:713:THR:OG1	2.25	0.54
28:T:158:DT:H2"	28:T:159:DT:O4'	2.07	0.54
5:M:204:GLY:O	5:M:207:LEU:HG	2.08	0.54
6:A:494:SER:OG	6:A:496:GLU:OE1	2.25	0.54
6:A:1148:ILE:N	6:A:1196:GLU:O	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:29:MET:HE1	14:K:97:LYS:HD2	1.89	0.54
9:E:20:LYS:HE3	9:E:34:GLU:HG2	1.89	0.54
11:H:41:ASP:OD2	11:H:122:LEU:N	2.29	0.54
15:L:62:LYS:H	15:L:63:ARG:NH1	2.06	0.54
23:2:47:ILE:HD12	23:2:104:PHE:HE2	1.73	0.54
1:Q:120:LYS:HG2	2:R:132:GLU:OE1	2.08	0.54
6:A:257:ARG:H	6:A:257:ARG:HE	1.55	0.54
6:A:1021:LEU:O	6:A:1024:SER:OG	2.18	0.54
9:E:56:LYS:NZ	9:E:84:ASP:H	2.05	0.54
11:H:100:THR:HG23	11:H:138:GLU:HA	1.88	0.54
17:0:245:ILE:HA	17:0:439:CYS:HB3	1.90	0.54
20:1:511:ALA:O	20:1:515:UNK:N	2.40	0.54
24:X:199:GLN:HA	24:X:202:PHE:HB2	1.90	0.54
1:Q:372:SER:HG	2:R:73:LEU:H	1.55	0.54
6:A:1043:ASP:N	6:A:1043:ASP:OD1	2.40	0.54
6:A:1161:THR:HG22	6:A:1163:ILE:N	2.23	0.54
6:A:1261:LYS:O	6:A:1264:GLU:HG3	2.08	0.54
7:B:345:LYS:HA	7:B:347:LYS:N	2.23	0.54
7:B:361:LEU:HB3	7:B:364:ILE:HG13	1.89	0.54
17:0:322:PRO:HB3	17:0:376:PHE:HB2	1.89	0.54
18:4:122:ASP:HA	18:4:125:LEU:HB2	1.90	0.54
21:7:637:MET:O	21:7:641:GLN:N	2.40	0.54
23:2:39:LEU:HD13	23:2:47:ILE:HG13	1.88	0.54
6:A:512:VAL:HA	6:A:519:PRO:HA	1.90	0.53
6:A:827:THR:O	6:A:831:THR:HG23	2.09	0.53
6:A:1348:LEU:HD23	6:A:1372:VAL:HG22	1.89	0.53
10:F:77:ASP:OD2	10:F:77:ASP:N	2.28	0.53
29:O:130:ASP:OD1	29:O:133:LYS:NZ	2.33	0.53
1:Q:375:LEU:HD21	2:R:134:VAL:HG21	1.90	0.53
4:G:50:ASP:OD1	4:G:53:ASN:N	2.35	0.53
5:M:236:LEU:O	5:M:239:ILE:HG12	2.08	0.53
6:A:980:ASP:OD1	6:A:1039:LYS:N	2.36	0.53
7:B:708:GLU:CD	7:B:708:GLU:H	2.09	0.53
7:B:808:ALA:O	7:B:812:LEU:HD22	2.09	0.53
20:1:303:UNK:O	20:1:305:UNK:N	2.42	0.53
4:G:84:GLY:HA2	4:G:146:LYS:NZ	2.23	0.53
6:A:31:SER:HB2	6:A:83:HIS:HB3	1.91	0.53
6:A:668:ASP:OD1	6:A:742:ASN:ND2	2.40	0.53
7:B:731:VAL:HG23	7:B:732:SER:H	1.74	0.53
9:E:97:VAL:O	9:E:101:GLN:NE2	2.41	0.53
9:E:143:ASN:OD1	9:E:145:THR:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:166:ILE:HG12	19:6:375:HIS:HB3	1.90	0.53
24:X:269:PRO:O	30:W:65:ARG:NH2	2.41	0.53
6:A:39:GLU:HG3	6:A:50:ILE:HD13	1.91	0.53
6:A:302:THR:HA	6:A:305:ASP:O	2.09	0.53
8:C:107:SER:OG	8:C:108:GLU:N	2.42	0.53
10:F:99:LEU:O	10:F:102:SER:OG	2.22	0.53
16:3:82:VAL:O	16:3:86:LYS:N	2.31	0.53
17:0:79:ILE:HD12	17:0:207:ILE:HG22	1.91	0.53
21:7:497:MET:HA	21:7:500:ARG:HE	1.73	0.53
27:N:16:DC:H2"	27:N:17:DG:N7	2.23	0.53
3:D:35:LEU:O	3:D:47:LEU:N	2.41	0.53
3:D:68:ARG:HG2	3:D:72:ARG:HH22	1.72	0.53
6:A:414:ASP:OD1	6:A:416:ARG:N	2.34	0.53
9:E:76:GLY:HA3	9:E:106:GLN:HB2	1.90	0.53
11:H:108:SER:OG	11:H:110:ASP:OD1	2.25	0.53
17:0:422:PRO:HA	17:0:433:PRO:HB3	1.91	0.53
23:2:24:ARG:HB3	23:2:219:VAL:HG11	1.90	0.53
27:N:5:DA:H61	28:T:161:DT:H3	1.55	0.53
29:O:141:ARG:NH1	29:O:144:GLN:OE1	2.38	0.53
29:O:176:ALA:HA	29:O:183:SER:HB2	1.90	0.53
2:R:94:LYS:HE3	2:R:107:LEU:HG	1.91	0.53
3:D:144:THR:HG23	4:G:105:PRO:HD3	1.91	0.53
4:G:10:ASN:HA	4:G:70:PHE:O	2.08	0.53
6:A:1209:MET:N	6:A:1231:ASP:OD1	2.28	0.53
6:A:1444:MET:CG	10:F:133:VAL:HG22	2.39	0.53
12:I:107:SER:O	12:I:107:SER:OG	2.26	0.53
15:L:61:THR:OG1	15:L:63:ARG:NH1	2.42	0.53
15:L:63:ARG:NE	15:L:63:ARG:HA	2.22	0.53
17:0:342:LEU:O	17:0:346:MET:N	2.41	0.53
24:X:203:LYS:HA	30:W:46:LEU:HD13	1.90	0.53
29:O:81:ASP:HB3	29:O:84:THR:HB	1.89	0.53
3:D:127:ASP:O	3:D:142:LYS:NZ	2.32	0.53
6:A:557:ASP:O	14:K:26:LYS:HB3	2.08	0.53
6:A:1301:GLU:HG3	6:A:1302:PRO:HD2	1.91	0.53
7:B:408:LEU:HD11	7:B:545:ILE:HD12	1.89	0.53
7:B:643:ASP:C	7:B:645:SER:N	2.62	0.53
6:A:1441:PHE:HZ	10:F:92:ARG:HB3	1.74	0.53
7:B:26:THR:N	7:B:29:ASP:OD2	2.42	0.53
9:E:38:PRO:HB2	9:E:41:ASP:OD1	2.09	0.53
9:E:101:GLN:N	9:E:101:GLN:OE1	2.42	0.53
12:I:7:CYS:O	12:I:9:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:208:TYR:HE2	17:0:213:LEU:HB2	1.73	0.53
17:0:308:GLU:CD	17:0:308:GLU:H	2.12	0.53
18:4:54:LEU:O	18:4:58:ILE:N	2.42	0.53
21:7:552:VAL:HG21	21:7:731:TYR:HD2	1.74	0.53
21:7:647:ASP:O	21:7:650:ASN:ND2	2.42	0.53
1:Q:333:LYS:HB2	7:B:70:ILE:HD11	1.90	0.53
2:R:134:VAL:N	2:R:216:GLY:O	2.32	0.53
3:D:195:ILE:HG21	3:D:198:LEU:HD12	1.89	0.53
6:A:254:GLU:OE1	7:B:935:ARG:NH1	2.42	0.53
7:B:892:LYS:NZ	7:B:909:ASP:OD2	2.41	0.53
7:B:894:ASP:N	7:B:894:ASP:OD1	2.41	0.53
12:I:18:GLU:HB3	12:I:20:LYS:HD3	1.91	0.53
18:4:78:ALA:HB2	18:4:152:ALA:HB2	1.90	0.53
19:6:291:LEU:HD13	19:6:297:LEU:HB3	1.91	0.53
30:W:124:CYS:N	30:W:129:THR:O	2.22	0.53
6:A:41:MET:O	6:A:50:ILE:HG13	2.07	0.53
6:A:53:LEU:HD12	6:A:54:ASN:H	1.73	0.53
6:A:420:ARG:NH2	6:A:423:ASP:OD2	2.27	0.53
6:A:1166:ASP:O	6:A:1170:ILE:HG12	2.09	0.53
7:B:137:TYR:N	7:B:137:TYR:CD1	2.76	0.53
7:B:345:LYS:N	7:B:346:GLU:HB3	2.23	0.53
7:B:706:GLN:N	7:B:710:LEU:HD23	2.21	0.53
11:H:84:ALA:H	14:K:54:ARG:HH22	1.57	0.53
17:0:53:LEU:HD13	17:0:86:LEU:HB2	1.91	0.53
20:1:370:UNK:C	20:1:372:VAL:H	2.22	0.53
21:7:212:PHE:O	21:7:216:ALA:N	2.34	0.53
21:7:615:LEU:HD12	21:7:618:TYR:HD2	1.74	0.53
23:2:19:GLN:HE21	23:2:85:HIS:CE1	2.26	0.53
26:V:62:VAL:HA	26:V:84:GLN:O	2.09	0.53
1:Q:103:LEU:HA	1:Q:384:PHE:O	2.09	0.52
3:D:34:GLN:O	3:D:47:LEU:HB2	2.09	0.52
3:D:154:PHE:O	3:D:155:ARG:NE	2.42	0.52
6:A:584:ASN:HA	6:A:610:GLY:HA3	1.89	0.52
6:A:847:ASP:N	6:A:847:ASP:OD1	2.40	0.52
7:B:1016:ALA:O	7:B:1020:ARG:HD2	2.09	0.52
8:C:235:VAL:HG21	13:J:6:ARG:NH2	2.24	0.52
12:I:25:LEU:O	12:I:37:GLU:HA	2.09	0.52
17:0:21:GLN:O	17:0:25:MET:N	2.29	0.52
29:O:172:LEU:HD13	29:O:193:LEU:HB2	1.90	0.52
30:W:44:LYS:HA	30:W:54:LEU:HD13	1.89	0.52
30:W:98:ILE:HB	30:W:186:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:71:VAL:HA	2:R:222:CYS:O	2.08	0.52
4:G:92:VAL:HG23	4:G:102:GLN:HB2	1.90	0.52
5:M:60:ARG:HD2	5:M:60:ARG:N	2.24	0.52
6:A:1212:VAL:O	6:A:1216:ILE:HG13	2.09	0.52
9:E:56:LYS:HZ1	9:E:84:ASP:H	1.56	0.52
12:I:7:CYS:H	12:I:12:ASN:H	1.58	0.52
17:0:137:THR:HA	17:0:142:LYS:HB3	1.91	0.52
1:Q:100:GLU:HA	2:R:95:ILE:O	2.10	0.52
1:Q:103:LEU:HD12	1:Q:384:PHE:HB2	1.90	0.52
1:Q:133:PHE:HE1	1:Q:359:ASN:HB2	1.74	0.52
4:G:60:ARG:HA	10:F:133:VAL:CG1	2.39	0.52
5:M:193:GLN:NE2	5:M:197:HIS:HA	2.22	0.52
6:A:218:ASP:N	6:A:218:ASP:OD1	2.42	0.52
6:A:1158:PRO:HB3	6:A:1188:GLN:NE2	2.22	0.52
6:A:1445:ILE:N	10:F:132:LEU:O	2.42	0.52
7:B:135:ARG:NH1	7:B:138:GLU:HB2	2.25	0.52
7:B:864:LYS:NZ	7:B:867:GLY:O	2.42	0.52
21:7:390:ALA:HB2	21:7:692:ARG:CZ	2.39	0.52
21:7:655:SER:HB2	21:7:657:VAL:HG22	1.91	0.52
29:O:67:LEU:HD13	29:O:70:ILE:HD11	1.91	0.52
29:O:160:ILE:N	29:O:217:ALA:O	2.41	0.52
6:A:60:SER:OG	6:A:65:LEU:O	2.24	0.52
6:A:287:HIS:HA	6:A:290:GLU:OE1	2.10	0.52
6:A:858:ASN:OD1	6:A:859:SER:N	2.43	0.52
6:A:1037:LEU:HD12	6:A:1042:PHE:HD1	1.74	0.52
27:N:10:DA:H2"	27:N:11:DA:N7	2.24	0.52
29:O:165:ASP:OD1	29:O:166:VAL:N	2.42	0.52
2:R:99:LYS:HB2	2:R:103:LYS:HE2	1.91	0.52
3:D:206:GLU:O	3:D:210:ILE:HG13	2.09	0.52
5:M:163:LEU:O	5:M:166:LYS:HG2	2.09	0.52
12:I:17:ARG:N	12:I:26:LEU:O	2.42	0.52
17:0:125:LYS:HE2	17:0:127:THR:HG23	1.92	0.52
17:0:703:ASP:HA	17:0:706:LEU:HD23	1.91	0.52
20:1:300:UNK:O	20:1:302:UNK:N	2.42	0.52
23:2:59:LEU:HB2	23:2:96:LEU:HB2	1.92	0.52
24:X:201:THR:HA	30:W:34:PHE:HB3	1.91	0.52
25:U:282:GLU:HB2	26:V:63:LYS:HG2	1.92	0.52
29:O:170:ILE:HG21	29:O:234:LEU:HD22	1.90	0.52
30:W:98:ILE:HG22	30:W:186:LEU:HD11	1.92	0.52
6:A:858:ASN:OD1	6:A:860:LEU:N	2.43	0.52
6:A:1129:GLU:O	6:A:1133:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1229:SER:HB3	6:A:1237:ILE:HD12	1.91	0.52
7:B:1097:HIS:CE1	31:P:9:G:H4'	2.45	0.52
11:H:56:THR:HA	11:H:145:ARG:HH11	1.72	0.52
24:X:207:CYS:HA	24:X:210:LEU:HD12	1.91	0.52
30:W:144:ARG:NH2	30:W:145:THR:H	2.07	0.52
4:G:9:LEU:O	4:G:72:VAL:N	2.42	0.52
5:M:271:GLY:HA2	5:M:277:ILE:CG1	2.33	0.52
6:A:23:SER:HG	6:A:26:GLU:H	1.53	0.52
6:A:72:GLU:O	6:A:76:GLU:HB3	2.09	0.52
6:A:1228:TRP:HA	6:A:1238:ILE:HA	1.91	0.52
11:H:57:VAL:HB	11:H:145:ARG:N	2.24	0.52
18:4:217:GLY:O	18:4:237:HIS:NE2	2.40	0.52
29:O:175:LEU:HD11	29:O:195:TYR:HE1	1.74	0.52
2:R:105:THR:OG1	2:R:119:GLU:OE2	2.14	0.52
3:D:63:LEU:HD13	3:D:130:LEU:HD13	1.92	0.52
6:A:353:ILE:HG13	6:A:482:PHE:HD1	1.75	0.52
6:A:860:LEU:HD11	6:A:1394:THR:HA	1.91	0.52
7:B:232:SER:O	7:B:261:ARG:NH2	2.42	0.52
7:B:950:ASP:OD2	7:B:967:ARG:NE	2.42	0.52
9:E:119:SER:O	9:E:122:LYS:HB2	2.10	0.52
11:H:57:VAL:HA	11:H:144:ILE:N	2.24	0.52
17:0:231:ILE:HA	17:0:455:SER:HB2	1.92	0.52
29:O:84:THR:O	29:O:88:HIS:ND1	2.43	0.52
6:A:244:PRO:O	6:A:247:ARG:N	2.40	0.52
6:A:821:ARG:HE	7:B:514:LEU:HB2	1.75	0.52
8:C:22:LEU:HG	8:C:25:VAL:HG21	1.91	0.52
14:K:12:LEU:HD11	14:K:18:LYS:HB2	1.90	0.52
17:0:657:ASP:O	17:0:661:HIS:ND1	2.35	0.52
17:0:719:GLN:OE1	17:0:722:ARG:NH1	2.43	0.52
19:6:352:CYS:HB3	19:6:366:CYS:SG	2.50	0.52
20:1:260:PHE:HE1	20:1:266:VAL:HG22	1.73	0.52
1:Q:381:ASP:OD1	1:Q:382:GLY:N	2.43	0.52
3:D:167:LEU:HA	3:D:170:THR:HG23	1.92	0.52
5:M:168:MET:O	5:M:172:MET:HG2	2.10	0.52
6:A:630:ILE:O	6:A:634:THR:OG1	2.28	0.52
7:B:46:GLN:OE1	7:B:47:GLN:HG2	2.10	0.52
7:B:647:GLY:C	7:B:649:LYS:H	2.11	0.52
7:B:936:ASP:OD1	7:B:938:SER:OG	2.14	0.52
7:B:1155:SER:OG	7:B:1156:ASP:N	2.43	0.52
9:E:81:GLU:HB3	9:E:110:PHE:HA	1.92	0.52
11:H:132:LEU:HB3	11:H:135:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:81:ARG:N	12:I:82:GLU:OE1	2.43	0.52
17:0:23:ASN:OD1	17:0:752:LYS:NZ	2.27	0.52
18:4:225:GLN:HE22	18:4:269:SER:HA	1.73	0.52
21:7:556:GLU:HA	21:7:707:SER:HB3	1.92	0.52
23:2:481:LEU:HA	23:2:493:ILE:HG21	1.92	0.52
26:V:85:VAL:N	26:V:106:ILE:O	2.29	0.52
3:D:130:LEU:HA	3:D:133:THR:HB	1.92	0.51
7:B:294:ASP:OD1	7:B:294:ASP:N	2.43	0.51
7:B:486:TYR:OH	7:B:1096:ARG:HB3	2.09	0.51
10:F:146:TRP:HE3	10:F:150:GLU:HG3	1.74	0.51
12:I:51:ASN:HB3	12:I:118:ARG:NH2	2.25	0.51
17:0:497:ILE:HB	17:0:682:ALA:HA	1.91	0.51
21:7:350:PRO:HD2	21:7:480:ARG:HH12	1.75	0.51
21:7:607:VAL:N	21:7:652:ILE:O	2.31	0.51
2:R:127:LYS:HA	2:R:220:HIS:ND1	2.25	0.51
2:R:129:VAL:HG11	2:R:220:HIS:HA	1.90	0.51
5:M:210:MET:HE3	5:M:210:MET:O	2.10	0.51
6:A:709:THR:N	6:A:712:GLU:OE2	2.30	0.51
6:A:1173:HIS:NE2	6:A:1227:ILE:HA	2.25	0.51
7:B:254:LEU:HG	7:B:255:GLN:N	2.24	0.51
10:F:135:ARG:HD2	10:F:143:PHE:CZ	2.45	0.51
11:H:57:VAL:C	11:H:143:LEU:HB2	2.31	0.51
12:I:26:LEU:HD23	12:I:37:GLU:HA	1.93	0.51
17:0:124:ARG:HH12	17:0:577:GLN:HB2	1.75	0.51
1:Q:339:ALA:O	1:Q:343:ARG:HG2	2.10	0.51
1:Q:367:ALA:HB3	7:B:369:GLY:O	2.10	0.51
2:R:303:LEU:O	2:R:307:PHE:N	2.32	0.51
5:M:280:VAL:HG12	5:M:309:ILE:HA	1.92	0.51
6:A:115:LEU:HD13	6:A:141:LEU:HB3	1.93	0.51
7:B:371:GLU:H	7:B:371:GLU:CD	2.08	0.51
7:B:422:LYS:O	7:B:425:THR:OG1	2.26	0.51
12:I:75:CYS:SG	12:I:78:CYS:N	2.83	0.51
17:0:181:LEU:HG	17:0:192:PRO:HB3	1.93	0.51
4:G:98:GLY:HA3	4:G:110:VAL:O	2.11	0.51
6:A:67:CYS:SG	6:A:80:HIS:HE1	2.16	0.51
6:A:1217:LYS:O	6:A:1221:LYS:HG3	2.10	0.51
6:A:1359:ASP:OD1	6:A:1361:SER:N	2.42	0.51
6:A:1444:MET:SD	10:F:133:VAL:HG22	2.50	0.51
7:B:70:ILE:HD12	7:B:89:GLU:OE2	2.10	0.51
7:B:704:ALA:HB2	7:B:738:PHE:CD2	2.45	0.51
9:E:45:LYS:HB3	9:E:46:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:12:DG:N2	28:T:155:DT:O2	2.43	0.51
29:O:115:ILE:HG12	29:O:121:MET:HG2	1.93	0.51
4:G:131:GLN:HG3	4:G:136:VAL:HG22	1.92	0.51
5:M:325:ASP:HB3	5:M:326:PRO:HD3	1.93	0.51
6:A:1442:ASP:CG	10:F:135:ARG:HA	2.31	0.51
9:E:83:CYS:SG	9:E:88:VAL:HG22	2.50	0.51
17:0:53:LEU:O	17:0:57:ILE:N	2.36	0.51
17:0:307:VAL:HG21	17:0:381:LEU:HB3	1.93	0.51
17:0:603:ARG:NH2	17:0:626:PRO:O	2.43	0.51
18:4:66:ALA:HA	18:4:117:ARG:NH2	2.25	0.51
18:4:84:LYS:HD3	18:4:132:LEU:HB2	1.93	0.51
21:7:264:PRO:O	21:7:268:VAL:N	2.43	0.51
23:2:92:SER:OG	23:2:93:SER:N	2.44	0.51
29:O:144:GLN:NE2	29:O:150:ALA:O	2.43	0.51
3:D:64:VAL:HG22	3:D:67:ARG:HH22	1.76	0.51
6:A:172:PRO:HB3	6:A:185:TRP:CD2	2.44	0.51
6:A:596:THR:O	6:A:598:LEU:N	2.44	0.51
7:B:102:VAL:O	7:B:109:THR:HA	2.10	0.51
7:B:645:SER:HG	7:B:648:HIS:CG	2.29	0.51
12:I:19:ASP:OD2	12:I:21:GLU:N	2.35	0.51
17:0:154:GLU:N	17:0:154:GLU:OE1	2.43	0.51
17:0:694:PRO:HG2	17:0:697:ILE:HB	1.92	0.51
3:D:69:ALA:HA	3:D:72:ARG:HB3	1.92	0.51
6:A:771:GLU:O	6:A:773:LYS:N	2.39	0.51
8:C:6:PRO:HB2	14:K:101:LEU:HG	1.93	0.51
9:E:88:VAL:HB	9:E:116:ILE:HD13	1.92	0.51
9:E:117:THR:O	9:E:120:ALA:N	2.43	0.51
10:F:134:ILE:HG22	10:F:135:ARG:H	1.75	0.51
11:H:57:VAL:HB	11:H:145:ARG:CA	2.40	0.51
17:0:643:ARG:HH11	17:0:650:GLU:HG3	1.75	0.51
25:U:285:TRP:HZ3	29:O:110:LYS:HE3	1.76	0.51
4:G:118:ASP:OD2	4:G:132:SER:OG	2.26	0.51
5:M:274:PRO:HA	5:M:277:ILE:HG12	1.92	0.51
6:A:226:GLU:OE2	6:A:230:ARG:NH2	2.42	0.51
6:A:727:ASP:OD1	6:A:727:ASP:N	2.42	0.51
6:A:851:HIS:O	6:A:854:ASN:N	2.43	0.51
6:A:857:ARG:HD3	6:A:861:GLY:O	2.11	0.51
7:B:360:PHE:O	7:B:374:LYS:NZ	2.37	0.51
11:H:95:TYR:O	11:H:143:LEU:HD23	2.10	0.51
12:I:80:SER:HG	12:I:82:GLU:H	1.56	0.51
15:L:61:THR:OG1	15:L:63:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:123:GLU:OE1	17:0:125:LYS:N	2.43	0.51
17:0:227:SER:HG	17:0:453:PHE:HE1	1.59	0.51
17:0:275:ARG:NH2	17:0:329:GLU:OE2	2.43	0.51
21:7:520:GLU:N	21:7:681:ARG:HH12	2.09	0.51
30:W:112:ASP:HB2	30:W:168:LYS:HG3	1.93	0.51
4:G:101:VAL:HG13	4:G:143:ILE:HD13	1.93	0.51
6:A:1233:ASP:OD1	6:A:1233:ASP:N	2.44	0.51
8:C:226:ASP:OD1	8:C:227:THR:OG1	2.25	0.51
12:I:8:ARG:CZ	12:I:8:ARG:HB3	2.40	0.51
17:0:72:CYS:HB3	17:0:210:TYR:CD1	2.46	0.51
6:A:335:ARG:HD2	7:B:1202:LEU:HD23	1.92	0.51
6:A:603:ASN:N	6:A:603:ASN:OD1	2.39	0.51
9:E:90:VAL:HA	9:E:120:ALA:HB2	1.93	0.51
14:K:60:ALA:O	14:K:73:LEU:HD12	2.10	0.51
17:0:502:ASP:OD1	17:0:521:ASN:ND2	2.44	0.51
18:4:58:ILE:HD12	18:4:125:LEU:HD13	1.93	0.51
19:6:120:ARG:HG2	19:6:309:PRO:HG3	1.92	0.51
19:6:159:GLU:O	19:6:163:GLN:NE2	2.44	0.51
20:1:501:UNK:O	20:1:505:THR:N	2.32	0.51
21:7:626:PHE:HB2	21:7:653:PHE:CD1	2.46	0.51
23:2:95:THR:OG1	23:2:96:LEU:N	2.44	0.51
4:G:23:LYS:HA	4:G:26:LEU:HB2	1.93	0.50
6:A:737:LEU:HD13	6:A:741:ASN:ND2	2.26	0.50
7:B:652:LYS:HE3	7:B:689:LEU:HD23	1.92	0.50
8:C:35:ARG:HD3	14:K:41:THR:OG1	2.11	0.50
17:0:120:VAL:HG12	17:0:129:VAL:HG13	1.93	0.50
29:O:175:LEU:HD12	29:O:179:HIS:HB2	1.93	0.50
1:Q:133:PHE:CE1	1:Q:359:ASN:HB2	2.46	0.50
6:A:862:ASN:OD1	6:A:862:ASN:N	2.41	0.50
9:E:59:SER:HG	9:E:82:PHE:H	1.53	0.50
18:4:202:SER:HB3	19:6:448:LEU:HD21	1.92	0.50
18:4:260:PRO:O	23:2:67:ASN:ND2	2.43	0.50
21:7:416:SER:OG	21:7:661:SER:OG	2.23	0.50
23:2:25:LEU:HD21	23:2:226:PHE:HE2	1.75	0.50
6:A:1228:TRP:HB3	6:A:1238:ILE:HG23	1.92	0.50
7:B:708:GLU:N	7:B:708:GLU:CD	2.64	0.50
15:L:38:LEU:HD23	15:L:39:SER:N	2.26	0.50
17:0:495:MET:HB2	17:0:680:VAL:HA	1.91	0.50
18:4:50:ILE:O	18:4:54:LEU:N	2.38	0.50
18:4:193:TYR:HE2	18:4:274:THR:HG21	1.77	0.50
18:4:302:GLY:HA2	19:6:319:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:477:LEU:HB3	21:7:505:ILE:HG12	1.94	0.50
21:7:619:ALA:HB3	21:7:626:PHE:CG	2.47	0.50
23:2:457:SER:N	23:2:493:ILE:O	2.41	0.50
27:N:11:DA:C5	27:N:12:DG:C6	2.99	0.50
4:G:97:HIS:CE1	30:W:146:GLU:HA	2.46	0.50
6:A:587:HIS:HA	6:A:607:ILE:O	2.11	0.50
7:B:882:THR:O	7:B:935:ARG:HA	2.11	0.50
7:B:1107:ALA:O	7:B:1108:ARG:HB3	2.12	0.50
8:C:79:GLN:OE1	8:C:79:GLN:N	2.44	0.50
17:0:310:PRO:HB2	17:0:408:LEU:HD21	1.93	0.50
17:0:515:ASP:N	17:0:515:ASP:OD1	2.45	0.50
17:0:555:GLN:HE22	17:0:564:TRP:HZ2	1.60	0.50
18:4:286:GLY:N	19:6:322:MET:O	2.44	0.50
19:6:137:LEU:HG	19:6:204:PRO:HG2	1.93	0.50
21:7:564:GLU:OE2	21:7:756:ARG:HB2	2.11	0.50
1:Q:409:ALA:HB1	7:B:323:VAL:CG1	2.42	0.50
6:A:75:ASN:HA	7:B:1116:ARG:HH12	1.77	0.50
6:A:164:ARG:O	6:A:166:GLY:N	2.42	0.50
7:B:93:GLY:N	7:B:131:ASP:O	2.42	0.50
11:H:84:ALA:HA	11:H:87:ARG:HG2	1.94	0.50
17:0:237:ALA:N	17:0:460:SER:OG	2.45	0.50
18:4:258:LEU:HB3	18:4:260:PRO:HD3	1.93	0.50
19:6:266:LEU:HA	19:6:291:LEU:HG	1.92	0.50
21:7:385:VAL:HG12	21:7:514:THR:HB	1.93	0.50
28:T:144:DA:H4'	29:O:125:GLY:HA2	1.93	0.50
29:O:133:LYS:HD3	29:O:155:PHE:CE2	2.47	0.50
3:D:67:ARG:HH11	3:D:130:LEU:HD21	1.76	0.50
6:A:43:GLU:OE1	6:A:43:GLU:N	2.36	0.50
6:A:1254:ALA:HB1	6:A:1256:GLU:HG3	1.93	0.50
7:B:327:ARG:O	7:B:331:LEU:HD12	2.11	0.50
7:B:497:ARG:HG2	7:B:498:THR:H	1.76	0.50
11:H:47:PHE:CE1	11:H:94:ASP:HB2	2.46	0.50
15:L:28:LYS:HG2	15:L:29:TYR:CE2	2.46	0.50
17:0:166:GLU:HG3	17:0:198:ARG:HH21	1.76	0.50
18:4:180:THR:OG1	18:4:214:LYS:NZ	2.35	0.50
19:6:427:TYR:N	19:6:436:PHE:O	2.44	0.50
21:7:536:TYR:OH	21:7:542:GLU:OE1	2.30	0.50
24:X:162:LEU:O	24:X:166:LEU:N	2.45	0.50
28:T:151:DC:H2"	28:T:152:DG:H8	1.77	0.50
29:O:162:GLY:N	29:O:214:LEU:O	2.44	0.50
29:O:178:SER:HB3	29:O:237:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:76:PHE:HZ	2:R:120:TYR:HE2	1.59	0.50
4:G:100:GLU:HA	4:G:109:PHE:HA	1.94	0.50
5:M:57:VAL:HG11	7:B:1113:VAL:HG13	1.93	0.50
6:A:1130:GLN:HA	6:A:1133:LEU:HD12	1.93	0.50
8:C:145:CYS:SG	8:C:146:LYS:N	2.85	0.50
9:E:79:TRP:HD1	9:E:96:PHE:HE1	1.58	0.50
14:K:14:GLU:OE1	14:K:14:GLU:N	2.45	0.50
15:L:40:LEU:HG	15:L:41:SER:O	2.11	0.50
17:0:349:LEU:HD23	17:0:349:LEU:H	1.77	0.50
17:0:360:LEU:HD11	17:0:410:SER:HA	1.93	0.50
18:4:244:LEU:O	18:4:248:LEU:N	2.34	0.50
19:6:269:GLN:HG3	19:6:288:TYR:CE2	2.44	0.50
19:6:403:CYS:SG	19:6:404:PHE:N	2.84	0.50
29:O:73:THR:HG23	29:O:158:GLN:HG3	1.93	0.50
4:G:166:ASP:O	4:G:168:LEU:HG	2.12	0.50
5:M:267:LYS:NZ	29:O:239:LYS:HB2	2.27	0.50
7:B:299:GLU:OE2	7:B:572:HIS:N	2.33	0.50
7:B:1051:THR:OG1	7:B:1053:GLU:N	2.45	0.50
9:E:77:SER:HG	9:E:105:PHE:HD1	1.58	0.50
9:E:95:THR:O	9:E:98:ILE:HG22	2.11	0.50
11:H:145:ARG:NH1	11:H:146:ARG:NH2	2.59	0.50
12:I:98:VAL:HG11	12:I:113:ASP:HB2	1.94	0.50
17:0:330:HIS:O	17:0:333:SER:OG	2.21	0.50
19:6:152:TYR:HD1	19:6:298:LYS:HD3	1.76	0.50
21:7:594:LEU:O	21:7:598:HIS:ND1	2.45	0.50
21:7:627:ILE:HG12	21:7:636:ARG:HG3	1.94	0.50
23:2:10:VAL:HG12	23:2:205:LEU:HD11	1.94	0.50
1:Q:116:THR:O	1:Q:390:ASP:HB3	2.12	0.50
7:B:137:TYR:O	7:B:140:ILE:HG13	2.11	0.50
17:0:509:ARG:HH11	17:0:685:ARG:HD3	1.77	0.50
23:2:51:VAL:HG13	23:2:109:ARG:HD2	1.94	0.50
23:2:108:LEU:HG	23:2:112:LEU:HD13	1.94	0.50
30:W:6:ASP:O	30:W:10:LYS:HG3	2.12	0.50
3:D:194:LEU:HD22	4:G:86:VAL:HG11	1.93	0.49
4:G:35:GLU:OE2	4:G:48:VAL:N	2.39	0.49
4:G:79:PHE:HE2	4:G:106:MET:HG2	1.77	0.49
5:M:273:SER:O	5:M:276:THR:HG22	2.12	0.49
6:A:249:SER:O	6:A:249:SER:OG	2.27	0.49
6:A:269:ILE:HD11	6:A:300:VAL:HA	1.94	0.49
6:A:390:GLN:O	6:A:393:ARG:HB3	2.12	0.49
6:A:1364:ASN:OD1	6:A:1365:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:363:HIS:CG	7:B:363:HIS:O	2.64	0.49
7:B:1074:ASN:HB2	7:B:1081:LEU:HD21	1.94	0.49
7:B:1179:GLN:HB3	7:B:1181:GLU:OE2	2.12	0.49
9:E:60:PHE:CZ	9:E:80:VAL:HG21	2.47	0.49
11:H:23:VAL:HA	11:H:42:ILE:O	2.11	0.49
12:I:19:ASP:OD2	12:I:23:ASN:N	2.34	0.49
12:I:80:SER:OG	12:I:82:GLU:OE1	2.23	0.49
15:L:47:ARG:HH22	15:L:54:ARG:CZ	2.25	0.49
17:0:239:ASN:OD1	17:0:664:GLN:NE2	2.45	0.49
21:7:302:GLU:HG2	21:7:322:SER:HB2	1.94	0.49
21:7:759:LEU:O	21:7:763:VAL:HG23	2.12	0.49
4:G:151:ILE:HB	4:G:158:HIS:HB2	1.93	0.49
5:M:157:CYS:C	5:M:159:ASP:H	2.15	0.49
6:A:1163:ILE:HG22	6:A:1165:GLU:H	1.76	0.49
6:A:1205:LYS:O	6:A:1274:ARG:NH1	2.45	0.49
9:E:76:GLY:H	9:E:106:GLN:HG2	1.77	0.49
9:E:79:TRP:HB2	9:E:105:PHE:CD2	2.47	0.49
15:L:47:ARG:HH12	15:L:54:ARG:NE	2.10	0.49
21:7:589:GLN:HB3	21:7:745:ILE:HD11	1.94	0.49
21:7:684:ALA:HB2	21:7:725:PHE:HZ	1.77	0.49
23:2:208:LEU:HD13	23:2:222:LEU:HD21	1.93	0.49
23:2:405:HIS:O	23:2:408:MET:N	2.45	0.49
6:A:594:GLY:O	6:A:596:THR:HG23	2.12	0.49
6:A:943:LEU:O	6:A:946:VAL:N	2.45	0.49
7:B:183:GLU:OE1	7:B:184:ALA:N	2.44	0.49
7:B:576:ASP:OD1	7:B:576:ASP:N	2.42	0.49
8:C:264:GLN:O	8:C:267:GLN:HB3	2.12	0.49
17:0:270:ARG:CZ	17:0:390:VAL:HA	2.42	0.49
17:0:564:TRP:CD2	20:1:239:PRO:HG3	2.46	0.49
27:N:12:DG:C5	27:N:13:DG:C6	3.00	0.49
30:W:140:LEU:HB2	30:W:147:PHE:HD1	1.76	0.49
1:Q:124:LYS:O	1:Q:126:LYS:NZ	2.28	0.49
2:R:98:ASN:OD1	2:R:103:LYS:HE3	2.12	0.49
3:D:24:ALA:N	3:D:28:GLN:HB2	2.27	0.49
4:G:14:HIS:HB3	4:G:17:PHE:HE1	1.77	0.49
4:G:108:VAL:HG22	4:G:159:ALA:HB3	1.94	0.49
6:A:607:ILE:HG23	6:A:612:ILE:HA	1.94	0.49
6:A:917:SER:OG	6:A:918:GLU:N	2.46	0.49
12:I:77:LYS:HG3	12:I:108:HIS:CD2	2.47	0.49
18:4:55:GLU:HA	18:4:58:ILE:HB	1.93	0.49
1:Q:343:ARG:NE	1:Q:343:ARG:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:405:THR:O	1:Q:408:GLU:N	2.46	0.49
6:A:425:GLN:O	6:A:427:GLN:NE2	2.45	0.49
6:A:463:ILE:HD11	6:A:469:ARG:HG3	1.95	0.49
6:A:810:PRO:HG3	7:B:1047:PHE:CD1	2.47	0.49
6:A:982:THR:OG1	6:A:983:ILE:N	2.44	0.49
7:B:994:TYR:HB2	7:B:999:MET:SD	2.52	0.49
9:E:78:LEU:HD12	9:E:107:THR:O	2.12	0.49
12:I:99:LEU:HB2	12:I:112:SER:HB3	1.95	0.49
15:L:28:LYS:HG2	15:L:29:TYR:CD2	2.47	0.49
17:0:619:THR:HG22	17:0:678:VAL:HB	1.94	0.49
21:7:406:SER:HB3	21:7:482:TRP:CE3	2.48	0.49
26:V:60:LEU:HA	26:V:86:THR:O	2.12	0.49
29:O:185:TYR:CG	29:O:187:PRO:HD3	2.48	0.49
29:O:204:LEU:HD23	29:O:214:LEU:HD11	1.92	0.49
3:D:61:GLU:O	3:D:64:VAL:HB	2.12	0.49
4:G:46:LEU:HD21	4:G:79:PHE:HB3	1.94	0.49
5:M:189:PHE:N	29:O:188:GLU:OE1	2.37	0.49
6:A:515:GLN:HG2	6:A:516:SER:OG	2.12	0.49
6:A:766:GLY:HA2	6:A:799:PHE:CE1	2.47	0.49
7:B:908:GLU:OE1	7:B:908:GLU:N	2.45	0.49
7:B:1101:ASP:N	7:B:1101:ASP:OD1	2.42	0.49
11:H:9:ILE:HD11	11:H:31:THR:HG21	1.95	0.49
11:H:84:ALA:H	14:K:54:ARG:HH12	1.59	0.49
12:I:54:GLU:OE1	12:I:120:GLN:HA	2.13	0.49
17:0:161:ASN:ND2	17:0:189:THR:O	2.46	0.49
21:7:606:ILE:HA	21:7:652:ILE:HG13	1.95	0.49
23:2:485:ASP:OD1	23:2:485:ASP:N	2.45	0.49
29:O:184:SER:H	29:O:193:LEU:HG	1.78	0.49
1:Q:116:THR:HA	2:R:136:THR:HG22	1.93	0.49
2:R:307:PHE:O	2:R:311:ASP:N	2.45	0.49
6:A:457:ALA:HB3	6:A:506:ALA:HA	1.93	0.49
7:B:27:ALA:O	7:B:30:SER:OG	2.29	0.49
15:L:62:LYS:H	15:L:63:ARG:HH12	1.60	0.49
17:0:312:LEU:O	17:0:314:GLN:N	2.44	0.49
17:0:318:THR:H	17:0:375:ARG:HH11	1.60	0.49
17:0:564:TRP:CE2	20:1:239:PRO:HG3	2.47	0.49
21:7:564:GLU:O	21:7:568:GLU:N	2.42	0.49
3:D:49:ALA:O	3:D:50:LEU:HD23	2.13	0.49
4:G:65:ASP:OD1	4:G:65:ASP:N	2.46	0.49
5:M:126:VAL:HG13	5:M:154:TYR:HE2	1.76	0.49
6:A:870:GLU:O	9:E:205:SER:OG	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1436:ILE:O	6:A:1437:GLY:C	2.51	0.49
7:B:643:ASP:OD2	7:B:654:ARG:NH2	2.29	0.49
17:0:211:HIS:O	17:0:215:ASP:N	2.38	0.49
21:7:438:PHE:HB3	21:7:459:MET:HG3	1.94	0.49
29:O:169:PRO:HA	29:O:208:VAL:O	2.13	0.49
4:G:65:ASP:O	4:G:67:SER:N	2.46	0.49
6:A:741:ASN:HD22	6:A:744:LYS:HB2	1.78	0.49
6:A:1218:GLN:O	6:A:1221:LYS:NZ	2.46	0.49
7:B:307:ASP:O	7:B:310:MET:N	2.45	0.49
9:E:185:ALA:O	9:E:189:GLY:N	2.46	0.49
14:K:10:PHE:HA	14:K:37:LYS:HB3	1.94	0.49
21:7:659:ASP:HB3	21:7:660:THR:HG22	1.95	0.49
25:U:253:ARG:HA	25:U:257:ARG:O	2.12	0.49
28:T:17:DG:H2'	28:T:18:DA:C4	2.47	0.49
4:G:7:LEU:HB2	4:G:74:TYR:CZ	2.48	0.49
5:M:180:CYS:SG	5:M:181:ARG:N	2.86	0.49
5:M:244:SER:CB	7:B:108:VAL:HA	2.43	0.49
6:A:36:ARG:O	6:A:270:LEU:HD21	2.12	0.49
6:A:316:GLN:O	6:A:318:SER:N	2.45	0.49
7:B:1122:ARG:HG3	7:B:1123:SER:N	2.26	0.49
7:B:1175:LEU:C	7:B:1177:HIS:H	2.16	0.49
8:C:91:HIS:HA	8:C:95:CYS:SG	2.53	0.49
9:E:67:GLU:O	9:E:70:SER:OG	2.25	0.49
19:6:129:THR:HG22	19:6:172:ILE:HD12	1.95	0.49
22:5:9:LEU:HD21	22:5:39:HIS:HD2	1.77	0.49
30:W:152:CYS:O	30:W:154:GLU:HG3	2.13	0.49
1:Q:337:GLU:OE1	1:Q:339:ALA:N	2.44	0.48
1:Q:377:SER:HB3	1:Q:385:THR:N	2.16	0.48
2:R:220:HIS:CG	2:R:221:GLU:N	2.81	0.48
6:A:924:LYS:HE3	6:A:984:LYS:HZ2	1.77	0.48
6:A:1072:ILE:O	6:A:1075:PRO:HD2	2.13	0.48
6:A:1225:PHE:CE2	6:A:1227:ILE:HD11	2.48	0.48
8:C:81:GLU:HG3	8:C:85:ASP:HB2	1.95	0.48
12:I:113:ASP:OD2	12:I:115:LYS:N	2.46	0.48
17:0:294:HIS:ND1	17:0:383:LEU:HD12	2.28	0.48
17:0:473:LEU:HB2	17:0:475:PHE:CD1	2.48	0.48
27:N:15:DG:N2	28:T:152:DG:O4'	2.45	0.48
1:Q:120:LYS:HG3	1:Q:393:TYR:O	2.13	0.48
6:A:39:GLU:OE2	6:A:50:ILE:HG21	2.12	0.48
6:A:404:TYR:HB2	6:A:433:GLU:HG3	1.95	0.48
6:A:786:HIS:CD2	6:A:786:HIS:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1198:ASP:OD2	6:A:1201:ALA:N	2.39	0.48
7:B:345:LYS:HA	7:B:347:LYS:H	1.78	0.48
12:I:18:GLU:O	12:I:20:LYS:HE3	2.14	0.48
17:0:512:ILE:O	17:0:513:ARG:NE	2.43	0.48
17:0:690:ARG:HG3	17:0:701:LEU:HD23	1.94	0.48
21:7:354:ILE:HD12	21:7:404:LYS:HA	1.95	0.48
26:V:82:ASN:HA	26:V:109:ASP:HA	1.93	0.48
29:O:196:ARG:HA	29:O:203:VAL:HA	1.95	0.48
1:Q:104:ARG:NH2	1:Q:105:ALA:HB3	2.28	0.48
3:D:159:THR:O	3:D:163:VAL:HG23	2.13	0.48
