



wwPDB EM Map/Model Validation Report ⓘ

Jun 14, 2016 – 02:12 PM EDT

PDB ID : 5IYB
EMDB ID: : EMD-8136
Title : Human core-PIC in the open state
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on : 2016-03-24
Resolution : 3.90 Å(reported)
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

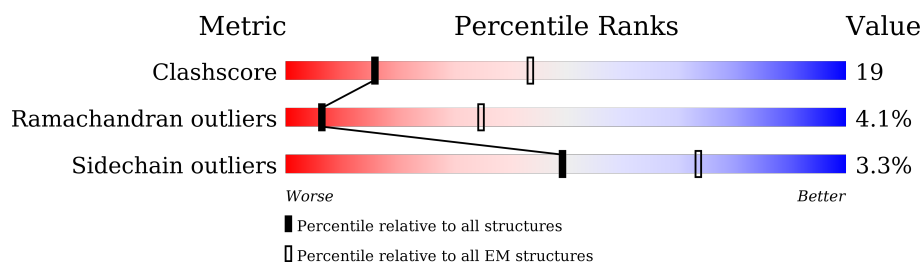
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	

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Mol	Chain	Length	Quality of chain
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	75	
23	Y	75	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 47728 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1454	Total	C	N	O	S	0	0
			11515	7234	2058	2150	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1165	Total	C	N	O	S	0	0
			9317	5878	1637	1738	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2213	1386	380	440	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	75	Total	C	N	O	P	0	0
			1553	735	297	447	74		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	75	Total	C	N	O	P	0	0
			1517	721	269	453	74		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	
24	U	1	Total	Mg	0
			1	1	

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	J	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	
25	B	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	C	1	Total	Zn	0
			1	1	
25	A	2	Total	Zn	0
			2	2	
25	U	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	

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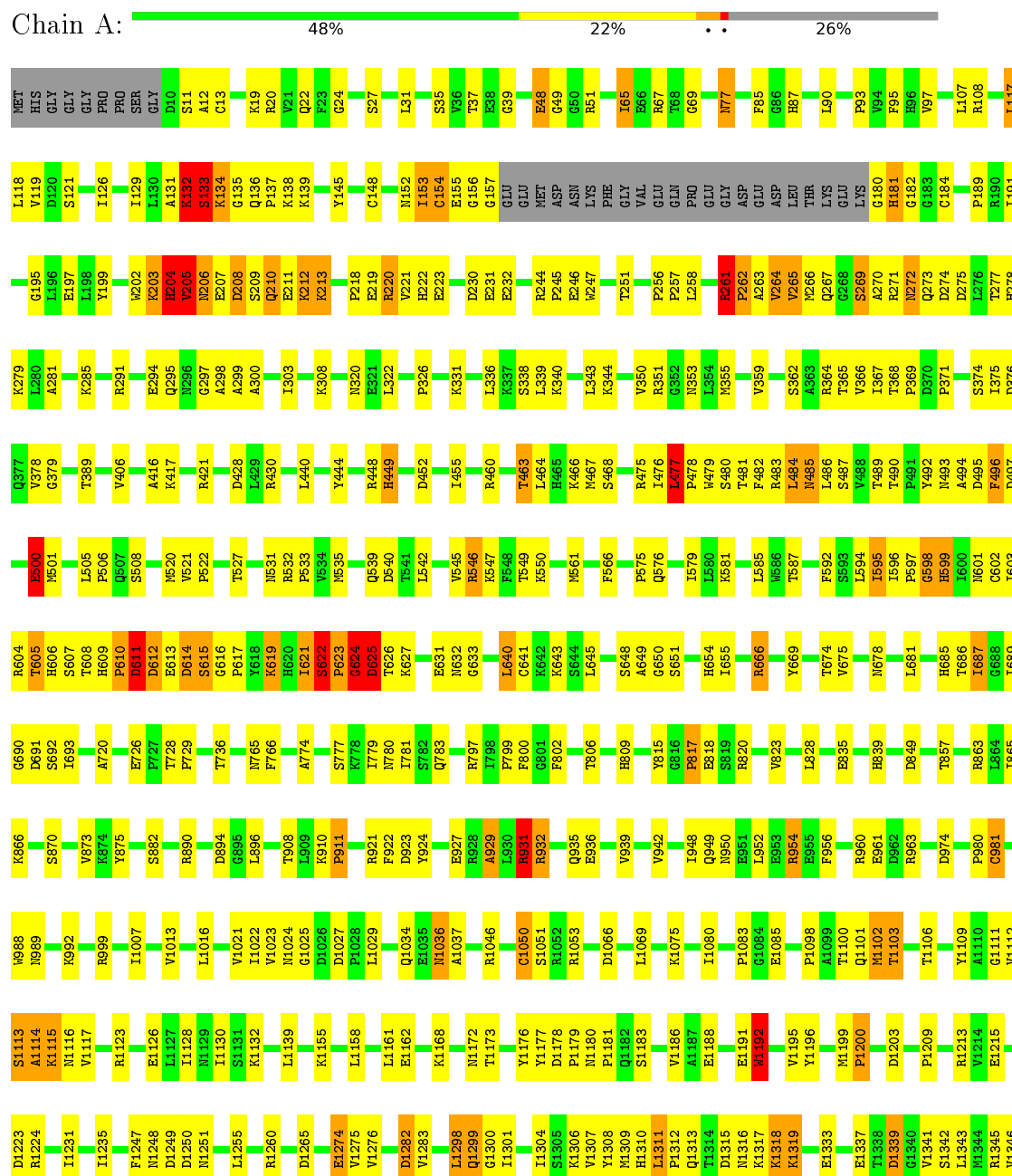
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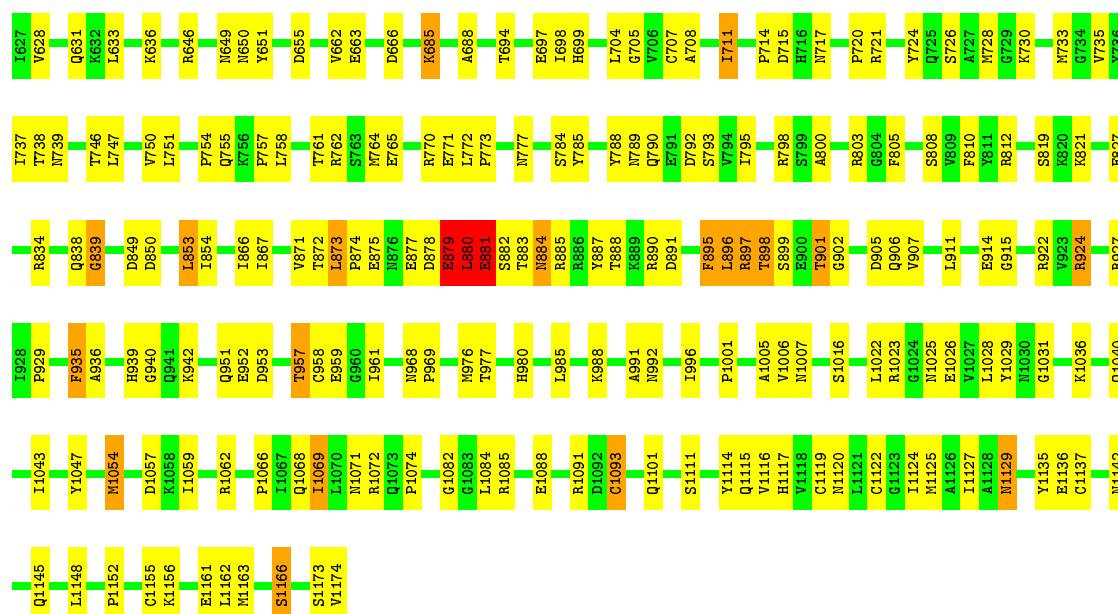
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
25	M	1	1	1	0

3 Residue-property plots

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

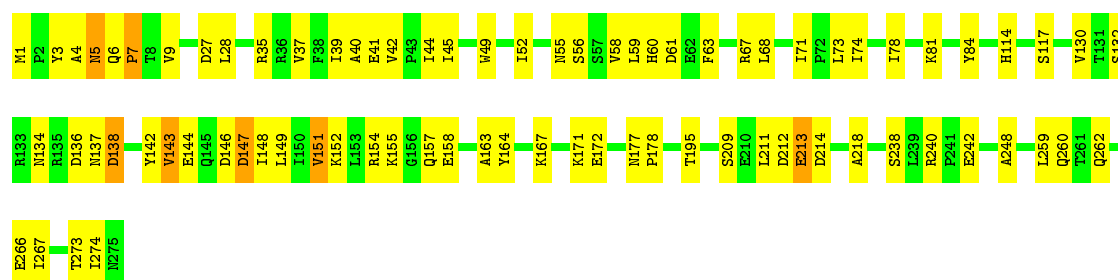
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 71% 27% .



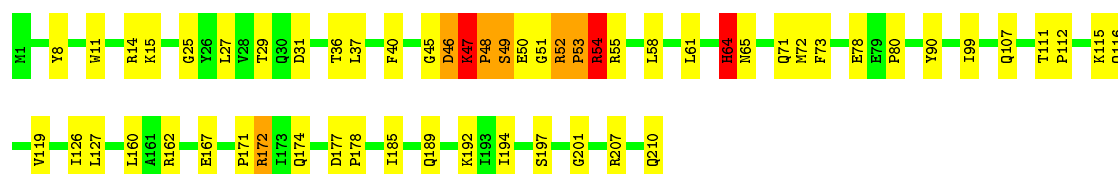
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 81% 10% 9%

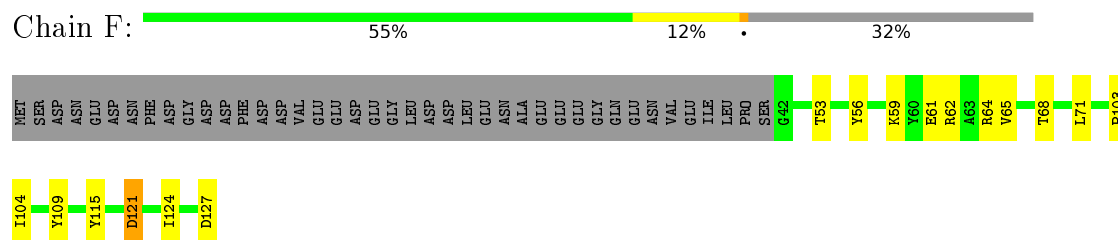


• Molecule 5: DNA-directed RNA polymerase II subunit RPB5

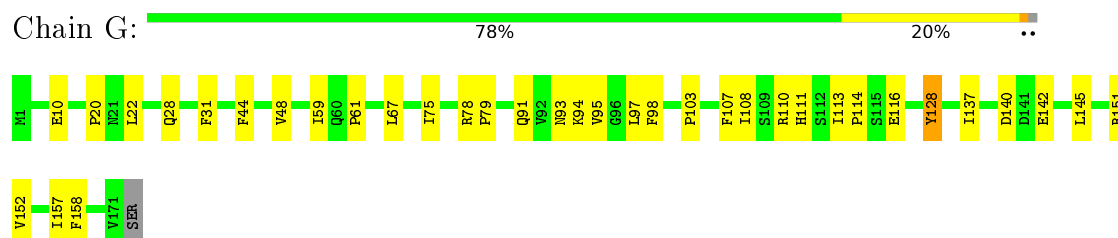
Chain E: 73% 23% . .



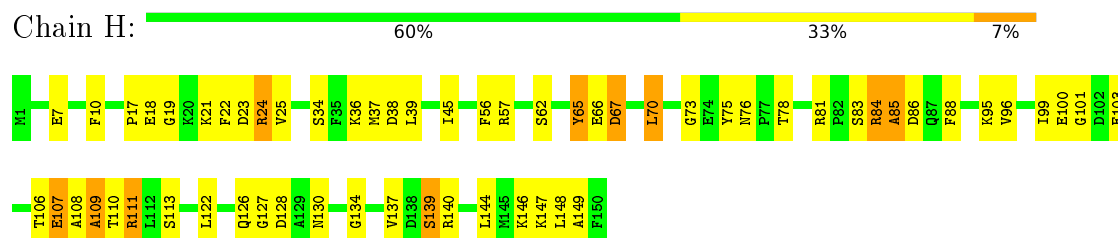
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6



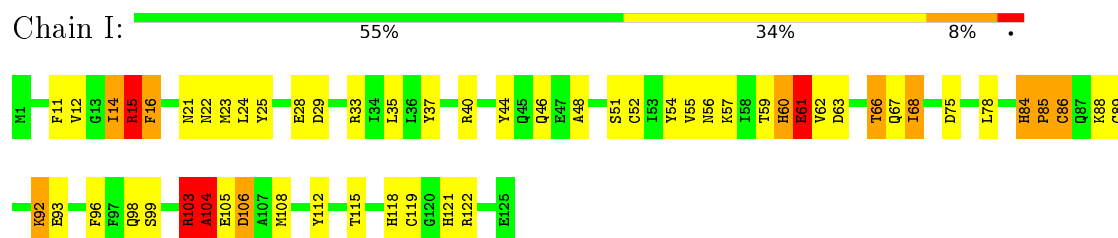
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



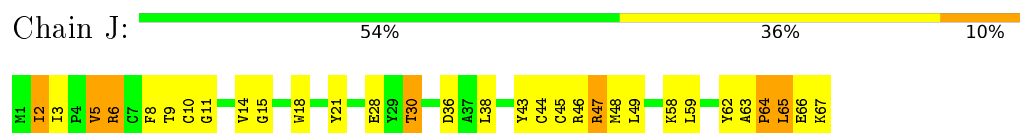
- Molecule 8: DNA-directed RNA polymerase II subunit RPB8



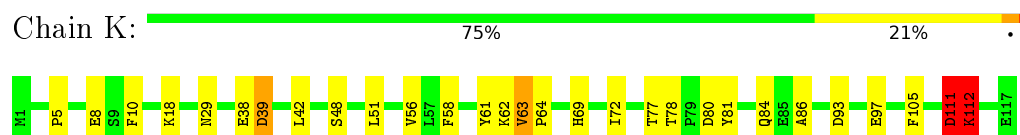
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



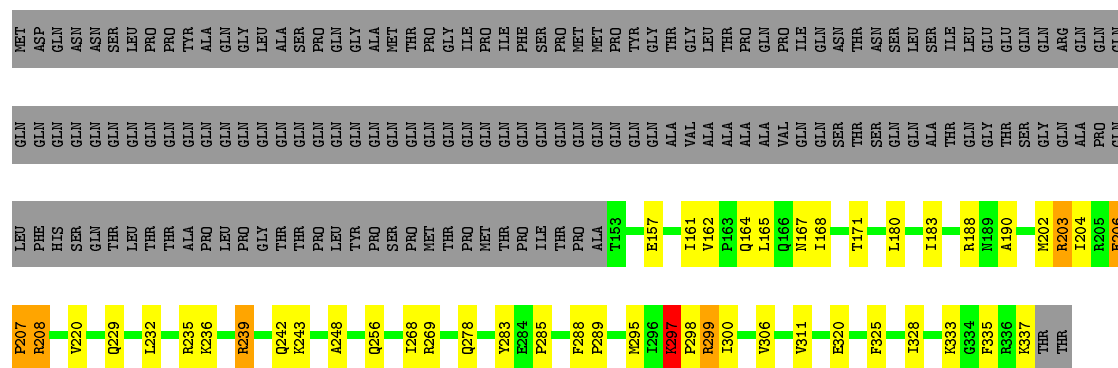
- Molecule 10: DNA-directed RNA polymerase II subunit RPB10



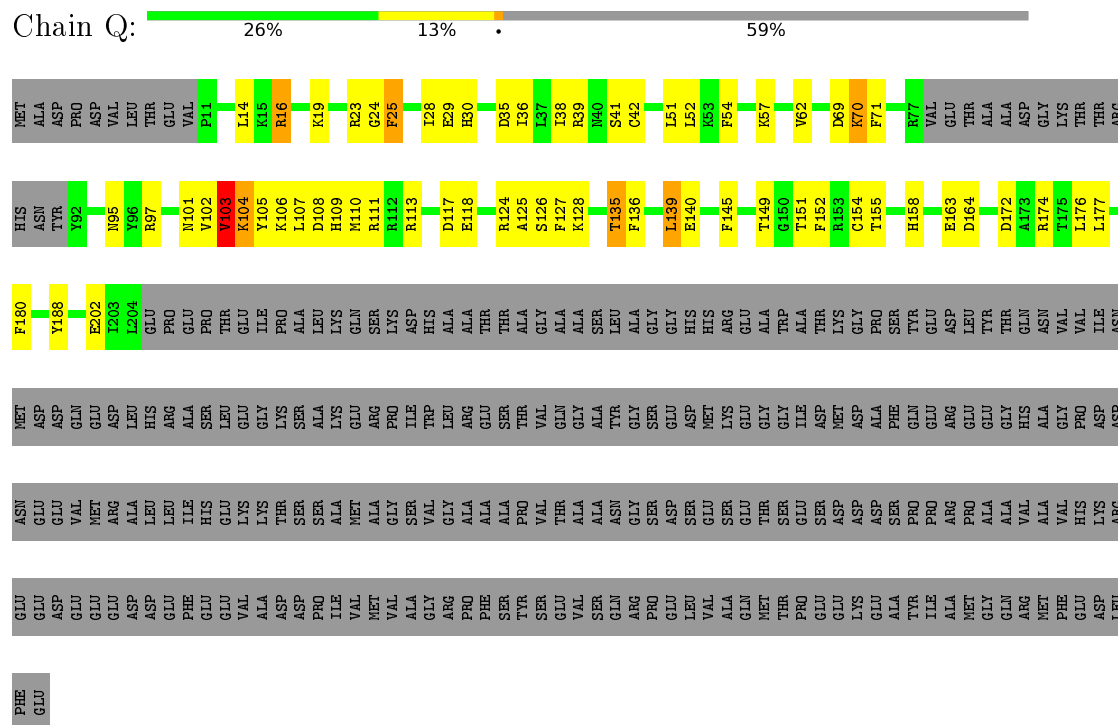
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



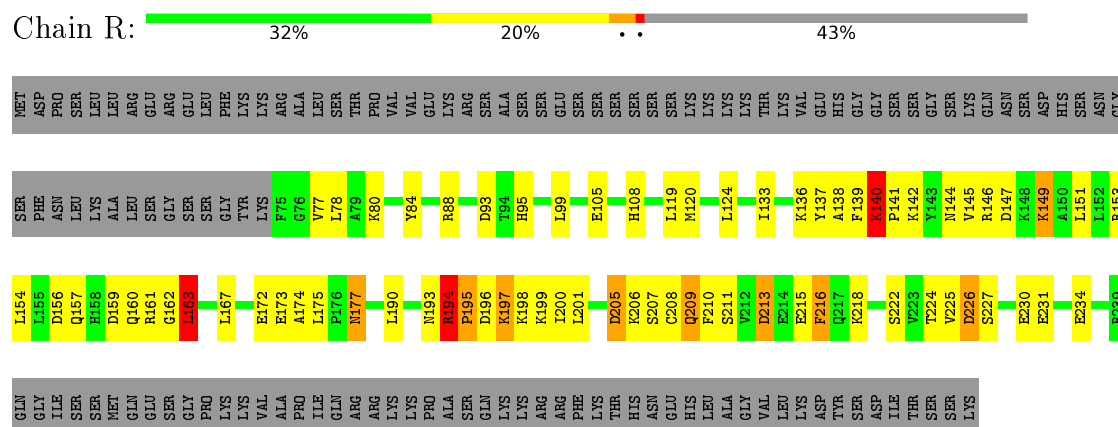
- Chain P: 40% 12% . 45%



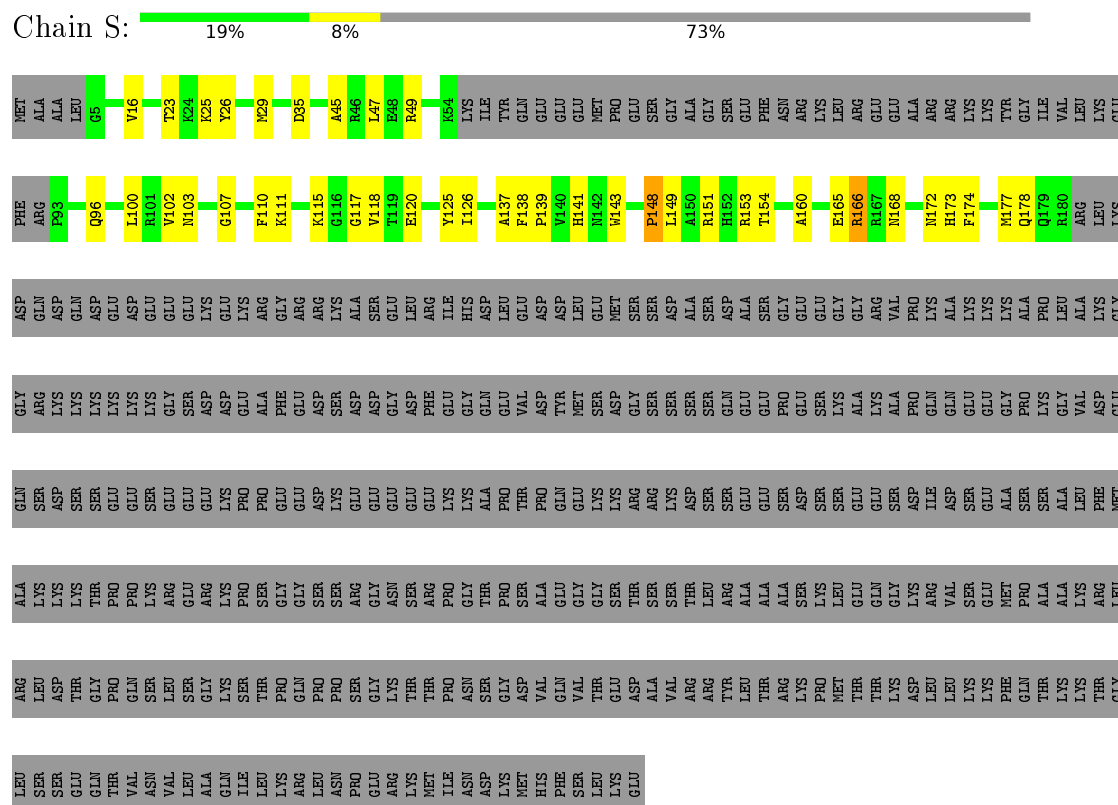
• Molecule 17: General transcription factor IIE subunit 1



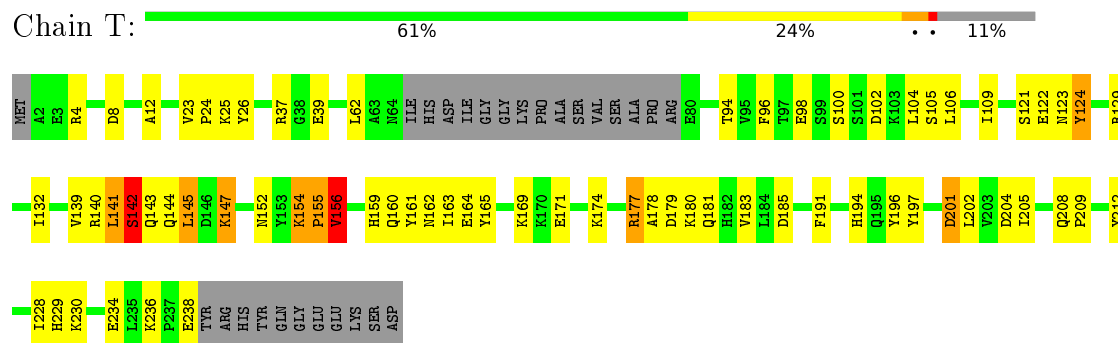
• Molecule 18: Transcription initiation factor IIE subunit beta



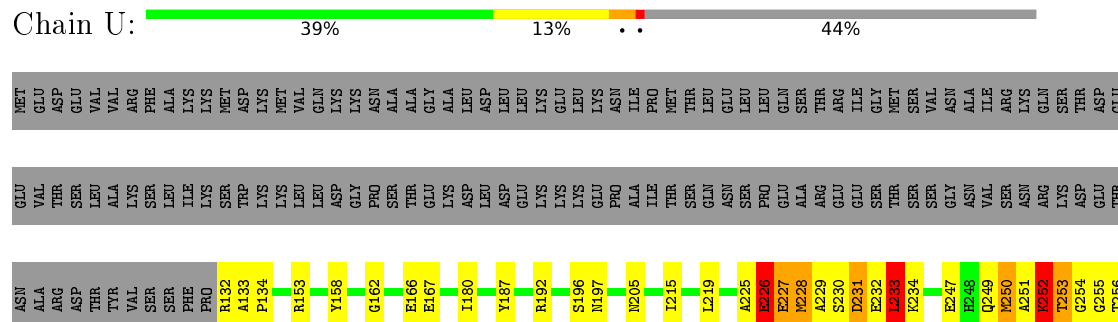
- Molecule 19: General transcription factor IIF subunit 1

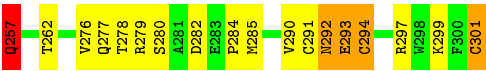


- Molecule 20: General transcription factor IIF subunit 2



- Molecule 21: Transcription elongation factor A protein 1

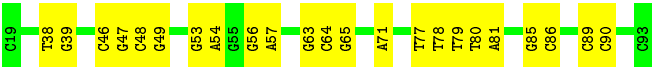




● Molecule 22: SCP-X



● Molecule 23: SCP-Y



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	79849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.47	1/11727 (0.0%)	0.78	20/15833 (0.1%)
10	J	0.55	0/542	0.89	0/730
11	K	0.39	0/956	0.63	0/1294
12	L	0.45	0/394	0.61	0/524
13	M	0.34	0/2429	0.72	10/3281 (0.3%)
14	N	0.25	0/945	0.58	1/1274 (0.1%)
15	O	0.24	0/816	0.48	0/1105
16	P	0.26	0/1489	0.74	1/2005 (0.0%)
17	Q	0.27	0/1507	0.60	0/2023
18	R	0.41	0/1380	0.88	3/1854 (0.2%)
19	S	0.26	0/1167	0.51	0/1576
2	B	0.56	1/9503 (0.0%)	0.81	8/12831 (0.1%)
20	T	0.32	0/1817	0.68	3/2445 (0.1%)
21	U	0.32	0/1358	0.64	2/1820 (0.1%)
22	X	0.62	0/1746	0.93	1/2698 (0.0%)
23	Y	0.60	0/1696	0.96	0/2612
3	C	0.49	0/2259	0.74	3/3073 (0.1%)
4	D	0.25	0/1077	0.47	0/1446
5	E	0.38	0/1753	0.76	4/2368 (0.2%)
6	F	0.43	0/700	0.67	0/946
7	G	0.27	0/1382	0.55	0/1874
8	H	0.35	0/1227	0.67	1/1654 (0.1%)
9	I	0.35	0/1038	1.06	6/1407 (0.4%)
All	All	0.45	2/48908 (0.0%)	0.76	63/66673 (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
14	N	0	4
18	R	0	2
19	S	0	1
2	B	0	1
20	T	0	1
5	E	0	1
8	H	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	500	GLU	CG-CD	6.64	1.61	1.51
2	B	1093	CYS	CB-SG	-5.22	1.73	1.81

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	84	HIS	C-N-CD	-25.40	64.71	120.60
16	P	206	GLU	C-N-CD	-22.56	70.96	120.60
1	A	261	ARG	C-N-CD	-21.04	74.32	120.60
18	R	194	ARG	C-N-CD	-20.97	74.47	120.60
5	E	52	ARG	C-N-CD	-14.21	89.34	120.60
1	A	1115	LYS	N-CA-C	-10.84	81.74	111.00
9	I	103	ARG	N-CA-C	-10.20	83.47	111.00
1	A	622	SER	C-N-CD	-9.92	98.78	120.60
13	M	87	GLY	N-CA-C	8.98	135.56	113.10
3	C	35	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	49	GLY	N-CA-C	-8.57	91.68	113.10
13	M	39	LEU	N-CA-C	8.47	133.88	111.00
9	I	61	GLU	N-CA-C	-8.14	89.02	111.00
5	E	64	HIS	C-N-CA	-7.85	102.07	121.70
2	B	249	LYS	N-CA-C	-7.79	89.97	111.00
13	M	91	ALA	N-CA-C	-7.53	90.67	111.00
1	A	622	SER	N-CA-C	-7.42	90.97	111.00
2	B	79	GLU	N-CA-C	7.28	130.65	111.00
21	U	257	GLN	N-CA-C	7.12	130.22	111.00
18	R	163	LEU	N-CA-C	-7.03	92.01	111.00
3	C	211	LEU	N-CA-C	-7.01	92.08	111.00
13	M	43	ASP	N-CA-C	-6.95	92.25	111.00
13	M	37	CYS	C-N-CA	-6.88	107.86	122.30
9	I	104	ALA	N-CA-C	-6.85	92.50	111.00
1	A	1311	LEU	CA-CB-CG	-6.57	100.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	38	GLY	N-CA-C	-6.57	96.68	113.10
14	N	356	GLY	N-CA-C	6.49	129.33	113.10
1	A	484	LEU	CB-CG-CD1	6.42	121.91	111.00
1	A	477	LEU	CB-CG-CD1	6.38	121.84	111.00
9	I	15	ARG	N-CA-C	-6.35	93.85	111.00
20	T	234	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	A	1311	LEU	CB-CG-CD1	-6.18	100.50	111.00
1	A	205	VAL	N-CA-C	6.09	127.43	111.00
13	M	94	ASP	N-CA-C	-5.95	94.93	111.00
2	B	289	ILE	CG1-CB-CG2	-5.90	98.42	111.40
13	M	89	GLY	N-CA-C	-5.86	98.44	113.10
2	B	922	ARG	NE-CZ-NH1	-5.82	117.39	120.30
20	T	234	GLU	CG-CD-OE1	5.81	129.93	118.30
1	A	204	HIS	N-CA-C	5.75	126.51	111.00
13	M	42	GLY	N-CA-C	5.68	127.30	113.10
2	B	76	GLY	N-CA-C	5.65	127.23	113.10
1	A	203	LYS	N-CA-C	5.59	126.10	111.00
20	T	142	SER	N-CA-C	5.59	126.10	111.00
18	R	140	LYS	C-N-CD	5.49	139.93	128.40
1	A	640	LEU	CB-CG-CD1	-5.47	101.69	111.00
3	C	35	ARG	NE-CZ-NH2	-5.47	117.56	120.30
5	E	47	LYS	C-N-CD	-5.42	108.68	120.60
5	E	54	ARG	N-CA-C	-5.41	96.41	111.00
21	U	299	LYS	CD-CE-NZ	5.33	123.96	111.70
22	X	30	DC	C1'-O4'-C4'	-5.30	104.80	110.10
1	A	614	ASP	N-CA-C	5.30	125.30	111.00
2	B	935	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	A	269	SER	N-CA-C	-5.27	96.78	111.00
2	B	879	GLU	N-CA-C	5.23	125.13	111.00
1	A	211	GLU	N-CA-C	-5.14	97.12	111.00
9	I	84	HIS	N-CA-C	5.11	124.80	111.00
2	B	924	ARG	NE-CZ-NH2	-5.11	117.75	120.30
13	M	93	PHE	N-CA-C	5.10	124.76	111.00
1	A	624	GLY	N-CA-C	5.10	125.84	113.10
8	H	85	ALA	N-CA-C	-5.09	97.27	111.00
1	A	1398	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	1192	TRP	CA-CB-CG	5.07	123.34	113.70
1	A	467	MET	CB-CG-SD	5.03	127.50	112.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	234	THR	Peptide
5	E	126	ILE	Peptide
8	H	111	ARG	Peptide
14	N	324	GLU	Peptide
14	N	355	ASP	Peptide
14	N	360	LEU	Mainchain
14	N	371	ILE	Peptide
18	R	146	ARG	Peptide
18	R	213	ASP	Sidechain
19	S	148	PRO	Peptide
20	T	123	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11606	518	0
2	B	9317	0	9306	377	0
3	C	2213	0	2153	68	0
4	D	1062	0	1042	10	0
5	E	1723	0	1745	61	0
6	F	689	0	715	16	0
7	G	1351	0	1358	33	0
8	H	1205	0	1168	60	0
9	I	1013	0	932	76	0
10	J	533	0	553	48	0
11	K	937	0	959	23	0
12	L	388	0	393	15	0
13	M	2391	0	2408	121	0
14	N	930	0	888	33	0
15	O	806	0	818	24	0
16	P	1462	0	1549	63	0
17	Q	1484	0	1496	169	0
18	R	1357	0	1380	175	0
19	S	1138	0	1103	24	0
20	T	1788	0	1819	91	0
21	U	1343	0	1338	60	0
22	X	1553	0	843	30	0
23	Y	1517	0	843	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	1	0	0	0	0
24	U	1	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	47728	0	46415	1755	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 19.