6:A:332:LYS:O	6:A:333:GLU:HB2	2.13	0.48
7:B:168:GLY:H	7:B:450:ALA:HB1	1.79	0.48
11:H:96:VAL:HG22	11:H:143:LEU:HD21	1.94	0.48
12:I:54:GLU:N	12:I:120:GLN:OE1	2.45	0.48
13:J:32:GLU:HA	13:J:35:ALA:HB3	1.95	0.48
17:0:76:MET:HB3	17:0:178:PHE:HE2	1.78	0.48
17:0:232:VAL:HG21	17:0:453:PHE:CD2	2.48	0.48
17:0:252:LEU:HB2	17:0:435:MET:HB2	1.95	0.48
23:2:475:ALA:O	23:2:479:GLY:N	2.43	0.48
27:N:21:DA:H4'	29:O:203:VAL:HG11	1.95	0.48
1:Q:375:LEU:HD21	2:R:68:VAL:HG21	1.94	0.48
5:M:129:ALA:O	5:M:133:ILE:HB	2.12	0.48
6:A:1163:ILE:HD12	6:A:1163:ILE:H	1.78	0.48
7:B:40:GLU:OE2	7:B:681:TRP:HD1	1.96	0.48
7:B:643:ASP:O	7:B:645:SER:N	2.47	0.48
10:F:135:ARG:HD2	10:F:143:PHE:CD1	2.48	0.48
11:H:34:ASP:OD2	11:H:34:ASP:N	2.45	0.48
17:0:190:LEU:HD12	17:0:195:ILE:HD11	1.94	0.48
17:0:244:CYS:O	17:0:247:SER:OG	2.30	0.48
21:7:414:SER:HB2	21:7:439:THR:HG23	1.95	0.48
21:7:555:ALA:N	21:7:705:PHE:O	2.46	0.48
23:2:53:ASN:ND2	23:2:55:ASN:OD1	2.47	0.48
29:O:114:LEU:HB2	29:O:122:VAL:HB	1.96	0.48
4:G:151:ILE:N	4:G:158:HIS:O	2.40	0.48
5:M:185:VAL:HG22	7:B:106:ASP:HB2	1.95	0.48
6:A:286:HIS:O	6:A:287:HIS:ND1	2.36	0.48
6:A:446:ARG:NH1	6:A:479:ASN:O	2.46	0.48
6:A:1445:ILE:CB	10:F:133:VAL:HG23	2.43	0.48
7:B:564:GLU:OE1	7:B:591:ARG:NE	2.46	0.48
11:H:58:THR:O	11:H:143:LEU:HD12	2.13	0.48
14:K:13:GLY:H	14:K:16:GLU:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:407:VAL:HG13	21:7:484:PHE:HB3	1.94	0.48
24:X:214:TRP:HD1	24:X:217:CYS:SG	2.37	0.48
3:D:71:LYS:O	3:D:75:LYS:HG3	2.13	0.48
4:G:102:GLN:HA	4:G:107:LYS:HA	1.94	0.48
5:M:241:ARG:O	5:M:245:HIS:ND1	2.47	0.48
6:A:896:ARG:HD2	6:A:897:TYR:CE2	2.49	0.48
6:A:1012:ARG:HB2	6:A:1012:ARG:CZ	2.44	0.48
6:A:1198:ASP:OD1	6:A:1200:ALA:N	2.46	0.48
9:E:56:LYS:HZ3	9:E:83:CYS:HA	1.77	0.48
17:0:83:LEU:HB3	17:0:177:SER:HA	1.96	0.48
17:0:244:CYS:HB2	17:0:442:ALA:HB1	1.95	0.48
17:0:431:PRO:HG3	24:X:252:LEU:HG	1.96	0.48
17:0:496:ILE:HG12	17:0:701:LEU:HD11	1.96	0.48
21:7:579:LEU:HD22	21:7:611:ASN:ND2	2.28	0.48
23:2:223:HIS:O	23:2:227:MET:N	2.47	0.48
1:Q:398:ARG:HD3	7:B:326:ASP:OD2	2.13	0.48
4:G:21:ARG:HD2	4:G:25:TYR:CE2	2.48	0.48
5:M:211:LYS:NZ	29:O:176:ALA:HB1	2.29	0.48
5:M:277:ILE:HA	5:M:280:VAL:HG22	1.96	0.48
6:A:39:GLU:CG	6:A:50:ILE:HD13	2.43	0.48
6:A:353:ILE:HG21	6:A:487:MET:SD	2.53	0.48
6:A:1435:PRO:HA	6:A:1439:GLY:O	2.14	0.48
7:B:405:ARG:O	7:B:406:LEU:HD23	2.14	0.48
7:B:586:TRP:NE1	7:B:588:GLY:O	2.34	0.48
7:B:1009:ASP:OD1	7:B:1009:ASP:N	2.34	0.48
11:H:33:GLN:HG3	11:H:129:TYR:CE1	2.49	0.48
11:H:81:PRO:O	11:H:83:GLN:N	2.47	0.48
17:0:537:MET:HB2	17:0:597:ILE:HG12	1.96	0.48
20:1:597:PHE:HE2	20:1:620:LEU:HD13	1.78	0.48
21:7:341:TYR:N	21:7:379:ALA:O	2.47	0.48
21:7:396:GLY:O	21:7:400:ALA:N	2.41	0.48
21:7:616:GLN:HE21	21:7:628:TYR:HD2	1.62	0.48
26:V:62:VAL:HG22	26:V:85:VAL:HG22	1.94	0.48
26:V:74:ASP:HB3	26:V:117:ASN:HB2	1.95	0.48
28:T:143:DT:O2	29:O:114:LEU:HD11	2.14	0.48
29:O:141:ARG:O	29:O:145:LYS:N	2.46	0.48
30:W:131:TYR:HD1	30:W:135:GLU:HB3	1.79	0.48
3:D:50:LEU:O	4:G:2:PHE:HB2	2.14	0.48
4:G:7:LEU:N	4:G:74:TYR:O	2.40	0.48
4:G:148:GLU:N	4:G:160:ILE:O	2.33	0.48
6:A:151:ASP:HB3	6:A:163:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:408:ASP:N	6:A:408:ASP:OD1	2.44	0.48
6:A:408:ASP:O	6:A:409:SER:OG	2.20	0.48
6:A:678:GLU:HG2	6:A:732:LEU:HD13	1.96	0.48
6:A:1089:VAL:HG12	6:A:1091:SER:HB3	1.95	0.48
7:B:37:PHE:CD2	7:B:38:PHE:N	2.81	0.48
7:B:569:TYR:CE2	7:B:571:PRO:HG3	2.49	0.48
17:0:85:GLU:O	17:0:89:LEU:HD13	2.13	0.48
18:4:28:VAL:O	18:4:76:ILE:N	2.40	0.48
18:4:67:PHE:CE1	23:2:44:LYS:HB3	2.48	0.48
1:Q:364:SER:N	1:Q:394:LYS:O	2.46	0.48
4:G:114:LEU:HD23	4:G:161:GLY:O	2.13	0.48
6:A:1139:GLU:O	6:A:1275:GLY:HA3	2.13	0.48
6:A:1239:ARG:HH22	6:A:1241:ARG:HH22	1.60	0.48
7:B:275:TYR:O	7:B:276:ILE:HD13	2.14	0.48
7:B:1051:THR:O	7:B:1055:ILE:HG13	2.14	0.48
8:C:163:ILE:HG13	8:C:165:LYS:H	1.78	0.48
11:H:56:THR:HB	11:H:93:TYR:CD1	2.47	0.48
18:4:246:GLN:HG3	20:1:503:VAL:HG11	1.94	0.48
20:1:557:CYS:HG	20:1:585:HIS:CD2	2.29	0.48
23:2:17:ILE:O	23:2:22:GLN:NE2	2.46	0.48
24:X:266:VAL:HG21	30:W:101:LYS:HG2	1.96	0.48
25:U:285:TRP:CH2	29:O:105:ARG:HB3	2.49	0.48
27:N:22:DT:OP2	29:O:196:ARG:NH1	2.46	0.48
2:R:121:ASP:N	2:R:225:MET:O	2.36	0.48
3:D:40:HIS:CE1	4:G:74:TYR:N	2.82	0.48
6:A:443:LEU:HD21	6:A:455:MET:HE2	1.96	0.48
6:A:483:ASP:O	31:P:10:A:H5”	2.13	0.48
6:A:926:GLN:NE2	6:A:926:GLN:O	2.46	0.48
7:B:128:LEU:HA	7:B:128:LEU:HD23	1.53	0.48
7:B:603:LEU:HD23	7:B:603:LEU:HA	1.58	0.48
8:C:186:LEU:HB3	8:C:188:HIS:CD2	2.49	0.48
17:0:346:MET:SD	17:0:433:PRO:HG2	2.54	0.48
17:0:369:ILE:HG21	17:0:374:LEU:HD13	1.95	0.48
28:T:24:DT:H4’	31:P:6:G:O6	2.13	0.48
1:Q:119:LEU:HD11	2:R:135:PHE:HB3	1.95	0.47
3:D:119:ARG:HB3	3:D:155:ARG:HH12	1.78	0.47
5:M:257:GLU:OE1	5:M:258:TYR:N	2.47	0.47
5:M:294:THR:O	5:M:296:ALA:N	2.47	0.47
6:A:50:ILE:C	6:A:52:GLY:H	2.18	0.47
6:A:346:ASP:OD1	6:A:346:ASP:N	2.46	0.47
6:A:446:ARG:HB2	6:A:487:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:784:LEU:HD23	6:A:784:LEU:HA	1.71	0.47
6:A:961:ARG:O	6:A:965:GLN:HG2	2.14	0.47
6:A:1134:ILE:HD13	6:A:1322:ILE:HG22	1.96	0.47
7:B:875:GLU:OE2	7:B:915:THR:OG1	2.18	0.47
8:C:99:LEU:HD13	8:C:120:ILE:HA	1.96	0.47
21:7:568:GLU:OE1	21:7:571:ARG:NH1	2.41	0.47
23:2:62:LEU:HA	23:2:65:TRP:CD1	2.48	0.47
30:W:11:ASN:HA	30:W:14:LYS:HD2	1.96	0.47
4:G:37:SER:O	4:G:44:TYR:HA	2.14	0.47
4:G:131:GLN:HG3	4:G:136:VAL:HG13	1.95	0.47
6:A:672:ASP:OD1	6:A:674:PRO:HD2	2.14	0.47
7:B:556:THR:O	7:B:559:SER:OG	2.30	0.47
7:B:834:ASN:HB3	7:B:840:ILE:HG13	1.95	0.47
7:B:1164:GLY:HA3	7:B:1190:ASP:OD2	2.14	0.47
11:H:55:LEU:HB2	11:H:144:ILE:O	2.13	0.47
11:H:102:TYR:CZ	11:H:115:TYR:HB3	2.49	0.47
11:H:116:TYR:HB2	11:H:123:MET:HE3	1.94	0.47
17:0:74:ARG:NH1	17:0:664:GLN:OE1	2.38	0.47
17:0:673:LYS:NZ	17:0:737:SER:O	2.40	0.47
18:4:71:ASN:OD1	18:4:71:ASN:N	2.44	0.47
21:7:609:SER:O	21:7:655:SER:HA	2.14	0.47
1:Q:139:LEU:HD23	2:R:212:THR:HG21	1.97	0.47
2:R:76:PHE:HZ	2:R:120:TYR:CE2	2.32	0.47
3:D:35:LEU:HG	3:D:36:LYS:HG3	1.96	0.47
3:D:147:TYR:HB2	4:G:104:GLY:HA2	1.95	0.47
5:M:242:PHE:HB3	5:M:302:LEU:HD21	1.96	0.47
6:A:567:LYS:CB	11:H:96:VAL:H	2.22	0.47
6:A:885:THR:O	6:A:940:ARG:NH1	2.42	0.47
6:A:1196:GLU:HA	6:A:1236:LEU:O	2.14	0.47
7:B:57:TYR:CD1	7:B:57:TYR:N	2.83	0.47
7:B:770:GLN:HB2	7:B:984:HIS:O	2.14	0.47
7:B:899:ILE:HD11	7:B:911:ILE:HA	1.96	0.47
8:C:162:GLY:HA3	8:C:170:TRP:CE2	2.49	0.47
8:C:181:ASP:OD1	8:C:184:ASN:N	2.46	0.47
14:K:99:GLY:O	14:K:103:THR:HG23	2.15	0.47
17:0:726:GLN:HA	19:6:290:ILE:HG12	1.96	0.47
19:6:129:THR:N	19:6:233:LEU:O	2.44	0.47
20:1:184:LEU:HD21	20:1:216:LEU:HB3	1.97	0.47
20:1:222:LEU:O	20:1:226:GLN:N	2.48	0.47
20:1:562:LYS:O	20:1:566:ILE:N	2.41	0.47
21:7:599:GLU:HG2	21:7:650:ASN:HD22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:285:TRP:CZ3	29:O:110:LYS:HE3	2.50	0.47
29:O:159:ASN:ND2	29:O:161:VAL:HG22	2.29	0.47
1:Q:120:LYS:NZ	1:Q:366:GLU:OE2	2.47	0.47
3:D:156:ASP:N	3:D:156:ASP:OD1	2.46	0.47
3:D:158:GLU:OE1	3:D:158:GLU:N	2.42	0.47
6:A:1207:LEU:HA	6:A:1211:GLN:HE22	1.80	0.47
7:B:329:THR:O	7:B:332:ASP:HB3	2.14	0.47
7:B:790:ASP:N	7:B:790:ASP:OD1	2.44	0.47
7:B:1162:ILE:HA	7:B:1162:ILE:HD13	1.60	0.47
9:E:93:MET:HE1	9:E:123:LEU:HD23	1.96	0.47
15:L:28:LYS:HB3	15:L:39:SER:HA	1.97	0.47
17:0:333:SER:HB2	17:0:337:ARG:HH22	1.80	0.47
17:0:436:ARG:NE	17:0:634:ILE:HG21	2.28	0.47
17:0:687:SER:HA	17:0:706:LEU:HD12	1.96	0.47
20:1:593:LEU:HA	20:1:596:LEU:HB2	1.95	0.47
1:Q:123:SER:HB3	1:Q:361:TRP:CH2	2.50	0.47
2:R:223:GLN:HG2	2:R:224:VAL:N	2.30	0.47
3:D:140:ASP:HA	3:D:143:ASN:ND2	2.30	0.47
4:G:81:PRO:HG3	4:G:106:MET:SD	2.54	0.47
5:M:267:LYS:HA	5:M:270:ALA:HB3	1.96	0.47
6:A:217:LYS:NZ	6:A:221:SER:OG	2.45	0.47
6:A:396:PRO:HG3	6:A:416:ARG:HG2	1.97	0.47
6:A:439:ASN:HA	6:A:459:ARG:HB3	1.96	0.47
7:B:955:THR:HB	15:L:55:ILE:HG22	1.96	0.47
9:E:78:LEU:HD11	9:E:109:ILE:HG12	1.97	0.47
12:I:51:ASN:HB3	12:I:118:ARG:CZ	2.44	0.47
13:J:53:HIS:CD2	13:J:54:VAL:H	2.32	0.47
17:0:325:ILE:HG22	17:0:331:PHE:HA	1.95	0.47
17:0:476:LYS:NZ	17:0:478:VAL:HG22	2.29	0.47
18:4:288:ILE:HD11	18:4:293:LEU:HD13	1.95	0.47
22:5:9:LEU:HD21	22:5:39:HIS:CD2	2.49	0.47
29:O:72:ALA:O	29:O:123:VAL:N	2.28	0.47
30:W:64:ASP:OD1	30:W:101:LYS:NZ	2.48	0.47
30:W:184:ASP:OD1	30:W:187:LYS:NZ	2.37	0.47
2:R:81:TRP:N	2:R:81:TRP:CD1	2.81	0.47
3:D:119:ARG:HD2	3:D:155:ARG:NH2	2.25	0.47
5:M:249:PRO:HB2	5:M:251:GLN:NE2	2.29	0.47
6:A:24:PRO:HD2	6:A:233:TRP:CD1	2.50	0.47
6:A:251:SER:HA	6:A:257:ARG:HA	1.96	0.47
6:A:446:ARG:HD2	6:A:480:ALA:HB2	1.95	0.47
7:B:585:VAL:HB	7:B:587:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:984:HIS:CD2	7:B:984:HIS:N	2.83	0.47
9:E:45:LYS:HB3	9:E:46:TYR:CD2	2.49	0.47
11:H:30:SER:HB3	11:H:36:CYS:O	2.15	0.47
12:I:51:ASN:HD22	12:I:118:ARG:HH12	1.62	0.47
17:0:37:ASN:ND2	17:0:476:LYS:O	2.47	0.47
17:0:643:ARG:HD2	17:0:650:GLU:HG3	1.97	0.47
19:6:171:ILE:HG21	19:6:196:LEU:HD11	1.95	0.47
20:1:491:UNK:O	20:1:493:UNK:N	2.47	0.47
21:7:206:ALA:O	21:7:210:ILE:N	2.32	0.47
21:7:510:LYS:HE3	21:7:531:ILE:HG12	1.96	0.47
21:7:527:LEU:HA	21:7:530:LEU:HB2	1.97	0.47
21:7:607:VAL:HA	21:7:671:ILE:HB	1.97	0.47
24:X:252:LEU:HB3	30:W:19:GLY:HA2	1.96	0.47
24:X:263:TRP:CZ3	30:W:179:ILE:HD11	2.49	0.47
27:N:17:DG:C4	27:N:18:DT:C4	3.03	0.47
1:Q:106:ILE:HD13	1:Q:385:THR:HG21	1.97	0.47
4:G:39:THR:HG1	4:G:41:LYS:H	1.60	0.47
6:A:525:GLN:OE1	7:B:836:GLU:N	2.47	0.47
6:A:1209:MET:HA	6:A:1212:VAL:HG23	1.95	0.47
6:A:1443:VAL:HG21	10:F:93:ILE:CD1	2.40	0.47
7:B:548:GLY:HA3	7:B:630:ALA:HB2	1.96	0.47
7:B:603:LEU:HB3	7:B:609:ILE:HG13	1.95	0.47
7:B:842:ASN:HB2	7:B:1009:ASP:HA	1.97	0.47
7:B:880:THR:O	7:B:880:THR:OG1	2.29	0.47
8:C:107:SER:OG	8:C:109:SER:N	2.48	0.47
10:F:93:ILE:HA	10:F:93:ILE:HD13	1.45	0.47
11:H:138:GLU:OE1	11:H:139:ASN:N	2.48	0.47
17:0:627:PHE:HD1	17:0:654:LEU:HD12	1.80	0.47
18:4:175:ARG:NH2	18:4:211:ASP:OD2	2.48	0.47
18:4:236:LEU:HB3	18:4:238:VAL:HG13	1.96	0.47
19:6:211:GLN:HB3	19:6:243:ASP:HA	1.96	0.47
21:7:133:TRP:N	21:7:142:ILE:O	2.45	0.47
21:7:678:GLY:HA2	21:7:679:SER:HA	1.67	0.47
23:2:250:LEU:O	23:2:254:ARG:N	2.37	0.47
25:U:258:TRP:CE2	26:V:66:LEU:HD23	2.50	0.47
29:O:141:ARG:HA	29:O:141:ARG:HD2	1.79	0.47
30:W:149:CYS:O	30:W:153:ASP:HA	2.14	0.47
1:Q:375:LEU:HA	1:Q:375:LEU:HD12	1.70	0.47
1:Q:377:SER:O	1:Q:384:PHE:HD1	1.98	0.47
5:M:299:GLY:HA2	5:M:304:VAL:HG22	1.97	0.47
6:A:567:LYS:HZ2	6:A:568:PRO:CD	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1257:ASP:N	6:A:1257:ASP:OD1	2.47	0.47
6:A:1271:ILE:HG22	6:A:1273:LEU:HD12	1.97	0.47
7:B:46:GLN:H	7:B:46:GLN:HG3	1.42	0.47
7:B:170:LEU:HD12	7:B:171:PRO:HD2	1.97	0.47
7:B:433:GLN:O	7:B:436:VAL:HG13	2.14	0.47
7:B:750:GLY:O	7:B:754:SER:OG	2.33	0.47
7:B:794:ASN:OD1	7:B:855:PHE:HD1	1.98	0.47
8:C:90:ASP:O	8:C:91:HIS:HB3	2.13	0.47
9:E:147:HIS:CD2	9:E:149:LEU:H	2.32	0.47
12:I:36:GLU:HB3	12:I:37:GLU:OE2	2.15	0.47
12:I:74:GLU:HB2	12:I:81:ARG:NH1	2.30	0.47
17:0:12:PHE:HE2	17:0:14:TYR:HB2	1.78	0.47
17:0:104:ARG:CZ	17:0:170:TYR:HB2	2.45	0.47
17:0:271:ILE:HA	17:0:388:LEU:HD22	1.97	0.47
21:7:545:GLN:HA	21:7:550:ALA:HA	1.97	0.47
21:7:709:VAL:HG13	21:7:715:GLU:HB3	1.97	0.47
23:2:353:SER:HB2	23:2:356:GLN:HB2	1.97	0.47
30:W:144:ARG:NH1	30:W:155:PRO:HG3	2.29	0.47
1:Q:120:LYS:HD3	1:Q:394:LYS:HD2	1.95	0.47
2:R:80:LYS:HB3	2:R:81:TRP:HD1	1.79	0.47
3:D:66:ARG:HH12	4:G:35:GLU:CD	2.18	0.47
3:D:130:LEU:O	3:D:134:THR:N	2.35	0.47
4:G:1:MET:N	4:G:80:LYS:O	2.35	0.47
5:M:267:LYS:HZ3	29:O:239:LYS:HB2	1.79	0.47
5:M:305:THR:HB	5:M:308:THR:H	1.80	0.47
6:A:871:ASP:OD1	6:A:872:GLY:N	2.48	0.47
6:A:1397:LEU:HB2	6:A:1426:GLU:HG3	1.96	0.47
17:0:581:LEU:O	17:0:585:THR:OG1	2.29	0.47
18:4:87:TYR:CE1	18:4:121:VAL:HG22	2.50	0.47
29:O:93:GLU:HG2	29:O:103:ILE:HD12	1.96	0.47
1:Q:117:HIS:ND1	1:Q:391:LYS:HB2	2.30	0.47
3:D:124:GLU:HA	3:D:127:ASP:HB2	1.97	0.47
5:M:286:ILE:HG13	5:M:291:ILE:HB	1.97	0.47
6:A:607:ILE:HG22	6:A:609:ASP:O	2.14	0.47
6:A:878:ILE:HD12	6:A:878:ILE:HG23	1.75	0.47
6:A:1034:GLU:O	6:A:1036:ARG:HG3	2.15	0.47
7:B:291:ILE:HD12	7:B:291:ILE:N	2.30	0.47
7:B:307:ASP:OD2	7:B:310:MET:HE3	2.15	0.47
7:B:706:GLN:HB2	7:B:710:LEU:HD23	1.96	0.47
11:H:125:LEU:HD12	11:H:125:LEU:HA	1.63	0.47
17:0:136:MET:HG3	17:0:154:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:176:ASN:HA	19:6:206:GLY:HA3	1.96	0.47
23:2:249:MET:O	23:2:253:MET:N	2.36	0.47
1:Q:106:ILE:HG13	1:Q:107:PRO:HD2	1.97	0.46
1:Q:142:LYS:O	1:Q:142:LYS:HG2	2.15	0.46
6:A:172:PRO:HB3	6:A:185:TRP:CE2	2.50	0.46
6:A:1121:GLU:O	6:A:1123:GLY:N	2.48	0.46
7:B:69:LEU:O	7:B:89:GLU:HA	2.15	0.46
7:B:547:VAL:N	7:B:612:GLU:OE2	2.45	0.46
7:B:1051:THR:OG1	7:B:1052:VAL:N	2.46	0.46
8:C:26:ASP:OD1	8:C:28:ALA:N	2.41	0.46
9:E:20:LYS:HE2	9:E:35:VAL:HA	1.96	0.46
15:L:47:ARG:HH22	15:L:54:ARG:NH1	2.13	0.46
17:0:416:PHE:HA	17:0:440:LEU:HG	1.97	0.46
18:4:130:TYR:O	18:4:134:GLU:N	2.48	0.46
18:4:303:ASN:N	18:4:303:ASN:OD1	2.48	0.46
21:7:582:ILE:O	21:7:587:LYS:HD2	2.15	0.46
29:O:175:LEU:HA	29:O:237:PHE:CD2	2.49	0.46
30:W:122:TYR:CD2	30:W:156:LEU:HB2	2.49	0.46
2:R:118:HIS:HB2	2:R:120:TYR:CE1	2.51	0.46
6:A:261:ASP:OD1	6:A:322:VAL:HG13	2.16	0.46
6:A:770:VAL:HA	6:A:822:GLU:OE1	2.15	0.46
6:A:873:MET:HE3	6:A:873:MET:HB3	1.75	0.46
6:A:1166:ASP:OD2	6:A:1194:ARG:NE	2.34	0.46
6:A:1174:PHE:CD1	6:A:1175:SER:N	2.79	0.46
6:A:1187:GLN:HE22	6:A:1188:GLN:NE2	2.13	0.46
7:B:805:THR:O	7:B:1044:ALA:N	2.35	0.46
7:B:990:ILE:HD12	7:B:990:ILE:HG23	1.65	0.46
7:B:1046:PRO:HB2	7:B:1047:PHE:CD2	2.50	0.46
15:L:27:LEU:HG	15:L:37:LYS:NZ	2.30	0.46
17:0:252:LEU:O	17:0:434:ILE:HA	2.16	0.46
17:0:534:PRO:HA	19:6:239:LEU:HG	1.97	0.46
18:4:64:HIS:O	18:4:71:ASN:ND2	2.31	0.46
21:7:422:GLN:HA	21:7:426:GLN:HE22	1.79	0.46
23:2:81:MET:HG2	23:2:86:LEU:HD11	1.97	0.46
25:U:253:ARG:HD3	25:U:255:LYS:H	1.80	0.46
25:U:269:ILE:O	25:U:272:ASN:ND2	2.48	0.46
29:O:175:LEU:HD11	29:O:195:TYR:CE1	2.51	0.46
1:Q:373:TYR:H	2:R:82:ARG:HH21	1.60	0.46
5:M:123:ASP:N	5:M:123:ASP:OD1	2.48	0.46
6:A:1406:VAL:HG13	6:A:1407:GLU:OE1	2.16	0.46
7:B:302:CYS:SG	7:B:307:ASP:HB3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1221:SER:O	7:B:1222:ARG:NE	2.40	0.46
8:C:60:ASP:O	8:C:63:ILE:N	2.48	0.46
17:0:694:PRO:O	17:0:698:ALA:N	2.31	0.46
18:4:194:ILE:HB	18:4:195:PRO:HD3	1.96	0.46
21:7:303:ARG:HB2	21:7:323:VAL:H	1.79	0.46
29:O:82:LEU:HD11	29:O:117:ALA:HB2	1.97	0.46
30:W:65:ARG:NE	30:W:93:HIS:HB3	2.30	0.46
2:R:138:GLN:H	2:R:138:GLN:CD	2.15	0.46
3:D:56:ARG:HE	3:D:148:LEU:HB3	1.79	0.46
3:D:156:ASP:O	3:D:158:GLU:N	2.48	0.46
6:A:74:MET:O	6:A:76:GLU:N	2.48	0.46
6:A:120:GLU:OE1	6:A:123:ARG:HD2	2.15	0.46
6:A:441:PRO:HA	6:A:458:HIS:O	2.15	0.46
7:B:1181:GLU:HA	7:B:1187:ASN:O	2.16	0.46
8:C:231:ASN:C	8:C:231:ASN:HD22	2.18	0.46
9:E:98:ILE:HA	9:E:101:GLN:NE2	2.31	0.46
13:J:23:ASN:HB3	13:J:27:GLU:OE2	2.15	0.46
17:0:681:LEU:HB3	17:0:686:PHE:CE2	2.50	0.46
20:1:260:PHE:HD1	20:1:266:VAL:HG13	1.80	0.46
20:1:517:UNK:O	20:1:519:UNK:N	2.49	0.46
21:7:420:TRP:HE1	21:7:661:SER:HG	0.57	0.46
21:7:660:THR:HA	21:7:661:SER:HA	1.75	0.46
28:T:145:DT:H1'	28:T:146:DA:C8	2.50	0.46
2:R:118:HIS:HB2	2:R:120:TYR:CZ	2.50	0.46
5:M:157:CYS:HB3	5:M:210:MET:CE	2.45	0.46
6:A:683:ILE:O	6:A:687:LYS:HG2	2.15	0.46
6:A:711:ARG:NH2	12:I:96:SER:O	2.46	0.46
6:A:1218:GLN:HA	6:A:1221:LYS:HD3	1.98	0.46
6:A:1441:PHE:CZ	10:F:92:ARG:HB3	2.51	0.46
7:B:468:GLU:H	7:B:471:LYS:HB2	1.80	0.46
7:B:1177:HIS:O	7:B:1179:GLN:HG3	2.15	0.46
10:F:97:ARG:O	10:F:101:ILE:HG13	2.16	0.46
11:H:36:CYS:HA	11:H:126:GLU:O	2.16	0.46
14:K:5:ASP:O	14:K:8:GLU:HG2	2.14	0.46
17:0:13:PRO:HG3	17:0:89:LEU:HD11	1.96	0.46
17:0:252:LEU:HD12	17:0:435:MET:HG3	1.96	0.46
17:0:465:PRO:HD2	17:0:656:PHE:HD2	1.80	0.46
17:0:473:LEU:HB2	17:0:475:PHE:CE1	2.50	0.46
18:4:61:LEU:HD11	18:4:73:VAL:HB	1.96	0.46
18:4:288:ILE:HB	18:4:295:VAL:HG22	1.97	0.46
21:7:443:LYS:HD3	21:7:444:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:587:LYS:HG3	21:7:708:LEU:HD23	1.96	0.46
21:7:636:ARG:HH12	21:7:657:VAL:HG23	1.81	0.46
21:7:751:ALA:O	21:7:756:ARG:NH2	2.46	0.46
23:2:243:SER:O	23:2:247:ARG:N	2.31	0.46
23:2:503:ASP:HA	23:2:506:LYS:HG2	1.97	0.46
26:V:65:ASN:O	26:V:81:LYS:N	2.39	0.46
4:G:40:GLY:H	4:G:154:VAL:HA	1.81	0.46
6:A:84:ILE:HD11	6:A:270:LEU:HD12	1.98	0.46
6:A:998:LEU:HA	6:A:1011:GLN:NE2	2.28	0.46
7:B:1114:LEU:HD12	7:B:1114:LEU:HA	1.61	0.46
7:B:1183:LYS:HB2	7:B:1183:LYS:HE3	1.71	0.46
11:H:145:ARG:NH1	11:H:146:ARG:CZ	2.79	0.46
13:J:58:GLU:O	13:J:61:LEU:N	2.48	0.46
21:7:552:VAL:HG11	21:7:731:TYR:CD2	2.50	0.46
21:7:692:ARG:NE	21:7:692:ARG:HA	2.30	0.46
28:T:159:DT:H2'	28:T:160:DT:C6	2.51	0.46
29:O:202:ILE:HG13	29:O:222:GLU:O	2.16	0.46
30:W:136:ALA:HB1	30:W:147:PHE:CD2	2.51	0.46
31:P:9:G:C6	31:P:10:A:C6	3.04	0.46
1:Q:104:ARG:HD2	1:Q:104:ARG:HA	1.55	0.46
1:Q:365:TYR:CE2	1:Q:367:ALA:HB2	2.50	0.46
2:R:80:LYS:HB3	2:R:81:TRP:CD1	2.51	0.46
2:R:94:LYS:H	2:R:94:LYS:HZ3	1.63	0.46
4:G:111:THR:HG22	4:G:112:LYS:H	1.79	0.46
6:A:872:GLY:O	6:A:1058:VAL:HG12	2.15	0.46
6:A:898:ARG:HB3	6:A:906:HIS:CD2	2.51	0.46
6:A:934:LYS:O	6:A:937:VAL:HG22	2.15	0.46
6:A:956:LEU:HD23	6:A:956:LEU:HA	1.63	0.46
9:E:39:LEU:O	9:E:42:PHE:HB3	2.15	0.46
11:H:57:VAL:O	11:H:58:THR:OG1	2.29	0.46
13:J:50:ILE:HA	13:J:50:ILE:HD13	1.60	0.46
13:J:61:LEU:HD23	13:J:61:LEU:HA	1.67	0.46
14:K:50:LEU:HD13	14:K:75:ILE:HD12	1.98	0.46
17:0:76:MET:HA	17:0:79:ILE:HB	1.97	0.46
19:6:164:ASN:ND2	19:6:305:VAL:O	2.49	0.46
21:7:342:ASP:OD1	21:7:342:ASP:N	2.46	0.46
21:7:438:PHE:HB2	21:7:455:SER:HB2	1.98	0.46
22:5:7:GLY:HA3	22:5:41:LEU:HD11	1.97	0.46
27:N:20:DT:C4	27:N:21:DA:N6	2.83	0.46
27:N:30:DA:C2	27:N:31:DT:C2	3.03	0.46
2:R:63:ARG:HG2	2:R:65:ASN:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:68:VAL:HG21	2:R:134:VAL:HG21	1.98	0.46
4:G:112:LYS:HA	4:G:112:LYS:HD2	1.74	0.46
5:M:276:THR:HA	5:M:279:VAL:HG12	1.98	0.46
6:A:882:SER:O	6:A:1025:ARG:NH2	2.40	0.46
6:A:1147:THR:HG23	12:I:48:LEU:HD11	1.98	0.46
6:A:1239:ARG:HH12	6:A:1241:ARG:NH1	2.13	0.46
7:B:185:THR:OG1	7:B:188:ASP:OD1	2.24	0.46
7:B:546:SER:OG	7:B:632:ARG:N	2.49	0.46
7:B:863:GLU:OE2	7:B:873:THR:HA	2.16	0.46
17:0:17:ILE:HG13	17:0:18:TYR:H	1.79	0.46
17:0:729:ASP:O	17:0:731:LYS:NZ	2.40	0.46
19:6:444:ILE:O	19:6:449:HIS:HA	2.16	0.46
21:7:578:MET:HA	21:7:581:TYR:CZ	2.50	0.46
22:5:58:LEU:HD23	23:2:450:ARG:HH11	1.80	0.46
27:N:17:DG:H22	28:T:149:DC:H42	1.63	0.46
27:N:22:DT:H1'	29:O:215:THR:OG1	2.16	0.46
29:O:67:LEU:HD11	29:O:220:ARG:HG3	1.98	0.46
29:O:161:VAL:HA	29:O:215:THR:HB	1.98	0.46
30:W:136:ALA:HB1	30:W:147:PHE:CG	2.51	0.46
1:Q:337:GLU:CD	1:Q:340:LYS:H	2.16	0.46
2:R:73:LEU:HD12	2:R:74:PRO:CD	2.46	0.46
2:R:74:PRO:HB2	2:R:76:PHE:HD1	1.80	0.46
6:A:578:LEU:HA	6:A:578:LEU:HD12	1.56	0.46
6:A:1100:ARG:NH1	6:A:1103:GLU:OE1	2.37	0.46
6:A:1167:GLU:HA	6:A:1170:ILE:HG12	1.97	0.46
6:A:1208:THR:OG1	6:A:1211:GLN:HG3	2.16	0.46
6:A:1221:LYS:HE2	6:A:1221:LYS:HB2	1.58	0.46
6:A:1286:LYS:HG3	6:A:1304:TRP:CH2	2.51	0.46
7:B:647:GLY:H	7:B:648:HIS:C	2.19	0.46
7:B:744:HIS:O	7:B:747:MET:HG2	2.15	0.46
7:B:1099:VAL:O	7:B:1101:ASP:N	2.49	0.46
7:B:1221:SER:C	7:B:1222:ARG:HE	2.18	0.46
9:E:87:SER:N	9:E:114:ASN:HB2	2.31	0.46
11:H:38:LEU:HD12	11:H:39:THR:N	2.31	0.46
12:I:33:SER:O	12:I:35:VAL:HG23	2.16	0.46
18:4:175:ARG:HH12	18:4:252:MET:HB3	1.80	0.46
23:2:10:VAL:HA	23:2:13:TYR:HB3	1.98	0.46
2:R:62:GLU:HG2	2:R:63:ARG:N	2.31	0.46
5:M:37:ARG:HG3	6:A:416:ARG:NH2	2.28	0.46
5:M:276:THR:O	5:M:280:VAL:HG13	2.16	0.46
6:A:43:GLU:OE2	6:A:48:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:557:ASP:OD1	6:A:559:VAL:N	2.48	0.46
6:A:809:THR:N	6:A:812:GLU:OE2	2.40	0.46
6:A:1035:TYR:N	6:A:1035:TYR:CD1	2.79	0.46
6:A:1266:THR:HG23	6:A:1270:ASN:OD1	2.16	0.46
7:B:365:THR:OG1	7:B:367:LEU:N	2.38	0.46
7:B:416:LEU:HD12	7:B:416:LEU:HA	1.69	0.46
7:B:487:THR:O	7:B:488:TYR:C	2.54	0.46
7:B:796:LEU:HD12	7:B:796:LEU:HA	1.68	0.46
7:B:838:SER:HB2	7:B:839:MET:CG	2.46	0.46
7:B:900:ALA:HB3	15:L:61:THR:HB	1.98	0.46
7:B:906:SER:O	7:B:941:LEU:HD21	2.16	0.46
17:0:527:VAL:HG22	17:0:531:LYS:HE3	1.98	0.46
28:T:149:DC:H2"	28:T:150:DG:C8	2.51	0.46
5:M:275:ILE:H	5:M:275:ILE:HD12	1.81	0.45
6:A:658:LEU:HG	6:A:659:HIS:ND1	2.31	0.45
6:A:1217:LYS:O	6:A:1221:LYS:N	2.49	0.45
7:B:234:ILE:H	7:B:234:ILE:HG12	1.43	0.45
8:C:174:ALA:HB3	8:C:233:GLU:O	2.16	0.45
9:E:119:SER:O	9:E:123:LEU:HD22	2.16	0.45
17:0:106:LEU:HD12	17:0:199:MET:HG3	1.97	0.45
17:0:508:SER:HB2	17:0:546:TYR:CE1	2.51	0.45
19:6:188:ASN:ND2	19:6:191:ASP:OD2	2.49	0.45
21:7:132:LEU:O	21:7:202:LYS:N	2.44	0.45
21:7:241:ILE:O	21:7:245:LEU:N	2.39	0.45
21:7:604:LYS:O	21:7:669:CYS:N	2.50	0.45
1:Q:110:ASP:O	1:Q:114:MET:HB2	2.16	0.45
1:Q:372:SER:HG	2:R:73:LEU:N	2.14	0.45
2:R:295:PRO:O	2:R:299:ILE:N	2.31	0.45
3:D:154:PHE:HB3	3:D:160:VAL:HG22	1.98	0.45
5:M:37:ARG:NH1	6:A:417:TYR:OH	2.48	0.45
5:M:127:GLN:HA	5:M:130:PHE:HB2	1.98	0.45
6:A:220:THR:OG1	6:A:221:SER:N	2.50	0.45
6:A:382:PRO:HG3	6:A:428:TYR:CZ	2.50	0.45
6:A:399:HIS:HB3	6:A:400:PRO:HD3	1.97	0.45
7:B:128:LEU:HB2	7:B:167:ILE:O	2.16	0.45
9:E:37:LEU:HD23	9:E:38:PRO:HD2	1.98	0.45
9:E:157:SER:N	9:E:160:GLU:OE1	2.49	0.45
10:F:136:ARG:O	10:F:137:TYR:CG	2.70	0.45
17:0:63:TYR:O	17:0:67:ARG:NH2	2.49	0.45
17:0:257:LEU:HA	17:0:260:ALA:HB3	1.97	0.45
17:0:446:ILE:HD12	17:0:473:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:251:ILE:HG12	19:6:276:LEU:HD13	1.99	0.45
20:1:466:UNK:O	20:1:468:UNK:N	2.49	0.45
21:7:362:ILE:HD11	21:7:367:GLU:HB3	1.98	0.45
2:R:70:LEU:HD12	2:R:71:VAL:H	1.81	0.45
4:G:83:LYS:HE3	4:G:150:CYS:HB2	1.97	0.45
5:M:251:GLN:NE2	5:M:252:VAL:HG23	2.31	0.45
6:A:229:SER:O	6:A:229:SER:OG	2.33	0.45
6:A:276:LEU:HD23	6:A:276:LEU:HA	1.56	0.45
6:A:559:VAL:HG13	11:H:78:SER:HA	1.98	0.45
6:A:904:THR:O	6:A:907:THR:HB	2.16	0.45
7:B:68:THR:HA	7:B:90:ILE:O	2.17	0.45
7:B:140:ILE:HA	7:B:141:ASP:HA	1.68	0.45
7:B:219:ALA:HB3	7:B:222:ILE:HD12	1.99	0.45
7:B:880:THR:OG1	7:B:934:LYS:NZ	2.33	0.45
7:B:1106:ARG:NH2	7:B:1109:GLY:O	2.49	0.45
9:E:4:GLU:N	9:E:4:GLU:OE1	2.49	0.45
9:E:94:LYS:HE3	9:E:123:LEU:HG	1.99	0.45
14:K:82:ASP:OD1	14:K:84:LYS:HG3	2.16	0.45
17:0:49:THR:HA	17:0:52:LEU:HB2	1.97	0.45
17:0:256:ALA:O	17:0:260:ALA:N	2.43	0.45
17:0:351:VAL:HB	17:0:421:GLU:HG2	1.97	0.45
17:0:487:LEU:HG	17:0:489:LYS:H	1.82	0.45
19:6:347:TYR:N	19:6:356:VAL:O	2.39	0.45
23:2:356:GLN:HE22	23:2:360:LEU:HD11	1.81	0.45
24:X:144:VAL:N	24:X:176:GLY:HA3	2.31	0.45
29:O:61:SER:OG	29:O:62:GLY:N	2.50	0.45
29:O:133:LYS:HB2	29:O:155:PHE:CZ	2.52	0.45
1:Q:378:VAL:HB	2:R:68:VAL:HA	1.97	0.45
6:A:55:ASP:HA	6:A:58:LEU:HD23	1.97	0.45
6:A:866:PHE:HE2	9:E:211:TYR:H	1.65	0.45
6:A:1312:ASN:OD1	6:A:1315:GLU:HG2	2.16	0.45
7:B:641:GLU:HB2	7:B:652:LYS:HG3	1.99	0.45
11:H:58:THR:H	11:H:143:LEU:HB2	1.80	0.45
15:L:31:CYS:HB2	15:L:48:CYS:HB2	1.57	0.45
17:0:217:LYS:HD3	17:0:308:GLU:HG3	1.98	0.45
18:4:146:ARG:HA	18:4:191:PHE:CZ	2.52	0.45
21:7:627:ILE:O	21:7:653:PHE:HB2	2.17	0.45
29:O:70:ILE:HG12	29:O:160:ILE:HG23	1.98	0.45
5:M:152:GLU:OE1	7:B:868:MET:HB2	2.17	0.45
6:A:23:SER:OG	6:A:23:SER:O	2.33	0.45
6:A:555:ASP:N	6:A:555:ASP:OD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:663:SER:OG	7:B:827:ILE:O	2.29	0.45
6:A:1038:THR:OG1	6:A:1040:GLN:N	2.50	0.45
7:B:793:ALA:HB3	7:B:856:PHE:HB2	1.98	0.45
17:0:2:LYS:HA	17:0:10:VAL:O	2.17	0.45
17:0:90:MET:HB2	17:0:175:VAL:HG21	1.99	0.45
17:0:285:GLU:OE2	17:0:288:LYS:NZ	2.31	0.45
17:0:507:SER:OG	17:0:508:SER:N	2.49	0.45
19:6:129:THR:OG1	19:6:234:ILE:HA	2.17	0.45
19:6:153:ALA:HA	19:6:156:PHE:HB3	1.97	0.45
21:7:519:ARG:NE	21:7:521:ASP:HB2	2.32	0.45
21:7:590:ALA:HA	21:7:739:LEU:HD11	1.99	0.45
21:7:625:PRO:HD2	21:7:649:ILE:HG12	1.98	0.45
23:2:28:SER:O	23:2:31:THR:OG1	2.35	0.45
24:X:207:CYS:SG	24:X:241:PRO:HA	2.56	0.45
24:X:259:PHE:CE1	30:W:109:LEU:HD11	2.49	0.45
30:W:17:VAL:HG21	30:W:29:LEU:HD22	1.97	0.45
30:W:149:CYS:H	30:W:154:GLU:N	2.14	0.45
1:Q:102:PRO:O	1:Q:103:LEU:HD13	2.16	0.45
2:R:63:ARG:HB3	2:R:66:ARG:NH1	2.32	0.45
3:D:141:LEU:O	3:D:145:MET:HG2	2.16	0.45
4:G:5:LYS:O	4:G:76:ALA:N	2.31	0.45