All (1755) 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)
17:Q:14:LEU:CD1	17:Q:102:VAL:HG23	1.29	1.58
17:Q:180:PHE:CZ	18:R:211:SER:CB	1.91	1.52
17:Q:180:PHE:CZ	18:R:211:SER:HB2	1.39	1.52
8:H:65:TYR:CE2	8:H:70:LEU:HB3	1.02	1.51
17:Q:14:LEU:HD11	17:Q:102:VAL:CG2	1.47	1.45
2:B:92:TYR:CG	20:T:145:LEU:HD13	1.51	1.43
17:Q:109:HIS:CE1	18:R:224:THR:HG21	1.51	1.43
17:Q:14:LEU:CD1	17:Q:102:VAL:CG2	1.98	1.42
8:H:65:TYR:CE2	8:H:70:LEU:CB	1.99	1.41
10:J:62:TYR:C	10:J:64:PRO:HD2	1.36	1.40
1:A:927:GLU:HB3	1:A:931:ARG:CG	1.48	1.39
8:H:65:TYR:HE2	8:H:70:LEU:CB	1.33	1.38
17:Q:180:PHE:HZ	18:R:211:SER:CB	1.27	1.37
13:M:10:LEU:O	13:M:12:ARG:N	1.57	1.36
17:Q:23:ARG:CZ	18:R:209:GLN:N	1.88	1.36
13:M:47:ASP:O	13:M:49:GLY:N	1.56	1.35
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.52	1.34
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	1.48	1.34
17:Q:105:TYR:CE1	18:R:231:GLU:CD	2.02	1.33
9:I:103:ARG:O	9:I:105:GLU:N	1.61	1.33
17:Q:105:TYR:CE1	17:Q:109:HIS:NE2	1.95	1.33
1:A:152:ASN:O	1:A:153:ILE:CG1	1.75	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:OE2	13:M:93:PHE:CE2	1.82	1.31
17:Q:180:PHE:CE2	18:R:211:SER:HB2	1.67	1.30
5:E:27:LEU:H	5:E:64:HIS:CB	1.42	1.29
1:A:1250:ASP:HB3	21:U:227:GLU:CD	1.22	1.29
17:Q:23:ARG:CD	18:R:207:SER:O	1.79	1.29
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.01	1.28
1:A:199:TYR:CE1	13:M:93:PHE:HZ	1.50	1.28
1:A:199:TYR:CZ	13:M:93:PHE:HZ	1.52	1.28
18:R:196:ASP:O	18:R:198:LYS:N	1.66	1.28
17:Q:23:ARG:NH2	18:R:209:GLN:H	1.30	1.27
1:A:199:TYR:OH	13:M:93:PHE:CZ	1.86	1.27
5:E:47:LYS:HB2	5:E:48:PRO:CD	1.62	1.26
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	1.52	1.23
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.52	1.23
2:B:92:TYR:CD2	20:T:145:LEU:HD13	1.74	1.23
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.53	1.22
1:A:262:PRO:HG2	1:A:274:ASP:CG	1.59	1.21
1:A:1319:LYS:HD3	1:A:1333:GLU:OE2	1.33	1.21
17:Q:23:ARG:NE	18:R:207:SER:O	1.72	1.21
17:Q:105:TYR:HE1	18:R:231:GLU:CG	1.51	1.21
2:B:132:VAL:HB	2:B:141:GLN:CG	1.71	1.21
1:A:1310:HIS:O	21:U:252:LYS:HG2	1.38	1.20
8:H:65:TYR:CZ	8:H:70:LEU:HB3	1.75	1.20
9:I:14:ILE:HG13	9:I:16:PHE:CE2	1.77	1.19
18:R:215:GLU:O	18:R:216:PHE:HB2	1.37	1.19
5:E:27:LEU:N	5:E:64:HIS:HB3	1.27	1.19
9:I:103:ARG:O	9:I:105:GLU:HG2	1.39	1.18
17:Q:109:HIS:CE1	18:R:224:THR:CG2	2.26	1.18
18:R:190:LEU:CD1	18:R:205:ASP:OD2	1.91	1.18
17:Q:109:HIS:ND1	18:R:224:THR:CG2	2.05	1.18
13:M:10:LEU:HD11	13:M:14:THR:HB	1.26	1.17
1:A:271:ARG:O	1:A:272:ASN:HB3	1.40	1.17
2:B:51:ILE:HG22	20:T:141:LEU:HD11	1.20	1.16
10:J:63:ALA:N	10:J:64:PRO:CD	2.06	1.16
1:A:202:TRP:CE3	1:A:212:LYS:HB3	1.80	1.16
1:A:157:GLY:N	1:A:181:HIS:NE2	1.93	1.15
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.60	1.15
13:M:178:LYS:O	20:T:154:LYS:HB3	1.46	1.15
2:B:491:ARG:O	2:B:492:ASP:HB2	1.44	1.14
1:A:1319:LYS:CD	1:A:1333:GLU:OE2	1.93	1.14
1:A:152:ASN:C	1:A:153:ILE:HG12	1.67	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:GLU:CB	1:A:931:ARG:HG2	1.77	1.14
17:Q:23:ARG:HH12	18:R:209:GLN:HB2	1.01	1.13
1:A:1319:LYS:HG2	1:A:1333:GLU:CG	1.78	1.12
17:Q:180:PHE:CE2	18:R:211:SER:CB	2.26	1.12
17:Q:29:GLU:OE2	18:R:194:ARG:NH2	1.81	1.11
1:A:1250:ASP:CB	21:U:227:GLU:CD	2.13	1.11
2:B:51:ILE:CG2	20:T:141:LEU:HD11	1.77	1.11
1:A:931:ARG:O	1:A:932:ARG:HB2	1.51	1.11
9:I:14:ILE:HG13	9:I:16:PHE:CZ	1.85	1.11
5:E:52:ARG:CB	5:E:53:PRO:HD2	1.75	1.11
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.33	1.11
2:B:225:LEU:HB2	2:B:228:SER:HB3	1.11	1.10
17:Q:14:LEU:HD12	17:Q:102:VAL:CG2	1.79	1.10
17:Q:101:ASN:O	17:Q:102:VAL:HG12	1.52	1.10
1:A:199:TYR:CE1	13:M:93:PHE:CZ	2.39	1.10
1:A:927:GLU:HB3	1:A:931:ARG:HG2	1.24	1.10
9:I:103:ARG:O	9:I:105:GLU:CG	1.98	1.10
1:A:927:GLU:HB3	1:A:931:ARG:CD	1.83	1.09
17:Q:180:PHE:CZ	18:R:211:SER:HB3	1.84	1.09
1:A:202:TRP:CE3	1:A:212:LYS:CB	2.34	1.09
10:J:62:TYR:C	10:J:64:PRO:CD	2.21	1.09
2:B:879:GLU:O	2:B:880:LEU:HB2	1.35	1.08
1:A:133:SER:OG	1:A:136:GLN:HB3	1.52	1.08
3:C:136:ASP:OD2	3:C:138:ASP:HB2	1.53	1.08
2:B:882:SER:O	2:B:887:TYR:CD1	2.06	1.08
17:Q:23:ARG:HD3	18:R:207:SER:O	1.43	1.08
1:A:1310:HIS:O	21:U:252:LYS:CG	2.02	1.07
1:A:611:ASP:OD2	1:A:627:LYS:HE3	1.51	1.07
17:Q:108:ASP:O	18:R:234:GLU:OE2	1.72	1.07
13:M:10:LEU:CD1	13:M:14:THR:HB	1.64	1.07
17:Q:105:TYR:CE1	18:R:231:GLU:CG	2.34	1.07
1:A:132:LYS:O	1:A:133:SER:HB2	1.25	1.06
17:Q:180:PHE:HZ	18:R:211:SER:CA	1.68	1.06
2:B:225:LEU:HB2	2:B:228:SER:CB	1.85	1.06
1:A:197:GLU:OE2	13:M:93:PHE:CZ	2.08	1.06
21:U:230:SER:O	21:U:231:ASP:HB2	1.50	1.05
1:A:152:ASN:O	1:A:153:ILE:HG12	0.89	1.05
5:E:49:SER:O	5:E:54:ARG:NH1	1.89	1.05
1:A:205:VAL:O	1:A:206:ASN:HB2	1.54	1.05
21:U:226:GLU:O	21:U:227:GLU:HB2	1.57	1.04
2:B:880:LEU:O	2:B:881:GLU:HB2	1.26	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:HB3	20:T:145:LEU:HB2	1.38	1.04
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.10	1.03
1:A:927:GLU:CB	1:A:931:ARG:CG	2.34	1.03
2:B:51:ILE:HG22	20:T:141:LEU:CD1	1.87	1.03
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.07	1.03
2:B:225:LEU:CB	2:B:228:SER:CB	2.37	1.03
1:A:132:LYS:O	1:A:133:SER:CB	2.05	1.02
1:A:265:VAL:O	1:A:272:ASN:OD1	1.77	1.02
1:A:202:TRP:CZ3	1:A:212:LYS:CG	2.42	1.02
2:B:78:VAL:O	2:B:79:GLU:CB	2.03	1.02
2:B:132:VAL:HB	2:B:141:GLN:HG3	1.06	1.02
2:B:52:GLN:HA	20:T:141:LEU:HD13	1.39	1.02
2:B:225:LEU:CB	2:B:228:SER:HB3	1.89	1.01
16:P:297:LYS:CB	16:P:298:PRO:CD	2.36	1.01
9:I:103:ARG:O	9:I:105:GLU:CA	2.09	1.01
9:I:105:GLU:O	9:I:106:ASP:HB2	1.60	1.00
1:A:1319:LYS:CG	1:A:1333:GLU:OE2	2.08	1.00
2:B:1066:PRO:HB3	13:M:46:ILE:HD13	1.39	1.00
17:Q:23:ARG:NH1	18:R:209:GLN:HB2	1.76	1.00
5:E:47:LYS:CB	5:E:48:PRO:HD2	1.91	0.99
9:I:103:ARG:C	9:I:105:GLU:N	2.01	0.99
5:E:27:LEU:N	5:E:64:HIS:CB	2.06	0.99
9:I:103:ARG:O	9:I:105:GLU:CB	2.10	0.99
1:A:199:TYR:OH	13:M:93:PHE:CE2	2.05	0.99
2:B:92:TYR:CG	20:T:145:LEU:CD1	2.44	0.99
5:E:52:ARG:CB	5:E:53:PRO:CD	2.40	0.99
20:T:154:LYS:H	20:T:154:LYS:HD2	1.28	0.99
13:M:94:ASP:OD1	13:M:99:SER:C	2.02	0.99
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	0.83	0.99
5:E:47:LYS:HB2	5:E:48:PRO:HD2	1.00	0.98
9:I:103:ARG:O	9:I:104:ALA:C	2.00	0.98
8:H:66:GLU:O	8:H:67:ASP:HB2	1.62	0.98
1:A:262:PRO:HG2	1:A:274:ASP:OD1	1.63	0.97
2:B:78:VAL:O	2:B:79:GLU:HB2	1.16	0.97
5:E:47:LYS:CB	5:E:48:PRO:CD	2.42	0.97
17:Q:109:HIS:ND1	18:R:224:THR:HG23	1.77	0.97
10:J:64:PRO:C	10:J:66:GLU:H	1.66	0.96
17:Q:113:ARG:HH22	18:R:218:LYS:HE2	1.15	0.96
17:Q:14:LEU:HD12	17:Q:102:VAL:HG21	1.44	0.96
17:Q:105:TYR:O	17:Q:109:HIS:CD2	2.19	0.96
1:A:495:ASP:O	1:A:497:ASP:N	1.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:195:PRO:CB	18:R:199:LYS:HD2	1.96	0.96
17:Q:23:ARG:CZ	18:R:208:CYS:C	2.34	0.95
18:R:225:VAL:HB	18:R:230:GLU:HG3	1.46	0.95
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.64	0.95
18:R:215:GLU:O	18:R:216:PHE:CB	2.10	0.95
17:Q:101:ASN:O	17:Q:102:VAL:CG1	2.13	0.95
2:B:74:ALA:HB2	20:T:201:ASP:HB3	1.47	0.95
21:U:231:ASP:O	21:U:232:GLU:CG	2.14	0.95
13:M:94:ASP:OD1	13:M:99:SER:O	1.85	0.95
15:O:3:TYR:O	15:O:5:LEU:N	2.01	0.94
2:B:225:LEU:HB3	2:B:228:SER:HB2	1.48	0.94
1:A:157:GLY:N	1:A:181:HIS:CD2	2.34	0.94
1:A:265:VAL:O	1:A:272:ASN:ND2	2.01	0.94
10:J:63:ALA:N	10:J:64:PRO:HD2	1.74	0.94
10:J:63:ALA:N	10:J:64:PRO:HD3	1.79	0.94
18:R:190:LEU:HD11	18:R:205:ASP:OD2	1.65	0.94
16:P:162:VAL:O	16:P:164:GLN:NE2	2.01	0.93
5:E:52:ARG:HB3	5:E:53:PRO:CD	1.94	0.93
1:A:1319:LYS:CD	1:A:1356:ARG:HH12	1.80	0.93
17:Q:105:TYR:CD1	18:R:231:GLU:OE2	2.21	0.93
17:Q:23:ARG:HH12	18:R:209:GLN:CB	1.80	0.93
2:B:92:TYR:HB3	20:T:145:LEU:CB	1.97	0.93
16:P:297:LYS:HE2	16:P:297:LYS:HA	1.48	0.93
1:A:265:VAL:O	1:A:272:ASN:CG	2.07	0.93
2:B:132:VAL:CB	2:B:141:GLN:HG3	1.97	0.92
16:P:297:LYS:HA	16:P:297:LYS:CE	1.97	0.92
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.34	0.92
1:A:927:GLU:HB3	1:A:931:ARG:CB	2.00	0.92
1:A:927:GLU:CB	1:A:931:ARG:HD3	1.98	0.92
2:B:490:GLY:O	2:B:491:ARG:HB2	1.66	0.92
17:Q:23:ARG:NH2	18:R:209:GLN:N	2.03	0.92
5:E:52:ARG:O	5:E:53:PRO:O	1.87	0.92
1:A:202:TRP:HE3	1:A:212:LYS:HB3	1.25	0.92
13:M:10:LEU:HD11	13:M:14:THR:CB	1.99	0.92
21:U:230:SER:O	21:U:231:ASP:CB	2.18	0.91
2:B:92:TYR:CD2	20:T:145:LEU:CD1	2.54	0.91
16:P:206:GLU:CG	16:P:236:LYS:NZ	2.26	0.91
17:Q:23:ARG:CZ	18:R:209:GLN:H	1.66	0.91
1:A:931:ARG:O	1:A:932:ARG:CB	2.18	0.90
20:T:177:ARG:C	20:T:179:ASP:H	1.74	0.90
1:A:210:GLN:OE1	1:A:212:LYS:HD3	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:94:ASP:HB3	13:M:97:GLY:O	1.71	0.90
1:A:1250:ASP:HB3	21:U:227:GLU:OE2	1.70	0.90
1:A:197:GLU:OE2	13:M:93:PHE:CD2	2.25	0.90
2:B:721:ARG:HG3	2:B:977:THR:HG22	1.52	0.89
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.51	0.89
2:B:880:LEU:O	2:B:881:GLU:CB	2.13	0.89
1:A:261:ARG:O	1:A:263:ALA:N	2.06	0.89
2:B:52:GLN:HA	20:T:141:LEU:CD1	2.01	0.89
1:A:1319:LYS:HG2	1:A:1333:GLU:HG2	1.52	0.89
5:E:48:PRO:O	5:E:49:SER:HB2	1.73	0.89
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.55	0.89
1:A:203:LYS:O	1:A:204:HIS:HB2	1.71	0.88
2:B:491:ARG:O	2:B:492:ASP:CB	2.20	0.88
1:A:212:LYS:CE	1:A:212:LYS:HA	2.02	0.87
20:T:177:ARG:NH1	20:T:209:PRO:O	2.07	0.87
17:Q:54:PHE:CD2	18:R:194:ARG:HD2	2.09	0.87
2:B:225:LEU:CB	2:B:228:SER:HB2	2.02	0.87
18:R:196:ASP:C	18:R:198:LYS:H	1.78	0.87
17:Q:105:TYR:CD1	18:R:231:GLU:CD	2.46	0.87
9:I:105:GLU:O	9:I:106:ASP:CB	2.22	0.86
13:M:10:LEU:C	13:M:12:ARG:N	2.19	0.86
17:Q:105:TYR:HE1	18:R:231:GLU:HG3	1.40	0.86
17:Q:113:ARG:NH2	18:R:218:LYS:CE	2.23	0.86
9:I:15:ARG:O	9:I:16:PHE:O	1.94	0.86
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.58	0.86
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.48	0.86
1:A:202:TRP:CZ3	1:A:212:LYS:HB3	2.10	0.86
2:B:751:LEU:HD12	2:B:808:SER:HB3	1.56	0.86
13:M:11:PRO:O	13:M:12:ARG:HB3	1.73	0.86
1:A:271:ARG:O	1:A:272:ASN:CB	2.19	0.86
2:B:1066:PRO:CB	13:M:46:ILE:HD13	2.05	0.85
10:J:62:TYR:O	10:J:64:PRO:HD2	1.74	0.85
18:R:225:VAL:CB	18:R:230:GLU:HG3	2.06	0.85
13:M:37:CYS:SG	13:M:39:LEU:HD22	2.17	0.85
1:A:210:GLN:NE2	1:A:212:LYS:HG2	1.91	0.85
3:C:136:ASP:OD2	3:C:138:ASP:CB	2.24	0.85
1:A:202:TRP:CZ3	1:A:212:LYS:HG3	2.11	0.85
15:O:3:TYR:HB3	15:O:98:CYS:SG	2.16	0.85
1:A:1319:LYS:HD3	1:A:1356:ARG:HH12	1.39	0.85
1:A:1313:GLN:HE22	1:A:1318:LYS:HD2	1.42	0.85
1:A:927:GLU:HB3	1:A:931:ARG:HD3	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:SER:O	5:E:54:ARG:CZ	2.24	0.85
2:B:879:GLU:O	2:B:880:LEU:CB	2.24	0.84
13:M:44:ARG:HE	13:M:46:ILE:CG2	1.89	0.84
21:U:231:ASP:O	21:U:232:GLU:HG2	1.77	0.84
1:A:202:TRP:CZ3	1:A:212:LYS:CB	2.61	0.84
1:A:477:LEU:HD11	1:A:483:ARG:HD3	1.58	0.84
17:Q:109:HIS:HA	18:R:234:GLU:OE1	1.76	0.84
1:A:608:THR:C	1:A:610:PRO:HD2	1.98	0.83
1:A:609:HIS:N	1:A:610:PRO:CD	2.41	0.83
2:B:179:LEU:HD11	2:B:771:GLU:HG2	1.59	0.83
1:A:927:GLU:CB	1:A:931:ARG:CD	2.50	0.83
17:Q:105:TYR:CD1	17:Q:109:HIS:NE2	2.32	0.83
2:B:92:TYR:CB	20:T:145:LEU:HD13	2.08	0.83
18:R:162:GLY:O	18:R:163:LEU:HB2	1.78	0.83
18:R:195:PRO:HB2	18:R:199:LYS:HD2	1.60	0.83
21:U:256:THR:O	21:U:257:GLN:HB2	1.76	0.83
17:Q:24:GLY:CA	18:R:210:PHE:HE2	1.92	0.83
2:B:1117:HIS:HB2	2:B:1127:ILE:HD13	1.61	0.83
9:I:57:LYS:O	9:I:59:THR:HG23	1.78	0.83
1:A:927:GLU:CG	1:A:931:ARG:HD3	2.08	0.82
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.55	0.82
3:C:209:SER:O	3:C:212:ASP:OD1	1.97	0.82
9:I:85:PRO:O	9:I:86:CYS:C	2.11	0.82
1:A:1313:GLN:NE2	1:A:1318:LYS:HB2	1.95	0.82
5:E:52:ARG:HG2	5:E:53:PRO:HD3	1.59	0.82
13:M:107:MET:HG2	23:Y:63:DG:H22	1.41	0.82
15:O:3:TYR:C	15:O:5:LEU:H	1.83	0.82
8:H:100:GLU:HG3	8:H:101:GLY:H	1.45	0.81
17:Q:23:ARG:HB2	18:R:207:SER:OG	1.80	0.81
21:U:231:ASP:O	21:U:232:GLU:HG3	1.79	0.81
2:B:290:TYR:HB3	2:B:562:ALA:HB1	1.62	0.81
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.12	0.81
14:N:332:GLU:HG2	15:O:92:LYS:HB3	1.63	0.81
9:I:14:ILE:HG12	9:I:16:PHE:CG	2.16	0.81
1:A:595:ILE:HG21	1:A:675:VAL:HG21	1.62	0.80
17:Q:23:ARG:NE	18:R:208:CYS:C	2.34	0.80
1:A:999:ARG:HE	8:H:99:ILE:HD12	1.43	0.80
17:Q:180:PHE:CE2	18:R:211:SER:HB3	2.09	0.80
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	2.01	0.80
1:A:927:GLU:HG2	1:A:931:ARG:HD3	1.64	0.80
1:A:1251:ASN:HA	21:U:234:LYS:HE3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:SER:O	1:A:1114:ALA:HB3	1.82	0.80
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.64	0.80
1:A:202:TRP:HE3	1:A:212:LYS:CB	1.84	0.80
11:K:111:ASP:O	11:K:112:LYS:HB2	1.80	0.80
17:Q:105:TYR:CE1	17:Q:109:HIS:CE1	2.70	0.80
1:A:1319:LYS:CD	1:A:1356:ARG:NH1	2.45	0.80
1:A:1022:ILE:H	1:A:1034:GLN:HE22	1.29	0.79
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.15	0.79
2:B:27:TRP:CE2	2:B:762:ARG:HG2	2.18	0.79
2:B:874:PRO:O	2:B:875:GLU:HB3	1.82	0.79
2:B:1068:GLN:O	2:B:1072:ARG:N	2.15	0.79
2:B:631:GLN:HB3	2:B:685:LYS:HE2	1.64	0.79
4:D:54:GLU:OE2	7:G:28:GLN:NE2	2.15	0.79
17:Q:23:ARG:NH1	18:R:209:GLN:N	2.31	0.78
1:A:624:GLY:O	1:A:626:THR:N	2.16	0.78
9:I:85:PRO:O	9:I:86:CYS:O	2.00	0.78
1:A:1251:ASN:ND2	21:U:227:GLU:O	2.12	0.78
2:B:52:GLN:CA	20:T:141:LEU:HD13	2.05	0.78
17:Q:111:ARG:NH1	17:Q:188:TYR:OH	2.16	0.78
20:T:177:ARG:O	20:T:179:ASP:N	2.14	0.78
2:B:882:SER:O	2:B:887:TYR:CE1	2.35	0.78
1:A:648:SER:O	1:A:651:SER:OG	2.02	0.78
3:C:212:ASP:O	3:C:214:ASP:N	2.16	0.78
17:Q:70:LYS:NZ	18:R:226:ASP:O	2.16	0.78
10:J:64:PRO:C	10:J:66:GLU:N	2.34	0.78
1:A:609:HIS:N	1:A:610:PRO:HD2	1.99	0.78
14:N:316:SER:OG	16:P:235:ARG:NH1	2.17	0.78
1:A:205:VAL:O	1:A:206:ASN:CB	2.31	0.77
2:B:483:ARG:HH11	2:B:526:LEU:HB2	1.48	0.77
8:H:65:TYR:HE2	8:H:70:LEU:CA	1.98	0.77
2:B:225:LEU:HD13	2:B:228:SER:OG	1.84	0.77
9:I:14:ILE:HG13	9:I:16:PHE:CD2	2.19	0.77
17:Q:54:PHE:HA	18:R:194:ARG:HD2	1.67	0.77
17:Q:23:ARG:NE	18:R:208:CYS:CA	2.48	0.77
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.17	0.77
5:E:61:LEU:HD13	5:E:73:PHE:HD1	1.49	0.77
1:A:608:THR:CB	1:A:610:PRO:HD2	2.14	0.76
2:B:803:ARG:NH2	2:B:951:GLN:OE1	2.16	0.76
11:K:39:ASP:N	11:K:39:ASP:OD1	2.18	0.76
2:B:133:ILE:HD13	2:B:139:GLN:HB3	1.66	0.76
7:G:111:HIS:NE2	17:Q:124:ARG:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:ARG:C	9:I:105:GLU:H	1.89	0.76
9:I:14:ILE:CG1	9:I:16:PHE:CE2	2.65	0.76
20:T:177:ARG:C	20:T:179:ASP:N	2.37	0.76
17:Q:105:TYR:O	17:Q:109:HIS:HD2	1.69	0.76
17:Q:39:ARG:NH2	18:R:159:ASP:OD2	2.18	0.76
17:Q:23:ARG:NH1	18:R:209:GLN:CB	2.43	0.76
13:M:182:ALA:HB2	20:T:154:LYS:HG3	1.68	0.76
17:Q:23:ARG:HE	18:R:208:CYS:CA	1.97	0.76
2:B:462:ALA:HB2	22:X:39:DT:H5"	1.67	0.76
17:Q:105:TYR:CE1	18:R:231:GLU:HG3	2.14	0.76
8:H:65:TYR:CZ	8:H:70:LEU:CB	2.50	0.75
13:M:11:PRO:O	13:M:12:ARG:CB	2.33	0.75
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.69	0.75
1:A:117:LEU:N	1:A:232:GLU:OE2	2.19	0.75
1:A:1319:LYS:HD3	1:A:1356:ARG:NH1	2.00	0.75
13:M:44:ARG:HE	13:M:46:ILE:HG22	1.52	0.75
17:Q:52:LEU:HB3	17:Q:54:PHE:HD1	1.50	0.75
17:Q:109:HIS:NE2	18:R:224:THR:HG21	2.00	0.75
17:Q:23:ARG:HE	18:R:208:CYS:HA	1.51	0.75
17:Q:24:GLY:C	18:R:210:PHE:HE2	1.89	0.75
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.21	0.75
5:E:55:ARG:HB3	5:E:78:GLU:OE2	1.87	0.75
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.69	0.75
14:N:320:VAL:HG11	16:P:236:LYS:HG2	1.68	0.75
17:Q:14:LEU:HD11	17:Q:102:VAL:CB	2.15	0.75
18:R:162:GLY:O	18:R:163:LEU:CB	2.32	0.75
5:E:27:LEU:H	5:E:64:HIS:HB3	0.74	0.75
17:Q:105:TYR:HE1	18:R:231:GLU:CB	2.00	0.75
1:A:1319:LYS:HD2	1:A:1356:ARG:HH12	1.52	0.74
1:A:331:LYS:NZ	23:Y:63:DG:O6	2.19	0.74
1:A:522:PRO:HA	1:A:666:ARG:HH21	1.52	0.74
2:B:735:VAL:HG22	2:B:750:VAL:HG13	1.67	0.74
5:E:40:PHE:CE2	5:E:46:ASP:OD2	2.40	0.74
13:M:15:CYS:SG	13:M:39:LEU:HD23	2.26	0.74
9:I:14:ILE:CG1	9:I:16:PHE:CD2	2.69	0.74
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.13	0.74
1:A:206:ASN:O	1:A:207:GLU:HB2	1.85	0.74
2:B:914:GLU:N	2:B:914:GLU:OE1	2.21	0.74
1:A:202:TRP:HZ3	1:A:212:LYS:HG3	1.52	0.74
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.17	0.74
8:H:65:TYR:OH	8:H:70:LEU:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:LEU:H	13:M:11:PRO:HD3	1.52	0.74
17:Q:108:ASP:C	18:R:234:GLU:OE2	2.25	0.74
1:A:212:LYS:HA	1:A:212:LYS:HE3	1.68	0.73
1:A:611:ASP:OD2	1:A:627:LYS:CE	2.35	0.73
17:Q:23:ARG:NH1	18:R:209:GLN:CA	2.51	0.73
17:Q:14:LEU:CD1	17:Q:102:VAL:HG21	1.99	0.73
17:Q:14:LEU:HD11	17:Q:102:VAL:HG23	0.74	0.73
18:R:225:VAL:CG1	18:R:230:GLU:HG3	2.18	0.73
17:Q:105:TYR:CZ	17:Q:109:HIS:NE2	2.53	0.73
1:A:261:ARG:C	1:A:263:ALA:H	1.91	0.73
9:I:104:ALA:O	9:I:105:GLU:HB2	1.86	0.73
21:U:231:ASP:C	21:U:232:GLU:HG2	2.09	0.73
1:A:264:VAL:O	1:A:266:MET:HG2	1.89	0.73
1:A:1177:TYR:H	9:I:51:SER:HB3	1.53	0.73
13:M:10:LEU:CD1	13:M:14:THR:CB	2.57	0.73
17:Q:14:LEU:CG	17:Q:102:VAL:HG23	2.16	0.73
2:B:52:GLN:CA	20:T:141:LEU:CD1	2.61	0.73
3:C:274:ILE:HD12	11:K:84:GLN:HB3	1.69	0.73
3:C:40:ALA:HB1	3:C:171:LYS:HB3	1.70	0.72
9:I:14:ILE:HG12	9:I:16:PHE:CD1	2.23	0.72
2:B:728:MET:HE2	2:B:942:LYS:HG2	1.70	0.72
10:J:64:PRO:O	10:J:66:GLU:N	2.21	0.72
13:M:37:CYS:SG	13:M:39:LEU:CD2	2.77	0.72
18:R:194:ARG:HG2	18:R:201:LEU:HD12	1.71	0.72
16:P:167:ASN:ND2	23:Y:79:DT:O2	2.22	0.72
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.71	0.72
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.71	0.72
21:U:252:LYS:O	21:U:253:THR:OG1	2.06	0.72
1:A:181:HIS:CD2	1:A:181:HIS:H	2.06	0.72
3:C:240:ARG:NH1	3:C:242:GLU:OE2	2.23	0.72
3:C:67:ARG:HH12	10:J:2:ILE:HG13	1.55	0.72
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.70	0.72
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.71	0.72
17:Q:101:ASN:C	17:Q:102:VAL:HG12	2.10	0.71
21:U:226:GLU:O	21:U:227:GLU:CB	2.36	0.71
1:A:269:SER:O	1:A:270:ALA:HB3	1.91	0.71
8:H:146:LYS:HE2	8:H:147:LYS:HG3	1.71	0.71
17:Q:102:VAL:O	17:Q:104:LYS:N	2.23	0.71
2:B:1085:ARG:NH2	23:Y:53:DG:OP2	2.24	0.71
8:H:66:GLU:O	8:H:67:ASP:CB	2.38	0.71
13:M:7:LEU:HD11	13:M:10:LEU:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:PRO:O	5:E:49:SER:CB	2.39	0.71
17:Q:29:GLU:CD	18:R:194:ARG:NH2	2.44	0.71
20:T:154:LYS:N	20:T:154:LYS:HD2	2.06	0.71
17:Q:23:ARG:HH21	18:R:208:CYS:HA	1.55	0.70
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.72	0.70
5:E:46:ASP:OD1	5:E:54:ARG:HG2	1.92	0.70
1:A:199:TYR:HE1	13:M:93:PHE:CZ	2.03	0.70
2:B:490:GLY:O	2:B:491:ARG:CB	2.37	0.70
3:C:212:ASP:C	3:C:214:ASP:H	1.93	0.70
2:B:777:ASN:O	10:J:47:ARG:NH1	2.24	0.70
18:R:190:LEU:HD12	18:R:205:ASP:OD2	1.86	0.70
17:Q:23:ARG:NH2	18:R:208:CYS:HA	2.05	0.70
1:A:960:ARG:NH2	1:A:961:GLU:OE2	2.24	0.70
2:B:48:ASP:OD1	2:B:159:THR:OG1	2.09	0.70
1:A:1319:LYS:HD2	1:A:1356:ARG:NH1	2.07	0.70
2:B:69:ALA:HB2	2:B:423:ILE:HB	1.74	0.70
3:C:56:SER:HG	3:C:158:GLU:H	1.40	0.70
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.74	0.70
2:B:988:LYS:NZ	2:B:1026:GLU:OE2	2.17	0.69
1:A:1251:ASN:ND2	21:U:227:GLU:HB3	2.07	0.69
13:M:47:ASP:C	13:M:49:GLY:N	2.39	0.69
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.72	0.69
1:A:1192:TRP:H	1:A:1192:TRP:HE3	1.40	0.69
1:A:153:ILE:O	1:A:154:CYS:C	2.31	0.69
13:M:47:ASP:O	13:M:49:GLY:CA	2.40	0.69
17:Q:180:PHE:HZ	18:R:211:SER:HA	1.55	0.69
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.58	0.69
1:A:262:PRO:O	1:A:263:ALA:HB3	1.93	0.69
13:M:178:LYS:O	20:T:154:LYS:CB	2.34	0.69
2:B:313:GLU:OE2	19:S:153:ARG:NH2	2.26	0.69
2:B:331:THR:HB	2:B:334:LYS:HB2	1.75	0.69
1:A:1313:GLN:NE2	1:A:1316:ASN:OD1	2.25	0.68
1:A:197:GLU:OE1	1:A:308:LYS:NZ	2.26	0.68
11:K:111:ASP:O	11:K:112:LYS:CB	2.41	0.68
2:B:225:LEU:HD13	2:B:228:SER:CB	2.24	0.68
2:B:323:SER:OG	2:B:335:ARG:NH1	2.27	0.68
17:Q:52:LEU:HB3	17:Q:54:PHE:CD1	2.28	0.68
1:A:271:ARG:HH12	2:B:821:LYS:HE2	1.58	0.68
21:U:251:ALA:O	21:U:252:LYS:HB2	1.92	0.68
1:A:210:GLN:CD	1:A:212:LYS:HD3	2.13	0.68
2:B:591:ARG:NH2	2:B:601:VAL:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.76	0.68
8:H:65:TYR:CE2	8:H:70:LEU:CG	2.77	0.68
3:C:212:ASP:C	3:C:214:ASP:N	2.47	0.68
18:R:194:ARG:CG	18:R:201:LEU:HD12	2.23	0.68
1:A:262:PRO:CG	1:A:274:ASP:CG	2.52	0.68
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.09	0.68
2:B:13:ASP:OD1	2:B:636:LYS:NZ	2.27	0.67
8:H:84:ARG:O	8:H:86:ASP:N	2.24	0.67
17:Q:23:ARG:NE	18:R:208:CYS:HA	2.09	0.67
1:A:207:GLU:O	1:A:209:SER:N	2.27	0.67
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.77	0.67
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.67
22:X:44:DC:H42	23:Y:48:DC:H42	1.41	0.67
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.25	0.67
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.76	0.67
2:B:1066:PRO:HB3	13:M:46:ILE:CD1	2.21	0.67
2:B:132:VAL:CB	2:B:141:GLN:CG	2.51	0.67
2:B:73:HIS:O	2:B:75:SER:N	2.28	0.67
21:U:153:ARG:NH2	21:U:166:GLU:OE2	2.28	0.67
1:A:210:GLN:CD	1:A:212:LYS:CD	2.63	0.67
14:N:324:GLU:HA	16:P:188:ARG:HH12	1.58	0.67
17:Q:23:ARG:HE	18:R:207:SER:C	1.98	0.67
20:T:140:ARG:O	20:T:142:SER:N	2.27	0.67
1:A:608:THR:OG1	1:A:610:PRO:HD2	1.94	0.67
15:O:3:TYR:CD1	15:O:98:CYS:SG	2.87	0.67
1:A:202:TRP:CE3	1:A:212:LYS:HB2	2.28	0.67
5:E:64:HIS:O	5:E:65:ASN:C	2.24	0.67
13:M:178:LYS:NZ	13:M:279:GLY:O	2.27	0.66
1:A:265:VAL:C	1:A:272:ASN:ND2	2.49	0.66
2:B:896:LEU:CD2	2:B:901:THR:HG21	2.25	0.66
1:A:1319:LYS:CG	1:A:1333:GLU:CG	2.61	0.66
2:B:225:LEU:O	2:B:227:ASN:N	2.28	0.66
1:A:1180:ASN:HB3	9:I:33:ARG:HH22	1.59	0.66
13:M:44:ARG:NE	13:M:46:ILE:CG2	2.58	0.66
16:P:203:ARG:HG3	16:P:203:ARG:HH21	1.59	0.66
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.79	0.66
20:T:177:ARG:NH2	20:T:212:TYR:HB2	2.10	0.66
1:A:133:SER:O	1:A:135:GLY:N	2.29	0.66
1:A:202:TRP:CZ3	1:A:212:LYS:HG2	2.29	0.66
1:A:460:ARG:NH2	1:A:493:ASN:HB2	2.10	0.66
9:I:60:HIS:CD2	9:I:62:VAL:HG12	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.77	0.66
2:B:761:THR:H	2:B:764:MET:HE3	1.61	0.66
17:Q:54:PHE:CD2	18:R:194:ARG:CD	2.77	0.66
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.30	0.65
1:A:1113:SER:O	1:A:1114:ALA:CB	2.44	0.65
9:I:84:HIS:CD2	9:I:84:HIS:H	2.15	0.65
17:Q:180:PHE:HE2	18:R:211:SER:CB	2.01	0.65
18:R:225:VAL:HB	18:R:230:GLU:CG	2.22	0.65
17:Q:57:LYS:NZ	22:X:27:DG:OP1	2.29	0.65
14:N:363:ARG:HD3	14:N:365:TYR:OH	1.97	0.65
17:Q:103:VAL:O	17:Q:106:LYS:N	2.29	0.65
8:H:65:TYR:OH	8:H:70:LEU:CB	2.43	0.65
13:M:89:GLY:O	13:M:90:ALA:HB3	1.95	0.65
9:I:14:ILE:CG1	9:I:16:PHE:CG	2.80	0.65
2:B:952:GLU:N	2:B:952:GLU:OE1	2.25	0.65
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.32	0.65
10:J:63:ALA:O	10:J:65:LEU:N	2.26	0.65
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.79	0.65
1:A:152:ASN:O	1:A:153:ILE:CB	2.42	0.64
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.30	0.64
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.30	0.64
5:E:52:ARG:CG	5:E:53:PRO:HD3	2.27	0.64
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.78	0.64
6:F:65:VAL:HG13	6:F:104:ILE:HD11	1.80	0.64
16:P:206:GLU:CB	16:P:236:LYS:HZ2	2.08	0.64
17:Q:24:GLY:HA2	18:R:210:PHE:CD2	2.33	0.64
20:T:154:LYS:H	20:T:154:LYS:CD	2.03	0.64
2:B:74:ALA:CB	20:T:201:ASP:HB3	2.22	0.64
1:A:1319:LYS:CD	1:A:1333:GLU:CD	2.56	0.64
1:A:22:GLN:HE22	1:A:1448:SER:HB2	1.63	0.64
1:A:863:ARG:NH2	1:A:1415:THR:OG1	2.31	0.64
17:Q:103:VAL:HG23	17:Q:107:LEU:HD12	1.80	0.64
1:A:522:PRO:CA	1:A:666:ARG:HH21	2.10	0.64
3:C:78:ILE:HD11	3:C:81:LYS:HE3	1.80	0.64
2:B:92:TYR:CB	20:T:145:LEU:HB2	2.24	0.64
1:A:271:ARG:HH22	2:B:821:LYS:NZ	1.95	0.64
10:J:62:TYR:HB3	10:J:64:PRO:CD	2.28	0.64
17:Q:36:ILE:O	17:Q:41:SER:OG	2.16	0.64
18:R:142:LYS:NZ	18:R:172:GLU:OE2	2.26	0.64
18:R:190:LEU:CD1	18:R:205:ASP:CG	2.65	0.64
1:A:609:HIS:O	1:A:610:PRO:O	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:GLN:HG3	2:B:141:GLN:O	1.96	0.63
16:P:298:PRO:O	16:P:300:ILE:HG12	1.97	0.63
18:R:190:LEU:CD1	18:R:205:ASP:HB2	2.28	0.63
1:A:1027:ASP:OD1	5:E:162:ARG:NH1	2.31	0.63
1:A:1179:PRO:HG2	9:I:33:ARG:HG3	1.80	0.63
1:A:133:SER:OG	1:A:136:GLN:CB	2.36	0.63
1:A:927:GLU:HB2	1:A:931:ARG:HG2	1.78	0.63
18:R:190:LEU:HD11	18:R:205:ASP:HB2	1.79	0.63
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.32	0.63
2:B:958:CYS:SG	2:B:959:GLU:N	2.72	0.63
9:I:84:HIS:CG	9:I:85:PRO:CD	2.70	0.63
20:T:177:ARG:HH22	20:T:212:TYR:HB2	1.63	0.63
2:B:1120:ASN:HB3	2:B:1145:GLN:HB3	1.81	0.63
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.64	0.63
1:A:460:ARG:HH21	1:A:493:ASN:HB2	1.61	0.63
9:I:14:ILE:CG1	9:I:16:PHE:CZ	2.72	0.63
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.63
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.81	0.63
1:A:326:PRO:HB3	13:M:87:GLY:CA	2.28	0.62
2:B:552:ASN:OD1	2:B:553:LEU:N	2.33	0.62
4:D:70:ARG:NH1	7:G:140:ASP:OD1	2.31	0.62
2:B:249:LYS:O	2:B:250:SER:HB2	1.99	0.62
9:I:14:ILE:HG13	9:I:16:PHE:CE1	2.33	0.62
23:Y:56:DG:H2''	23:Y:57:DA:H5'	1.80	0.62
1:A:1112:VAL:HG12	1:A:1311:LEU:HD21	1.81	0.62
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.34	0.62
13:M:10:LEU:N	13:M:11:PRO:HD3	2.14	0.62
21:U:231:ASP:C	21:U:232:GLU:CG	2.67	0.62
1:A:923:ASP:O	1:A:932:ARG:NH1	2.32	0.62
1:A:950:ASN:OD1	1:A:954:ARG:NH1	2.33	0.62
2:B:422:PHE:O	2:B:426:GLY:N	2.28	0.62
20:T:202:LEU:HD12	20:T:205:ILE:HD11	1.81	0.62
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.39	0.62
1:A:244:ARG:HG2	1:A:245:PRO:HD2	1.81	0.62
1:A:339:LEU:HD11	2:B:1161:GLU:HG2	1.81	0.62
15:O:3:TYR:C	15:O:5:LEU:N	2.51	0.62
16:P:206:GLU:C	16:P:208:ARG:H	2.02	0.62
20:T:139:VAL:HG13	20:T:142:SER:OG	1.99	0.62
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.30	0.62
17:Q:103:VAL:CG2	17:Q:104:LYS:N	2.62	0.62
1:A:93:PRO:HB3	1:A:251:THR:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.63	0.62
2:B:761:THR:H	2:B:764:MET:CE	2.13	0.62
9:I:14:ILE:CG1	9:I:16:PHE:CE1	2.83	0.62
1:A:779:ILE:O	1:A:783:GLN:HG3	2.00	0.61
1:A:896:LEU:HD23	1:A:1080:ILE:HD12	1.82	0.61
7:G:78:ARG:NH1	7:G:79:PRO:O	2.33	0.61
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.65	0.61
16:P:162:VAL:O	16:P:162:VAL:HG23	2.00	0.61
19:S:111:LYS:HE3	19:S:149:LEU:HD21	1.82	0.61
2:B:924:ARG:NH1	3:C:60:HIS:HB2	2.16	0.61
1:A:1313:GLN:HE22	1:A:1318:LYS:CD	2.11	0.61
1:A:1102:MET:HB2	1:A:1389:ASP:OD1	2.00	0.61
13:M:44:ARG:NE	13:M:46:ILE:HG22	2.15	0.61
1:A:1298:LEU:O	1:A:1300:GLY:N	2.31	0.61
20:T:145:LEU:HG	20:T:145:LEU:O	2.00	0.61
10:J:3:ILE:HD12	10:J:15:GLY:HA2	1.81	0.61
20:T:236:LYS:NZ	20:T:238:GLU:O	2.33	0.61
14:N:344:ARG:NH2	23:Y:79:DT:OP2	2.30	0.61
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.82	0.61
1:A:927:GLU:H	1:A:931:ARG:HG2	1.65	0.61
1:A:890:ARG:CZ	1:A:1023:VAL:HB	2.30	0.61
17:Q:23:ARG:CB	18:R:207:SER:OG	2.48	0.61
20:T:144:GLN:O	20:T:145:LEU:HB2	1.99	0.61
2:B:901:THR:OG1	2:B:902:GLY:N	2.31	0.61
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.83	0.61
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.66	0.61
18:R:190:LEU:HD11	18:R:205:ASP:CB	2.31	0.61
18:R:190:LEU:HD13	18:R:205:ASP:OD2	1.97	0.61
3:C:67:ARG:HH21	3:C:148:ILE:HD11	1.65	0.60
6:F:62:ARG:NH1	6:F:127:ASP:O	2.27	0.60
1:A:1192:TRP:O	1:A:1196:TYR:N	2.34	0.60
1:A:603:ILE:HD11	1:A:988:TRP:CE2	2.35	0.60
8:H:23:ASP:O	8:H:25:VAL:N	2.32	0.60
17:Q:54:PHE:HA	18:R:194:ARG:CD	2.31	0.60
1:A:133:SER:O	1:A:134:LYS:C	2.36	0.60
1:A:927:GLU:HB3	1:A:931:ARG:HB2	1.82	0.60
2:B:1040:GLN:CD	2:B:1040:GLN:H	2.05	0.60
1:A:267:GLN:H	13:M:49:GLY:HA2	1.66	0.60
1:A:857:THR:HG21	1:A:1100:THR:HA	1.84	0.60
18:R:138:ALA:C	18:R:140:LYS:H	2.05	0.60
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:62:LYS:HE2	11:K:72:ILE:HD11	1.82	0.60
1:A:621:ILE:HG22	1:A:621:ILE:O	2.02	0.60
14:N:22:ILE:HD11	14:N:43:LYS:HB2	1.83	0.60
1:A:1319:LYS:CG	1:A:1333:GLU:HG2	2.29	0.60
1:A:622:SER:O	1:A:623:PRO:C	2.41	0.60
18:R:144:ASN:ND2	18:R:173:GLU:OE2	2.28	0.60
1:A:95:PHE:CE2	1:A:218:PRO:HG3	2.37	0.60
17:Q:35:ASP:OD1	18:R:161:ARG:NH2	2.33	0.60
22:X:47:DG:H2"	22:X:48:DA:H5"	1.84	0.60
1:A:65:ILE:HD11	1:A:263:ALA:O	2.02	0.59
2:B:225:LEU:C	2:B:227:ASN:N	2.54	0.59
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.84	0.59
3:C:117:SER:HB3	3:C:130:VAL:HG21	1.83	0.59
5:E:160:LEU:HD21	5:E:167:GLU:HG3	1.84	0.59
8:H:65:TYR:CE2	8:H:70:LEU:HD23	2.37	0.59
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.85	0.59
8:H:95:LYS:HB3	8:H:139:SER:HA	1.85	0.59
14:N:321:SER:OG	16:P:243:LYS:NZ	2.26	0.59
1:A:65:ILE:CD1	1:A:263:ALA:O	2.51	0.59
1:A:643:LYS:HD3	21:U:301:CYS:SG	2.43	0.59
17:Q:117:ASP:OD1	17:Q:174:ARG:NH1	2.35	0.59
18:R:93:ASP:O	18:R:140:LYS:NZ	2.35	0.59
22:X:50:DC:H2"	22:X:51:DG:C8	2.37	0.59
1:A:522:PRO:HA	1:A:666:ARG:NH2	2.17	0.59
1:A:375:ILE:HD11	1:A:669:TYR:HB3	1.85	0.59
16:P:206:GLU:HA	16:P:206:GLU:OE2	2.02	0.59
17:Q:54:PHE:CD2	18:R:194:ARG:NE	2.70	0.59
17:Q:23:ARG:CZ	18:R:208:CYS:HA	2.32	0.59
1:A:202:TRP:CE3	1:A:212:LYS:CG	2.81	0.59
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.85	0.59
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.67	0.59
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.85	0.59
1:A:1021:VAL:HA	1:A:1034:GLN:NE2	2.18	0.59
8:H:84:ARG:HB3	8:H:86:ASP:HB2	1.84	0.59
13:M:44:ARG:HE	13:M:46:ILE:HG23	1.65	0.59
17:Q:103:VAL:O	17:Q:105:TYR:N	2.36	0.59
20:T:142:SER:OG	20:T:143:GLN:OE1	2.17	0.59
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.34	0.59
2:B:297:MET:SD	2:B:373:LEU:HD22	2.42	0.59
13:M:44:ARG:NE	13:M:46:ILE:HG23	2.18	0.59
1:A:1114:ALA:C	1:A:1116:ASN:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PHE:CZ	1:A:815:TYR:HE1	2.21	0.58
2:B:883:THR:O	2:B:885:ARG:N	2.36	0.58
10:J:62:TYR:CA	10:J:64:PRO:HD2	2.30	0.58
17:Q:23:ARG:CZ	18:R:208:CYS:CA	2.80	0.58
18:R:225:VAL:HG12	18:R:227:SER:H	1.67	0.58
1:A:720:ALA:HB1	9:I:108:MET:HG2	1.84	0.58
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.85	0.58
13:M:41:VAL:HG23	13:M:41:VAL:O	2.03	0.58
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.84	0.58
21:U:132:ARG:N	21:U:167:GLU:OE2	2.36	0.58
20:T:4:ARG:NE	20:T:102:ASP:OD2	2.35	0.58
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.38	0.58
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.86	0.58
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.86	0.58
13:M:178:LYS:C	20:T:154:LYS:HB3	2.22	0.58
19:S:49:ARG:NH1	19:S:96:GLN:O	2.36	0.58
20:T:26:TYR:HE2	20:T:124:TYR:HH	1.52	0.58
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.11	0.58
1:A:353:ASN:HD21	2:B:1071:ASN:HD21	1.50	0.58
1:A:364:ARG:NH2	1:A:500:GLU:OE1	2.37	0.58
2:B:471:ASN:OD1	2:B:472:ARG:N	2.37	0.58
8:H:84:ARG:C	8:H:86:ASP:N	2.56	0.58
1:A:1416:ARG:HB3	1:A:1433:GLU:OE1	2.03	0.58
1:A:69:GLY:HA2	1:A:77:ASN:HA	1.85	0.58
2:B:289:ILE:O	2:B:291:ASP:N	2.35	0.58
9:I:14:ILE:CG1	9:I:16:PHE:CD1	2.86	0.58
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.85	0.58
7:G:31:PHE:HE1	7:G:48:VAL:HB	1.68	0.58
8:H:106:THR:O	8:H:108:ALA:N	2.33	0.58
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.38	0.58
1:A:417:LYS:HG2	1:A:449:HIS:CE1	2.39	0.58
1:A:799:PRO:O	1:A:806:THR:HG22	2.02	0.58
13:M:10:LEU:N	13:M:11:PRO:CD	2.67	0.57
18:R:144:ASN:OD1	18:R:145:VAL:N	2.36	0.57
17:Q:54:PHE:CG	18:R:194:ARG:HD2	2.39	0.57
1:A:156:GLY:N	1:A:181:HIS:CE1	2.73	0.57
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.87	0.57
2:B:834:ARG:O	2:B:885:ARG:NH1	2.38	0.57
2:B:685:LYS:HA	2:B:688:ALA:HB3	1.85	0.57
18:R:195:PRO:HB3	18:R:199:LYS:HD2	1.86	0.57
17:Q:180:PHE:CZ	18:R:211:SER:CA	2.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:99:LEU:HD12	18:R:124:LEU:HD12	1.86	0.57
1:A:1310:HIS:O	21:U:252:LYS:HG3	2.00	0.57
1:A:480:SER:HB3	2:B:1059:ILE:HD12	1.86	0.57
2:B:755:GLN:HB2	2:B:777:ASN:ND2	2.19	0.57
22:X:13:DA:H2"	22:X:14:DA:C8	2.40	0.57
2:B:228:SER:O	2:B:405:ARG:NH1	2.36	0.57
17:Q:103:VAL:O	17:Q:104:LYS:C	2.43	0.57
1:A:35:SER:OG	1:A:37:THR:HG22	2.04	0.57
2:B:51:ILE:HG23	20:T:141:LEU:HD11	1.80	0.57
1:A:152:ASN:C	1:A:153:ILE:CG1	2.47	0.57
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.38	0.57
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.38	0.57
1:A:1251:ASN:OD1	21:U:197:ASN:ND2	2.35	0.57
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.37	0.57
1:A:181:HIS:CD2	1:A:181:HIS:N	2.73	0.57
2:B:895:PHE:CD1	2:B:895:PHE:N	2.73	0.57
5:E:27:LEU:N	5:E:64:HIS:HB2	2.12	0.57
17:Q:28:ILE:HG21	18:R:190:LEU:HD13	1.85	0.56
18:R:84:TYR:OH	18:R:88:ARG:NH1	2.38	0.56
2:B:326:ALA:HB2	2:B:338:TYR:CE2	2.40	0.56
2:B:483:ARG:NH1	2:B:526:LEU:HB2	2.20	0.56
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.87	0.56
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.38	0.56
1:A:631:GLU:HG3	1:A:988:TRP:CH2	2.40	0.56
2:B:1129:ASN:HA	2:B:1135:TYR:HD1	1.69	0.56
1:A:1085:GLU:OE2	6:F:59:LYS:HE2	2.05	0.56
1:A:264:VAL:HG23	1:A:265:VAL:N	2.20	0.56
1:A:611:ASP:CG	1:A:626:THR:OG1	2.43	0.56
2:B:882:SER:O	2:B:887:TYR:CG	2.56	0.56
5:E:52:ARG:CB	5:E:53:PRO:HD3	2.34	0.56
1:A:1299:GLN:HG2	1:A:1300:GLY:N	2.21	0.56
1:A:279:LYS:HB2	1:A:336:LEU:HD21	1.88	0.56
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.87	0.56
2:B:883:THR:O	2:B:884:ASN:C	2.41	0.56
7:G:93:ASN:OD1	7:G:94:LYS:N	2.38	0.56
9:I:75:ASP:HB3	9:I:78:LEU:HD12	1.86	0.56
3:C:148:ILE:HG12	10:J:5:VAL:HG22	1.86	0.56
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.39	0.56
2:B:74:ALA:HB2	20:T:201:ASP:CB	2.29	0.56
3:C:142:TYR:O	3:C:144:GLU:N	2.39	0.56
17:Q:24:GLY:HA2	18:R:210:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:115:LYS:NZ	19:S:117:GLY:O	2.32	0.56
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.87	0.56
2:B:800:ALA:O	2:B:805:PHE:HB3	2.05	0.56
14:N:333:ASN:OD1	14:N:361:ASN:N	2.26	0.56
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.45	0.56
1:A:294:GLU:HA	1:A:298:ALA:HB2	1.88	0.56
1:A:464:LEU:HD21	1:A:1100:THR:HG21	1.88	0.56
2:B:720:PRO:O	2:B:724:TYR:HD2	1.88	0.56
12:L:26:ASN:HB3	12:L:28:ILE:HG13	1.87	0.56
1:A:631:GLU:HG3	1:A:988:TRP:HH2	1.69	0.56
2:B:225:LEU:O	2:B:228:SER:N	2.39	0.56
2:B:329:GLY:H	2:B:335:ARG:HH21	1.54	0.56
1:A:269:SER:O	1:A:270:ALA:CB	2.55	0.55
3:C:130:VAL:O	3:C:134:ASN:ND2	2.39	0.55
13:M:44:ARG:HG3	13:M:46:ILE:HG23	1.88	0.55
1:A:929:ALA:C	1:A:931:ARG:H	2.07	0.55
17:Q:16:ARG:HD2	17:Q:19:LYS:HB2	1.86	0.55
2:B:577:HIS:HD1	2:B:579:ASP:H	1.51	0.55
2:B:704:LEU:HD22	2:B:708:ALA:CB	2.36	0.55
3:C:154:ARG:N	3:C:157:GLN:OE1	2.38	0.55
21:U:227:GLU:O	21:U:228:MET:C	2.44	0.55
1:A:212:LYS:HA	1:A:212:LYS:NZ	2.20	0.55
1:A:606:HIS:HB2	1:A:627:LYS:HA	1.87	0.55
1:A:800:PHE:HZ	1:A:815:TYR:HE1	1.53	0.55
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.87	0.55
3:C:117:SER:OG	3:C:147:ASP:OD2	2.16	0.55
10:J:10:CYS:SG	10:J:11:GLY:N	2.79	0.55
17:Q:109:HIS:HE1	18:R:231:GLU:CB	2.19	0.55
19:S:172:ASN:OD1	19:S:173:HIS:N	2.38	0.55
2:B:92:TYR:HE1	20:T:143:GLN:HE21	1.54	0.55
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.24	0.55
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.92	0.55
1:A:1307:VAL:HG11	1:A:1339:ASP:OD2	2.06	0.55
1:A:611:ASP:CG	1:A:626:THR:HG1	2.10	0.55
1:A:611:ASP:O	1:A:612:ASP:HB2	2.05	0.55
12:L:19:CYS:SG	12:L:20:GLY:N	2.80	0.55
15:O:64:THR:HG21	16:P:188:ARG:HD2	1.89	0.55
1:A:138:LYS:HB2	1:A:1445:HIS:CE1	2.41	0.55
1:A:875:TYR:O	6:F:53:THR:HG22	2.06	0.55
5:E:45:GLY:C	5:E:47:LYS:H	2.10	0.55
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:89:GLY:O	13:M:90:ALA:CB	2.55	0.55
18:R:151:LEU:HD13	18:R:154:LEU:HD13	1.89	0.55
17:Q:113:ARG:HB2	18:R:222:SER:O	2.07	0.55
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.70	0.55
21:U:226:GLU:OE1	21:U:226:GLU:N	2.39	0.55
2:B:77:GLU:CG	2:B:78:VAL:H	2.15	0.55
13:M:10:LEU:O	13:M:11:PRO:C	2.34	0.55
16:P:206:GLU:C	16:P:208:ARG:N	2.60	0.55
23:Y:48:DC:H2"	23:Y:49:DG:C8	2.41	0.55
5:E:55:ARG:CB	5:E:78:GLU:OE2	2.55	0.55
13:M:94:ASP:OD2	13:M:100:LYS:N	2.39	0.55
1:A:460:ARG:NE	1:A:492:TYR:O	2.32	0.55
2:B:151:LYS:N	2:B:441:SER:OG	2.38	0.55
19:S:126:ILE:O	19:S:137:ALA:HA	2.07	0.55
1:A:121:SER:HA	1:A:126:ILE:HG21	1.87	0.54
1:A:1310:HIS:HB3	21:U:252:LYS:HD3	1.88	0.54
1:A:364:ARG:HE	1:A:500:GLU:CD	2.10	0.54
5:E:185:ILE:HG13	5:E:189:GLN:OE1	2.07	0.54
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.36	0.54
18:R:190:LEU:HD11	18:R:205:ASP:CG	2.25	0.54
1:A:1111:GLY:HA2	21:U:254:GLY:HA2	1.90	0.54
1:A:208:ASP:OD1	1:A:209:SER:N	2.41	0.54
1:A:678:ASN:O	1:A:681:LEU:HB3	2.06	0.54
1:A:685:HIS:HB3	2:B:784:SER:OG	2.07	0.54
2:B:704:LEU:HD22	2:B:708:ALA:HB1	1.89	0.54
5:E:177:ASP:OD1	5:E:178:PRO:HD2	2.08	0.54
16:P:206:GLU:O	16:P:208:ARG:N	2.40	0.54
17:Q:103:VAL:HG23	17:Q:104:LYS:N	2.21	0.54
19:S:47:LEU:HD23	20:T:104:LEU:HD13	1.89	0.54
21:U:251:ALA:O	21:U:252:LYS:CB	2.53	0.54
1:A:262:PRO:O	1:A:263:ALA:CB	2.55	0.54
1:A:870:SER:HB2	1:A:882:SER:HB3	1.90	0.54
2:B:879:GLU:HG2	2:B:879:GLU:O	2.07	0.54
9:I:15:ARG:HG3	9:I:15:ARG:O	2.07	0.54
19:S:103:ASN:HB2	19:S:107:GLY:HA3	1.89	0.54
13:M:290:ARG:NH1	22:X:4:DG:OP1	2.39	0.54
1:A:219:GLU:O	1:A:222:HIS:HB3	2.08	0.54
2:B:240:LEU:O	2:B:253:GLY:HA2	2.07	0.54
18:R:78:LEU:HD11	18:R:124:LEU:HD21	1.89	0.54
1:A:924:TYR:OH	1:A:949:GLN:HA	2.08	0.54
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:290:ARG:HH12	22:X:4:DG:P	2.31	0.54
1:A:1103:THR:HG23	1:A:1106:THR:H	1.71	0.54
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.40	0.54
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.90	0.54
2:B:116:ARG:HH12	12:L:42:ARG:HH11	1.54	0.54
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.54
14:N:323:GLU:HG3	14:N:325:GLY:HA3	1.89	0.54
1:A:549:THR:HG21	1:A:640:LEU:HG	1.90	0.54
1:A:1316:ASN:HA	21:U:292:ASN:O	2.07	0.54
1:A:1341:VAL:O	1:A:1343:LEU:N	2.38	0.54
1:A:133:SER:C	1:A:135:GLY:N	2.60	0.54
1:A:603:ILE:HD11	1:A:988:TRP:NE1	2.23	0.54
8:H:65:TYR:CE2	8:H:70:LEU:CD2	2.91	0.54
18:R:225:VAL:HG11	18:R:230:GLU:HG3	1.90	0.54
13:M:179:GLU:CA	20:T:154:LYS:HG2	2.33	0.54
1:A:1132:LYS:N	22:X:46:DC:OP1	2.37	0.54
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.23	0.54
2:B:649:ASN:OD1	2:B:650:ASN:N	2.41	0.54
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.42	0.54
17:Q:109:HIS:HE1	18:R:231:GLU:HA	1.73	0.54
1:A:266:MET:O	1:A:272:ASN:ND2	2.41	0.53
1:A:597:PRO:O	1:A:599:HIS:N	2.40	0.53
2:B:1152:PRO:HG2	2:B:1155:CYS:HB2	1.90	0.53
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.90	0.53
12:L:27:GLU:O	12:L:29:LYS:N	2.41	0.53
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.40	0.53
1:A:156:GLY:CA	1:A:181:HIS:NE2	2.72	0.53
1:A:203:LYS:O	1:A:204:HIS:CB	2.51	0.53
2:B:853:LEU:HD12	12:L:46:LYS:HE3	1.91	0.53
9:I:103:ARG:C	9:I:105:GLU:HG2	2.25	0.53
13:M:7:LEU:CD1	13:M:10:LEU:HD13	2.39	0.53
20:T:147:LYS:HG2	20:T:147:LYS:O	2.07	0.53
17:Q:25:PHE:CZ	17:Q:110:MET:HE3	2.44	0.53
1:A:389:THR:HB	1:A:417:LYS:HD3	1.90	0.53
1:A:602:CYS:HB2	1:A:655:ILE:HD12	1.91	0.53
2:B:92:TYR:HE2	2:B:146:LYS:NZ	2.06	0.53
2:B:73:HIS:C	2:B:75:SER:H	2.11	0.53
17:Q:105:TYR:CE1	18:R:231:GLU:HB2	2.43	0.53
1:A:521:VAL:C	1:A:666:ARG:HH21	2.12	0.53
1:A:624:GLY:C	1:A:626:THR:H	2.11	0.53
2:B:874:PRO:O	2:B:875:GLU:CB	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:LYS:NZ	4:D:124:ASP:OD2	2.28	0.53
18:R:140:LYS:HB3	18:R:141:PRO:HD3	1.89	0.53
17:Q:23:ARG:HH22	18:R:209:GLN:H	1.40	0.53
1:A:535:MET:O	1:A:669:TYR:OH	2.25	0.53
17:Q:23:ARG:NH2	18:R:208:CYS:CA	2.72	0.53
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.43	0.53
13:M:44:ARG:HH11	13:M:46:ILE:HG22	1.74	0.53
13:M:7:LEU:HD11	13:M:10:LEU:CD1	2.39	0.53
20:T:228:ILE:O	20:T:230:LYS:N	2.38	0.53
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.90	0.53
2:B:739:ASN:HB3	10:J:62:TYR:CZ	2.44	0.53
16:P:161:ILE:O	16:P:161:ILE:HG12	2.08	0.53
2:B:195:ILE:HD11	2:B:481:HIS:HE2	1.74	0.53
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.24	0.53
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.91	0.53
9:I:14:ILE:HA	9:I:16:PHE:CE1	2.43	0.53
17:Q:23:ARG:NE	18:R:207:SER:C	2.56	0.53
17:Q:29:GLU:CD	18:R:194:ARG:HH21	2.09	0.53
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.91	0.53
2:B:160:TYR:HE1	20:T:144:GLN:HG2	1.74	0.53
2:B:248:LYS:O	2:B:249:LYS:HB2	2.07	0.53
8:H:108:ALA:O	8:H:110:THR:N	2.42	0.53
3:C:58:VAL:HG21	10:J:59:LEU:HB3	1.90	0.53
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.91	0.53
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.91	0.53
21:U:290:VAL:HG22	21:U:297:ARG:HG2	1.90	0.52
1:A:1248:ASN:HD21	1:A:1255:LEU:HA	1.75	0.52
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.09	0.52
1:A:428:ASP:OD1	1:A:430:ARG:N	2.37	0.52
2:B:27:TRP:CD2	2:B:762:ARG:HG2	2.43	0.52
7:G:94:LYS:HG3	7:G:95:VAL:HG23	1.90	0.52
9:I:60:HIS:CD2	9:I:62:VAL:CG1	2.92	0.52
2:B:489:ILE:HG13	2:B:490:GLY:H	1.74	0.52
10:J:62:TYR:CB	10:J:64:PRO:CD	2.87	0.52
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.92	0.52
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.91	0.52
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.35	0.52
1:A:11:SER:O	1:A:13:CYS:N	2.43	0.52
1:A:522:PRO:HG3	1:A:666:ARG:HG2	1.89	0.52
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.23	0.52
16:P:269:ARG:HB3	16:P:335:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:ASN:OD1	1:A:1173:THR:N	2.43	0.52
2:B:225:LEU:CD1	2:B:228:SER:HB3	2.39	0.52
2:B:289:ILE:HD13	2:B:297:MET:SD	2.50	0.52
3:C:212:ASP:O	3:C:213:GLU:C	2.48	0.52
1:A:476:ILE:HD12	1:A:476:ILE:N	2.25	0.52
1:A:927:GLU:N	1:A:931:ARG:HG2	2.24	0.52