4:G:142:ARG:O	4:G:170:ALA:HA	2.17	0.45
6:A:326:ARG:HG2	6:A:1406:VAL:HG11	1.98	0.45
6:A:352:VAL:HG21	7:B:1099:VAL:HG12	1.99	0.45
6:A:863:VAL:HG11	6:A:866:PHE:CE1	2.51	0.45
7:B:37:PHE:C	7:B:39:ARG:H	2.20	0.45
7:B:110:HIS:ND1	7:B:111:ALA:O	2.43	0.45
7:B:254:LEU:HD13	7:B:360:PHE:HE1	1.82	0.45
7:B:979:LYS:HD3	31:P:10:A:OP1	2.17	0.45
7:B:1159:ARG:HG2	7:B:1160:VAL:N	2.31	0.45
8:C:3:GLU:HG2	14:K:100:ALA:HB1	1.98	0.45
10:F:112:GLU:OE2	10:F:123:LYS:NZ	2.40	0.45
25:U:263:LYS:NZ	25:U:278:LYS:HG2	2.32	0.45
1:Q:378:VAL:HA	1:Q:384:PHE:CE1	2.52	0.45
4:G:14:HIS:HB3	4:G:17:PHE:CE1	2.52	0.45
4:G:132:SER:OG	4:G:133:SER:N	2.50	0.45
5:M:251:GLN:HA	5:M:254:THR:HG22	1.99	0.45
6:A:217:LYS:HE2	6:A:217:LYS:HB2	1.64	0.45
6:A:391:LEU:O	6:A:394:ASN:N	2.48	0.45
6:A:407:ARG:HA	6:A:430:TRP:CG	2.52	0.45
7:B:878:GLN:C	7:B:879:ARG:HE	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:3:GLU:C	8:C:7:GLN:HE22	2.13	0.45
11:H:99:GLY:HA3	11:H:118:PHE:CD2	2.52	0.45
17:0:343:LYS:HG2	17:0:347:LYS:NZ	2.31	0.45
19:6:239:LEU:HD11	19:6:268:ALA:HB1	1.99	0.45
20:1:193:LYS:O	20:1:196:GLN:HG3	2.17	0.45
20:1:633:TYR:O	20:1:637:TYR:N	2.36	0.45
21:7:393:THR:HG23	21:7:486:ILE:HG21	1.98	0.45
28:T:147:DT:H1'	29:O:207:PHE:CE1	2.51	0.45
29:O:172:LEU:HD21	29:O:206:ILE:HG22	1.99	0.45
29:O:214:LEU:HB3	29:O:223:ILE:HD12	1.97	0.45
30:W:134:LEU:O	30:W:138:GLN:HG2	2.17	0.45
2:R:110:GLU:HG2	2:R:117:PRO:N	2.32	0.45
3:D:26:THR:OG1	3:D:26:THR:O	2.25	0.45
5:M:310:LYS:HA	5:M:313:TYR:HB3	1.97	0.45
6:A:288:ALA:HA	6:A:291:GLU:OE1	2.16	0.45
6:A:830:LYS:HB2	6:A:1082:ASN:ND2	2.32	0.45
6:A:841:LEU:HA	6:A:841:LEU:HD23	1.59	0.45
6:A:1292:PRO:HA	6:A:1298:TYR:HA	1.97	0.45
7:B:872:GLU:HG2	7:B:916:THR:HG22	1.96	0.45
7:B:890:TYR:OH	7:B:936:ASP:OD2	2.34	0.45
7:B:894:ASP:OD2	15:L:58:LYS:NZ	2.36	0.45
12:I:78:CYS:SG	12:I:80:SER:N	2.76	0.45
13:J:22:LEU:O	13:J:26:GLN:HG2	2.16	0.45
15:L:32:ALA:HB3	15:L:55:ILE:HG13	1.97	0.45
17:0:376:PHE:HB3	17:0:379:GLU:OE2	2.17	0.45
18:4:239:GLU:CD	18:4:239:GLU:H	2.20	0.45
29:O:69:ASN:HA	29:O:126:ALA:O	2.17	0.45
29:O:164:CYS:O	29:O:211:LYS:HA	2.17	0.45
29:O:164:CYS:SG	29:O:212:ILE:HB	2.56	0.45
30:W:99:LYS:HA	30:W:186:LEU:HD13	1.98	0.45
6:A:333:GLU:HA	6:A:338:GLY:HA3	1.97	0.45
6:A:1192:LEU:HD11	6:A:1194:ARG:HB2	1.99	0.45
6:A:1199:ARG:HA	6:A:1236:LEU:HD11	1.98	0.45
6:A:1211:GLN:HG3	6:A:1211:GLN:H	1.45	0.45
6:A:1441:PHE:HD2	6:A:1441:PHE:C	2.20	0.45
7:B:333:PHE:O	7:B:333:PHE:HD1	2.00	0.45
7:B:712:PRO:HD2	7:B:733:HIS:HD2	1.81	0.45
7:B:785:TYR:CD2	7:B:786:ASN:N	2.85	0.45
8:C:208:GLU:H	8:C:208:GLU:HG3	1.34	0.45
11:H:145:ARG:HD3	11:H:145:ARG:HA	1.51	0.45
12:I:68:LEU:HA	12:I:68:LEU:HD23	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:18:LYS:NZ	14:K:38:GLU:OE2	2.26	0.45
15:L:62:LYS:HB2	15:L:63:ARG:HH22	1.82	0.45
17:0:79:ILE:HD13	17:0:79:ILE:HA	1.85	0.45
18:4:29:ILE:O	18:4:178:VAL:HA	2.17	0.45
30:W:123:MET:CG	30:W:157:VAL:HB	2.47	0.45
1:Q:398:ARG:HE	1:Q:398:ARG:HB2	1.59	0.45
5:M:130:PHE:CG	5:M:151:LYS:HE2	2.52	0.45
5:M:215:ARG:HD3	5:M:215:ARG:HA	1.56	0.45
5:M:282:ILE:O	5:M:286:ILE:HG22	2.17	0.45
6:A:544:ASP:OD1	6:A:545:GLN:N	2.47	0.45
7:B:70:ILE:HA	7:B:89:GLU:OE2	2.17	0.45
7:B:238:ALA:HB2	7:B:385:LEU:HB2	1.98	0.45
7:B:294:ASP:H	12:I:12:ASN:HD22	1.62	0.45
7:B:647:GLY:C	7:B:649:LYS:N	2.70	0.45
7:B:797:TYR:HB3	7:B:798:TYR:CD2	2.52	0.45
7:B:1095:LEU:HD23	7:B:1095:LEU:HA	1.63	0.45
8:C:262:LEU:HA	8:C:262:LEU:HD23	1.64	0.45
9:E:83:CYS:SG	9:E:85:GLU:N	2.90	0.45
17:0:656:PHE:HA	17:0:692:GLN:HG2	1.98	0.45
18:4:86:LEU:HA	18:4:128:GLU:HB3	1.98	0.45
19:6:154:ILE:HG23	19:6:193:ILE:HD12	2.00	0.45
20:1:588:ASP:O	20:1:592:LYS:N	2.35	0.45
23:2:25:LEU:HD21	23:2:226:PHE:CE2	2.51	0.45
23:2:56:GLU:OE1	23:2:99:ASN:HB3	2.17	0.45
27:N:13:DG:H2"	27:N:14:DC:O4'	2.16	0.45
28:T:22:DT:H2'	28:T:23:DC:H5'	1.99	0.45
31:P:6:G:C2	31:P:7:A:C8	3.05	0.45
1:Q:120:LYS:HE2	1:Q:394:LYS:NZ	2.32	0.44
2:R:99:LYS:HB2	2:R:103:LYS:CE	2.46	0.44
4:G:35:GLU:CD	4:G:47:CYS:HA	2.37	0.44
6:A:219:PHE:CD1	6:A:220:THR:N	2.79	0.44
6:A:549:MET:HE2	6:A:577:ILE:HG21	1.97	0.44
6:A:635:ARG:HA	6:A:635:ARG:NH1	2.33	0.44
6:A:1025:ARG:HD3	6:A:1025:ARG:HA	1.69	0.44
6:A:1034:GLU:HB2	6:A:1035:TYR:CD1	2.51	0.44
6:A:1098:VAL:N	6:A:1099:PRO:HD2	2.32	0.44
6:A:1100:ARG:NH2	6:A:1351:GLU:OE1	2.42	0.44
6:A:1286:LYS:HG3	6:A:1304:TRP:CZ3	2.52	0.44
7:B:380:TYR:CZ	7:B:384:ARG:HD3	2.51	0.44
7:B:492:LEU:HD23	7:B:492:LEU:HA	1.68	0.44
7:B:820:GLY:N	7:B:1091:TYR:OH	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1152:MET:HE3	7:B:1152:MET:HB3	1.82	0.44
9:E:197:LYS:HA	9:E:211:TYR:HD1	1.81	0.44
11:H:100:THR:OG1	11:H:138:GLU:HG2	2.18	0.44
15:L:47:ARG:HH12	15:L:54:ARG:CZ	2.30	0.44
17:0:223:SER:HB2	17:0:226:VAL:HG22	1.99	0.44
17:0:333:SER:HB2	17:0:337:ARG:NH2	2.32	0.44
17:0:490:LYS:NZ	17:0:700:GLY:HA2	2.32	0.44
17:0:694:PRO:HB2	17:0:696:TRP:CD1	2.52	0.44
18:4:247:TYR:CZ	20:1:503:VAL:HG22	2.53	0.44
21:7:457:TYR:OH	21:7:488:ASP:N	2.50	0.44
21:7:524:ILE:H	21:7:524:ILE:HD12	1.82	0.44
27:N:22:DT:O2	29:O:215:THR:OG1	2.21	0.44
29:O:170:ILE:HD13	29:O:234:LEU:HD22	1.99	0.44
29:O:227:PHE:HA	29:O:230:ILE:HG22	1.98	0.44
30:W:5:ILE:O	30:W:9:VAL:HG23	2.17	0.44
30:W:38:LEU:O	30:W:86:TYR:HA	2.17	0.44
3:D:138:ASN:O	3:D:141:LEU:HB3	2.17	0.44
3:D:154:PHE:CD2	3:D:160:VAL:HG13	2.52	0.44
6:A:20:GLY:O	7:B:1213:THR:OG1	2.31	0.44
6:A:29:ALA:HB1	7:B:1184:GLY:HA2	1.99	0.44
6:A:265:LYS:HD2	6:A:265:LYS:HA	1.74	0.44
6:A:854:ASN:O	6:A:867:ILE:HA	2.16	0.44
6:A:993:LEU:HD23	6:A:1022:LEU:HD21	1.99	0.44
6:A:1277:GLU:OE1	6:A:1277:GLU:N	2.47	0.44
7:B:98:THR:OG1	7:B:99:LYS:O	2.31	0.44
8:C:62:PHE:CE1	8:C:66:ARG:HD2	2.51	0.44
11:H:62:SER:OG	11:H:63:LEU:HG	2.17	0.44
14:K:87:LEU:HD12	14:K:87:LEU:HA	1.78	0.44
15:L:48:CYS:O	15:L:48:CYS:SG	2.76	0.44
17:0:436:ARG:HE	17:0:634:ILE:CG2	2.30	0.44
20:1:235:UNK:HA	20:1:381:LEU:HD11	1.99	0.44
21:7:557:VAL:N	21:7:707:SER:O	2.49	0.44
22:5:13:ASP:OD1	22:5:15:SER:OG	2.30	0.44
25:U:249:ASP:OD1	26:V:119:LYS:NZ	2.47	0.44
1:Q:117:HIS:HE1	1:Q:390:ASP:OD2	2.00	0.44
3:D:56:ARG:CB	3:D:148:LEU:HD22	2.46	0.44
4:G:116:PRO:HD3	4:G:164:LYS:HA	1.99	0.44
5:M:38:PHE:HD1	5:M:56:LEU:HD23	1.82	0.44
6:A:67:CYS:O	6:A:71:GLN:N	2.50	0.44
6:A:83:HIS:HD2	6:A:238:CYS:SG	2.41	0.44
6:A:426:LEU:H	6:A:426:LEU:HG	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1223:ASP:HB2	6:A:1224:LEU:HD12	1.99	0.44
6:A:1441:PHE:C	6:A:1441:PHE:CD2	2.90	0.44
7:B:95:ILE:HD12	7:B:129:PHE:O	2.17	0.44
7:B:1060:ARG:HD2	7:B:1060:ARG:HA	1.55	0.44
8:C:50:GLU:OE2	15:L:66:GLN:HA	2.17	0.44
9:E:118:PRO:O	9:E:121:MET:HB2	2.17	0.44
14:K:49:GLU:HG2	14:K:94:ILE:HG13	2.00	0.44
17:0:37:ASN:ND2	17:0:475:PHE:HD2	2.16	0.44
17:0:107:GLY:HA2	17:0:207:ILE:HB	1.99	0.44
17:0:714:ILE:HA	17:0:717:THR:HG22	1.99	0.44
17:0:734:GLU:O	17:0:738:VAL:N	2.51	0.44
19:6:244:PRO:HB3	20:1:230:PRO:HB3	2.00	0.44
19:6:441:ASP:HA	19:6:444:ILE:HD12	2.00	0.44
20:1:280:GLU:HA	20:1:284:TRP:CD1	2.52	0.44
21:7:622:MET:H	21:7:622:MET:HG3	1.67	0.44
29:O:185:TYR:CD2	29:O:187:PRO:HD3	2.53	0.44
2:R:75:MET:CE	2:R:75:MET:H	2.30	0.44
2:R:119:GLU:HB3	2:R:233:TYR:N	2.32	0.44
3:D:168:LYS:HD3	3:D:168:LYS:HA	1.84	0.44
4:G:35:GLU:OE1	4:G:47:CYS:HA	2.17	0.44
4:G:114:LEU:HD21	4:G:160:ILE:HG23	2.00	0.44
6:A:332:LYS:HG3	6:A:333:GLU:OE1	2.17	0.44
6:A:473:SER:OG	6:A:650:GLN:NE2	2.50	0.44
6:A:965:GLN:HG2	6:A:965:GLN:H	1.47	0.44
6:A:1059:HIS:ND1	10:F:87:LYS:HG2	2.33	0.44
7:B:240:ILE:O	7:B:240:ILE:HG13	2.17	0.44
7:B:860:MET:SD	7:B:861:ASP:N	2.90	0.44
8:C:127:ARG:O	8:C:129:ILE:N	2.51	0.44
15:L:30:ILE:HG22	15:L:31:CYS:O	2.18	0.44
17:0:110:SER:OG	17:0:111:ARG:N	2.51	0.44
23:2:431:GLN:NE2	23:2:435:PRO:HD2	2.31	0.44
1:Q:135:LEU:HD23	1:Q:136:PRO:HA	1.99	0.44
3:D:76:LYS:HA	3:D:76:LYS:HD2	1.68	0.44
6:A:332:LYS:HD2	6:A:332:LYS:HA	1.59	0.44
6:A:1227:ILE:O	6:A:1239:ARG:N	2.30	0.44
6:A:1404:GLU:O	6:A:1408:ILE:HG12	2.18	0.44
6:A:1443:VAL:HG12	6:A:1443:VAL:O	2.16	0.44
7:B:901:PRO:O	15:L:61:THR:HG22	2.17	0.44
7:B:911:ILE:HG12	7:B:939:THR:O	2.18	0.44
7:B:1155:SER:OG	7:B:1156:ASP:OD1	2.34	0.44
8:C:195:GLN:N	8:C:200:GLU:OE2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:69:ILE:HA	9:E:72:PHE:O	2.17	0.44
14:K:49:GLU:O	14:K:52:ASN:HB2	2.16	0.44
14:K:57:LEU:N	14:K:76:GLN:O	2.44	0.44
17:0:666:LEU:HD11	17:0:681:LEU:HD21	1.99	0.44
21:7:606:ILE:HD13	21:7:665:PRO:HG2	1.99	0.44
23:2:90:ASN:ND2	23:2:99:ASN:OD1	2.51	0.44
25:U:258:TRP:NE1	26:V:66:LEU:HD23	2.32	0.44
1:Q:141:ARG:HB3	1:Q:348:TYR:CB	2.47	0.44
3:D:52:LEU:O	3:D:152:SER:OG	2.25	0.44
4:G:153:GLN:HE21	4:G:153:GLN:HB2	1.48	0.44
5:M:268:GLU:HB3	5:M:315:ILE:HD11	2.00	0.44
6:A:1217:LYS:C	6:A:1221:LYS:HG3	2.38	0.44
7:B:103:ASN:HB2	7:B:169:ARG:HH22	1.82	0.44
7:B:260:GLY:O	7:B:267:ARG:HD3	2.18	0.44
8:C:59:ALA:O	8:C:62:PHE:HB3	2.18	0.44
11:H:101:ALA:HB2	11:H:116:TYR:CE2	2.52	0.44
12:I:101:PHE:N	12:I:110:PHE:O	2.42	0.44
18:4:90:SER:HB3	19:6:407:GLN:NE2	2.32	0.44
20:1:264:PRO:O	20:1:268:LYS:HG2	2.18	0.44
21:7:599:GLU:HA	21:7:650:ASN:HD22	1.83	0.44
21:7:604:LYS:HD3	21:7:694:LYS:NZ	2.33	0.44
21:7:612:VAL:HG13	21:7:629:GLY:HA3	2.00	0.44
23:2:109:ARG:NH1	23:2:109:ARG:HA	2.33	0.44
24:X:201:THR:HA	30:W:34:PHE:CB	2.48	0.44
27:N:20:DT:H4'	29:O:194:ILE:HD11	1.99	0.44
29:O:200:PRO:HG2	29:O:226:ALA:HB2	1.99	0.44
29:O:220:ARG:HG2	29:O:224:TYR:CE2	2.53	0.44
30:W:122:TYR:CZ	30:W:147:PHE:HE2	2.35	0.44
1:Q:106:ILE:HG23	1:Q:107:PRO:O	2.18	0.44
5:M:132:LYS:O	5:M:135:MET:HG2	2.18	0.44
6:A:206:GLU:HG3	6:A:207:ILE:H	1.82	0.44
6:A:526:ASP:OD1	7:B:1013:ASN:ND2	2.41	0.44
6:A:567:LYS:C	6:A:567:LYS:HD3	2.38	0.44
6:A:878:ILE:HG22	6:A:879:GLU:N	2.33	0.44
6:A:1207:LEU:HA	6:A:1207:LEU:HD23	1.68	0.44
7:B:215:GLN:NE2	7:B:479:VAL:HG12	2.32	0.44
7:B:838:SER:HB2	7:B:839:MET:HG2	1.99	0.44
7:B:1110:PRO:O	7:B:1119:VAL:HG13	2.16	0.44
12:I:42:LEU:HD12	12:I:43:VAL:N	2.33	0.44
17:0:342:LEU:HA	17:0:345:ARG:HB2	1.99	0.44
17:0:701:LEU:HD12	17:0:705:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:709:SER:O	17:0:713:ALA:N	2.42	0.44
18:4:136:GLU:HA	18:4:140:ILE:CG1	2.44	0.44
19:6:164:ASN:O	19:6:167:SER:OG	2.31	0.44
19:6:349:CYS:SG	19:6:368:LEU:HD11	2.58	0.44
20:1:260:PHE:CG	20:1:267:LYS:HD3	2.53	0.44
24:X:219:GLU:O	24:X:223:GLN:HG2	2.18	0.44
27:N:31:DT:C2	27:N:32:DG:C8	3.06	0.44
29:O:74:VAL:HG11	29:O:152:PHE:CE1	2.53	0.44
30:W:28:VAL:HG11	30:W:58:ILE:HD13	1.98	0.44
1:Q:104:ARG:HA	2:R:92:LEU:HB3	2.00	0.44
2:R:94:LYS:NZ	2:R:94:LYS:H	2.15	0.44
3:D:67:ARG:HB3	3:D:67:ARG:CZ	2.48	0.44
4:G:98:GLY:O	4:G:130:TYR:OH	2.36	0.44
4:G:148:GLU:HG3	4:G:162:SER:HB3	1.99	0.44
5:M:186:ALA:HB2	5:M:237:THR:OG1	2.17	0.44
5:M:186:ALA:HB1	5:M:238:TYR:CG	2.53	0.44
6:A:286:HIS:C	6:A:287:HIS:HD1	2.18	0.44
6:A:333:GLU:N	6:A:333:GLU:OE2	2.50	0.44
6:A:598:LEU:HD23	6:A:598:LEU:HA	1.77	0.44
6:A:811:GLN:O	6:A:814:PHE:N	2.51	0.44
7:B:370:PHE:HD1	7:B:373:ARG:HE	1.61	0.44
7:B:461:LEU:HD23	7:B:461:LEU:HA	1.70	0.44
10:F:128:LYS:NZ	10:F:148:VAL:O	2.49	0.44
12:I:108:HIS:CE1	12:I:110:PHE:HB3	2.53	0.44
17:0:276:LYS:HE2	17:0:276:LYS:HB2	1.89	0.44
21:7:695:ARG:HD3	21:7:695:ARG:HA	1.80	0.44
25:U:258:TRP:HB2	25:U:283:ALA:H	1.82	0.44
30:W:192:SER:HB3	30:W:194:ILE:HG13	1.99	0.44
3:D:37:GLN:CD	4:G:5:LYS:HZ1	2.20	0.44
4:G:50:ASP:OD2	4:G:53:ASN:HB2	2.18	0.44
6:A:69:THR:HA	6:A:71:GLN:NE2	2.32	0.44
6:A:276:LEU:HD11	6:A:293:GLU:HA	2.00	0.44
6:A:372:LYS:HD3	6:A:397:ASN:O	2.18	0.44
6:A:567:LYS:HG2	6:A:568:PRO:HD2	2.00	0.44
6:A:964:ILE:HD13	6:A:964:ILE:HA	1.69	0.44
6:A:1084:PHE:CD2	6:A:1086:PHE:HB2	2.53	0.44
6:A:1377:THR:O	6:A:1379:GLY:N	2.51	0.44
6:A:1381:LEU:HA	6:A:1381:LEU:HD23	1.77	0.44
7:B:68:THR:HG22	7:B:91:SER:HA	1.99	0.44
7:B:1084:GLN:NE2	8:C:191:TYR:HA	2.32	0.44
8:C:220:ASP:OD1	8:C:222:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:107:VAL:HG12	10:F:109:VAL:H	1.83	0.44
11:H:13:SER:N	11:H:27:GLU:O	2.50	0.44
11:H:82:PRO:CA	11:H:87:ARG:HD2	2.48	0.44
13:J:25:LEU:HA	13:J:25:LEU:HD23	1.67	0.44
18:4:210:ILE:HD13	18:4:227:THR:HG21	1.99	0.44
24:X:268:LEU:HD21	30:W:101:LYS:HE3	1.99	0.44
27:N:21:DA:N3	29:O:205:LEU:HD11	2.32	0.44
30:W:9:VAL:HG22	30:W:189:ILE:HD13	1.99	0.44
6:A:141:LEU:HD23	6:A:141:LEU:HA	1.79	0.43
6:A:1230:GLU:O	6:A:1233:ASP:N	2.43	0.43
7:B:129:PHE:CD1	7:B:166:PHE:HA	2.52	0.43
7:B:408:LEU:HA	7:B:408:LEU:HD23	1.56	0.43
11:H:111:LEU:HD23	11:H:111:LEU:HA	1.60	0.43
12:I:58:VAL:HG11	12:I:109:ILE:HD11	1.99	0.43
12:I:99:LEU:HA	12:I:99:LEU:HD23	1.74	0.43
12:I:104:LEU:HA	12:I:104:LEU:HD13	1.55	0.43
19:6:134:GLU:N	19:6:206:GLY:O	2.45	0.43
21:7:409:VAL:HA	21:7:486:ILE:HB	2.00	0.43
23:2:146:ILE:HD12	23:2:146:ILE:HA	1.89	0.43
24:X:157:ASP:O	24:X:161:GLU:N	2.45	0.43
3:D:66:ARG:HG2	3:D:133:THR:HG22	2.00	0.43
4:G:59:GLY:O	10:F:133:VAL:HG11	2.18	0.43
6:A:445:ASN:HA	6:A:454:SER:O	2.18	0.43
6:A:732:LEU:HA	6:A:732:LEU:HD23	1.69	0.43
6:A:781:ASP:HB3	6:A:790:ASP:OD1	2.18	0.43
6:A:785:PRO:HG2	6:A:786:HIS:CD2	2.53	0.43
6:A:1079:MET:HE2	6:A:1359:ASP:HB3	1.99	0.43
6:A:1161:THR:HG22	6:A:1163:ILE:H	1.81	0.43
7:B:766:ARG:HD3	7:B:766:ARG:HA	1.62	0.43
7:B:1037:LEU:HD23	7:B:1037:LEU:HA	1.67	0.43
8:C:69:LEU:O	13:J:6:ARG:HD2	2.18	0.43
9:E:30:ILE:HG23	9:E:34:GLU:OE1	2.18	0.43
17:0:195:ILE:O	17:0:199:MET:HG2	2.18	0.43
17:0:224:ASN:HD21	17:0:228:LYS:NZ	2.15	0.43
17:0:327:ARG:HB3	17:0:330:HIS:HB3	2.00	0.43
18:4:86:LEU:HD11	18:4:132:LEU:HD13	1.99	0.43
20:1:346:ASP:HB2	20:1:347:PRO:HD3	1.99	0.43
21:7:604:LYS:HD3	21:7:694:LYS:HZ1	1.83	0.43
5:M:174:ALA:O	5:M:178:ILE:HG12	2.17	0.43
6:A:315:LEU:HA	6:A:321:PRO:HA	2.00	0.43
6:A:811:GLN:O	6:A:812:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:901:LEU:HD22	6:A:919:ILE:HG22	2.00	0.43
6:A:1208:THR:N	6:A:1211:GLN:OE1	2.40	0.43
7:B:230:ALA:N	7:B:231:PRO:HD2	2.33	0.43
7:B:1084:GLN:HE22	8:C:191:TYR:HA	1.82	0.43
14:K:14:GLU:N	14:K:16:GLU:OE1	2.52	0.43
14:K:29:ASN:HD22	14:K:79:GLU:HA	1.83	0.43
15:L:47:ARG:N	15:L:53:HIS:O	2.45	0.43
17:0:171:LEU:HD11	17:0:195:ILE:HG21	2.00	0.43
17:0:465:PRO:HD2	17:0:656:PHE:CD2	2.54	0.43
17:0:720:PHE:CZ	17:0:724:MET:HG3	2.53	0.43
18:4:119:ARG:HH22	18:4:123:GLU:HG2	1.82	0.43
21:7:341:TYR:CD2	21:7:343:PHE:HD1	2.35	0.43
21:7:421:ARG:NH1	21:7:437:VAL:HG11	2.33	0.43
2:R:73:LEU:HA	2:R:224:VAL:HB	2.00	0.43
5:M:248:LEU:HA	5:M:249:PRO:HD3	1.86	0.43
6:A:107:CYS:HB3	6:A:111:GLY:N	2.34	0.43
6:A:130:ASP:CG	6:A:133:LYS:HB2	2.39	0.43
6:A:657:LEU:HA	6:A:657:LEU:HD12	1.68	0.43
6:A:673:GLY:O	6:A:676:MET:N	2.51	0.43
6:A:903:ASN:O	6:A:907:THR:OG1	2.36	0.43
7:B:59:LEU:HD12	7:B:59:LEU:HA	1.50	0.43
7:B:96:TYR:N	7:B:129:PHE:O	2.36	0.43
7:B:710:LEU:HA	7:B:710:LEU:HD13	1.55	0.43
7:B:806:THR:OG1	7:B:809:MET:HG3	2.18	0.43
7:B:884:ARG:HB2	7:B:936:ASP:H	1.83	0.43
7:B:1174:LYS:N	7:B:1179:GLN:O	2.51	0.43
8:C:22:LEU:HD12	8:C:22:LEU:HA	1.52	0.43
8:C:67:LEU:HD23	8:C:67:LEU:HA	1.64	0.43
9:E:28:TYR:HA	9:E:64:PRO:HA	1.99	0.43
9:E:46:TYR:O	9:E:54:GLN:N	2.48	0.43
11:H:93:TYR:CG	11:H:143:LEU:HD22	2.53	0.43
17:0:116:LEU:HD23	17:0:158:TYR:CE2	2.53	0.43
17:0:460:SER:HB2	17:0:463:ILE:HG13	1.99	0.43
18:4:258:LEU:CB	18:4:260:PRO:HD3	2.49	0.43
27:N:17:DG:H2"	27:N:18:DT:O4'	2.18	0.43
27:N:17:DG:H2'	27:N:18:DT:C6	2.53	0.43
28:T:146:DA:H5'	29:O:68:GLN:CD	2.39	0.43
28:T:150:DG:C4	28:T:151:DC:N3	2.87	0.43
3:D:153:ARG:HH22	3:D:182:SER:C	2.22	0.43
4:G:4:ILE:HG23	4:G:49:LEU:HD11	2.01	0.43
5:M:156:LEU:HD23	5:M:156:LEU:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:944:ARG:NH1	6:A:1296:GLY:O	2.49	0.43
7:B:605:ARG:NH2	7:B:691:GLU:OE2	2.50	0.43
7:B:614:SER:C	7:B:615:MET:HG3	2.38	0.43
7:B:1096:ARG:O	7:B:1097:HIS:CG	2.72	0.43
8:C:10:ILE:HG13	14:K:108:GLU:HG2	2.01	0.43
10:F:146:TRP:CD1	10:F:146:TRP:N	2.87	0.43
11:H:83:GLN:O	11:H:85:GLY:N	2.50	0.43
18:4:78:ALA:HB2	18:4:152:ALA:CB	2.49	0.43
19:6:126:LEU:HB3	19:6:160:PHE:CZ	2.54	0.43
19:6:237:GLY:HA2	19:6:266:LEU:HB2	2.01	0.43
23:2:378:ILE:HD12	23:2:382:SER:HB2	2.00	0.43
28:T:152:DG:C5	28:T:153:DC:C4	3.06	0.43
1:Q:399:ASN:OD1	1:Q:402:ALA:HA	2.19	0.43
2:R:118:HIS:CG	2:R:120:TYR:HH	2.36	0.43
5:M:26:GLU:OE2	6:A:407:ARG:NH1	2.52	0.43
5:M:40:GLU:N	5:M:40:GLU:OE2	2.52	0.43
6:A:359:LEU:HA	6:A:359:LEU:HD12	1.60	0.43
6:A:450:LEU:O	6:A:451:HIS:CD2	2.72	0.43
6:A:1046:LEU:HD12	6:A:1046:LEU:HA	1.70	0.43
6:A:1256:GLU:C	6:A:1258:HIS:H	2.22	0.43
6:A:1333:ILE:HA	6:A:1333:ILE:HD13	1.83	0.43
8:C:165:LYS:NZ	14:K:9:LEU:O	2.30	0.43
9:E:153:HIS:O	9:E:154:ILE:HD13	2.19	0.43
12:I:19:ASP:CB	12:I:24:ARG:H	2.19	0.43
17:0:350:HIS:ND1	30:W:184:ASP:OD2	2.52	0.43
19:6:124:ARG:HA	19:6:229:THR:N	2.33	0.43
19:6:129:THR:HA	19:6:172:ILE:HB	2.00	0.43
21:7:546:LYS:HA	21:7:546:LYS:HD2	1.84	0.43
28:T:137:DA:C2	28:T:138:DG:C4	3.07	0.43
29:O:205:LEU:O	29:O:213:VAL:N	2.41	0.43
4:G:97:HIS:H	4:G:97:HIS:CD2	2.36	0.43
4:G:131:GLN:N	4:G:131:GLN:OE1	2.51	0.43
6:A:118:HIS:C	6:A:123:ARG:HH12	2.22	0.43
6:A:360:GLU:HB2	6:A:363:GLN:OE1	2.18	0.43
6:A:1191:TRP:HD1	6:A:1256:GLU:OE1	2.01	0.43
7:B:245:GLU:H	7:B:245:GLU:CD	2.18	0.43
7:B:355:ILE:HD13	7:B:355:ILE:HA	1.79	0.43
7:B:706:GLN:H	7:B:710:LEU:CD2	2.27	0.43
7:B:848:ARG:HB3	13:J:8:PHE:HD1	1.83	0.43
11:H:84:ALA:N	14:K:54:ARG:HH12	2.17	0.43
15:L:33:GLU:HB2	15:L:53:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:659:MET:HA	17:0:662:ALA:HB3	1.99	0.43
25:U:262:LEU:O	25:U:279:ALA:N	2.49	0.43
28:T:137:DA:C4	28:T:138:DG:C8	3.07	0.43
1:Q:342:LEU:O	1:Q:346:GLU:HG3	2.18	0.43
3:D:215:SER:HA	3:D:218:GLU:HG2	2.01	0.43
6:A:935:GLN:NE2	6:A:935:GLN:O	2.51	0.43
6:A:1047:SER:OG	6:A:1048:ASN:N	2.52	0.43
6:A:1333:ILE:HD13	6:A:1381:LEU:HD12	2.00	0.43
8:C:136:ASP:OD2	8:C:140:ASN:N	2.52	0.43
11:H:61:SER:O	11:H:139:ASN:ND2	2.48	0.43
13:J:22:LEU:HA	13:J:22:LEU:HD23	1.70	0.43
18:4:28:VAL:HG13	18:4:57:LEU:HD21	2.00	0.43
19:6:231:GLU:HA	19:6:260:ARG:O	2.19	0.43
21:7:387:PRO:HB3	21:7:540:TRP:CH2	2.54	0.43
21:7:443:LYS:HD3	21:7:444:GLU:N	2.34	0.43
21:7:584:ASN:HB3	21:7:587:LYS:HB3	2.01	0.43
23:2:428:GLU:OE1	23:2:428:GLU:N	2.52	0.43
28:T:21:DC:H2'	28:T:22:DT:H6	1.81	0.43
28:T:147:DT:H5'	29:O:211:LYS:HE2	2.00	0.43
29:O:102:VAL:N	29:O:115:ILE:O	2.37	0.43
30:W:179:ILE:HG23	30:W:183:ILE:HG23	2.00	0.43
1:Q:353:GLU:OE1	1:Q:353:GLU:N	2.52	0.43
1:Q:376:LEU:HD12	2:R:69:TRP:HB3	2.00	0.43
2:R:79:GLU:N	2:R:79:GLU:OE1	2.52	0.43
3:D:142:LYS:HA	3:D:142:LYS:HD3	1.74	0.43
4:G:138:THR:O	4:G:141:SER:OG	2.17	0.43
5:M:177:LEU:HD11	5:M:181:ARG:HH21	1.83	0.43
6:A:573:SER:OG	6:A:574:GLY:N	2.51	0.43
6:A:913:LEU:HD11	6:A:981:LEU:O	2.18	0.43
7:B:102:VAL:CG1	7:B:112:LEU:HD22	2.48	0.43
8:C:143:LEU:HG	13:J:2:ILE:HD11	2.00	0.43
8:C:215:GLU:N	8:C:215:GLU:CD	2.71	0.43
9:E:215:MET:HE3	9:E:215:MET:HB3	1.91	0.43
11:H:24:CYS:HB2	11:H:44:VAL:HG11	2.01	0.43
15:L:29:TYR:O	15:L:30:ILE:HD13	2.18	0.43
17:0:428:ALA:O	17:0:430:VAL:HG13	2.19	0.43
18:4:25:LEU:HB3	18:4:174:SER:HB3	2.00	0.43
18:4:236:LEU:HD22	18:4:238:VAL:HG12	2.00	0.43
21:7:303:ARG:HG3	21:7:320:ASN:C	2.39	0.43
21:7:385:VAL:HG23	21:7:538:ALA:N	2.34	0.43
21:7:548:HIS:HB3	21:7:693:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:586:THR:O	21:7:590:ALA:N	2.37	0.43
24:X:260:VAL:HG22	30:W:20:PHE:HA	2.01	0.43
1:Q:141:ARG:HB3	1:Q:348:TYR:HB2	2.00	0.43
1:Q:362:VAL:O	1:Q:395:PHE:HA	2.19	0.43
3:D:123:LEU:HD22	3:D:149:THR:HB	2.00	0.43
3:D:188:ALA:O	3:D:192:LYS:HG3	2.18	0.43
4:G:38:CYS:O	4:G:155:SER:HA	2.18	0.43
6:A:116:ASP:HA	6:A:117:GLU:HA	1.61	0.43
6:A:933:TYR:O	6:A:937:VAL:HG13	2.18	0.43
6:A:981:LEU:HD21	6:A:1039:LYS:HA	2.01	0.43
6:A:1032:LEU:HD23	6:A:1032:LEU:HA	1.77	0.43
6:A:1032:LEU:O	6:A:1036:ARG:HG2	2.18	0.43
9:E:180:ARG:HH12	9:E:192:ARG:HB2	1.83	0.43
12:I:55:THR:H	12:I:120:GLN:CD	2.22	0.43
14:K:108:GLU:HA	14:K:111:LEU:HD22	2.00	0.43
17:0:524:SER:HA	17:0:527:VAL:HG12	2.01	0.43
18:4:28:VAL:HG22	18:4:57:LEU:HD11	2.01	0.43
18:4:117:ARG:HA	18:4:120:ASN:ND2	2.33	0.43
19:6:173:ILE:HG13	19:6:180:GLN:HB2	2.01	0.43
20:1:258:ASN:O	20:1:261:GLU:HG3	2.18	0.43
29:O:132:SER:O	29:O:136:SER:OG	2.37	0.43
1:Q:108:LYS:HE2	1:Q:108:LYS:HB2	1.76	0.42
1:Q:127:ILE:HG12	1:Q:129:PRO:HD3	2.01	0.42
3:D:44:GLU:HG2	3:D:45:GLU:N	2.34	0.42
3:D:208:GLU:C	3:D:212:LYS:HZ3	2.22	0.42
6:A:70:CYS:O	6:A:72:GLU:N	2.47	0.42
6:A:1224:LEU:O	6:A:1226:VAL:HG23	2.19	0.42
6:A:1436:ILE:HA	6:A:1436:ILE:HD13	1.76	0.42
7:B:234:ILE:HG21	7:B:257:LYS:HB3	2.01	0.42
7:B:578:THR:HG23	7:B:622:LYS:C	2.40	0.42
7:B:847:ASP:HB3	8:C:167:HIS:CE1	2.54	0.42
7:B:1010:LEU:HD12	7:B:1010:LEU:HA	1.64	0.42
8:C:4:GLU:OE1	8:C:4:GLU:N	2.51	0.42
8:C:179:GLU:HG2	8:C:180:TYR:N	2.34	0.42
8:C:190:ASP:OD1	8:C:191:TYR:N	2.52	0.42
9:E:81:GLU:HG2	9:E:96:PHE:CD1	2.54	0.42
10:F:99:LEU:O	10:F:103:MET:HG3	2.18	0.42
21:7:230:ASN:O	21:7:345:ASN:HB3	2.19	0.42
21:7:449:GLU:HG3	21:7:453:VAL:HG22	2.00	0.42
23:2:481:LEU:HD21	23:2:491:PHE:CG	2.54	0.42
29:O:113:ALA:HB2	29:O:139:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:O:123:VAL:HG21	29:O:136:SER:OG	2.19	0.42
5:M:215:ARG:O	5:M:218:SER:OG	2.35	0.42
6:A:214:ILE:HG22	6:A:218:ASP:OD1	2.18	0.42
6:A:446:ARG:HB2	6:A:487:MET:CE	2.49	0.42
6:A:457:ALA:O	6:A:507:VAL:HG23	2.19	0.42
6:A:860:LEU:HB2	6:A:862:ASN:OD1	2.19	0.42
6:A:1022:LEU:HA	6:A:1022:LEU:HD12	1.72	0.42
6:A:1104:ILE:HG22	6:A:1105:LEU:HD23	2.01	0.42
6:A:1263:ILE:O	6:A:1267:MET:HG2	2.19	0.42
6:A:1442:ASP:HA	10:F:134:ILE:O	2.19	0.42
7:B:555:ILE:HA	7:B:558:LEU:HD12	2.01	0.42
7:B:617:ARG:NH2	12:I:61:ASP:OD1	2.42	0.42
7:B:1072:MET:HE2	7:B:1072:MET:HB3	1.95	0.42
18:4:33:ALA:O	18:4:37:TRP:N	2.30	0.42
19:6:133:SER:HB2	19:6:207:ASN:HA	2.01	0.42
20:1:613:THR:O	20:1:617:LYS:N	2.52	0.42
21:7:397:ILE:HD12	21:7:430:LEU:HD22	1.99	0.42
21:7:403:ILE:HD11	21:7:407:VAL:HG22	2.01	0.42
23:2:481:LEU:HD13	23:2:484:LYS:HB3	2.02	0.42
24:X:193:LEU:O	24:X:197:ARG:HG3	2.19	0.42
30:W:8:ILE:O	30:W:12:LEU:N	2.52	0.42
1:Q:121:PHE:HD1	1:Q:361:TRP:CD2	2.37	0.42
4:G:64:THR:C	4:G:66:GLY:H	2.22	0.42
5:M:157:CYS:HB2	5:M:163:LEU:HD11	2.01	0.42
6:A:61:ILE:HA	6:A:74:MET:HE1	2.02	0.42
6:A:436:ILE:HD12	6:A:436:ILE:HG23	1.71	0.42
6:A:1266:THR:HB	6:A:1267:MET:HE2	2.01	0.42
7:B:334:ILE:H	7:B:334:ILE:HG12	1.65	0.42
7:B:563:MET:HA	7:B:589:VAL:O	2.18	0.42
9:E:101:GLN:CD	9:E:101:GLN:N	2.70	0.42
10:F:96:THR:O	10:F:100:GLN:HG3	2.19	0.42
11:H:42:ILE:HG23	11:H:95:TYR:CE2	2.55	0.42
11:H:54:SER:HB3	11:H:146:ARG:HD3	2.01	0.42
15:L:31:CYS:SG	15:L:34:CYS:SG	3.17	0.42
17:0:52:LEU:HD22	17:0:233:ILE:HD13	2.02	0.42
17:0:236:GLU:HB3	17:0:238:HIS:HE1	1.84	0.42
17:0:338:LEU:HD23	17:0:342:LEU:HD23	2.01	0.42
19:6:233:LEU:HA	19:6:262:LYS:O	2.20	0.42
19:6:233:LEU:HD21	19:6:264:LEU:HD22	2.01	0.42
20:1:256:ILE:HG13	20:1:257:LEU:N	2.34	0.42
21:7:659:ASP:HA	21:7:660:THR:HA	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:2:110:ASN:O	23:2:115:GLY:N	2.52	0.42
29:O:175:LEU:HA	29:O:237:PHE:CE2	2.54	0.42
2:R:126:LYS:HG2	2:R:128:VAL:O	2.19	0.42
3:D:204:ASP:O	3:D:207:LEU:HB2	2.19	0.42
4:G:146:LYS:O	4:G:161:GLY:HA2	2.20	0.42
5:M:118:VAL:O	5:M:124:ASN:HB3	2.19	0.42
6:A:367:PRO:HG3	6:A:466:SER:O	2.19	0.42
6:A:501:LEU:HD23	6:A:501:LEU:HA	1.65	0.42
6:A:562:THR:HA	11:H:79:TRP:HB2	2.02	0.42
6:A:664:THR:OG1	6:A:668:ASP:OD2	2.28	0.42
7:B:933:SER:OG	7:B:934:LYS:N	2.52	0.42
7:B:1207:LEU:HD23	7:B:1207:LEU:HA	1.57	0.42
17:0:173:LYS:HD2	17:0:173:LYS:HA	1.86	0.42
17:0:349:LEU:HB3	30:W:180:GLN:HG2	2.01	0.42
17:0:372:LYS:HB2	17:0:373:PRO:HD3	2.01	0.42
19:6:216:MET:HE3	19:6:220:LEU:HD13	2.01	0.42
19:6:352:CYS:SG	19:6:354:SER:OG	2.57	0.42
21:7:606:ILE:HG12	21:7:652:ILE:HD11	2.01	0.42
23:2:410:ARG:HA	23:2:413:GLU:HB2	2.01	0.42
25:U:252:THR:OG1	25:U:259:LYS:HB2	2.20	0.42
27:N:31:DT:O2	28:T:135:DA:H2	2.03	0.42
28:T:141:DT:H2"	29:O:99:PHE:CG	2.54	0.42
28:T:146:DA:C6	28:T:147:DT:C4	3.07	0.42
4:G:57:GLN:HG2	4:G:58:ARG:N	2.34	0.42
6:A:123:ARG:NH1	6:A:123:ARG:HB2	2.33	0.42
6:A:135:PHE:HB2	6:A:222:LEU:O	2.20	0.42
6:A:351:THR:O	6:A:486:GLU:HB3	2.20	0.42
6:A:593:GLU:C	6:A:593:GLU:CD	2.77	0.42
6:A:1001:ARG:NH1	10:F:82:THR:HA	2.33	0.42
6:A:1211:GLN:HA	6:A:1214:GLU:HG2	2.00	0.42
6:A:1389:PHE:CG	6:A:1390:ASN:N	2.87	0.42
6:A:1390:ASN:O	6:A:1399:ARG:HD2	2.20	0.42