2:B:133:ILE:HD13	2:B:139:GLN:CB	2.39	0.52
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.45	0.52
1:A:271:ARG:HH22	2:B:821:LYS:CE	2.21	0.52
16:P:162:VAL:C	16:P:164:GLN:HE21	2.05	0.52
18:R:194:ARG:CG	18:R:201:LEU:CD1	2.88	0.52
1:A:1162:GLU:HA	1:A:1304:ILE:HD11	1.92	0.52
17:Q:102:VAL:O	17:Q:102:VAL:HG13	2.10	0.52
1:A:625:ASP:OD2	8:H:22:PHE:CE1	2.63	0.52
2:B:952:GLU:HG3	3:C:39:ILE:HG23	1.91	0.52
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.43	0.52
17:Q:69:ASP:O	17:Q:70:LYS:HB2	2.10	0.52
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.92	0.51
2:B:329:GLY:H	2:B:335:ARG:NH2	2.07	0.51
2:B:160:TYR:CE1	20:T:144:GLN:HG2	2.46	0.51
2:B:991:ALA:HB1	10:J:43:TYR:HB2	1.90	0.51
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.51
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.75	0.51
1:A:264:VAL:CG2	1:A:265:VAL:N	2.73	0.51
1:A:927:GLU:CA	1:A:931:ARG:HG2	2.40	0.51
2:B:92:TYR:HB3	20:T:145:LEU:CG	2.41	0.51
1:A:156:GLY:HA2	1:A:181:HIS:CD2	2.46	0.51
1:A:489:THR:OG1	1:A:494:ALA:O	2.28	0.51
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.93	0.51
2:B:72:GLN:NE2	2:B:77:GLU:O	2.44	0.51
2:B:116:ARG:NH1	12:L:42:ARG:HH11	2.09	0.51
18:R:190:LEU:CD1	18:R:205:ASP:CB	2.88	0.51
1:A:689:ILE:HD13	2:B:985:LEU:HD22	1.93	0.51
18:R:190:LEU:HD12	18:R:205:ASP:CG	2.29	0.51
22:X:39:DT:H2"	22:X:40:DT:H5"	1.92	0.51
1:A:261:ARG:C	1:A:263:ALA:N	2.60	0.51
2:B:45:ASP:OD2	2:B:531:TYR:OH	2.25	0.51
5:E:29:THR:HG22	5:E:31:ASP:H	1.75	0.51
15:O:66:ARG:HB3	15:O:73:THR:HB	1.93	0.51
17:Q:110:MET:SD	18:R:222:SER:HB2	2.50	0.51
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.91	0.51
3:C:4:ALA:HB2	11:K:93:ASP:OD2	2.11	0.51
5:E:47:LYS:NZ	5:E:52:ARG:O	2.41	0.51
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.46	0.51
1:A:153:ILE:O	1:A:154:CYS:O	2.29	0.51
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.51	0.51
2:B:193:VAL:N	2:B:468:GLN:O	2.41	0.51
2:B:866:ILE:HG13	2:B:867:ILE:N	2.25	0.51
13:M:17:ASN:OD1	13:M:18:HIS:N	2.44	0.51
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.46	0.51
1:A:1313:GLN:CD	1:A:1318:LYS:HB2	2.31	0.50
1:A:271:ARG:HH12	2:B:821:LYS:CE	2.24	0.50
1:A:281:ALA:O	1:A:285:LYS:HG3	2.12	0.50
2:B:714:PRO:O	2:B:717:ASN:HB2	2.11	0.50
7:G:151:ARG:HB2	7:G:158:PHE:CE1	2.46	0.50
8:H:106:THR:O	8:H:107:GLU:HB2	2.09	0.50
10:J:28:GLU:HG2	10:J:30:THR:HG22	1.93	0.50
17:Q:108:ASP:OD1	17:Q:111:ARG:NH2	2.19	0.50
2:B:92:TYR:CD1	20:T:145:LEU:HD13	2.30	0.50
1:A:202:TRP:HZ3	1:A:212:LYS:CG	2.09	0.50
1:A:1319:LYS:CG	1:A:1333:GLU:OE1	2.58	0.50
1:A:1427:LEU:HD23	1:A:1456:GLU:HB3	1.93	0.50
1:A:180:GLY:C	1:A:182:GLY:H	2.15	0.50
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.50
2:B:746:THR:HG22	2:B:812:ARG:NH1	2.27	0.50
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.93	0.50
22:X:13:DA:N6	23:Y:80:DT:O4	2.44	0.50
1:A:131:ALA:O	1:A:133:SER:N	2.45	0.50
2:B:157:ARG:N	2:B:161:CYS:SG	2.71	0.50
2:B:225:LEU:CD1	2:B:228:SER:CB	2.89	0.50
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.46	0.50
2:B:738:THR:HG22	2:B:772:LEU:HD21	1.93	0.50
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.92	0.50
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.50
20:T:177:ARG:HE	20:T:208:GLN:HB2	1.77	0.50
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.93	0.50
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.76	0.50
2:B:499:ARG:HH11	2:B:520:VAL:HG22	1.76	0.50
2:B:529:MET:HE2	2:B:623:ARG:HB2	1.94	0.50
2:B:803:ARG:HH12	2:B:951:GLN:HE22	1.59	0.50
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:242:GLN:HG3	16:P:248:ALA:HB3	1.94	0.50
17:Q:180:PHE:CZ	18:R:211:SER:HA	2.39	0.50
1:A:614:ASP:O	1:A:615:SER:OG	2.21	0.50
2:B:1069:ILE:HG12	13:M:48:VAL:CG1	2.42	0.50
2:B:1124:ILE:H	2:B:1124:ILE:HD12	1.76	0.50
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.42	0.50
2:B:628:VAL:HG12	2:B:633:LEU:HD23	1.94	0.50
2:B:838:GLN:O	2:B:891:ASP:N	2.40	0.50
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.47	0.50
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.93	0.50
1:A:924:TYR:CE1	1:A:949:GLN:HG2	2.47	0.50
3:C:67:ARG:HH22	10:J:2:ILE:HG13	1.77	0.50
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.47	0.50
13:M:52:TRP:CD1	13:M:67:VAL:HG22	2.47	0.50
20:T:160:GLN:HA	20:T:163:ILE:HD12	1.94	0.50
2:B:35:ASP:CG	2:B:646:ARG:HH12	2.15	0.49
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.76	0.49
13:M:60:ALA:O	13:M:62:LYS:N	2.45	0.49
16:P:203:ARG:HG3	16:P:203:ARG:NH2	2.25	0.49
1:A:980:PRO:HB2	1:A:981:CYS:SG	2.51	0.49
2:B:1117:HIS:O	2:B:1127:ILE:HG12	2.11	0.49
7:G:91:GLN:HG2	17:Q:145:PHE:CE1	2.47	0.49
8:H:17:PRO:O	8:H:19:GLY:N	2.45	0.49
9:I:85:PRO:C	9:I:86:CYS:O	2.49	0.49
1:A:1250:ASP:C	21:U:227:GLU:HG3	2.33	0.49
8:H:103:GLU:HA	8:H:108:ALA:HB1	1.95	0.49
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.59	0.49
1:A:138:LYS:HB2	1:A:1445:HIS:HE1	1.76	0.49
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.94	0.49
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.45	0.49
1:A:326:PRO:HB3	13:M:87:GLY:N	2.27	0.49
16:P:206:GLU:CD	16:P:236:LYS:NZ	2.66	0.49
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.47	0.49
1:A:133:SER:O	1:A:136:GLN:N	2.35	0.49
1:A:624:GLY:C	1:A:626:THR:N	2.66	0.49
3:C:44:ILE:HD11	3:C:238:SER:HB2	1.94	0.49
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.95	0.49
13:M:179:GLU:HA	20:T:154:LYS:CG	2.36	0.49
22:X:46:DC:H42	23:Y:47:DG:H22	1.59	0.49
1:A:1192:TRP:HE1	1:A:1248:ASN:HB3	1.77	0.49
1:A:1392:TYR:OH	1:A:1394:ASN:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PHE:HZ	1:A:815:TYR:CE1	2.28	0.49
2:B:77:GLU:HB3	2:B:78:VAL:HG23	1.93	0.49
13:M:79:ASP:N	13:M:79:ASP:OD1	2.46	0.49
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.48	0.49
1:A:362:SER:HB3	2:B:1084:LEU:HD12	1.95	0.49
2:B:35:ASP:OD2	2:B:646:ARG:NH1	2.37	0.49
2:B:563:ASP:OD1	2:B:610:ARG:NH1	2.45	0.49
16:P:311:VAL:HG11	23:Y:81:DA:C2	2.47	0.49
16:P:311:VAL:HG11	23:Y:81:DA:H2	1.78	0.49
7:G:98:PHE:CZ	17:Q:152:PHE:HE1	2.31	0.49
19:S:118:VAL:HG13	19:S:120:GLU:HG3	1.95	0.49
2:B:20:ASP:OD1	2:B:21:LEU:N	2.45	0.49
2:B:509:VAL:HG11	2:B:524:LYS:HB3	1.94	0.49
2:B:905:ASP:OD1	2:B:924:ARG:NH1	2.46	0.49
3:C:7:PRO:HG3	11:K:97:GLU:HG2	1.94	0.49
5:E:192:LYS:HE3	5:E:194:ILE:HD11	1.93	0.49
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.95	0.49
13:M:297:PRO:HG3	13:M:310:VAL:HG11	1.93	0.49
13:M:57:ASN:ND2	23:Y:54:DA:OP2	2.44	0.49
1:A:262:PRO:CG	1:A:274:ASP:OD1	2.50	0.49
2:B:351:VAL:HG11	2:B:361:LYS:HA	1.94	0.49
3:C:267:ILE:HG21	3:C:274:ILE:HD13	1.93	0.49
22:X:40:DT:H1'	22:X:41:DT:H3'	1.95	0.49
1:A:27:SER:O	1:A:31:LEU:N	2.42	0.49
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.43	0.49
2:B:223:SER:O	2:B:224:CYS:HB3	2.12	0.49
2:B:191:GLU:OE2	2:B:472:ARG:NH1	2.46	0.49
3:C:68:LEU:O	3:C:71:ILE:HG12	2.13	0.49
8:H:108:ALA:O	8:H:109:ALA:C	2.52	0.49
8:H:37:MET:HG2	8:H:127:GLY:HA3	1.95	0.49
17:Q:103:VAL:HG23	17:Q:107:LEU:CD1	2.43	0.49
1:A:1408:ARG:NH2	1:A:1421:ARG:O	2.45	0.48
1:A:460:ARG:HB2	1:A:501:MET:SD	2.52	0.48
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.94	0.48
9:I:61:GLU:O	9:I:63:ASP:N	2.45	0.48
13:M:94:ASP:OD1	13:M:100:LYS:N	2.45	0.48
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.48	0.48
1:A:817:PRO:HG2	1:A:818:GLU:OE1	2.12	0.48
1:A:873:VAL:HB	1:A:1083:PRO:HA	1.93	0.48
11:K:61:TYR:HA	11:K:72:ILE:O	2.14	0.48
14:N:312:GLU:HB3	14:N:313:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:101:ASN:O	17:Q:102:VAL:HG13	2.08	0.48
17:Q:102:VAL:O	17:Q:102:VAL:HG22	2.11	0.48
17:Q:105:TYR:CE1	18:R:231:GLU:OE1	2.59	0.48
1:A:484:LEU:HD23	1:A:484:LEU:N	2.28	0.48
1:A:809:HIS:CE1	2:B:697:GLU:OE2	2.67	0.48
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.95	0.48
5:E:11:TRP:O	5:E:15:LYS:HG2	2.14	0.48
5:E:47:LYS:HB2	5:E:48:PRO:HD3	1.78	0.48
1:A:924:TYR:CZ	1:A:949:GLN:HA	2.48	0.48
17:Q:28:ILE:HG21	18:R:205:ASP:OD2	2.13	0.48
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.97	0.48
1:A:266:MET:C	1:A:272:ASN:ND2	2.64	0.48
5:E:52:ARG:CG	5:E:53:PRO:CD	2.87	0.48
8:H:111:ARG:HB3	8:H:127:GLY:O	2.13	0.48
18:R:88:ARG:NH1	18:R:105:GLU:OE2	2.42	0.48
20:T:37:ARG:HH22	20:T:62:LEU:HB2	1.78	0.48
21:U:292:ASN:O	21:U:294:CYS:N	2.47	0.48
1:A:220:ARG:O	1:A:221:VAL:C	2.52	0.48
3:C:155:LYS:HB3	10:J:65:LEU:HD22	1.95	0.48
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.79	0.48
1:A:1155:LYS:HD3	21:U:249:GLN:OE1	2.13	0.48
1:A:1186:VAL:HG12	1:A:1188:GLU:HG2	1.96	0.48
1:A:546:ARG:HB3	1:A:640:LEU:O	2.13	0.48
2:B:225:LEU:C	2:B:227:ASN:H	2.17	0.48
18:R:93:ASP:HB3	18:R:95:HIS:CE1	2.47	0.48
1:A:379:GLY:HA2	1:A:475:ARG:O	2.14	0.48
2:B:225:LEU:O	2:B:226:GLU:C	2.50	0.48
2:B:26:CYS:SG	2:B:27:TRP:N	2.87	0.48
13:M:235:ILE:HD11	13:M:300:PHE:CE1	2.49	0.48
17:Q:28:ILE:CG2	18:R:205:ASP:OD2	2.61	0.48
20:T:194:HIS:HD1	20:T:196:TYR:H	1.62	0.48
1:A:1036:ASN:ND2	1:A:1037:ALA:N	2.62	0.48
1:A:1213:ARG:NH2	1:A:1215:GLU:OE2	2.46	0.48
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.45	0.48
1:A:463:THR:HG22	1:A:468:SER:HB3	1.94	0.48
2:B:202:THR:O	2:B:204:THR:N	2.47	0.48
1:A:1410:HIS:N	5:E:174:GLN:HE22	2.12	0.48
7:G:114:PRO:HB2	7:G:116:GLU:HG2	1.95	0.48
17:Q:36:ILE:HD13	17:Q:52:LEU:HD21	1.96	0.48
21:U:290:VAL:HG13	21:U:297:ARG:HG2	1.96	0.48
1:A:1313:GLN:NE2	1:A:1318:LYS:HD2	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.44	0.48
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.48
20:T:177:ARG:CZ	20:T:212:TYR:HB2	2.44	0.48
2:B:232:THR:OG1	2:B:233:SER:N	2.46	0.47
9:I:15:ARG:NH1	9:I:46:GLN:OE1	2.47	0.47
1:A:297:GLY:HA3	17:Q:57:LYS:HG3	1.96	0.47
18:R:157:GLN:OE1	18:R:162:GLY:HA2	2.14	0.47
22:X:38:DT:H2'	22:X:39:DT:C6	2.49	0.47
1:A:1109:TYR:O	21:U:256:THR:HG22	2.14	0.47
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.96	0.47
8:H:56:PHE:HA	8:H:148:LEU:HA	1.96	0.47
13:M:289:TYR:HA	13:M:292:ILE:HG12	1.96	0.47
19:S:174:PHE:O	19:S:178:GLN:HG2	2.14	0.47
20:T:94:THR:HG22	20:T:109:ILE:HA	1.96	0.47
1:A:490:THR:HG23	21:U:282:ASP:HB3	1.96	0.47
8:H:17:PRO:C	8:H:19:GLY:H	2.17	0.47
19:S:25:LYS:HD3	19:S:141:HIS:CD2	2.49	0.47
20:T:139:VAL:CG1	20:T:142:SER:OG	2.62	0.47
1:A:90:LEU:O	1:A:291:ARG:NH2	2.47	0.47
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.49	0.47
13:M:235:ILE:HD11	13:M:300:PHE:HE1	1.79	0.47
16:P:239:ARG:HD2	16:P:239:ARG:HA	1.57	0.47
13:M:178:LYS:NZ	23:Y:86:DC:OP1	2.45	0.47
1:A:689:ILE:O	1:A:692:SER:OG	2.29	0.47
2:B:474:THR:HG23	2:B:477:SER:H	1.78	0.47
2:B:936:ALA:HB2	2:B:942:LYS:HA	1.97	0.47
3:C:143:VAL:HG23	3:C:144:GLU:H	1.80	0.47
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.97	0.47
13:M:22:ILE:HG23	13:M:35:PRO:HG2	1.96	0.47
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.96	0.47
15:O:50:GLN:O	15:O:53:ARG:NH1	2.47	0.47
1:A:1036:ASN:HD22	1:A:1036:ASN:C	2.18	0.47
1:A:117:LEU:HD23	1:A:119:VAL:H	1.80	0.47
1:A:766:PHE:CE1	1:A:781:ILE:HG12	2.49	0.47
2:B:1069:ILE:HA	2:B:1072:ARG:HE	1.80	0.47
2:B:119:THR:HG23	2:B:187:ILE:HA	1.97	0.47
2:B:414:GLU:HG2	2:B:436:LYS:HD3	1.95	0.47
2:B:628:VAL:HG22	2:B:694:THR:C	2.35	0.47
2:B:715:ASP:OD1	2:B:715:ASP:N	2.46	0.47
10:J:44:CYS:O	10:J:47:ARG:HG3	2.15	0.47
3:C:61:ASP:OD2	12:L:48:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:C	1:A:181:HIS:CD2	2.87	0.47
1:A:406:VAL:HG21	1:A:440:LEU:HD11	1.97	0.47
1:A:522:PRO:HG3	1:A:666:ARG:HE	1.79	0.47
2:B:127:ASP:OD2	2:B:144:HIS:NE2	2.47	0.47
3:C:242:GLU:N	3:C:242:GLU:OE1	2.46	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.15	0.47
15:O:66:ARG:N	15:O:73:THR:O	2.48	0.47
16:P:206:GLU:OE1	16:P:236:LYS:NZ	2.47	0.47
17:Q:109:HIS:HE1	18:R:231:GLU:CA	2.28	0.47
1:A:1251:ASN:HD21	21:U:227:GLU:HB3	1.79	0.47
1:A:220:ARG:HD2	1:A:223:GLU:OE1	2.14	0.47
2:B:101:ARG:O	13:M:175:ARG:NH2	2.45	0.47
8:H:128:ASP:N	8:H:128:ASP:OD1	2.46	0.47
9:I:93:GLU:O	9:I:115:THR:HG22	2.15	0.47
16:P:206:GLU:CB	16:P:236:LYS:NZ	2.75	0.47
18:R:193:ASN:HB3	18:R:197:LYS:HA	1.95	0.47
21:U:252:LYS:HA	21:U:252:LYS:HD2	1.44	0.47
2:B:1115:GLN:OE1	2:B:1115:GLN:N	2.47	0.47
2:B:274:ARG:HE	2:B:308:ALA:HB1	1.79	0.47
1:A:1177:TYR:N	9:I:51:SER:HB3	2.27	0.47
1:A:1450:PRO:O	1:A:1452:LYS:HG3	2.15	0.47
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.47
1:A:691:ASP:OD1	1:A:765:ASN:N	2.48	0.47
2:B:854:ILE:O	2:B:907:VAL:HG21	2.15	0.47
10:J:63:ALA:H	10:J:64:PRO:HD3	1.75	0.47
13:M:10:LEU:O	13:M:12:ARG:CA	2.53	0.47
13:M:205:SER:OG	16:P:278:GLN:NE2	2.43	0.47
13:M:86:LYS:NZ	22:X:35:DT:H3	2.12	0.47
16:P:297:LYS:C	16:P:299:ARG:H	2.17	0.47
1:A:532:ARG:HB3	1:A:649:ALA:HB2	1.96	0.47
1:A:809:HIS:HE1	2:B:697:GLU:OE2	1.98	0.47
2:B:41:ARG:HA	2:B:41:ARG:HD2	1.68	0.47
7:G:110:ARG:HA	7:G:113:ILE:HD12	1.97	0.47
13:M:169:ARG:HH11	13:M:206:VAL:HG21	1.79	0.47
22:X:44:DC:H2'	22:X:45:DG:C8	2.49	0.47
23:Y:71:DA:H2'	23:Y:71:DA:OP2	2.15	0.47
6:F:56:TYR:CD1	6:F:124:ILE:HB	2.50	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.80	0.46
3:C:171:LYS:HE3	11:K:10:PHE:HB3	1.96	0.46
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.50	0.46
16:P:161:ILE:HG23	16:P:161:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLU:HG2	1:A:247:TRP:CD1	2.49	0.46
1:A:606:HIS:O	1:A:608:THR:N	2.45	0.46
1:A:625:ASP:OD2	8:H:22:PHE:HE1	1.98	0.46
2:B:1028:LEU:HD12	2:B:1028:LEU:HA	1.51	0.46
2:B:298:MET:O	2:B:301:VAL:HG12	2.16	0.46
13:M:12:ARG:NH1	13:M:23:LEU:O	2.48	0.46
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.15	0.46
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.96	0.46
2:B:101:ARG:HB3	13:M:131:PRO:HG2	1.96	0.46
18:R:177:ASN:C	18:R:177:ASN:HD22	2.19	0.46
1:A:890:ARG:NH2	1:A:1023:VAL:HB	2.30	0.46
1:A:1013:VAL:HG11	1:A:1046:ARG:HG2	1.97	0.46
1:A:1192:TRP:HA	1:A:1195:VAL:HB	1.98	0.46
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.55	0.46
2:B:187:ILE:HD11	2:B:448:LEU:HD23	1.98	0.46
2:B:646:ARG:HA	2:B:649:ASN:HB3	1.98	0.46
3:C:49:TRP:O	3:C:163:ALA:HA	2.16	0.46
16:P:207:PRO:O	16:P:208:ARG:O	2.34	0.46
19:S:165:GLU:HA	19:S:168:ASN:HB2	1.97	0.46
22:X:31:DG:H2''	22:X:32:DA:O5'	2.16	0.46
1:A:1408:ARG:HD2	1:A:1422:GLN:HE22	1.80	0.46
2:B:163:LEU:HD12	2:B:163:LEU:N	2.31	0.46
2:B:613:ARG:HD3	2:B:615:TYR:CE2	2.50	0.46
1:A:581:LYS:NZ	8:H:86:ASP:O	2.49	0.46
9:I:98:GLN:NE2	9:I:108:MET:SD	2.89	0.46
1:A:561:MET:HG2	11:K:58:PHE:CD1	2.50	0.46
18:R:149:LYS:HD2	18:R:175:LEU:H	1.81	0.46
17:Q:24:GLY:O	18:R:210:PHE:HE2	1.99	0.46
20:T:179:ASP:O	20:T:181:GLN:N	2.48	0.46
22:X:37:DT:H4'	22:X:38:DT:H4'	1.98	0.46
3:C:6:GLN:HG3	3:C:6:GLN:O	2.16	0.46
1:A:1484:MET:CE	7:G:20:PRO:HD3	2.45	0.46
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.85	0.46
13:M:37:CYS:SG	13:M:39:LEU:HB2	2.55	0.46
18:R:138:ALA:O	18:R:140:LYS:N	2.49	0.46
1:A:1181:PRO:C	1:A:1183:SER:H	2.18	0.46
1:A:1128:ILE:HD11	1:A:1401:LEU:HD21	1.97	0.46
1:A:197:GLU:OE2	13:M:93:PHE:CE1	2.66	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HE3	1.98	0.46
3:C:262:GLN:O	3:C:266:GLU:HG2	2.16	0.46
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:182:ALA:CB	20:T:154:LYS:HG3	2.42	0.46
1:A:592:PHE:CZ	1:A:595:ILE:HD11	2.50	0.46
1:A:533:PRO:CG	1:A:654:HIS:HB2	2.46	0.46
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.79	0.46
2:B:195:ILE:HG21	2:B:486:ASN:HB2	1.97	0.46
5:E:172:ARG:HD2	5:E:210:GLN:HB3	1.98	0.46
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.48	0.46
13:M:44:ARG:NH1	13:M:46:ILE:HG22	2.30	0.46
20:T:191:PHE:HA	20:T:197:TYR:HE2	1.81	0.46
1:A:777:SER:OG	1:A:779:ILE:HG22	2.15	0.46
2:B:285:LEU:O	2:B:289:ILE:HG22	2.16	0.46
2:B:992:ASN:O	10:J:46:ARG:NH2	2.48	0.46
3:C:149:LEU:HD23	10:J:2:ILE:HD13	1.98	0.46
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.81	0.46
1:A:1050:CYS:HB3	1:A:1053:ARG:HG2	1.98	0.45
1:A:609:HIS:N	1:A:610:PRO:HD3	2.29	0.45
1:A:693:ILE:HG21	2:B:1023:ARG:NE	2.32	0.45
2:B:646:ARG:HG2	2:B:646:ARG:O	2.16	0.45
2:B:754:PRO:HB2	2:B:773:PRO:CG	2.45	0.45
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.51	0.45
18:R:120:MET:SD	18:R:137:TYR:OH	2.69	0.45
1:A:1319:LYS:H	1:A:1356:ARG:HH22	1.64	0.45
1:A:546:ARG:HB2	1:A:546:ARG:HE	1.59	0.45
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.45
5:E:14:ARG:NH1	5:E:58:LEU:O	2.49	0.45
5:E:25:GLY:O	5:E:65:ASN:HA	2.16	0.45
5:E:55:ARG:HD2	5:E:78:GLU:OE1	2.17	0.45
13:M:10:LEU:H	13:M:11:PRO:CD	2.24	0.45
15:O:3:TYR:CB	15:O:98:CYS:SG	2.98	0.45
18:R:78:LEU:HB2	18:R:119:LEU:HD22	1.98	0.45
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.81	0.45
1:A:546:ARG:HG3	1:A:547:LYS:H	1.82	0.45
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.98	0.45
1:A:595:ILE:HD12	1:A:595:ILE:C	2.37	0.45
1:A:999:ARG:HE	8:H:99:ILE:CD1	2.22	0.45
2:B:487:SER:HA	2:B:488:PRO:HD3	1.67	0.45
2:B:898:THR:OG1	2:B:899:SER:N	2.49	0.45
8:H:24:ARG:O	8:H:45:ILE:N	2.49	0.45
21:U:280:SER:HB2	21:U:284:PRO:HA	1.98	0.45
2:B:739:ASN:HB3	10:J:62:TYR:OH	2.16	0.45
2:B:758:LEU:O	2:B:996:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:TYR:CD1	6:F:115:TYR:HB3	2.51	0.45
1:A:1408:ARG:HD2	1:A:1422:GLN:NE2	2.30	0.45
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.39	0.45
1:A:728:THR:HG23	1:A:736:THR:HG23	1.99	0.45
1:A:97:VAL:HG21	1:A:322:LEU:HD21	1.99	0.45
2:B:1066:PRO:HA	13:M:46:ILE:HG21	1.98	0.45
2:B:1062:ARG:HH11	2:B:1082:GLY:HA2	1.80	0.45
2:B:250:SER:HB3	2:B:251:ALA:H	1.40	0.45
3:C:44:ILE:HD11	3:C:238:SER:CB	2.46	0.45
8:H:75:TYR:HD1	8:H:75:TYR:H	1.65	0.45
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.99	0.45
17:Q:23:ARG:CD	18:R:207:SER:C	2.76	0.45
20:T:177:ARG:HH22	20:T:212:TYR:CB	2.29	0.45
20:T:26:TYR:HE2	20:T:124:TYR:OH	2.00	0.45
1:A:1112:VAL:HB	21:U:253:THR:HB	1.99	0.45
21:U:255:GLY:HA3	21:U:257:GLN:OE1	2.16	0.45
22:X:12:DT:H2"	22:X:13:DA:H8	1.81	0.45
1:A:210:GLN:HB2	1:A:212:LYS:HD2	1.99	0.45
4:D:26:PHE:HE2	7:G:78:ARG:HG2	1.82	0.45
8:H:23:ASP:N	8:H:23:ASP:OD1	2.49	0.45
18:R:225:VAL:HB	18:R:230:GLU:CB	2.47	0.45
1:A:527:THR:HG22	1:A:532:ARG:O	2.17	0.45
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.16	0.45
2:B:51:ILE:HG23	2:B:51:ILE:HD12	1.64	0.45
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.16	0.45
10:J:62:TYR:CB	10:J:64:PRO:HD2	2.46	0.45
13:M:37:CYS:SG	13:M:39:LEU:HD23	2.56	0.45
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.98	0.45
2:B:225:LEU:HD13	2:B:228:SER:HB3	1.98	0.45
3:C:146:ASP:O	3:C:148:ILE:N	2.49	0.45
13:M:246:PRO:HB2	16:P:306:VAL:HG21	1.99	0.45
23:Y:80:DT:H2"	23:Y:81:DA:C8	2.52	0.45
1:A:611:ASP:OD2	1:A:627:LYS:HG3	2.17	0.45
1:A:522:PRO:N	1:A:666:ARG:HH21	2.15	0.45
2:B:514:THR:HG21	2:B:521:GLY:HA2	1.99	0.45
2:B:51:ILE:HG22	20:T:141:LEU:HD13	1.89	0.45
2:B:952:GLU:HG3	3:C:39:ILE:CG2	2.46	0.45
5:E:172:ARG:CD	5:E:210:GLN:HB3	2.47	0.45
9:I:14:ILE:HA	9:I:16:PHE:CD1	2.52	0.45
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.31	0.45
14:N:324:GLU:HA	16:P:188:ARG:NH1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:ARG:O	1:A:932:ARG:CG	2.65	0.45
2:B:100:GLU:O	2:B:103:GLY:N	2.40	0.45
2:B:295:PRO:HB2	9:I:11:PHE:CD2	2.46	0.45
2:B:453:TRP:CG	2:B:463:ARG:HB2	2.52	0.45
2:B:1101:GLN:OE1	6:F:64:ARG:NH1	2.50	0.45
15:O:3:TYR:HD1	15:O:98:CYS:SG	2.38	0.45
20:T:152:ASN:N	20:T:152:ASN:OD1	2.49	0.45
23:Y:56:DG:C2'	23:Y:57:DA:H5'	2.46	0.45
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.99	0.44
1:A:1195:VAL:HG12	21:U:192:ARG:HD3	1.98	0.44
1:A:267:GLN:H	13:M:49:GLY:CA	2.29	0.44
1:A:37:THR:O	1:A:39:GLY:N	2.50	0.44
1:A:495:ASP:HB3	2:B:792:ASP:OD2	2.16	0.44
2:B:319:ASN:OD1	2:B:332:LYS:HG3	2.18	0.44
2:B:968:ASN:CG	2:B:969:PRO:HD2	2.37	0.44
3:C:149:LEU:HD23	10:J:2:ILE:CD1	2.47	0.44
3:C:45:ILE:HG22	3:C:73:LEU:HD12	1.98	0.44
6:F:64:ARG:HH22	7:G:61:PRO:HB3	1.82	0.44
11:K:29:ASN:ND2	11:K:78:THR:O	2.50	0.44
18:R:77:VAL:HA	18:R:80:LYS:HE3	1.99	0.44
19:S:166:ARG:HG3	19:S:166:ARG:HH11	1.83	0.44
20:T:177:ARG:NH1	20:T:212:TYR:HB2	2.32	0.44
1:A:1274:GLU:O	1:A:1276:VAL:N	2.48	0.44
1:A:477:LEU:HB2	1:A:478:PRO:HD2	2.00	0.44
1:A:666:ARG:HA	1:A:666:ARG:HD3	1.28	0.44
1:A:686:THR:OG1	1:A:687:ILE:N	2.49	0.44
2:B:403:LEU:O	2:B:407:MET:HG2	2.17	0.44
2:B:896:LEU:HD23	2:B:901:THR:HG21	1.97	0.44
8:H:130:ASN:O	8:H:134:GLY:N	2.50	0.44
10:J:6:ARG:H	10:J:14:VAL:H	1.65	0.44
10:J:21:TYR:CG	10:J:49:LEU:HD21	2.52	0.44
15:O:64:THR:CG2	16:P:188:ARG:HB3	2.47	0.44
17:Q:71:PHE:CE1	17:Q:106:LYS:HE3	2.52	0.44
17:Q:35:ASP:CG	18:R:161:ARG:HH22	2.18	0.44
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.17	0.44
1:A:610:PRO:O	1:A:612:ASP:N	2.50	0.44
1:A:797:ARG:NH2	1:A:820:ARG:HB2	2.33	0.44
3:C:71:ILE:HG13	3:C:71:ILE:O	2.16	0.44
7:G:97:LEU:HD23	7:G:108:ILE:HD12	1.97	0.44
14:N:11:PRO:HA	14:N:14:TYR:HD2	1.81	0.44
14:N:32:ASP:HB3	14:N:34:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:354:LYS:HA	14:N:369:LYS:HA	1.99	0.44
18:R:138:ALA:C	18:R:140:LYS:N	2.69	0.44
18:R:153:ARG:O	18:R:157:GLN:N	2.46	0.44
1:A:156:GLY:CA	1:A:181:HIS:CD2	3.00	0.44
1:A:416:ALA:HA	1:A:448:ARG:HA	2.00	0.44
2:B:116:ARG:O	2:B:117:ASN:HB2	2.18	0.44
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.47	0.44
10:J:67:LYS:HB3	12:L:23:HIS:HE1	1.82	0.44
14:N:332:GLU:CD	15:O:92:LYS:HD3	2.38	0.44
1:A:19:LYS:HD3	2:B:1174:VAL:HG23	1.98	0.44
1:A:275:ASP:HA	1:A:278:HIS:HB2	1.99	0.44
1:A:932:ARG:HD2	1:A:939:VAL:HG21	1.99	0.44
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.57	0.44
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.99	0.44
7:G:152:VAL:HG22	7:G:157:ILE:HG13	1.98	0.44
10:J:21:TYR:HB2	10:J:38:LEU:CD1	2.47	0.44
14:N:315:ASN:HA	16:P:239:ARG:HH12	1.82	0.44
14:N:349:TRP:HB3	14:N:351:PHE:CE1	2.53	0.44
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.99	0.44
18:R:163:LEU:HD12	18:R:163:LEU:HA	1.76	0.44
13:M:252:SER:OG	23:Y:85:DG:OP1	2.30	0.44
1:A:1319:LYS:HD2	1:A:1319:LYS:HA	1.37	0.44
1:A:389:THR:HB	1:A:417:LYS:CD	2.48	0.44
1:A:51:ARG:NH2	2:B:878:ASP:OD1	2.51	0.44
1:A:522:PRO:CA	1:A:666:ARG:HE	2.31	0.44
2:B:1125:MET:HG3	2:B:1163:MET:HE1	1.98	0.44
1:A:19:LYS:HD2	2:B:1173:SER:H	1.82	0.44
2:B:302:LYS:HE2	9:I:23:MET:SD	2.57	0.44
2:B:87:LYS:NZ	2:B:89:GLU:OE2	2.51	0.44
5:E:27:LEU:H	5:E:64:HIS:CA	2.20	0.44
8:H:113:SER:OG	8:H:126:GLN:HG2	2.17	0.44
3:C:67:ARG:NH1	10:J:2:ILE:HG13	2.28	0.44
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.99	0.44
2:B:380:ARG:NE	2:B:609:GLU:OE1	2.48	0.44
2:B:62:ALA:N	2:B:63:PRO:HD3	2.33	0.44
9:I:35:LEU:HB3	9:I:48:ALA:HB3	1.99	0.44
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.99	0.44
17:Q:51:LEU:HD11	18:R:163:LEU:HD11	1.99	0.44
1:A:608:THR:OG1	1:A:610:PRO:CD	2.63	0.44
1:A:608:THR:OG1	1:A:610:PRO:HG2	2.18	0.44
2:B:80:GLU:OE1	2:B:134:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:PRO:CB	8:H:122:LEU:HD13	2.48	0.44
9:I:57:LYS:HB3	9:I:59:THR:HG22	2.00	0.44
18:R:157:GLN:HG2	18:R:160:GLN:HB3	1.99	0.44
20:T:8:ASP:HB3	20:T:105:SER:HA	1.99	0.44
13:M:99:SER:HG	22:X:33:DA:H61	1.66	0.44
1:A:1467:GLY:O	1:A:1470:CYS:HB2	2.17	0.44
1:A:272:ASN:O	1:A:273:GLN:C	2.54	0.44
1:A:505:LEU:HA	1:A:506:PRO:HD2	1.83	0.44
1:A:521:VAL:O	1:A:666:ARG:NH2	2.50	0.44
1:A:927:GLU:O	1:A:931:ARG:CB	2.66	0.44
2:B:243:GLY:N	2:B:252:ILE:HG21	2.32	0.44
2:B:42:GLN:HG2	2:B:526:LEU:HD11	2.00	0.44
2:B:872:THR:HG23	2:B:888:THR:O	2.18	0.44
3:C:56:SER:OG	3:C:158:GLU:N	2.27	0.44
1:A:326:PRO:HB3	13:M:87:GLY:HA2	1.99	0.43
2:B:73:HIS:C	2:B:75:SER:N	2.71	0.43
8:H:34:SER:HB2	8:H:36:LYS:NZ	2.33	0.43
8:H:85:ALA:HB1	8:H:144:LEU:CD2	2.48	0.43
9:I:119:CYS:HB3	9:I:121:HIS:H	1.82	0.43
12:L:27:GLU:O	12:L:28:ILE:C	2.57	0.43
17:Q:109:HIS:CE1	18:R:231:GLU:HG3	2.52	0.43
23:Y:64:DC:N4	23:Y:65:DG:O6	2.51	0.43
1:A:1249:ASP:HB2	21:U:196:SER:HB2	2.00	0.43
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.43
2:B:1040:GLN:N	2:B:1040:GLN:CD	2.71	0.43
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.99	0.43
2:B:803:ARG:HH21	3:C:177:ASN:HD22	1.66	0.43
10:J:62:TYR:HB2	10:J:64:PRO:HG2	2.00	0.43
13:M:86:LYS:HA	13:M:86:LYS:HD3	1.75	0.43
16:P:298:PRO:HB2	16:P:320:GLU:HB3	1.99	0.43
17:Q:23:ARG:CZ	18:R:209:GLN:HB2	2.45	0.43
20:T:177:ARG:NE	20:T:208:GLN:HB2	2.33	0.43
2:B:698:ILE:O	2:B:699:HIS:HB2	2.17	0.43
3:C:147:ASP:OD2	3:C:148:ILE:HG22	2.17	0.43
3:C:259:LEU:HD22	11:K:42:LEU:HD11	2.00	0.43
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.53	0.43
18:R:195:PRO:CG	18:R:199:LYS:HD2	2.47	0.43
20:T:165:TYR:O	20:T:169:LYS:HG2	2.18	0.43
21:U:257:GLN:HA	21:U:257:GLN:NE2	2.33	0.43
1:A:1301:ILE:HG21	1:A:1345:ARG:CZ	2.48	0.43
1:A:640:LEU:HD13	1:A:645:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.84	0.43
2:B:22:TRP:O	2:B:24:GLU:N	2.51	0.43
17:Q:54:PHE:CA	18:R:194:ARG:HD2	2.42	0.43
21:U:225:ALA:HB3	21:U:228:MET:HA	1.99	0.43
1:A:350:VAL:HG11	1:A:1431:SER:HA	1.99	0.43
1:A:486:LEU:HD12	1:A:496:PHE:CE2	2.54	0.43
1:A:922:PHE:CE2	1:A:932:ARG:NH1	2.86	0.43
2:B:1069:ILE:HG12	13:M:48:VAL:HG11	2.01	0.43
2:B:871:VAL:HG13	2:B:890:ARG:HB2	2.01	0.43
13:M:32:MET:O	13:M:40:VAL:HA	2.19	0.43
7:G:158:PHE:CE1	17:Q:139:LEU:HB2	2.53	0.43
1:A:368:THR:OG1	1:A:483:ARG:NH1	2.51	0.43
2:B:225:LEU:HB3	2:B:228:SER:CB	2.18	0.43
3:C:260:GLN:O	3:C:260:GLN:HG3	2.17	0.43
4:D:71:PHE:HE1	7:G:142:GLU:HG2	1.83	0.43
10:J:66:GLU:HB3	12:L:23:HIS:CE1	2.54	0.43
17:Q:109:HIS:CE1	18:R:231:GLU:HB2	2.54	0.43
17:Q:128:LYS:N	17:Q:163:GLU:O	2.51	0.43
1:A:1168:LYS:HD3	1:A:1306:LYS:HG2	2.01	0.43
1:A:206:ASN:C	1:A:208:ASP:H	2.22	0.43
1:A:485:ASN:OD1	1:A:486:LEU:N	2.52	0.43
2:B:953:ASP:O	2:B:1031:GLY:HA3	2.19	0.43
10:J:44:CYS:SG	10:J:45:CYS:N	2.92	0.43
11:K:5:PRO:HD2	11:K:8:GLU:OE1	2.19	0.43
17:Q:24:GLY:C	18:R:210:PHE:CE2	2.80	0.43
1:A:1410:HIS:HB2	5:E:174:GLN:NE2	2.34	0.43
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.92	0.43
1:A:220:ARG:O	1:A:223:GLU:N	2.52	0.43
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.54	0.43
2:B:1005:ALA:O	2:B:1007:ASN:N	2.52	0.43
8:H:66:GLU:HG2	8:H:66:GLU:O	2.17	0.43
9:I:35:LEU:HD12	9:I:35:LEU:HA	1.84	0.43
11:K:112:LYS:HD3	11:K:112:LYS:O	2.19	0.43
14:N:22:ILE:HG13	14:N:43:LYS:HD2	2.00	0.43
17:Q:109:HIS:HE1	18:R:231:GLU:HB2	1.83	0.43
17:Q:110:MET:CE	18:R:222:SER:OG	2.66	0.43
19:S:23:THR:O	20:T:100:SER:OG	2.23	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.18	0.43
21:U:247:GLU:HA	21:U:250:MET:HG2	2.00	0.43
1:A:155:GLU:C	1:A:181:HIS:CE1	2.92	0.43
1:A:566:PHE:HB3	1:A:674:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:VAL:HA	2:B:1111:SER:HB3	2.00	0.43
2:B:51:ILE:HD13	2:B:51:ILE:HA	1.89	0.43
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.83	0.43
18:R:161:ARG:C	18:R:163:LEU:H	2.22	0.43
23:Y:46:DC:H2"	23:Y:47:DG:C8	2.53	0.43
23:Y:89:DC:H2"	23:Y:90:DC:C5	2.54	0.43
1:A:210:GLN:CD	1:A:212:LYS:HG2	2.37	0.43
2:B:711:ILE:HG21	2:B:711:ILE:HD13	1.76	0.43
2:B:707:CYS:SG	2:B:730:LYS:NZ	2.92	0.43
2:B:819:SER:H	2:B:827:GLU:HB2	1.84	0.43
6:F:121:ASP:N	6:F:121:ASP:OD1	2.51	0.43
9:I:16:PHE:HB3	9:I:22:ASN:O	2.19	0.43
12:L:38:GLU:O	13:M:226:LYS:NZ	2.32	0.43
14:N:28:ILE:HD13	15:O:35:GLN:HG2	2.01	0.43
16:P:298:PRO:O	16:P:299:ARG:C	2.56	0.43
16:P:325:PHE:HA	16:P:328:ILE:HG22	2.01	0.43
19:S:45:ALA:HA	19:S:102:VAL:HA	2.00	0.43
21:U:158:TYR:O	21:U:162:GLY:N	2.47	0.43
1:A:613:GLU:HG2	21:U:262:THR:HB	2.01	0.43
22:X:44:DC:N4	23:Y:48:DC:H42	2.14	0.43
1:A:1282:ASP:OD1	1:A:1283:VAL:HG23	2.19	0.42
1:A:865:ILE:HD12	1:A:866:LYS:N	2.34	0.42
1:A:936:GLU:HB2	1:A:939:VAL:HG23	2.00	0.42
2:B:1114:TYR:HE2	2:B:1156:LYS:HD3	1.84	0.42
2:B:235:ILE:HD11	2:B:347:MET:HG3	1.99	0.42
2:B:875:GLU:HA	2:B:875:GLU:OE1	2.19	0.42
12:L:35:ARG:NH1	12:L:42:ARG:HE	2.17	0.42
1:A:197:GLU:HG3	1:A:199:TYR:HE1	1.84	0.42
1:A:366:VAL:HB	1:A:481:THR:HG22	2.01	0.42
2:B:475:PHE:CE2	2:B:479:LEU:HD22	2.55	0.42
2:B:771:GLU:OE2	10:J:58:LYS:HE3	2.20	0.42
8:H:100:GLU:HG3	8:H:101:GLY:N	2.25	0.42
9:I:57:LYS:C	9:I:59:THR:N	2.68	0.42
1:A:561:MET:SD	11:K:51:LEU:HD21	2.59	0.42
17:Q:35:ASP:HA	17:Q:38:ILE:HD12	2.01	0.42
20:T:98:GLU:HA	20:T:104:LEU:HD23	2.01	0.42
1:A:1050:CYS:SG	1:A:1051:SER:N	2.92	0.42
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.74	0.42
1:A:608:THR:CA	1:A:610:PRO:HD2	2.49	0.42
1:A:689:ILE:HG13	1:A:690:GLY:N	2.34	0.42
2:B:1119:CYS:HB3	2:B:1122:CYS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:798:ARG:NH2	3:C:172:GLU:O	2.49	0.42
4:D:126:GLU:O	4:D:130:ILE:N	2.43	0.42
5:E:61:LEU:HD11	5:E:71:GLN:HG3	2.00	0.42
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.20	0.42
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.54	0.42
1:A:927:GLU:O	1:A:931:ARG:HB3	2.19	0.42
2:B:1162:LEU:HD23	2:B:1162:LEU:HA	1.67	0.42
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.02	0.42
7:G:31:PHE:CE1	7:G:48:VAL:HB	2.52	0.42
20:T:25:LYS:HA	20:T:25:LYS:HD2	1.82	0.42
1:A:1161:LEU:HD11	1:A:1346:VAL:HG22	2.02	0.42
1:A:546:ARG:HG3	1:A:547:LYS:N	2.34	0.42
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.34	0.42
2:B:1043:ILE:HG21	2:B:1043:ILE:HD13	1.74	0.42
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.01	0.42
2:B:757:PRO:HA	2:B:1047:TYR:CD2	2.54	0.42
2:B:961:ILE:HG13	2:B:961:ILE:H	1.55	0.42
1:A:780:ASN:ND2	2:B:976:MET:SD	2.89	0.42
5:E:11:TRP:CZ2	5:E:36:THR:HA	2.54	0.42
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.55	0.42
16:P:204:ILE:HD12	16:P:206:GLU:HB2	2.00	0.42
17:Q:172:ASP:O	17:Q:176:LEU:N	2.39	0.42
1:A:522:PRO:CG	1:A:666:ARG:HE	2.33	0.42
2:B:751:LEU:HD12	2:B:751:LEU:HA	1.81	0.42
3:C:84:TYR:CE1	3:C:167:LYS:HE3	2.55	0.42
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.55	0.42
2:B:282:ARG:HH11	9:I:21:ASN:HD21	1.67	0.42
9:I:68:ILE:HG23	9:I:122:ARG:HD2	2.00	0.42
16:P:157:GLU:CD	16:P:333:LYS:HD3	2.40	0.42
17:Q:105:TYR:CE1	18:R:231:GLU:CB	2.86	0.42
22:X:15:DA:H2"	22:X:16:DA:C8	2.55	0.42
1:A:483:ARG:NH2	2:B:788:TYR:CE2	2.87	0.42
2:B:453:TRP:HB2	2:B:463:ARG:HB2	2.01	0.42
2:B:501:LEU:CD1	2:B:505:LEU:HD22	2.50	0.42
2:B:873:LEU:CB	2:B:874:PRO:CD	2.96	0.42
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.34	0.42
9:I:28:GLU:HG3	9:I:29:ASP:N	2.34	0.42
18:R:213:ASP:C	18:R:215:GLU:H	2.22	0.42
22:X:0:DG:H2"	22:X:1:DA:C8	2.55	0.42
23:Y:80:DT:H2'	23:Y:80:DT:H6	1.71	0.42
1:A:1130:ILE:HD12	1:A:1411:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:LEU:HD21	1:A:1308:TYR:CE2	2.54	0.42
1:A:693:ILE:HG21	2:B:1023:ARG:HE	1.85	0.42
1:A:24:GLY:O	2:B:1166:SER:HB3	2.20	0.42
2:B:728:MET:HE2	2:B:942:LYS:CG	2.45	0.42
13:M:35:PRO:HB2	13:M:36:GLU:OE1	2.19	0.42
13:M:106:THR:HA	23:Y:63:DG:H21	1.84	0.42
1:A:1176:TYR:HE1	9:I:52:CYS:HB2	1.85	0.42
1:A:118:LEU:HD12	1:A:148:CYS:HB3	2.02	0.42
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.91	0.42
2:B:414:GLU:HA	2:B:417:ILE:HG22	2.02	0.42
1:A:1484:MET:HE3	7:G:20:PRO:HD3	2.02	0.42
1:A:67:ARG:HH21	13:M:45:VAL:HB	1.85	0.42
14:N:333:ASN:HB3	14:N:359:ASN:O	2.20	0.42
14:N:314:LEU:HD12	16:P:242:GLN:NE2	2.34	0.42
16:P:295:MET:HG3	16:P:297:LYS:H	1.85	0.42
7:G:91:GLN:HG2	17:Q:145:PHE:CZ	2.54	0.42
17:Q:30:HIS:CE1	17:Q:62:VAL:HG22	2.54	0.42
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.85	0.42
1:A:1311:LEU:HA	1:A:1312:PRO:HD2	1.97	0.42
1:A:136:GLN:HG3	1:A:139:LYS:H	1.85	0.42
1:A:542:LEU:O	1:A:545:VAL:HG12	2.20	0.42
2:B:728:MET:SD	2:B:940:GLY:HA2	2.59	0.42
8:H:85:ALA:CB	8:H:144:LEU:CD2	2.98	0.42
21:U:225:ALA:O	21:U:227:GLU:N	2.51	0.42
1:A:1098:PRO:HA	1:A:1101:GLN:OE1	2.20	0.41
1:A:478:PRO:O	1:A:479:TRP:HB2	2.20	0.41
1:A:522:PRO:CB	1:A:666:ARG:HE	2.33	0.41
1:A:692:SER:O	1:A:828:LEU:HD22	2.20	0.41
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.84	0.41
10:J:5:VAL:HG12	10:J:6:ARG:HG3	2.02	0.41
11:K:63:VAL:HA	11:K:64:PRO:HD3	1.95	0.41
14:N:308:GLN:NE2	14:N:313:PRO:O	2.46	0.41
17:Q:136:PHE:HD1	17:Q:140:GLU:OE1	2.03	0.41
18:R:133:ILE:HG13	18:R:136:LYS:HG3	2.02	0.41
20:T:121:SER:OG	20:T:122:GLU:N	2.52	0.41
22:X:58:DC:H2"	22:X:59:DG:C8	2.54	0.41
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.17	0.41
1:A:1036:ASN:ND2	1:A:1036:ASN:C	2.73	0.41
1:A:1413:ALA:O	1:A:1418:GLY:HA3	2.19	0.41
1:A:929:ALA:C	1:A:931:ARG:N	2.73	0.41
2:B:65:ILE:O	2:B:85:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ALA:CB	20:T:201:ASP:CB	2.96	0.41
3:C:27:ASP:OD1	3:C:28:LEU:N	2.53	0.41
5:E:73:PHE:HD2	5:E:90:TYR:OH	2.02	0.41
8:H:96:VAL:HB	8:H:137:VAL:O	2.20	0.41
9:I:119:CYS:C	9:I:121:HIS:H	2.24	0.41
16:P:288:PHE:HA	16:P:289:PRO:HD3	1.96	0.41
17:Q:154:CYS:SG	17:Q:155:THR:N	2.93	0.41
18:R:196:ASP:C	18:R:198:LYS:N	2.45	0.41
2:B:92:TYR:CD1	20:T:145:LEU:CD1	2.96	0.41
1:A:823:VAL:HG13	1:A:835:GLU:HB3	2.02	0.41
1:A:924:TYR:OH	1:A:952:LEU:HB2	2.21	0.41
2:B:251:ALA:O	2:B:254:GLN:NE2	2.53	0.41
2:B:529:MET:HB2	2:B:624:PRO:HD2	2.03	0.41
5:E:11:TRP:HZ2	5:E:36:THR:HA	1.86	0.41
1:A:1473:LEU:HB3	7:G:59:ILE:HD12	2.01	0.41
18:R:167:LEU:HD22	18:R:200:ILE:HB	2.02	0.41
19:S:16:VAL:O	20:T:39:GLU:HA	2.19	0.41
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.55	0.41
2:B:92:TYR:HE1	20:T:143:GLN:NE2	2.15	0.41
20:T:179:ASP:OD1	20:T:183:VAL:HG23	2.21	0.41
21:U:233:LEU:HB3	21:U:234:LYS:H	1.77	0.41
1:A:133:SER:C	1:A:135:GLY:H	2.23	0.41
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.55	0.41
2:B:451:GLY:HA2	2:B:467:SER:HB3	2.01	0.41
2:B:849:ASP:OD1	2:B:850:ASP:N	2.53	0.41
3:C:52:ILE:HG21	3:C:55:ASN:HB2	2.01	0.41
3:C:71:ILE:HG22	3:C:148:ILE:HG21	2.02	0.41
9:I:84:HIS:N	9:I:84:HIS:CD2	2.85	0.41
13:M:11:PRO:O	13:M:12:ARG:CG	2.68	0.41
13:M:95:GLU:O	13:M:96:PHE:HD1	2.02	0.41
14:N:360:LEU:O	14:N:361:ASN:CB	2.69	0.41
16:P:283:TYR:CD2	16:P:285:PRO:HD3	2.55	0.41
17:Q:24:GLY:O	18:R:210:PHE:CE2	2.73	0.41
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.55	0.41
1:A:364:ARG:NE	1:A:500:GLU:CD	2.73	0.41
1:A:608:THR:OG1	1:A:610:PRO:CG	2.68	0.41
1:A:592:PHE:CZ	1:A:640:LEU:HD11	2.55	0.41
1:A:927:GLU:HG3	1:A:929:ALA:H	1.86	0.41
2:B:274:ARG:HA	2:B:278:PHE:O	2.20	0.41
3:C:42:VAL:CB	3:C:178:PRO:HG3	2.45	0.41
9:I:11:PHE:CD1	9:I:55:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ILE:HD13	10:J:15:GLY:HA3	2.03	0.41
12:L:26:ASN:C	12:L:28:ILE:H	2.24	0.41
17:Q:23:ARG:CG	18:R:208:CYS:O	2.69	0.41
21:U:133:ALA:HA	21:U:134:PRO:HD3	1.89	0.41
1:A:1432:PHE:HD1	1:A:1433:GLU:HB2	1.84	0.41
1:A:265:VAL:HG23	1:A:266:MET:H	1.85	0.41
1:A:378:VAL:O	1:A:475:ARG:N	2.53	0.41
1:A:366:VAL:O	1:A:481:THR:HB	2.21	0.41
1:A:546:ARG:NH2	1:A:550:LYS:HD2	2.35	0.41
1:A:623:PRO:HB3	8:H:122:LEU:HD13	2.03	0.41
1:A:974:ASP:HB2	1:A:1317:LYS:NZ	2.36	0.41
2:B:800:ALA:C	2:B:805:PHE:HB3	2.41	0.41
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.56	0.41
13:M:47:ASP:O	13:M:48:VAL:C	2.38	0.41
15:O:79:VAL:HG21	15:O:93:VAL:HG12	2.01	0.41
20:T:143:GLN:OE1	20:T:143:GLN:N	2.54	0.41
22:X:13:DA:H2"	22:X:14:DA:H8	1.83	0.41
23:Y:38:DT:H2"	23:Y:39:DG:C8	2.56	0.41
1:A:1024:ASN:OD1	1:A:1025:GLY:N	2.54	0.41
1:A:1179:PRO:HA	1:A:1209:PRO:HA	2.03	0.41
1:A:1299:GLN:HG2	1:A:1300:GLY:H	1.85	0.41
1:A:483:ARG:HH21	2:B:788:TYR:HE2	1.68	0.41
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.03	0.41
2:B:479:LEU:HA	2:B:479:LEU:HD12	1.84	0.41
2:B:733:MET:HE3	2:B:1054:MET:HE3	2.02	0.41
1:A:271:ARG:NH1	2:B:821:LYS:HE2	2.31	0.41
8:H:78:THR:HG21	11:K:78:THR:CG2	2.51	0.41
9:I:15:ARG:C	9:I:16:PHE:O	2.53	0.41
13:M:200:LYS:HE2	13:M:200:LYS:HB3	1.75	0.41
16:P:190:ALA:HB2	16:P:202:MET:HG2	2.01	0.41
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.68	0.41
20:T:155:PRO:O	20:T:156:VAL:HG22	2.21	0.41
20:T:159:HIS:ND1	20:T:160:GLN:N	2.65	0.41
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.21	0.41
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.51	0.41
1:A:598:GLY:HA2	1:A:633:GLY:HA3	2.02	0.41
2:B:181:PRO:HD3	2:B:475:PHE:HE1	1.86	0.41
2:B:631:GLN:HE21	2:B:685:LYS:HD2	1.86	0.41
2:B:895:PHE:HB2	2:B:896:LEU:H	1.67	0.41
2:B:897:ARG:O	2:B:898:THR:C	2.59	0.41
4:D:73:ARG:HD3	4:D:141:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:197:SER:HB3	5:E:201:GLY:H	1.85	0.41
8:H:108:ALA:C	8:H:110:THR:N	2.74	0.41
13:M:25:GLU:HG2	13:M:32:MET:SD	2.61	0.41
15:O:17:GLU:O	15:O:21:GLU:HG2	2.21	0.41
16:P:268:ILE:O	16:P:337:LYS:HE3	2.21	0.41
21:U:278:THR:HG22	21:U:285:MET:SD	2.60	0.41
1:A:1464:ALA:O	1:A:1466:ALA:N	2.52	0.41
1:A:256:PRO:HG2	1:A:261:ARG:HD3	2.02	0.41
1:A:608:THR:HB	1:A:610:PRO:HD2	1.97	0.41
2:B:237:VAL:HG12	2:B:372:LEU:HD22	2.02	0.41
2:B:38:GLY:H	2:B:41:ARG:HG2	1.85	0.41
2:B:422:PHE:CZ	2:B:429:PHE:HB2	2.55	0.41
2:B:527:ALA:HA	2:B:705:GLY:HA2	2.02	0.41
2:B:877:GLU:OE1	2:B:877:GLU:N	2.54	0.41
4:D:103:LEU:HD13	4:D:114:LEU:HD13	2.02	0.41
5:E:111:THR:HG23	22:X:56:DC:H4'	2.02	0.41
5:E:8:TYR:HD1	5:E:37:LEU:HD22	1.86	0.41
6:F:68:THR:HG21	7:G:59:ILE:HG21	2.02	0.41
6:F:71:LEU:HA	6:F:71:LEU:HD12	1.81	0.41
20:T:161:TYR:O	20:T:164:GLU:HB3	2.21	0.41
23:Y:77:DT:C6	23:Y:78:DT:H72	2.56	0.41
1:A:297:GLY:HA3	17:Q:57:LYS:CG	2.50	0.41
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.02	0.41
2:B:38:GLY:H	2:B:41:ARG:CG	2.34	0.41
1:A:576:GLN:HB2	8:H:73:GLY:O	2.20	0.41
8:H:81:ARG:C	8:H:83:SER:H	2.25	0.41
10:J:8:PHE:H	10:J:48:MET:HE3	1.85	0.41
18:R:151:LEU:HB3	18:R:154:LEU:HB3	2.03	0.41
18:R:194:ARG:HG3	18:R:201:LEU:CD1	2.50	0.41
22:X:43:DT:H2''	22:X:44:DC:C4'	2.51	0.41
1:A:367:ILE:HG21	1:A:367:ILE:HD13	1.87	0.41
1:A:616:GLY:O	1:A:619:LYS:HB2	2.21	0.41
2:B:927:ARG:NH2	2:B:1057:ASP:OD1	2.54	0.41
2:B:166:LEU:HB3	2:B:170:ASP:HB2	2.02	0.41
2:B:280:SER:HB2	2:B:283:ASP:OD2	2.21	0.41
2:B:422:PHE:C	2:B:422:PHE:CD1	2.92	0.41
2:B:496:ALA:CB	2:B:498:PRO:HD2	2.50	0.41
2:B:561:ILE:HA	2:B:561:ILE:HD12	1.95	0.41
3:C:1:MET:HB3	3:C:3:TYR:CE2	2.56	0.41
5:E:116:GLN:O	5:E:119:VAL:HB	2.21	0.41
5:E:61:LEU:HD12	5:E:72:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:15:CYS:SG	13:M:39:LEU:CD2	3.04	0.41
13:M:36:GLU:N	13:M:36:GLU:OE1	2.54	0.41
17:Q:109:HIS:CE1	18:R:231:GLU:CB	3.02	0.41
19:S:143:TRP:C	19:S:143:TRP:CD1	2.95	0.41
1:A:455:ILE:HD13	1:A:520:MET:HE1	2.02	0.40
2:B:191:GLU:OE1	2:B:472:ARG:HD2	2.21	0.40
2:B:299:GLU:OE2	2:B:302:LYS:HE3	2.21	0.40
2:B:626:LEU:HG	2:B:698:ILE:HG22	2.03	0.40
5:E:171:PRO:HB2	5:E:207:ARG:HD2	2.02	0.40
7:G:128:TYR:O	7:G:137:ILE:N	2.53	0.40
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.86	0.40
13:M:91:ALA:O	13:M:92:SER:C	2.58	0.40
16:P:171:THR:HG23	16:P:256:GLN:HG3	2.02	0.40
18:R:194:ARG:HA	18:R:194:ARG:HD3	1.61	0.40
18:R:194:ARG:HB2	18:R:201:LEU:HG	2.02	0.40
21:U:247:GLU:OE1	21:U:250:MET:HG3	2.22	0.40
21:U:252:LYS:HB3	21:U:253:THR:H	1.67	0.40
1:A:823:VAL:HA	1:A:835:GLU:HG2	2.03	0.40
2:B:751:LEU:CD1	2:B:808:SER:HB3	2.39	0.40
5:E:80:PRO:HA	5:E:107:GLN:HB3	2.03	0.40
1:A:1473:LEU:HD23	6:F:104:ILE:HD12	2.02	0.40
9:I:44:TYR:OH	9:I:46:GLN:NE2	2.47	0.40
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.86	0.40
18:R:194:ARG:HG3	18:R:201:LEU:HD12	2.03	0.40
1:A:539:GLN:HB3	2:B:790:GLN:HG2	2.03	0.40
1:A:595:ILE:HD12	1:A:596:ILE:N	2.36	0.40
1:A:921:ARG:HG3	1:A:956:PHE:CZ	2.57	0.40
2:B:957:THR:HG21	2:B:1026:GLU:OE1	2.22	0.40
2:B:229:SER:HA	2:B:405:ARG:HH22	1.84	0.40
2:B:406:GLY:HA2	2:B:409:LYS:HE2	2.04	0.40
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.86	0.40
8:H:85:ALA:HB3	8:H:144:LEU:HD21	2.04	0.40
9:I:66:THR:C	9:I:68:ILE:H	2.24	0.40
16:P:206:GLU:HB3	16:P:236:LYS:NZ	2.36	0.40
20:T:23:VAL:HA	20:T:24:PRO:HD3	1.94	0.40
20:T:174:LYS:HG2	22:X:19:DG:H4'	2.02	0.40
1:A:320:ASN:HB2	1:A:338:SER:HB3	2.03	0.40
1:A:604:ARG:HG2	1:A:605:THR:H	1.87	0.40
2:B:853:LEU:HB3	2:B:867:ILE:HG12	2.03	0.40
10:J:62:TYR:HB3	10:J:64:PRO:HD3	2.00	0.40
16:P:229:GLN:HA	16:P:232:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:149:THR:HG23	17:Q:151:THR:H	1.86	0.40
22:X:31:DG:H2'	22:X:32:DA:C5'	2.52	0.40
22:X:64:DG:H2'	22:X:65:DA:C8	2.57	0.40
1:A:1376:LYS:HD2	1:A:1379:GLU:OE2	2.22	0.40
1:A:485:ASN:OD1	1:A:487:SER:N	2.49	0.40
1:A:369:PRO:HB3	1:A:486:LEU:CD1	2.52	0.40
2:B:499:ARG:NH2	2:B:522:LEU:HD11	2.37	0.40
1:A:1471:PHE:HZ	6:F:61:GLU:HA	1.87	0.40
8:H:62:SER:O	8:H:140:ARG:NH2	2.54	0.40
9:I:88:LYS:HD3	9:I:119:CYS:SG	2.61	0.40
17:Q:113:ARG:NH1	18:R:218:LYS:HG3	2.37	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	A	1450/1970 (74%)	1258 (87%)	126 (9%)	66 (5%)	3	33
2	B	1163/1174 (99%)	1012 (87%)	109 (9%)	42 (4%)	4	40
3	C	273/275 (99%)	241 (88%)	23 (8%)	9 (3%)	5	42
4	D	127/142 (89%)	118 (93%)	9 (7%)	0	100	100
5	E	208/210 (99%)	188 (90%)	14 (7%)	6 (3%)	6	45
6	F	84/127 (66%)	78 (93%)	6 (7%)	0	100	100
7	G	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
8	H	148/150 (99%)	117 (79%)	23 (16%)	8 (5%)	2	30
9	I	123/125 (98%)	91 (74%)	19 (15%)	13 (11%)	0	11
10	J	65/67 (97%)	51 (78%)	8 (12%)	6 (9%)	1	16
11	K	115/117 (98%)	110 (96%)	1 (1%)	4 (4%)	4	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	44/58 (76%)	31 (70%)	8 (18%)	5 (11%)	0	9
13	M	308/316 (98%)	266 (86%)	28 (9%)	14 (4%)	3	33
14	N	109/376 (29%)	99 (91%)	8 (7%)	2 (2%)	11	54
15	O	97/109 (89%)	92 (95%)	4 (4%)	1 (1%)	19	64
16	P	183/339 (54%)	170 (93%)	9 (5%)	4 (2%)	8	50
17	Q	176/439 (40%)	151 (86%)	17 (10%)	8 (4%)	3	33
18	R	163/291 (56%)	126 (77%)	26 (16%)	11 (7%)	1	25
19	S	134/517 (26%)	123 (92%)	8 (6%)	3 (2%)	8	50
20	T	218/249 (88%)	189 (87%)	19 (9%)	10 (5%)	3	33
21	U	168/301 (56%)	145 (86%)	10 (6%)	13 (8%)	1	20
All	All	5525/7524 (73%)	4820 (87%)	480 (9%)	225 (4%)	6	36