7:B:757:PRO:CG	7:B:983:ARG:HH21	2.32	0.42
8:C:241:ASP:OD2	14:K:109:TRP:NE1	2.53	0.42
9:E:186:LEU:O	9:E:189:GLY:N	2.52	0.42
10:F:71:GLU:HA	10:F:72:LYS:HA	1.74	0.42
11:H:135:LEU:HA	11:H:135:LEU:HD23	1.66	0.42
12:I:5:ARG:HB3	12:I:5:ARG:CZ	2.48	0.42
12:I:24:ARG:H	12:I:24:ARG:HG3	1.72	0.42
12:I:77:LYS:HE2	12:I:77:LYS:HB3	1.69	0.42
16:3:140:ASN:O	16:3:144:ILE:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:57:ILE:HG22	17:0:93:ARG:HH21	1.84	0.42
17:0:525:MET:O	17:0:529:PHE:HD2	2.02	0.42
17:0:685:ARG:HB3	17:0:689:LYS:NZ	2.35	0.42
18:4:279:THR:HG21	18:4:281:ARG:HE	1.85	0.42
19:6:136:MET:O	19:6:145:ARG:HB2	2.19	0.42
21:7:352:LEU:O	21:7:404:LYS:NZ	2.53	0.42
21:7:408:ILE:HG13	21:7:485:ILE:HG13	2.02	0.42
28:T:147:DT:H5'	29:O:211:LYS:HG3	2.01	0.42
30:W:122:TYR:HD2	30:W:156:LEU:HB2	1.83	0.42
1:Q:114:MET:HA	2:R:137:GLU:O	2.19	0.42
1:Q:119:LEU:HB2	2:R:133:TYR:H	1.85	0.42
1:Q:124:LYS:HG2	1:Q:126:LYS:HZ2	1.84	0.42
3:D:166:LEU:O	3:D:170:THR:HG23	2.18	0.42
4:G:119:LEU:HA	4:G:132:SER:HA	2.00	0.42
5:M:200:THR:HA	5:M:203:PHE:HB3	2.00	0.42
6:A:329:LEU:HD22	6:A:335:ARG:HB2	2.02	0.42
6:A:662:PHE:HD2	7:B:829:CYS:SG	2.43	0.42
6:A:668:ASP:CG	6:A:742:ASN:HD22	2.22	0.42
6:A:709:THR:HB	6:A:712:GLU:HG3	2.01	0.42
6:A:1140:HIS:NE2	6:A:1272:THR:OG1	2.35	0.42
6:A:1359:ASP:OD1	6:A:1360:GLY:N	2.52	0.42
7:B:1074:ASN:OD1	7:B:1076:HIS:N	2.53	0.42
8:C:76:ASP:C	8:C:129:ILE:HD11	2.40	0.42
10:F:116:ASP:HB3	10:F:119:ARG:CG	2.49	0.42
10:F:140:ASP:OD1	10:F:142:SER:N	2.35	0.42
12:I:21:GLU:N	12:I:21:GLU:CD	2.73	0.42
14:K:36:GLU:HB3	14:K:37:LYS:HE2	2.01	0.42
18:4:67:PHE:CD1	18:4:253:PHE:HZ	2.37	0.42
21:7:350:PRO:HG2	21:7:480:ARG:HH22	1.85	0.42
21:7:355:ASP:OD2	21:7:357:LYS:NZ	2.49	0.42
21:7:594:LEU:HD22	21:7:598:HIS:HE1	1.85	0.42
24:X:206:SER:OG	24:X:207:CYS:N	2.52	0.42
29:O:160:ILE:O	29:O:215:THR:HA	2.20	0.42
29:O:163:SER:HB3	29:O:213:VAL:HG13	2.01	0.42
4:G:26:LEU:HA	4:G:26:LEU:HD23	1.64	0.42
5:M:268:GLU:C	5:M:270:ALA:H	2.23	0.42
6:A:149:GLU:O	6:A:164:ARG:NH1	2.52	0.42
7:B:192:LEU:HD23	7:B:192:LEU:HA	1.73	0.42
8:C:80:LEU:HD12	8:C:80:LEU:HA	1.78	0.42
8:C:101:LEU:HD12	8:C:101:LEU:HA	1.79	0.42
8:C:137:LYS:HE3	8:C:137:LYS:HB3	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:108:SER:OG	11:H:109:LYS:N	2.51	0.42
12:I:59:VAL:HG23	12:I:61:ASP:N	2.34	0.42
14:K:16:GLU:OE1	14:K:16:GLU:N	2.52	0.42
21:7:626:PHE:O	21:7:628:TYR:HD1	2.03	0.42
1:Q:342:LEU:HB3	1:Q:343:ARG:HH22	1.85	0.42
2:R:92:LEU:HD12	2:R:93:GLY:O	2.19	0.42
3:D:37:GLN:HG2	3:D:47:LEU:HA	2.00	0.42
6:A:871:ASP:OD1	6:A:871:ASP:C	2.57	0.42
6:A:912:LEU:O	6:A:979:SER:HB3	2.20	0.42
6:A:1148:ILE:HG23	12:I:49:ILE:HG13	2.02	0.42
6:A:1172:LEU:O	6:A:1174:PHE:N	2.53	0.42
7:B:125:SER:HA	7:B:171:PRO:HA	2.01	0.42
7:B:590:HIS:CD2	7:B:591:ARG:O	2.73	0.42
7:B:1132:GLU:H	7:B:1132:GLU:HG2	1.62	0.42
8:C:214:ASN:HB3	8:C:217:ASP:OD2	2.19	0.42
9:E:79:TRP:CD1	9:E:96:PHE:HE1	2.36	0.42
11:H:26:ILE:HD13	11:H:26:ILE:HA	1.56	0.42
11:H:50:ALA:H	11:H:53:ASP:CG	2.15	0.42
11:H:110:ASP:O	11:H:111:LEU:HD23	2.19	0.42
15:L:31:CYS:SG	15:L:34:CYS:CA	3.06	0.42
15:L:34:CYS:SG	15:L:36:SER:CB	3.08	0.42
19:6:142:ARG:NH1	19:6:294:GLU:OE2	2.52	0.42
21:7:431:GLN:N	21:7:431:GLN:OE1	2.53	0.42
21:7:477:LEU:HA	21:7:482:TRP:NE1	2.34	0.42
23:2:19:GLN:HG3	23:2:85:HIS:CG	2.55	0.42
29:O:63:ILE:HB	29:O:227:PHE:CZ	2.54	0.42
30:W:5:ILE:HG13	30:W:192:SER:OG	2.20	0.42
3:D:174:PRO:O	3:D:177:VAL:HG22	2.19	0.42
4:G:3:PHE:O	4:G:77:VAL:HA	2.20	0.42
5:M:166:LYS:HA	5:M:166:LYS:HD3	1.83	0.42
6:A:10:PRO:HD2	7:B:1191:ILE:O	2.20	0.42
6:A:21:LEU:HD11	6:A:1414:ALA:HA	2.01	0.42
6:A:279:LEU:HB3	6:A:289:ILE:CD1	2.50	0.42
6:A:374:LEU:HA	6:A:374:LEU:HD23	1.79	0.42
6:A:451:HIS:HB3	6:A:453:MET:N	2.35	0.42
6:A:525:GLN:CD	7:B:836:GLU:HG2	2.40	0.42
7:B:319:GLU:HG2	12:I:15:TYR:OH	2.20	0.42
13:J:23:ASN:O	13:J:27:GLU:HG2	2.20	0.42
14:K:19:LEU:HA	14:K:19:LEU:HD23	1.74	0.42
17:0:360:LEU:O	17:0:364:LYS:N	2.46	0.42
19:6:451:CYS:HB3	19:6:454:CYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:581:TYR:CE1	21:7:714:GLN:HB3	2.55	0.42
27:N:23:DA:N1	28:T:144:DA:N6	2.68	0.42
28:T:157:DT:C4	28:T:158:DT:C4	3.07	0.42
3:D:40:HIS:CE1	4:G:6:ASP:HB3	2.54	0.42
4:G:64:THR:OG1	4:G:65:ASP:N	2.53	0.42
5:M:54:ASP:OD1	5:M:55:LYS:N	2.53	0.42
5:M:283:TYR:HA	5:M:286:ILE:HG22	2.01	0.42
6:A:507:VAL:O	6:A:510:GLN:N	2.37	0.42
6:A:803:SER:HG	6:A:805:LEU:H	1.63	0.42
6:A:1111:MET:HB3	6:A:1111:MET:HE2	1.40	0.42
6:A:1153:TYR:CD1	6:A:1163:ILE:HD11	2.55	0.42
6:A:1409:LEU:HA	6:A:1409:LEU:HD23	1.62	0.42
6:A:1442:ASP:HB2	10:F:136:ARG:CA	2.50	0.42
7:B:852:ARG:HH11	7:B:852:ARG:HD3	1.69	0.42
8:C:5:GLY:HA3	8:C:6:PRO:HD3	1.87	0.42
9:E:88:VAL:HG21	9:E:110:PHE:HE1	1.83	0.42
11:H:79:TRP:CH2	11:H:81:PRO:HA	2.54	0.42
17:0:428:ALA:O	30:W:11:ASN:HB3	2.20	0.42
17:0:726:GLN:NE2	19:6:290:ILE:HG13	2.35	0.42
21:7:410:LEU:O	21:7:488:ASP:N	2.53	0.42
23:2:422:LEU:HA	23:2:425:ASN:OD1	2.20	0.42
23:2:446:LEU:O	23:2:450:ARG:N	2.42	0.42
27:N:29:DT:C2	28:T:138:DG:C2	3.08	0.42
28:T:146:DA:H2	29:O:207:PHE:HZ	1.68	0.42
29:O:179:HIS:CD2	29:O:237:PHE:HE2	2.38	0.42
2:R:99:LYS:HD2	2:R:99:LYS:HA	1.89	0.41
3:D:176:GLU:H	3:D:176:GLU:HG3	1.59	0.41
5:M:188:THR:HG23	29:O:188:GLU:CD	2.41	0.41
6:A:129:LYS:HB2	6:A:129:LYS:HE2	1.84	0.41
6:A:968:GLN:O	6:A:972:HIS:N	2.53	0.41
6:A:1267:MET:HE2	6:A:1267:MET:N	2.35	0.41
7:B:45:SER:OG	7:B:46:GLN:N	2.53	0.41
7:B:68:THR:O	7:B:69:LEU:HD23	2.20	0.41
7:B:420:LEU:HD11	7:B:456:GLY:HA3	2.01	0.41
7:B:468:GLU:O	7:B:471:LYS:N	2.53	0.41
7:B:471:LYS:HB3	7:B:471:LYS:HE2	1.75	0.41
7:B:586:TRP:CD1	7:B:586:TRP:C	2.91	0.41
7:B:647:GLY:N	7:B:648:HIS:C	2.73	0.41
7:B:910:VAL:HA	7:B:940:PRO:HA	2.02	0.41
11:H:58:THR:O	11:H:143:LEU:N	2.51	0.41
11:H:61:SER:HB2	11:H:139:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:17:ARG:HD3	12:I:28:GLU:OE2	2.20	0.41
14:K:47:ARG:HE	14:K:47:ARG:HB3	1.61	0.41
17:0:584:GLU:HG3	17:0:585:THR:N	2.35	0.41
17:0:590:CYS:SG	17:0:596:ALA:HB3	2.60	0.41
18:4:299:ILE:N	18:4:300:PRO:HD2	2.34	0.41
21:7:420:TRP:O	21:7:423:GLN:HG2	2.20	0.41
23:2:365:HIS:ND1	23:2:365:HIS:O	2.53	0.41
23:2:503:ASP:OD1	23:2:507:ARG:NH1	2.53	0.41
29:O:106:ILE:HD11	29:O:135:ALA:HA	2.02	0.41
1:Q:337:GLU:OE2	1:Q:339:ALA:HB3	2.20	0.41
3:D:40:HIS:CE1	4:G:74:TYR:H	2.37	0.41
3:D:167:LEU:HA	3:D:170:THR:CG2	2.50	0.41
3:D:188:ALA:HB1	3:D:207:LEU:HD12	2.02	0.41
6:A:57:ARG:HB2	6:A:68:GLN:CB	2.50	0.41
6:A:102:VAL:O	6:A:105:CYS:N	2.49	0.41
6:A:239:LEU:HD12	6:A:239:LEU:HA	1.76	0.41
6:A:496:GLU:H	6:A:496:GLU:CD	2.17	0.41
6:A:595:THR:H	6:A:595:THR:HG23	1.55	0.41
6:A:1127:ASP:CG	6:A:1130:GLN:H	2.23	0.41
6:A:1150:SER:O	12:I:45:ARG:HA	2.20	0.41
6:A:1225:PHE:CZ	6:A:1227:ILE:HD11	2.56	0.41
7:B:48:LEU:HA	7:B:48:LEU:HD23	1.69	0.41
7:B:555:ILE:H	7:B:555:ILE:HG13	1.42	0.41
7:B:710:LEU:O	7:B:733:HIS:HB3	2.20	0.41
7:B:755:ILE:HD12	7:B:755:ILE:HG23	1.82	0.41
7:B:882:THR:O	7:B:884:ARG:N	2.53	0.41
9:E:43:LYS:O	9:E:47:CYS:HB2	2.20	0.41
9:E:48:ASP:N	9:E:52:ARG:O	2.37	0.41
10:F:97:ARG:HD2	10:F:97:ARG:HA	1.71	0.41
12:I:68:LEU:HB3	12:I:84:VAL:HG13	2.02	0.41
16:3:128:LYS:O	16:3:132:LYS:N	2.47	0.41
17:0:184:TYR:CE1	17:0:188:LYS:HG3	2.54	0.41
17:0:357:LYS:HB2	17:0:413:GLU:OE1	2.20	0.41
17:0:581:LEU:HA	17:0:584:GLU:HG2	2.00	0.41
19:6:120:ARG:HE	19:6:307:PRO:HB2	1.85	0.41
27:N:17:DG:N3	28:T:150:DG:N2	2.67	0.41
28:T:140:DT:H2'	28:T:141:DT:H71	2.02	0.41
30:W:144:ARG:NH2	30:W:146:GLU:H	2.17	0.41
31:P:6:G:C6	31:P:7:A:H1'	2.55	0.41
1:Q:106:ILE:HB	1:Q:385:THR:HG21	2.02	0.41
5:M:272:LYS:H	29:O:208:VAL:HG11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:49:LYS:HE3	6:A:49:LYS:HB3	1.86	0.41
6:A:49:LYS:HD3	6:A:55:ASP:O	2.20	0.41
6:A:178:GLY:C	6:A:179:LEU:HD13	2.40	0.41
6:A:664:THR:HG22	7:B:1014:PRO:HB3	2.02	0.41
6:A:982:THR:HG23	6:A:985:ASP:OD2	2.20	0.41
7:B:135:ARG:NH1	7:B:137:TYR:O	2.53	0.41
7:B:782:LEU:HD23	7:B:782:LEU:HA	1.67	0.41
7:B:842:ASN:HB3	7:B:845:SER:HB3	2.02	0.41
7:B:1187:ASN:HD21	7:B:1190:ASP:CB	2.26	0.41
8:C:54:ASN:OD1	8:C:55:THR:N	2.53	0.41
11:H:40:LEU:HD12	11:H:41:ASP:H	1.85	0.41
12:I:74:GLU:HB2	12:I:81:ARG:CZ	2.50	0.41
17:0:69:ILE:HB	17:0:205:ILE:HG13	2.02	0.41
18:4:55:GLU:O	18:4:59:VAL:HG23	2.21	0.41
18:4:114:UNK:C	18:4:116:ARG:N	2.83	0.41
30:W:65:ARG:HG2	30:W:93:HIS:HB3	2.03	0.41
5:M:318:GLU:OE1	5:M:319:HIS:ND1	2.53	0.41
6:A:72:GLU:OE2	6:A:80:HIS:NE2	2.52	0.41
6:A:1142:THR:OG1	6:A:1143:LEU:N	2.52	0.41
6:A:1263:ILE:HD12	6:A:1263:ILE:HA	1.84	0.41
7:B:89:GLU:O	7:B:135:ARG:N	2.48	0.41
7:B:120:ARG:HE	7:B:120:ARG:HB3	1.67	0.41
7:B:585:VAL:HB	7:B:587:HIS:HE1	1.84	0.41
7:B:794:ASN:C	7:B:795:ILE:HD12	2.40	0.41
7:B:838:SER:HB3	7:B:988:GLY:HA3	2.02	0.41
7:B:976:ILE:CD1	7:B:992:ILE:HA	2.51	0.41
7:B:997:GLU:HG2	7:B:998:ASP:N	2.35	0.41
17:0:19:PRO:HG3	17:0:739:TRP:CE2	2.56	0.41
17:0:413:GLU:O	17:0:414:GLU:HG3	2.20	0.41
17:0:495:MET:HA	17:0:705:ASP:OD2	2.19	0.41
18:4:34:PRO:HD2	18:4:80:SER:CB	2.50	0.41
18:4:175:ARG:NE	18:4:256:PRO:HG3	2.26	0.41
21:7:564:GLU:OE1	21:7:757:ARG:HB2	2.21	0.41
22:5:8:ALA:HB2	22:5:44:PRO:HG3	2.02	0.41
23:2:394:ASP:OD1	23:2:395:GLN:N	2.54	0.41
30:W:44:LYS:NZ	30:W:51:LYS:HG2	2.34	0.41
1:Q:333:LYS:H	7:B:70:ILE:HG12	1.84	0.41
1:Q:352:MET:HG2	1:Q:361:TRP:HB2	2.02	0.41
2:R:96:ARG:O	2:R:104:ILE:HG23	2.20	0.41
3:D:183:LEU:HD12	3:D:195:ILE:HD11	2.03	0.41
4:G:110:VAL:HA	4:G:161:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:414:ASP:OD1	6:A:415:LEU:N	2.53	0.41
6:A:495:GLU:O	6:A:498:ARG:HG3	2.21	0.41
6:A:618:GLU:OE1	6:A:620:LYS:N	2.44	0.41
6:A:752:LYS:HD3	6:A:752:LYS:HA	1.86	0.41
6:A:765:VAL:HG23	6:A:802:ASN:O	2.20	0.41
6:A:843:LYS:HD2	6:A:843:LYS:HA	1.71	0.41
6:A:1235:LYS:HB2	6:A:1237:ILE:HD11	2.03	0.41
6:A:1407:GLU:CD	6:A:1407:GLU:N	2.73	0.41
7:B:20:ASP:OD2	7:B:21:GLU:N	2.52	0.41
7:B:1035:ALA:O	7:B:1039:GLY:N	2.53	0.41
8:C:201:TRP:HA	8:C:202:PRO:HD3	1.96	0.41
10:F:147:SER:O	10:F:149:GLU:N	2.54	0.41
11:H:89:LEU:C	11:H:91:ASP:H	2.24	0.41
12:I:52:ILE:HA	12:I:120:GLN:O	2.20	0.41
14:K:7:PHE:HA	14:K:10:PHE:CZ	2.55	0.41
17:0:108:LEU:HD22	17:0:200:ILE:HD11	2.02	0.41
17:0:132:LYS:HE3	17:0:132:LYS:HB2	1.89	0.41
17:0:267:LEU:HD22	17:0:399:LEU:HD13	2.00	0.41
17:0:527:VAL:O	17:0:531:LYS:HG3	2.20	0.41
17:0:575:ASP:OD1	17:0:575:ASP:N	2.54	0.41
17:0:632:SER:OG	17:0:633:ARG:N	2.53	0.41
18:4:67:PHE:HE1	23:2:44:LYS:HB3	1.85	0.41
18:4:180:THR:HG23	18:4:214:LYS:HA	2.01	0.41
23:2:100:LEU:HA	23:2:100:LEU:HD23	1.79	0.41
24:X:193:LEU:HD21	24:X:228:SER:HA	2.02	0.41
27:N:18:DT:C4	28:T:148:DA:N1	2.88	0.41
1:Q:104:ARG:O	1:Q:385:THR:HG23	2.21	0.41
1:Q:134:HIS:HB3	1:Q:354:ASP:OD1	2.20	0.41
2:R:124:LEU:HD22	2:R:220:HIS:NE2	2.36	0.41
6:A:139:TRP:O	6:A:143:LYS:HB3	2.19	0.41
6:A:217:LYS:HG3	6:A:218:ASP:H	1.85	0.41
6:A:595:THR:HG21	6:A:604:GLY:HA3	2.02	0.41
6:A:726:ARG:HE	6:A:726:ARG:HB3	1.60	0.41
6:A:1155:ASP:HB3	6:A:1241:ARG:HH21	1.86	0.41
7:B:301:ILE:HD13	7:B:382:ILE:HG21	2.02	0.41
7:B:523:CYS:HB2	7:B:750:GLY:HA3	2.02	0.41
10:F:138:LEU:HA	10:F:138:LEU:HD13	1.56	0.41
10:F:147:SER:O	10:F:150:GLU:HG2	2.20	0.41
11:H:95:TYR:HA	11:H:95:TYR:HD1	1.73	0.41
11:H:136:LYS:HE2	11:H:136:LYS:HB2	1.80	0.41
17:0:709:SER:HB3	17:0:712:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:228:THR:H	18:4:228:THR:HG22	1.62	0.41
20:1:194:VAL:HA	20:1:197:GLU:HG2	2.01	0.41
23:2:337:GLY:O	23:2:406:PRO:HB2	2.21	0.41
23:2:419:LYS:NZ	23:2:426:CYS:O	2.35	0.41
23:2:435:PRO:O	23:2:439:ASP:N	2.40	0.41
2:R:66:ARG:O	2:R:217:THR:N	2.54	0.41
2:R:74:PRO:HB2	2:R:76:PHE:CE1	2.56	0.41
4:G:31:LEU:HD11	4:G:51:TYR:CE1	2.55	0.41
4:G:97:HIS:NE2	30:W:145:THR:O	2.52	0.41
6:A:404:TYR:CD1	6:A:414:ASP:HA	2.56	0.41
6:A:1435:PRO:O	6:A:1436:ILE:HD13	2.21	0.41
7:B:356:LEU:HD23	7:B:356:LEU:N	2.36	0.41
7:B:693:ILE:HA	7:B:693:ILE:HD13	1.75	0.41
7:B:1151:LEU:HD12	7:B:1151:LEU:HA	1.74	0.41
19:6:243:ASP:O	20:1:389:LEU:HD22	2.20	0.41
21:7:562:THR:OG1	21:7:563:ALA:N	2.52	0.41
24:X:258:GLU:O	24:X:262:MET:N	2.51	0.41
25:U:267:VAL:HG12	25:U:269:ILE:HG13	2.03	0.41
26:V:69:TYR:HB2	26:V:76:TRP:HZ3	1.83	0.41
27:N:37:DG:C2	27:N:38:DT:C2	3.08	0.41
28:T:18:DA:N3	28:T:18:DA:H3'	2.36	0.41
1:Q:97:GLU:OE2	1:Q:99:ASN:N	2.54	0.41
1:Q:125:LYS:O	1:Q:127:ILE:N	2.54	0.41
1:Q:141:ARG:NE	1:Q:348:TYR:O	2.53	0.41
1:Q:333:LYS:N	7:B:70:ILE:HG12	2.36	0.41
6:A:369:SER:N	14:K:2:ASN:OD1	2.40	0.41
6:A:839:ARG:O	6:A:843:LYS:HG2	2.20	0.41
6:A:1067:LEU:HD12	6:A:1067:LEU:HA	1.83	0.41
6:A:1193:LEU:HD12	6:A:1194:ARG:N	2.35	0.41
6:A:1341:ILE:HD12	6:A:1341:ILE:HA	1.85	0.41
6:A:1425:SER:O	6:A:1429:ILE:HG13	2.21	0.41
6:A:1441:PHE:HZ	10:F:92:ARG:CB	2.33	0.41
7:B:239:GLU:HG2	7:B:240:ILE:N	2.36	0.41
7:B:1079:LYS:HG2	7:B:1080:LYS:N	2.36	0.41
7:B:1156:ASP:N	7:B:1156:ASP:OD1	2.50	0.41
7:B:1173:ALA:O	7:B:1175:LEU:N	2.53	0.41
9:E:65:THR:O	9:E:68:SER:OG	2.25	0.41
13:J:30:LEU:HD12	13:J:30:LEU:HA	1.52	0.41
17:0:120:VAL:HG21	34:0:801:SF4:S4	2.61	0.41
17:0:636:LYS:O	17:0:640:GLU:HG2	2.21	0.41
19:6:137:LEU:HD23	19:6:137:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:562:LYS:HD2	20:1:562:LYS:HA	1.94	0.41
21:7:583:MET:HB3	21:7:763:VAL:HG21	2.02	0.41
21:7:633:GLN:O	21:7:637:MET:HG2	2.21	0.41
23:2:273:LYS:HG3	23:2:276:LEU:HD23	2.03	0.41
24:X:224:LEU:O	24:X:229:LYS:N	2.53	0.41
27:N:19:DA:N6	28:T:146:DA:H61	2.19	0.41
28:T:144:DA:H1'	29:O:69:ASN:ND2	2.36	0.41
29:O:74:VAL:HA	29:O:154:ASP:O	2.20	0.41
29:O:194:ILE:HD12	29:O:205:LEU:HD22	2.03	0.41
1:Q:106:ILE:HD12	1:Q:106:ILE:HA	1.87	0.41
1:Q:376:LEU:O	1:Q:378:VAL:N	2.53	0.41
2:R:69:TRP:CH2	2:R:220:HIS:HD2	2.39	0.41
5:M:266:ILE:O	5:M:266:ILE:HG23	2.21	0.41
6:A:147:VAL:HG23	6:A:148:CYS:N	2.36	0.41
6:A:217:LYS:NZ	6:A:218:ASP:HA	2.36	0.41
6:A:340:LEU:HD13	6:A:1429:ILE:HG23	2.02	0.41
6:A:420:ARG:HB3	6:A:423:ASP:CB	2.50	0.41
6:A:834:THR:HB	6:A:1077:THR:HG22	2.01	0.41
6:A:857:ARG:CZ	10:F:139:PRO:HG2	2.51	0.41
6:A:878:ILE:CG2	6:A:955:PRO:HB2	2.51	0.41
6:A:899:VAL:HG13	6:A:1029:ARG:HH11	1.85	0.41
6:A:1189:SER:HB3	6:A:1242:VAL:O	2.21	0.41
6:A:1359:ASP:CG	6:A:1361:SER:H	2.24	0.41
7:B:69:LEU:HD23	7:B:69:LEU:HA	1.70	0.41
7:B:193:LYS:HZ1	13:J:65:PRO:HD3	1.86	0.41
7:B:386:LEU:HD22	7:B:386:LEU:HA	1.85	0.41
7:B:519:TRP:CD1	7:B:519:TRP:C	2.94	0.41
7:B:637:LEU:HD23	7:B:637:LEU:HA	1.63	0.41
7:B:644:GLU:HG2	7:B:648:HIS:NE2	2.36	0.41
7:B:815:ARG:HE	7:B:815:ARG:HB3	1.39	0.41
8:C:29:MET:HE2	8:C:29:MET:HB2	1.92	0.41
8:C:51:VAL:HG13	15:L:65:VAL:HG13	2.03	0.41
8:C:58:LEU:HD23	8:C:58:LEU:HA	1.79	0.41
8:C:106:GLU:H	8:C:106:GLU:HG2	1.69	0.41
9:E:71:LYS:HE2	9:E:71:LYS:HB3	1.82	0.41
9:E:180:ARG:NH1	9:E:192:ARG:HB2	2.36	0.41
11:H:89:LEU:C	11:H:91:ASP:N	2.75	0.41
11:H:104:PHE:HE1	11:H:136:LYS:HD3	1.86	0.41
15:L:31:CYS:SG	15:L:34:CYS:CB	3.08	0.41
17:0:48:LYS:O	17:0:52:LEU:HB2	2.21	0.41
19:6:365:CYS:O	20:1:559:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:361:GLN:H	21:7:361:GLN:HG2	1.68	0.41
21:7:528:ASN:O	21:7:532:GLY:N	2.53	0.41
21:7:671:ILE:HG13	21:7:706:TYR:HB2	2.02	0.41
23:2:143:TRP:O	23:2:146:ILE:HG22	2.21	0.41
27:N:21:DA:H5"	29:O:196:ARG:HH22	1.86	0.41
28:T:130:DG:C2	28:T:131:DT:C2	3.08	0.41
29:O:73:THR:HG1	29:O:158:GLN:CD	2.25	0.41
29:O:94:TYR:HB2	29:O:102:VAL:HA	2.02	0.41
29:O:182:PHE:O	29:O:195:TYR:HA	2.21	0.41
29:O:204:LEU:HD22	29:O:230:ILE:HG21	2.02	0.41
29:O:206:ILE:HG23	29:O:212:ILE:CD1	2.49	0.41
30:W:113:LEU:HG	30:W:165:ASN:OD1	2.21	0.41
1:Q:123:SER:H	1:Q:361:TRP:HH2	1.69	0.41
2:R:64:SER:HA	2:R:214:ILE:HG22	2.02	0.41
2:R:105:THR:OG1	2:R:120:TYR:O	2.38	0.41
5:M:51:VAL:HG12	6:A:412:ARG:O	2.21	0.41
5:M:132:LYS:HE3	5:M:132:LYS:HB2	1.89	0.41
6:A:84:ILE:O	6:A:239:LEU:N	2.50	0.41
6:A:151:ASP:HB3	6:A:162:VAL:O	2.21	0.41
6:A:288:ALA:HA	6:A:291:GLU:CD	2.41	0.41
6:A:340:LEU:HD23	6:A:340:LEU:HA	1.73	0.41
6:A:901:LEU:HA	6:A:901:LEU:HD23	1.87	0.41
6:A:1284:MET:HE3	6:A:1284:MET:HB3	1.85	0.41
6:A:1444:MET:CE	10:F:133:VAL:HG13	2.50	0.41
7:B:387:LEU:HD12	7:B:387:LEU:HA	1.64	0.41
7:B:864:LYS:HA	7:B:872:GLU:CD	2.42	0.41
11:H:102:TYR:CE1	11:H:115:TYR:HB3	2.56	0.41
17:0:293:LEU:HD22	17:0:319:GLU:HG3	2.03	0.41
17:0:611:ASP:OD1	17:0:612:PHE:N	2.54	0.41
19:6:346:GLY:HA2	19:6:358:SER:N	2.36	0.41
21:7:370:LEU:HD22	21:7:374:PHE:CZ	2.56	0.41
21:7:409:VAL:O	21:7:455:SER:N	2.40	0.41
21:7:417:VAL:HG13	21:7:454:VAL:HG22	2.02	0.41
27:N:23:DA:H4'	29:O:158:GLN:O	2.21	0.41
3:D:63:LEU:HB3	3:D:130:LEU:HD13	2.04	0.40
5:M:167:SER:C	5:M:169:GLU:H	2.24	0.40
6:A:114:LEU:HB3	6:A:145:LYS:HG2	2.03	0.40
6:A:220:THR:C	6:A:222:LEU:N	2.75	0.40
6:A:407:ARG:HA	6:A:430:TRP:CD1	2.56	0.40
6:A:497:THR:HG22	7:B:1146:PHE:HA	2.03	0.40
6:A:1077:THR:H	6:A:1077:THR:HG23	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1109:LYS:HE2	6:A:1109:LYS:HB2	1.69	0.40
6:A:1224:LEU:HA	6:A:1241:ARG:O	2.22	0.40
6:A:1443:VAL:HG13	10:F:148:VAL:HG13	2.03	0.40
7:B:65:GLU:OE2	7:B:247:GLY:HA2	2.21	0.40
7:B:731:VAL:O	7:B:732:SER:OG	2.31	0.40
7:B:806:THR:HG22	7:B:1045:SER:HA	2.02	0.40
7:B:901:PRO:HA	7:B:949:VAL:HG12	2.04	0.40
8:C:153:LEU:HD11	8:C:155:LEU:HD23	2.01	0.40
11:H:4:THR:HG21	11:H:7:ASP:HB2	2.02	0.40
11:H:55:LEU:O	11:H:146:ARG:CZ	2.69	0.40
15:L:40:LEU:HD12	15:L:40:LEU:HA	1.81	0.40
17:0:285:GLU:HA	17:0:288:LYS:HD2	2.03	0.40
17:0:523:GLY:HA3	17:0:559:ILE:HG12	2.03	0.40
17:0:732:ASP:OD1	17:0:733:GLN:N	2.54	0.40
20:1:253:ARG:HA	20:1:256:ILE:HG12	2.03	0.40
20:1:273:ASN:HB3	20:1:277:ASN:O	2.20	0.40
20:1:278:PHE:O	20:1:283:PHE:HB2	2.21	0.40
23:2:382:SER:HA	23:2:385:ARG:HH11	1.86	0.40
27:N:21:DA:H5"	29:O:196:ARG:NH2	2.37	0.40
29:O:172:LEU:O	29:O:176:ALA:N	2.54	0.40
29:O:185:TYR:CZ	29:O:187:PRO:HB3	2.56	0.40
31:P:6:G:H3'	31:P:6:G:N3	2.36	0.40
5:M:142:LEU:HD12	5:M:142:LEU:HA	1.73	0.40
6:A:409:SER:OG	6:A:411:ASP:OD1	2.38	0.40
6:A:849:MET:HB2	6:A:1063:MET:SD	2.61	0.40
6:A:1017:LEU:HA	6:A:1017:LEU:HD12	1.88	0.40
6:A:1242:VAL:HG12	6:A:1243:VAL:H	1.86	0.40
7:B:232:SER:O	7:B:261:ARG:CZ	2.69	0.40
7:B:483:LEU:HA	7:B:483:LEU:HD12	1.63	0.40
7:B:552:MET:HA	7:B:555:ILE:CD1	2.51	0.40
7:B:861:ASP:CG	7:B:914:LYS:HZ3	2.19	0.40
7:B:1030:LEU:HA	7:B:1030:LEU:HD12	1.78	0.40
8:C:22:LEU:O	8:C:228:PHE:N	2.48	0.40
8:C:183:TRP:CZ2	8:C:207:CYS:HB3	2.56	0.40
9:E:52:ARG:HE	9:E:52:ARG:HB2	1.70	0.40
11:H:24:CYS:SG	11:H:44:VAL:HG11	2.61	0.40
12:I:19:ASP:HB2	12:I:24:ARG:NH1	2.36	0.40
17:0:210:TYR:OH	17:0:235:ASP:O	2.33	0.40
17:0:506:ILE:O	17:0:683:ASP:HA	2.21	0.40
18:4:138:LYS:O	18:4:142:GLN:N	2.55	0.40
19:6:144:ASN:HD21	19:6:146:HIS:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:181:LEU:HD11	19:6:184:GLN:HA	2.02	0.40
21:7:409:VAL:HB	21:7:454:VAL:HA	2.02	0.40
21:7:460:VAL:HG13	21:7:474:MET:SD	2.62	0.40
23:2:58:PRO:HB3	23:2:95:THR:HG21	2.02	0.40
25:U:250:LYS:O	25:U:261:SER:N	2.45	0.40
28:T:25:DC:H6	28:T:25:DC:H5"	1.86	0.40
29:O:120:LYS:HA	29:O:120:LYS:HD3	1.86	0.40
29:O:138:LYS:O	29:O:142:ILE:HG13	2.21	0.40
6:A:525:GLN:NE2	7:B:836:GLU:HG2	2.36	0.40
6:A:927:VAL:HA	6:A:930:ASP:OD2	2.22	0.40
6:A:1063:MET:SD	6:A:1436:ILE:HG23	2.61	0.40
6:A:1084:PHE:HD2	6:A:1086:PHE:HB2	1.86	0.40
6:A:1153:TYR:HB2	6:A:1192:LEU:HD23	2.03	0.40
7:B:282:ILE:HG13	7:B:283:VAL:N	2.36	0.40
7:B:1032:SER:HB2	7:B:1089:PRO:HG2	2.04	0.40
8:C:90:ASP:OD1	8:C:90:ASP:C	2.60	0.40
9:E:31:THR:OG1	9:E:34:GLU:N	2.41	0.40
9:E:140:LEU:HA	9:E:140:LEU:HD23	1.81	0.40
15:L:25:ALA:HB3	15:L:37:LYS:NZ	2.37	0.40
17:0:19:PRO:HG3	17:0:739:TRP:CD2	2.57	0.40
17:0:332:VAL:O	17:0:336:LYS:HG3	2.21	0.40
17:0:375:ARG:HG3	17:0:410:SER:OG	2.22	0.40
19:6:127:ILE:HG21	19:6:220:LEU:HD23	2.02	0.40
19:6:128:LEU:HD12	19:6:233:LEU:HD13	2.03	0.40
19:6:174:MET:HG2	19:6:209:SER:H	1.87	0.40
19:6:298:LYS:HA	19:6:298:LYS:HD2	1.82	0.40
21:7:585:PRO:HB3	21:7:750:TYR:HB2	2.03	0.40
22:5:3:ARG:HH11	23:2:460:SER:HB2	1.86	0.40
24:X:207:CYS:HB3	24:X:242:ARG:H	1.86	0.40
26:V:84:GLN:HB3	26:V:105:VAL:HG12	2.02	0.40
2:R:76:PHE:CZ	2:R:120:TYR:HE2	2.38	0.40
2:R:135:PHE:HA	2:R:215:VAL:H	1.86	0.40
3:D:68:ARG:HG2	3:D:72:ARG:NH2	2.36	0.40
4:G:61:ILE:HG12	10:F:133:VAL:HG12	2.03	0.40
4:G:151:ILE:HA	4:G:151:ILE:HD13	1.80	0.40
5:M:37:ARG:HD2	5:M:37:ARG:HA	1.53	0.40
5:M:283:TYR:O	5:M:287:LEU:HG	2.21	0.40
6:A:107:CYS:HB2	6:A:148:CYS:SG	2.61	0.40
6:A:968:GLN:HA	6:A:973:ILE:CD1	2.51	0.40
6:A:1143:LEU:O	6:A:1146:VAL:HG12	2.21	0.40
6:A:1335:ILE:HA	6:A:1335:ILE:HD13	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:258:LEU:HD13	7:B:269:ILE:HG12	2.02	0.40
7:B:399:ASP:O	7:B:400:HIS:C	2.60	0.40
7:B:1223:ASP:N	7:B:1223:ASP:OD1	2.54	0.40
8:C:66:ARG:HH11	8:C:66:ARG:HD3	1.67	0.40
8:C:94:LYS:HE3	8:C:94:LYS:HB2	1.89	0.40
8:C:118:LEU:HA	8:C:118:LEU:HD23	1.56	0.40
8:C:176:ILE:HG12	8:C:232:VAL:HG22	2.03	0.40
8:C:243:VAL:HG12	8:C:244:VAL:N	2.37	0.40
9:E:77:SER:O	9:E:106:GLN:HB3	2.20	0.40
9:E:178:ILE:HG23	9:E:214:CYS:HA	2.03	0.40
10:F:140:ASP:OD1	10:F:142:SER:OG	2.35	0.40
11:H:10:PHE:HB3	11:H:28:ALA:HB1	2.03	0.40
11:H:57:VAL:O	11:H:93:TYR:CZ	2.74	0.40
14:K:42:LEU:HA	14:K:42:LEU:HD12	1.78	0.40
15:L:34:CYS:SG	15:L:36:SER:HB3	2.62	0.40
15:L:61:THR:HG1	15:L:63:ARG:HG2	1.87	0.40
17:0:37:ASN:HD22	17:0:475:PHE:HD2	1.69	0.40
17:0:614:HIS:HB3	17:0:618:ARG:NH2	2.36	0.40
18:4:159:TYR:HE1	19:6:407:GLN:HB2	1.86	0.40
25:U:286:VAL:OXT	29:O:110:LYS:HD2	2.21	0.40
29:O:75:THR:HG22	29:O:77:GLY:H	1.86	0.40
1:Q:118:LEU:HB2	1:Q:392:VAL:HA	2.04	0.40
1:Q:139:LEU:HA	1:Q:351:VAL:O	2.22	0.40
3:D:206:GLU:HA	3:D:209:ARG:NE	2.37	0.40
6:A:325:ILE:O	6:A:328:ARG:N	2.52	0.40
6:A:336:ILE:HG23	6:A:336:ILE:HD12	1.82	0.40
6:A:563:PRO:HB3	6:A:572:TRP:CE2	2.57	0.40
6:A:1348:LEU:HA	6:A:1348:LEU:HD12	1.72	0.40
6:A:1442:ASP:OD1	6:A:1442:ASP:C	2.60	0.40
7:B:126:SER:O	7:B:170:LEU:N	2.41	0.40
7:B:313:MET:HG3	7:B:390:LEU:HD21	2.02	0.40
7:B:1059:LEU:HD12	7:B:1059:LEU:HA	1.80	0.40
8:C:62:PHE:HE1	8:C:66:ARG:HD2	1.87	0.40
8:C:231:ASN:C	8:C:231:ASN:ND2	2.75	0.40
10:F:94:LEU:HD23	10:F:94:LEU:HA	1.87	0.40
10:F:135:ARG:HD2	10:F:143:PHE:CE2	2.57	0.40
10:F:140:ASP:CG	10:F:142:SER:HG	2.25	0.40
15:L:26:THR:HA	15:L:62:LYS:NZ	2.36	0.40
17:0:57:ILE:HD11	17:0:86:LEU:HD11	2.03	0.40
17:0:565:LYS:HE3	17:0:565:LYS:HB2	1.86	0.40
17:0:620:VAL:O	17:0:680:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:392:LYS:HE2	21:7:392:LYS:HB3	1.83	0.40
21:7:641:GLN:O	21:7:645:TYR:HB3	2.22	0.40
27:N:19:DA:N3	29:O:190:PHE:HD1	2.18	0.40
28:T:148:DA:H2'	28:T:148:DA:H5'	1.89	0.40
29:O:136:SER:HB2	29:O:152:PHE:CE1	2.47	0.40
30:W:49:ILE:HD11	30:W:54:LEU:HD12	2.02	0.40
30:W:102:VAL:HG13	30:W:179:ILE:HG12	2.04	0.40
30:W:131:TYR:HA	30:W:135:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	Q	140/735 (19%)	119 (85%)	21 (15%)	0	100	100
2	R	142/398 (36%)	126 (89%)	16 (11%)	0	100	100
3	D	153/221 (69%)	140 (92%)	13 (8%)	0	100	100
4	G	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
5	M	228/345 (66%)	196 (86%)	29 (13%)	3 (1%)	12	42
6	A	1395/1733 (80%)	1227 (88%)	161 (12%)	7 (0%)	29	64
7	B	1096/1224 (90%)	942 (86%)	149 (14%)	5 (0%)	29	64
8	C	264/318 (83%)	241 (91%)	22 (8%)	1 (0%)	34	69
9	E	212/215 (99%)	199 (94%)	13 (6%)	0	100	100
10	F	83/155 (54%)	73 (88%)	10 (12%)	0	100	100
11	H	129/146 (88%)	97 (75%)	31 (24%)	1 (1%)	19	54
12	I	117/122 (96%)	95 (81%)	22 (19%)	0	100	100
13	J	63/70 (90%)	52 (82%)	11 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	K	112/120 (93%)	101 (90%)	11 (10%)	0	100	100
15	L	44/70 (63%)	30 (68%)	14 (32%)	0	100	100
16	3	70/321 (22%)	65 (93%)	5 (7%)	0	100	100
17	0	752/778 (97%)	701 (93%)	51 (7%)	0	100	100
18	4	279/338 (82%)	246 (88%)	33 (12%)	0	100	100
19	6	336/461 (73%)	295 (88%)	39 (12%)	2 (1%)	25	59
20	1	256/543 (47%)	237 (93%)	17 (7%)	2 (1%)	19	54
21	7	630/843 (75%)	578 (92%)	52 (8%)	0	100	100
22	5	64/72 (89%)	59 (92%)	5 (8%)	0	100	100
23	2	456/513 (89%)	412 (90%)	44 (10%)	0	100	100
24	X	145/328 (44%)	126 (87%)	19 (13%)	0	100	100
25	U	44/286 (15%)	39 (89%)	5 (11%)	0	100	100
26	V	45/122 (37%)	45 (100%)	0	0	100	100
29	O	178/240 (74%)	165 (93%)	13 (7%)	0	100	100
30	W	189/482 (39%)	179 (95%)	10 (5%)	0	100	100
All	All	7791/11370 (68%)	6941 (89%)	829 (11%)	21 (0%)	44	73

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	M	269	ILE
5	M	270	ALA
6	A	68	GLN
6	A	72	GLU
6	A	609	ASP
7	B	837	ASP
7	B	838	SER
19	6	411	PRO
6	A	466	SER
11	H	58	THR
7	B	1046	PRO
5	M	158	HIS
6	A	47	ARG
8	C	175	ALA
6	A	958	VAL
7	B	991	GLY
19	6	112	LYS

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Mol	Chain	Res	Type
20	1	229	GLY
6	A	957	PRO
7	B	712	PRO
20	1	351	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	Q	108/641 (17%)	84 (78%)	24 (22%)	1 4
2	R	78/362 (22%)	62 (80%)	16 (20%)	1 5
3	D	139/200 (70%)	126 (91%)	13 (9%)	8 32
4	G	152/152 (100%)	137 (90%)	15 (10%)	8 29
5	M	202/299 (68%)	171 (85%)	31 (15%)	2 12
6	A	1224/1520 (80%)	1032 (84%)	192 (16%)	2 11
7	B	967/1061 (91%)	833 (86%)	134 (14%)	3 15
8	C	234/274 (85%)	198 (85%)	36 (15%)	2 11
9	E	196/197 (100%)	169 (86%)	27 (14%)	3 16
10	F	75/137 (55%)	63 (84%)	12 (16%)	2 11
11	H	117/128 (91%)	95 (81%)	22 (19%)	1 6
12	I	113/116 (97%)	83 (74%)	30 (26%)	0 1
13	J	60/65 (92%)	51 (85%)	9 (15%)	3 12
14	K	99/102 (97%)	89 (90%)	10 (10%)	7 28
15	L	40/57 (70%)	28 (70%)	12 (30%)	0 0
16	3	1/303 (0%)	1 (100%)	0	100 100
17	0	686/707 (97%)	657 (96%)	29 (4%)	30 62
18	4	198/298 (66%)	185 (93%)	13 (7%)	16 47
19	6	247/406 (61%)	237 (96%)	10 (4%)	31 65
20	1	169/396 (43%)	160 (95%)	9 (5%)	22 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	7	414/737 (56%)	394 (95%)	20 (5%)	25 58
22	5	53/66 (80%)	53 (100%)	0	100 100
23	2	258/468 (55%)	250 (97%)	8 (3%)	40 70
24	X	54/295 (18%)	54 (100%)	0	100 100
25	U	42/260 (16%)	41 (98%)	1 (2%)	49 76
26	V	46/108 (43%)	44 (96%)	2 (4%)	29 62
29	O	152/205 (74%)	144 (95%)	8 (5%)	22 54
30	W	155/429 (36%)	147 (95%)	8 (5%)	23 55
All	All	6279/9989 (63%)	5588 (89%)	691 (11%)	10 25