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	48	GLU
1	A	133	SER
1	A	153	ILE
1	A	204	HIS
1	A	208	ASP
1	A	262	PRO
1	A	272	ASN
1	A	295	GLN
1	A	344	LYS
1	A	496	PHE
1	A	598	GLY
1	A	605	THR
1	A	607	SER
1	A	610	PRO
1	A	623	PRO
1	A	625	ASP
1	A	911	PRO
1	A	1117	VAL
1	A	1200	PRO
1	A	1299	GLN
1	A	1342	SER
2	B	61	ASP

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Mol	Chain	Res	Type
2	B	63	PRO
2	B	74	ALA
2	B	78	VAL
2	B	79	GLU
2	B	141	GLN
2	B	203	ASN
2	B	231	PRO
2	B	249	LYS
2	B	251	ALA
2	B	491	ARG
2	B	492	ASP
2	B	880	LEU
2	B	881	GLU
2	B	898	THR
2	B	901	THR
2	B	1136	GLU
2	B	1166	SER
3	C	143	VAL
5	E	47	LYS
5	E	49	SER
5	E	53	PRO
5	E	54	ARG
8	H	18	GLU
8	H	65	TYR
8	H	67	ASP
9	I	15	ARG
9	I	16	PHE
9	I	85	PRO
9	I	86	CYS
9	I	99	SER
9	I	104	ALA
9	I	106	ASP
9	I	118	HIS
10	J	64	PRO
12	L	28	ILE
13	M	10	LEU
13	M	11	PRO
13	M	12	ARG
13	M	48	VAL
13	M	87	GLY
14	N	355	ASP
15	O	4	GLN