All (691) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	98	TYR
1	Q	104	ARG
1	Q	110	ASP
1	Q	111	LEU
1	Q	112	GLU
1	Q	114	MET
1	Q	118	LEU
1	Q	122	GLN
1	Q	126	LYS
1	Q	130	VAL
1	Q	132	ASP
1	Q	133	PHE
1	Q	135	LEU
1	Q	331	GLN
1	Q	336	ASP
1	Q	350	TRP
1	Q	352	MET
1	Q	355	PHE
1	Q	359	ASN
1	Q	380	ASP
1	Q	396	THR
1	Q	398	ARG
1	Q	399	ASN
1	Q	403	THR
2	R	71	VAL
2	R	79	GLU

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Mol	Chain	Res	Type
2	R	83	ASP
2	R	92	LEU
2	R	94	LYS
2	R	108	LEU
2	R	109	ASN
2	R	121	ASP
2	R	125	THR
2	R	127	LYS
2	R	128	VAL
2	R	130	GLU
2	R	138	GLN
2	R	211	LYS
2	R	217	THR
2	R	225	MET
3	D	26	THR
3	D	50	LEU
3	D	61	GLU
3	D	132	GLN
3	D	140	ASP
3	D	144	THR
3	D	153	ARG
3	D	157	GLN
3	D	160	VAL
3	D	169	SER
3	D	177	VAL
3	D	187	THR
3	D	203	SER
4	G	13	LEU
4	G	21	ARG
4	G	39	THR
4	G	49	LEU
4	G	58	ARG
4	G	64	THR
4	G	65	ASP
4	G	83	LYS
4	G	97	HIS
4	G	111	THR
4	G	145	VAL
4	G	151	ILE
4	G	153	GLN
4	G	154	VAL
4	G	155	SER

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Mol	Chain	Res	Type
5	M	22	LEU
5	M	40	GLU
5	M	47	LEU
5	M	51	VAL
5	M	58	ASP
5	M	123	ASP
5	M	125	GLU
5	M	133	ILE
5	M	134	THR
5	M	142	LEU
5	M	158	HIS
5	M	160	GLU
5	M	162	THR
5	M	170	SER
5	M	175	SER
5	M	177	LEU
5	M	184	GLU
5	M	187	ARG
5	M	195	LEU
5	M	196	ILE
5	M	197	HIS
5	M	215	ARG
5	M	250	MET
5	M	257	GLU
5	M	267	LYS
5	M	284	LEU
5	M	286	ILE
5	M	291	ILE
5	M	298	VAL
5	M	305	THR
5	M	311	SER
6	A	13	THR
6	A	22	PHE
6	A	23	SER
6	A	37	PHE
6	A	41	MET
6	A	45	GLN
6	A	47	ARG
6	A	49	LYS
6	A	57	ARG
6	A	58	LEU
6	A	61	ILE

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Mol	Chain	Res	Type
6	A	63	ARG
6	A	64	ASN
6	A	68	GLN
6	A	71	GLN
6	A	72	GLU
6	A	84	ILE
6	A	93	VAL
6	A	96	ILE
6	A	110	CYS
6	A	115	LEU
6	A	116	ASP
6	A	117	GLU
6	A	129	LYS
6	A	140	THR
6	A	144	THR
6	A	145	LYS
6	A	147	VAL
6	A	152	VAL
6	A	174	ILE
6	A	175	ARG
6	A	179	LEU
6	A	203	SER
6	A	217	LYS
6	A	219	PHE
6	A	221	SER
6	A	225	ASN
6	A	235	ILE
6	A	236	LEU
6	A	237	THR
6	A	252	PHE
6	A	253	ASN
6	A	254	GLU
6	A	257	ARG
6	A	266	LEU
6	A	269	ILE
6	A	275	SER
6	A	280	GLU
6	A	286	HIS
6	A	299	HIS
6	A	318	SER
6	A	333	GLU
6	A	352	VAL

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Mol	Chain	Res	Type
6	A	354	SER
6	A	359	LEU
6	A	366	VAL
6	A	381	THR
6	A	385	ILE
6	A	389	THR
6	A	398	GLU
6	A	407	ARG
6	A	408	ASP
6	A	411	ASP
6	A	419	LYS
6	A	438	ASP
6	A	440	ASP
6	A	447	GLN
6	A	449	SER
6	A	450	LEU
6	A	469	ARG
6	A	470	LEU
6	A	472	LEU
6	A	476	SER
6	A	486	GLU
6	A	488	ASN
6	A	496	GLU
6	A	497	THR
6	A	502	SER
6	A	524	VAL
6	A	529	CYS
6	A	538	ASP
6	A	546	VAL
6	A	562	THR
6	A	566	ILE
6	A	567	LYS
6	A	573	SER
6	A	579	SER
6	A	589	GLN
6	A	599	SER
6	A	612	ILE
6	A	624	SER
6	A	634	THR
6	A	635	ARG
6	A	644	LYS
6	A	672	ASP

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Mol	Chain	Res	Type
6	A	677	ARG
6	A	678	GLU
6	A	681	GLU
6	A	685	GLU
6	A	716	ASP
6	A	728	LYS
6	A	739	ASP
6	A	740	LEU
6	A	754	SER
6	A	764	CYS
6	A	781	ASP
6	A	783	THR
6	A	788	SER
6	A	790	ASP
6	A	803	SER
6	A	808	LEU
6	A	827	THR
6	A	830	LYS
6	A	853	ASP
6	A	862	ASN
6	A	867	ILE
6	A	879	GLU
6	A	889	SER
6	A	899	VAL
6	A	903	ASN
6	A	905	ASP
6	A	909	ASP
6	A	912	LEU
6	A	914	GLU
6	A	915	SER
6	A	948	VAL
6	A	963	ILE
6	A	965	GLN
6	A	972	HIS
6	A	979	SER
6	A	982	THR
6	A	985	ASP
6	A	998	LEU
6	A	1000	LEU
6	A	1006	ILE
6	A	1015	VAL
6	A	1025	ARG

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Mol	Chain	Res	Type
6	A	1038	THR
6	A	1043	ASP
6	A	1046	LEU
6	A	1056	SER
6	A	1085	HIS
6	A	1089	VAL
6	A	1106	ASN
6	A	1117	THR
6	A	1135	ARG
6	A	1138	ILE
6	A	1142	THR
6	A	1160	SER
6	A	1172	LEU
6	A	1174	PHE
6	A	1192	LEU
6	A	1196	GLU
6	A	1197	LEU
6	A	1198	ASP
6	A	1204	ASP
6	A	1208	THR
6	A	1211	GLN
6	A	1212	VAL
6	A	1219	THR
6	A	1223	ASP
6	A	1232	ASN
6	A	1237	ILE
6	A	1240	CYS
6	A	1257	ASP
6	A	1261	LYS
6	A	1263	ILE
6	A	1265	ASN
6	A	1274	ARG
6	A	1278	ASN
6	A	1290	LYS
6	A	1291	VAL
6	A	1299	VAL
6	A	1327	ILE
6	A	1329	THR
6	A	1334	ASP
6	A	1358	SER
6	A	1362	TYR
6	A	1368	MET

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Mol	Chain	Res	Type
6	A	1372	VAL
6	A	1382	THR
6	A	1383	SER
6	A	1386	ARG
6	A	1391	ARG
6	A	1392	SER
6	A	1400	CYS
6	A	1406	VAL
6	A	1407	GLU
6	A	1411	GLU
6	A	1425	SER
6	A	1430	LEU
6	A	1441	PHE
7	B	26	THR
7	B	30	SER
7	B	37	PHE
7	B	46	GLN
7	B	50	SER
7	B	70	ILE
7	B	98	THR
7	B	104	GLU
7	B	135	ARG
7	B	137	TYR
7	B	167	ILE
7	B	183	GLU
7	B	188	ASP
7	B	195	CYS
7	B	199	MET
7	B	208	SER
7	B	209	GLU
7	B	211	VAL
7	B	223	VAL
7	B	234	ILE
7	B	235	SER
7	B	240	ILE
7	B	253	THR
7	B	254	LEU
7	B	294	ASP
7	B	304	ASP
7	B	312	GLU
7	B	333	PHE
7	B	334	ILE

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Mol	Chain	Res	Type
7	B	345	LYS
7	B	347	LYS
7	B	357	GLN
7	B	364	ILE
7	B	365	THR
7	B	376	PHE
7	B	385	LEU
7	B	386	LEU
7	B	393	LYS
7	B	396	ASP
7	B	420	LEU
7	B	428	ILE
7	B	431	TYR
7	B	435	THR
7	B	448	ILE
7	B	455	SER
7	B	457	LEU
7	B	466	TRP
7	B	480	SER
7	B	481	GLN
7	B	487	THR
7	B	493	SER
7	B	513	GLN
7	B	516	ASN
7	B	527	THR
7	B	529	GLU
7	B	531	GLN
7	B	555	ILE
7	B	568	ASP
7	B	574	SER
7	B	583	ASN
7	B	614	SER
7	B	617	ARG
7	B	624	LEU
7	B	625	LYS
7	B	628	THR
7	B	641	GLU
7	B	642	ASP
7	B	649	LYS
7	B	668	ASP
7	B	683	SER
7	B	685	LEU

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Mol	Chain	Res	Type
7	B	690	VAL
7	B	698	GLU
7	B	708	GLU
7	B	722	ASP
7	B	731	VAL
7	B	733	HIS
7	B	736	THR
7	B	737	THR
7	B	764	SER
7	B	771	SER
7	B	783	THR
7	B	789	MET
7	B	812	LEU
7	B	815	ARG
7	B	825	VAL
7	B	836	GLU
7	B	837	ASP
7	B	845	SER
7	B	848	ARG
7	B	852	ARG
7	B	864	LYS
7	B	868	MET
7	B	875	GLU
7	B	879	ARG
7	B	882	THR
7	B	887	HIS
7	B	891	ASP
7	B	893	LEU
7	B	894	ASP
7	B	896	ASP
7	B	908	GLU
7	B	909	ASP
7	B	935	ARG
7	B	944	THR
7	B	951	GLN
7	B	955	THR
7	B	958	GLN
7	B	962	LYS
7	B	963	PHE
7	B	982	SER
7	B	989	THR
7	B	995	ARG

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Mol	Chain	Res	Type
7	B	996	ARG
7	B	1002	THR
7	B	1007	VAL
7	B	1009	ASP
7	B	1022	THR
7	B	1032	SER
7	B	1048	THR
7	B	1051	THR
7	B	1052	VAL
7	B	1061	GLU
7	B	1101	ASP
7	B	1111	MET
7	B	1115	THR
7	B	1123	SER
7	B	1129	ARG
7	B	1151	LEU
7	B	1162	ILE
7	B	1183	LYS
7	B	1191	ILE
7	B	1218	THR
7	B	1224	PHE
8	C	14	SER
8	C	18	VAL
8	C	21	ILE
8	C	25	VAL
8	C	26	ASP
8	C	35	ARG
8	C	41	ILE
8	C	52	GLU
8	C	54	ASN
8	C	60	ASP
8	C	76	ASP
8	C	87	PHE
8	C	90	ASP
8	C	93	ASP
8	C	107	SER
8	C	115	SER
8	C	119	VAL
8	C	125	MET
8	C	136	ASP
8	C	137	LYS
8	C	138	GLU

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Mol	Chain	Res	Type
8	C	156	THR
8	C	186	LEU
8	C	195	GLN
8	C	196	ASP
8	C	197	SER
8	C	204	SER
8	C	208	GLU
8	C	211	ASP
8	C	215	GLU
8	C	231	ASN
8	C	235	VAL
8	C	240	VAL
8	C	244	VAL
8	C	258	ILE
8	C	268	ASP
9	E	2	ASP
9	E	4	GLU
9	E	5	ASN
9	E	17	ARG
9	E	19	VAL
9	E	31	THR
9	E	37	LEU
9	E	41	ASP
9	E	54	GLN
9	E	61	GLN
9	E	66	GLU
9	E	67	GLU
9	E	68	SER
9	E	84	ASP
9	E	85	GLU
9	E	92	THR
9	E	98	ILE
9	E	101	GLN
9	E	105	PHE
9	E	107	THR
9	E	131	THR
9	E	134	THR
9	E	149	LEU
9	E	155	ARG
9	E	202	SER
9	E	205	SER
9	E	215	MET

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Mol	Chain	Res	Type
10	F	71	GLU
10	F	93	ILE
10	F	96	THR
10	F	111	LEU
10	F	112	GLU
10	F	122	MET
10	F	128	LYS
10	F	132	LEU
10	F	133	VAL
10	F	134	ILE
10	F	142	SER
10	F	155	LEU
11	H	9	ILE
11	H	15	VAL
11	H	16	ASP
11	H	26	ILE
11	H	27	GLU
11	H	30	SER
11	H	32	THR
11	H	44	VAL
11	H	55	LEU
11	H	58	THR
11	H	88	SER
11	H	92	ASP
11	H	94	ASP
11	H	95	TYR
11	H	105	GLU
11	H	108	SER
11	H	112	ILE
11	H	128	ASN
11	H	130	ARG
11	H	142	LEU
11	H	143	LEU
11	H	145	ARG
12	I	3	THR
12	I	5	ARG
12	I	9	ASP
12	I	10	CYS
12	I	17	ARG
12	I	19	ASP
12	I	22	ASN
12	I	24	ARG

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Mol	Chain	Res	Type
12	I	25	LEU
12	I	28	GLU
12	I	29	CYS
12	I	32	CYS
12	I	37	GLU
12	I	40	SER
12	I	48	LEU
12	I	49	ILE
12	I	51	ASN
12	I	60	GLN
12	I	67	THR
12	I	70	ARG
12	I	71	SER
12	I	77	LYS
12	I	78	CYS
12	I	80	SER
12	I	88	SER
12	I	104	LEU
12	I	111	THR
12	I	118	ARG
12	I	119	THR
12	I	120	GLN
13	J	3	VAL
13	J	5	VAL
13	J	7	CYS
13	J	9	SER
13	J	10	CYS
13	J	20	SER
13	J	38	ARG
13	J	50	ILE
13	J	64	ASN
14	K	6	ARG
14	K	20	LYS
14	K	54	ARG
14	K	77	THR
14	K	82	ASP
14	K	93	SER
14	K	101	LEU
14	K	104	ASN
14	K	106	GLU
14	K	114	LEU
15	L	27	LEU

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Mol	Chain	Res	Type
15	L	31	CYS
15	L	34	CYS
15	L	35	SER
15	L	42	ARG
15	L	43	THR
15	L	44	ASP
15	L	46	VAL
15	L	48	CYS
15	L	50	ASP
15	L	53	HIS
15	L	55	ILE
17	0	5	ILE
17	0	49	THR
17	0	109	THR
17	0	115	CYS
17	0	140	GLN
17	0	142	LYS
17	0	162	LEU
17	0	175	VAL
17	0	221	ARG
17	0	241	ASP
17	0	253	THR
17	0	259	ARG
17	0	315	ASP
17	0	325	ILE
17	0	344	THR
17	0	349	LEU
17	0	388	LEU
17	0	393	VAL
17	0	395	ASP
17	0	414	GLU
17	0	419	ILE
17	0	421	GLU
17	0	511	GLU
17	0	532	ILE
17	0	572	GLU
17	0	584	GLU
17	0	585	THR
17	0	647	ARG
17	0	656	PHE
18	4	52	LYS
18	4	123	GLU

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Mol	Chain	Res	Type
18	4	125	LEU
18	4	132	LEU
18	4	149	LEU
18	4	176	LEU
18	4	180	THR
18	4	223	PHE
18	4	228	THR
18	4	252	MET
18	4	263	VAL
18	4	276	CYS
18	4	287	PHE
19	6	118	TYR
19	6	123	ILE
19	6	166	ILE
19	6	230	ARG
19	6	270	VAL
19	6	310	VAL
19	6	372	LEU
19	6	384	MET
19	6	440	CYS
19	6	448	LEU
20	1	189	LYS
20	1	261	GLU
20	1	277	ASN
20	1	282	GLU
20	1	321	PHE
20	1	331	HIS
20	1	339	LEU
20	1	348	VAL
20	1	381	LEU
21	7	313	VAL
21	7	323	VAL
21	7	393	THR
21	7	408	ILE
21	7	431	GLN
21	7	435	CYS
21	7	437	VAL
21	7	447	GLN
21	7	453	VAL
21	7	478	THR
21	7	490	VAL
21	7	514	THR

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Mol	Chain	Res	Type
21	7	534	LYS
21	7	573	THR
21	7	605	ILE
21	7	610	ASP
21	7	620	LEU
21	7	634	GLN
21	7	680	ARG
21	7	692	ARG
23	2	21	VAL
23	2	60	LEU
23	2	72	LEU
23	2	87	LEU
23	2	92	SER
23	2	385	ARG
23	2	410	ARG
23	2	484	LYS
25	U	264	ASP
26	V	57	GLN
26	V	76	TRP
29	O	91	ASN
29	O	136	SER
29	O	161	VAL
29	O	181	THR
29	O	182	PHE
29	O	183	SER
29	O	218	LYS
29	O	221	GLU
30	W	15	PHE
30	W	58	ILE
30	W	123	MET
30	W	126	ILE
30	W	133	GLN
30	W	147	PHE
30	W	149	CYS
30	W	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	138	GLN
3	D	28	GLN
3	D	40	HIS

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Mol	Chain	Res	Type
3	D	179	GLN
4	G	97	HIS
4	G	131	GLN
4	G	153	GLN
5	M	124	ASN
6	A	68	GLN
6	A	80	HIS
6	A	282	ASN
6	A	339	ASN
6	A	451	HIS
6	A	741	ASN
6	A	935	GLN
6	A	1078	GLN
6	A	1173	HIS
6	A	1188	GLN
6	A	1218	GLN
6	A	1232	ASN
6	A	1278	ASN
7	B	178	ASN
7	B	481	GLN
7	B	686	ASN
7	B	794	ASN
7	B	1177	HIS
7	B	1179	GLN
8	C	231	ASN
11	H	128	ASN
12	I	12	ASN
12	I	89	GLN
17	0	60	GLN
17	0	224	ASN
17	0	283	GLN
17	0	521	ASN
17	0	726	GLN
18	4	225	GLN
19	6	351	ASN
20	1	331	HIS
21	7	331	GLN
21	7	611	ASN
23	2	90	ASN
23	2	99	ASN
23	2	356	GLN
24	X	265	ASN

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Mol	Chain	Res	Type
29	O	68	GLN
29	O	158	GLN
30	W	138	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	P	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	P	8	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 16 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	$\#\|Z\| > 2$
34	SF4	0	801	17	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
34	SF4	0	801	17	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	0	801	SF4	2	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
20	1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	355:UNK	C	368:UNK	N	14.81
1	1	519:UNK	C	537:GLU	N	11.86

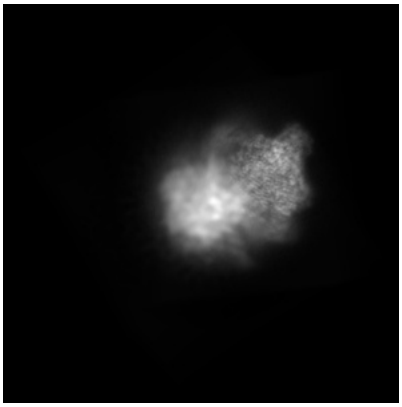
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23908. These allow visual inspection of the internal detail of the map and identification of artifacts.

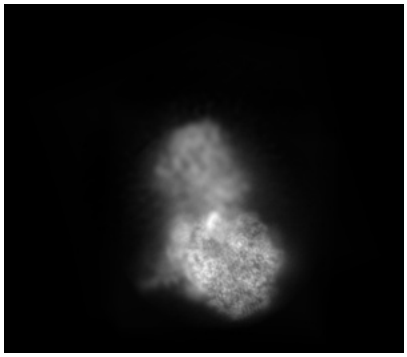
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

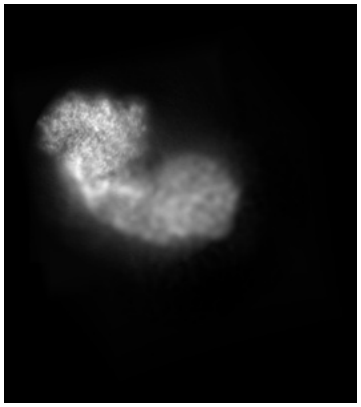
6.1.1 Primary map



X



Y

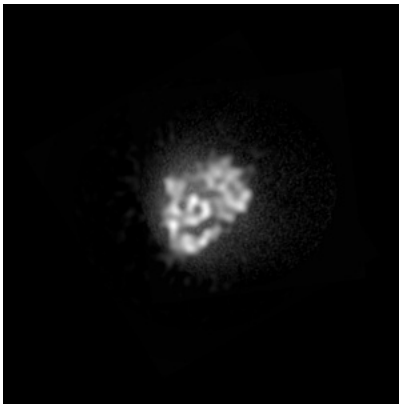


Z

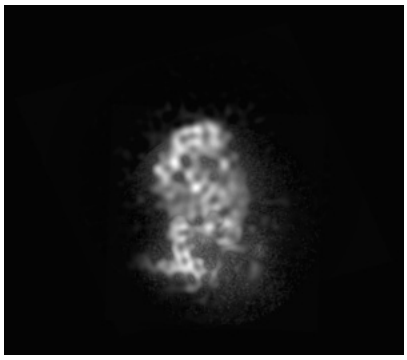
The images above show the map projected in three orthogonal directions.

6.2 Central slices

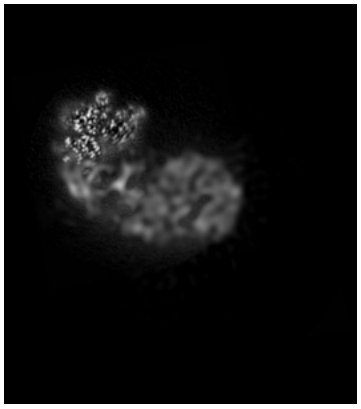
6.2.1 Primary map



X Index: 209



Y Index: 237

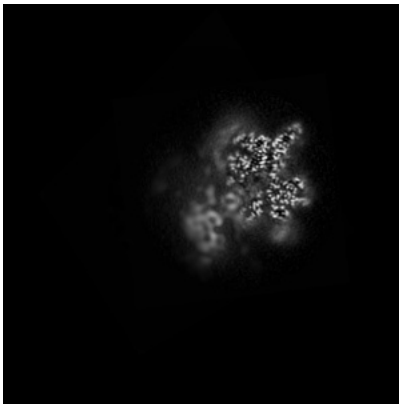


Z Index: 240

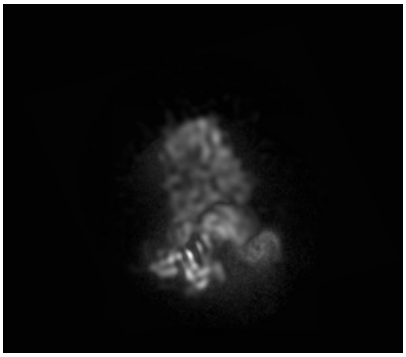
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

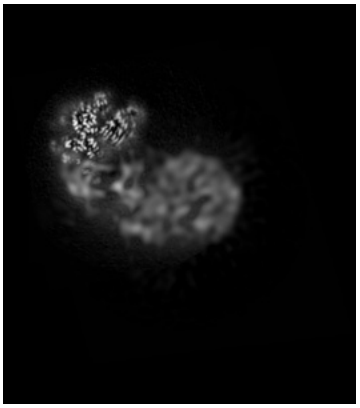
6.3.1 Primary map



X Index: 109



Y Index: 253

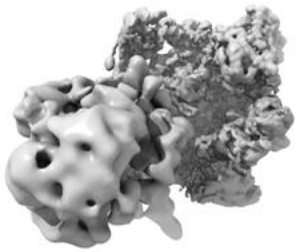


Z Index: 242

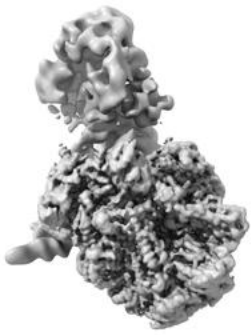
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

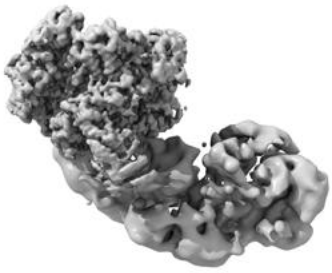
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

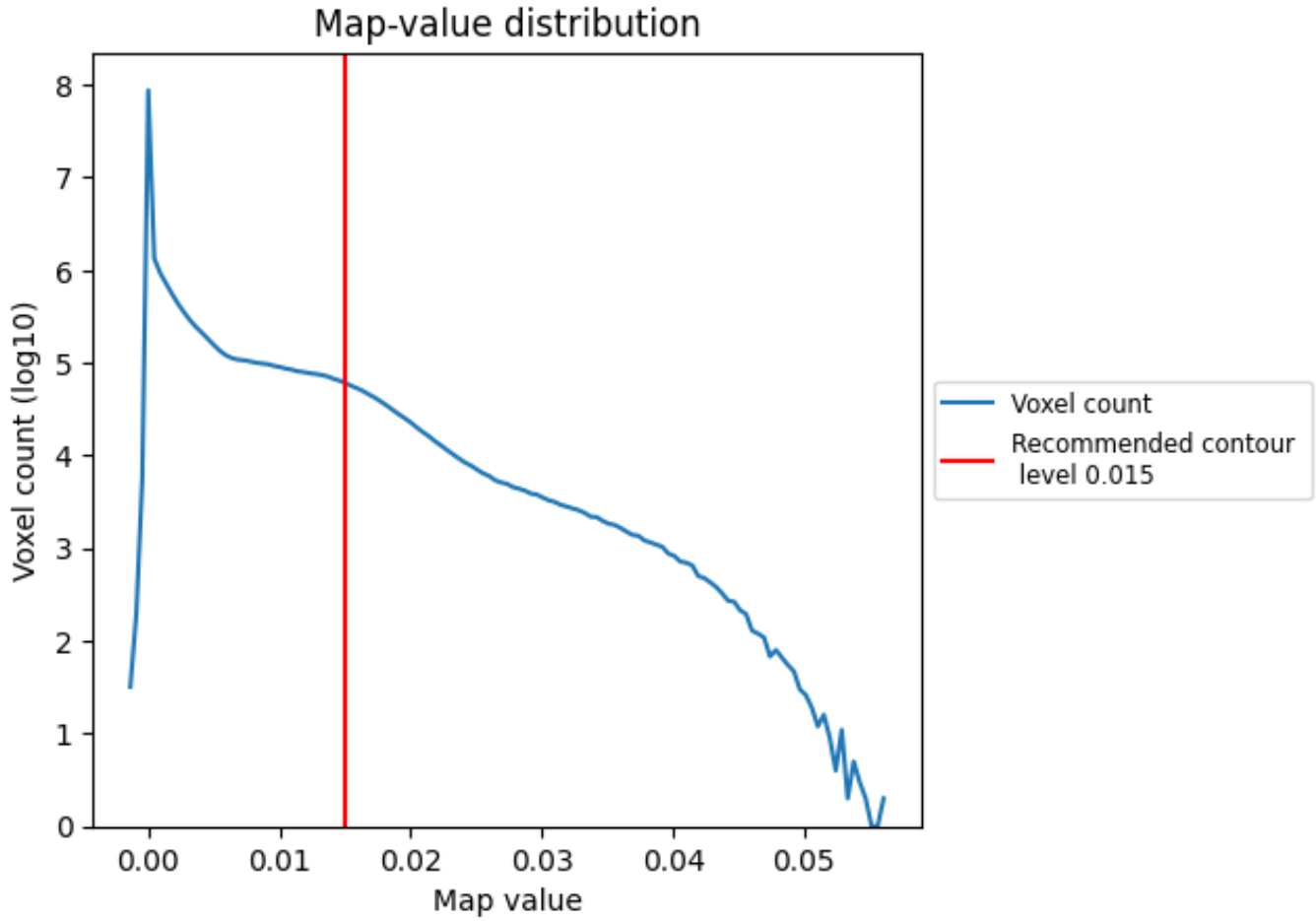
6.5 Mask visualisation (i)

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

7 Map analysis

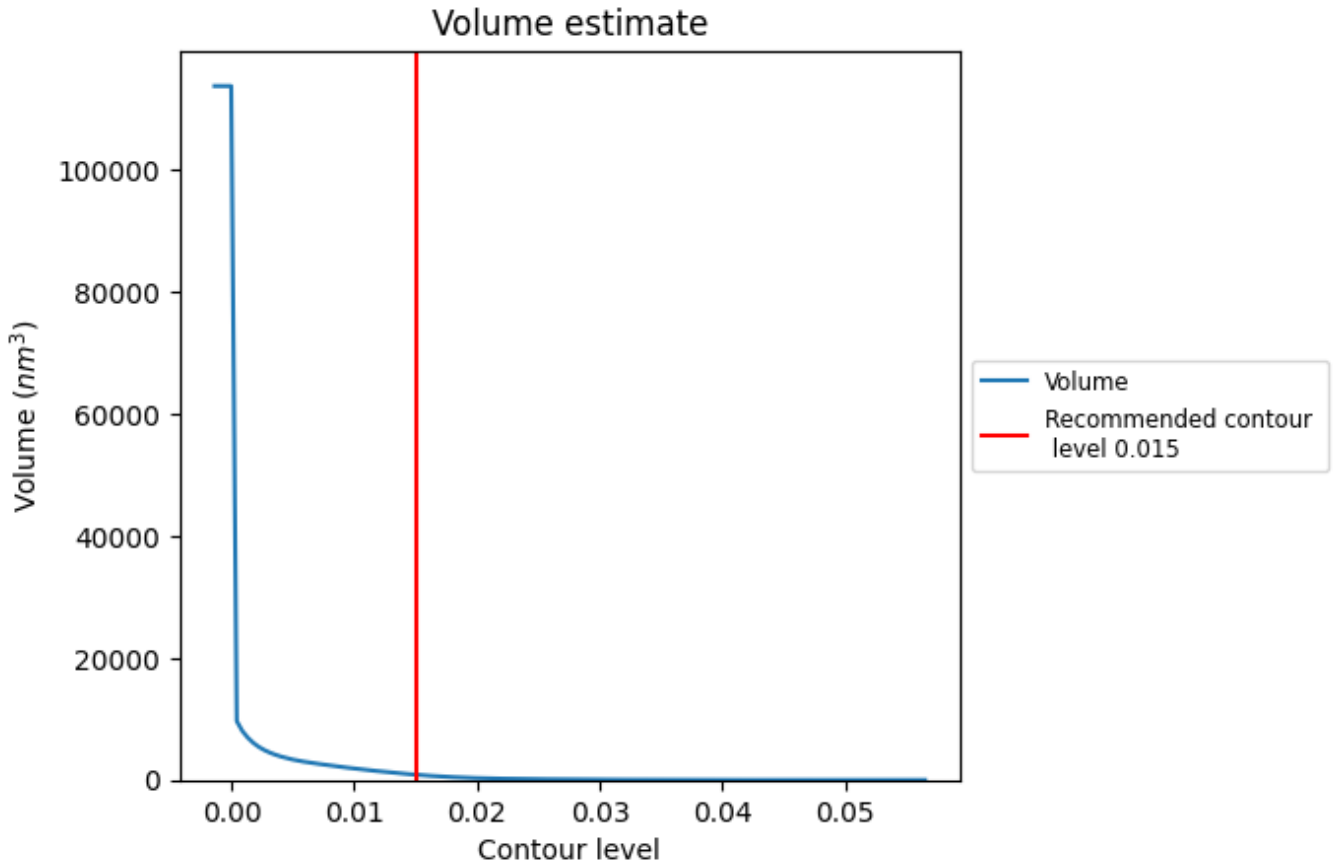
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 863 nm^3; this corresponds to an approximate mass of 779 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.

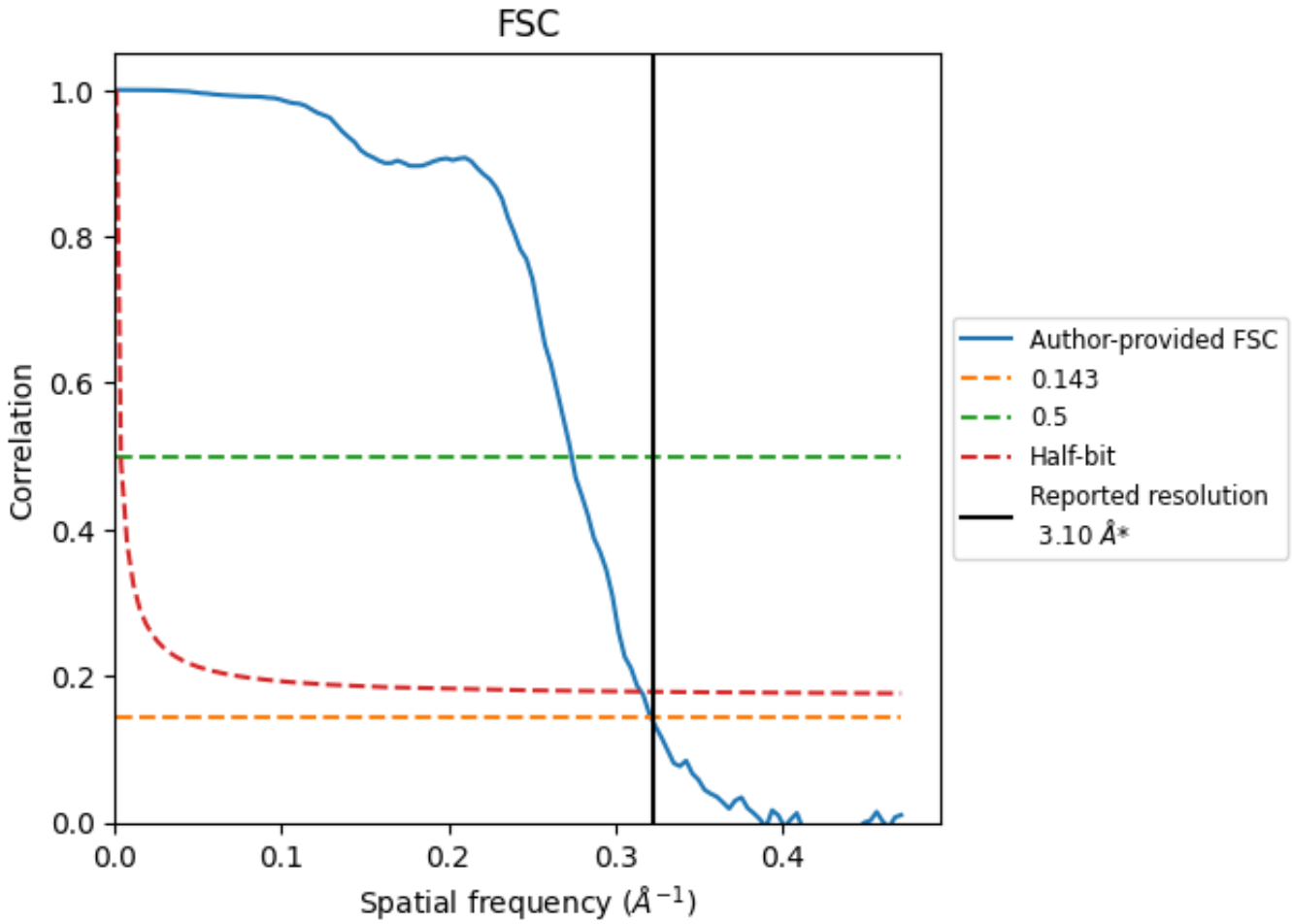
7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

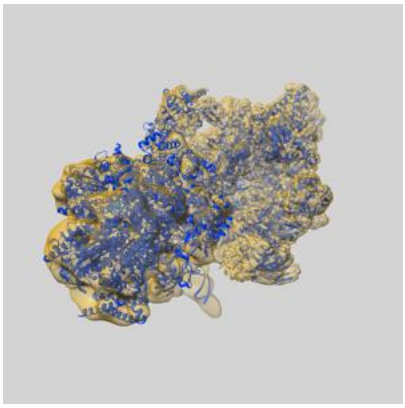
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.65	3.17
Unmasked-calculated*	-	-	-

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

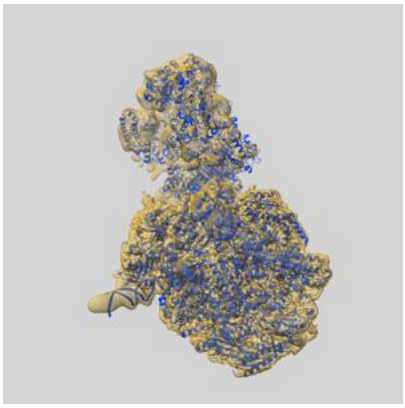
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23908 and PDB model 7ML4. Per-residue inclusion information can be found in section 3 on page 12.

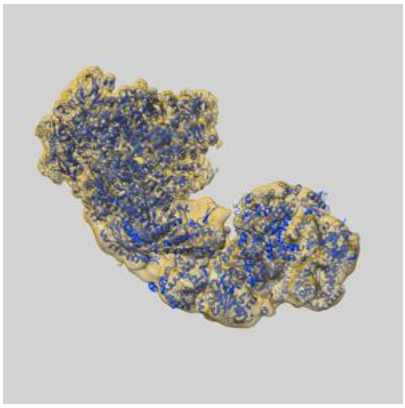
9.1 Map-model overlay



X



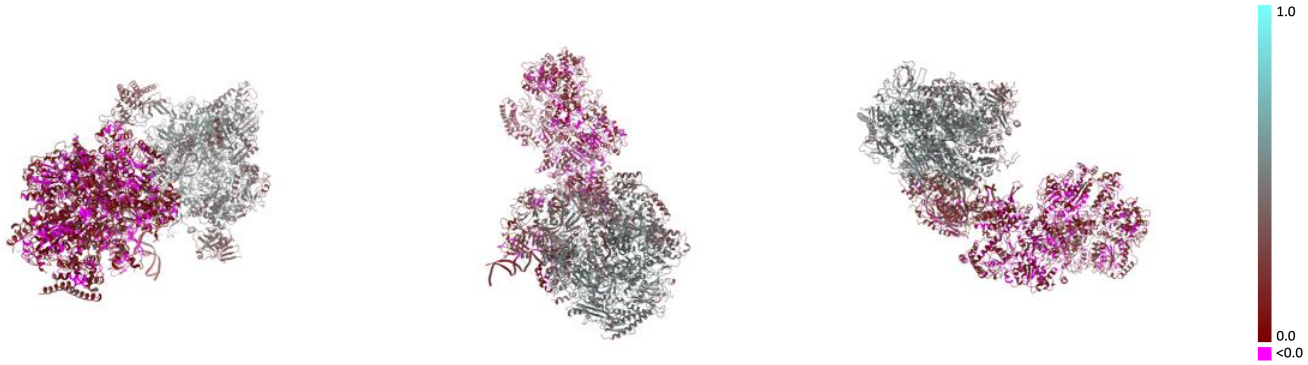
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

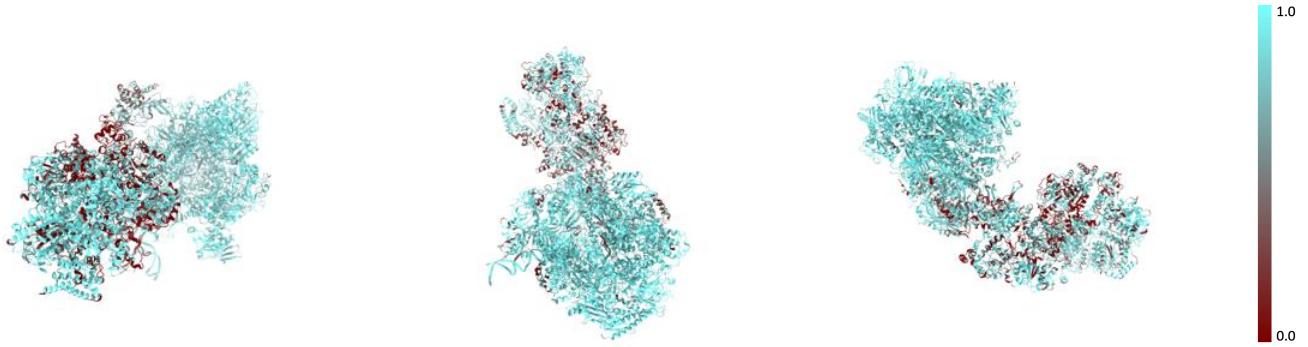
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

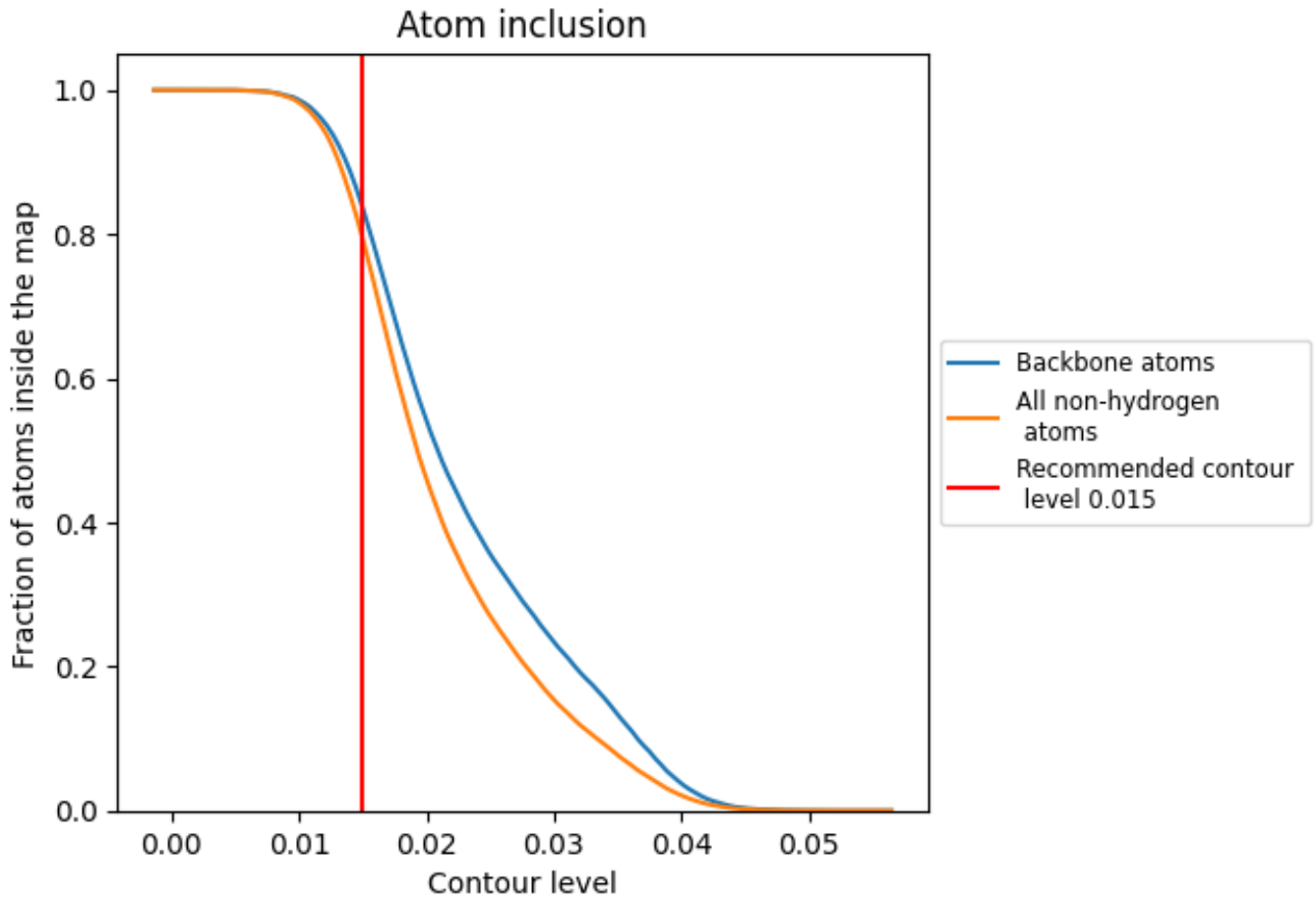
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7934	0.2810
0	0.6656	0.0610
1	0.5789	0.0820
2	0.6947	0.0880
3	0.4377	0.1210
4	0.7977	0.0710
5	0.4675	0.0950
6	0.7829	0.0790
7	0.4377	0.0470
A	0.9260	0.4730
B	0.9413	0.4960
C	0.9570	0.4930
D	0.4631	0.2750
E	0.9251	0.4610
F	0.9537	0.5000
G	0.6800	0.3600
H	0.9413	0.4440
I	0.8647	0.4200
J	0.9787	0.5080
K	0.8775	0.4750
L	0.9601	0.4430
M	0.7543	0.1890
N	0.9166	0.1710
O	0.8963	0.0690
P	0.6545	0.2610
Q	0.8946	0.3570
R	0.8488	0.2590
T	0.8461	0.1830
U	0.6488	0.0900
V	0.7878	0.1090
W	0.6687	0.1000
X	0.7939	0.0640