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Mol	Chain	Res	Type
16	P	207	PRO
16	P	208	ARG
17	Q	25	PHE
17	Q	103	VAL
17	Q	118	GLU
18	R	140	LYS
18	R	163	LEU
18	R	195	PRO
18	R	197	LYS
20	T	124	TYR
20	T	142	SER
20	T	145	LEU
21	U	227	GLU
21	U	231	ASP
21	U	257	GLN
21	U	277	GLN
21	U	293	GLU
1	A	77	ASN
1	A	134	LYS
1	A	154	CYS
1	A	195	GLY
1	A	206	ASN
1	A	213	LYS
1	A	299	ALA
1	A	452	ASP
1	A	531	ASN
1	A	611	ASP
1	A	929	ALA
1	A	931	ARG
1	A	932	ARG
1	A	1275	VAL
1	A	1315	ASP
2	B	23	GLN
2	B	250	SER
2	B	428	ASP
2	B	518	HIS
2	B	527	ALA
2	B	549	SER
2	B	561	ILE
2	B	879	GLU
3	C	5	ASN
3	C	213	GLU

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Mol	Chain	Res	Type
5	E	48	PRO
8	H	109	ALA
8	H	149	ALA
9	I	92	LYS
9	I	103	ARG
10	J	2	ILE
12	L	25	GLU
13	M	90	ALA
13	M	92	SER
13	M	93	PHE
16	P	297	LYS
16	P	299	ARG
17	Q	70	LYS
17	Q	104	LYS
17	Q	125	ALA
18	R	147	ASP
18	R	216	PHE
20	T	141	LEU
20	T	155	PRO
20	T	156	VAL
20	T	171	GLU
20	T	180	LYS
20	T	229	HIS
21	U	226	GLU
21	U	252	LYS
21	U	253	THR
1	A	184	CYS
1	A	210	GLN
1	A	374	SER
1	A	599	HIS
1	A	624	GLY
1	A	894	ASP
1	A	1102	MET
1	A	1103	THR
1	A	1265	ASP
1	A	1435	THR
2	B	77	GLU
2	B	513	GLU
2	B	685	LYS
2	B	873	LEU
2	B	884	ASN
8	H	24	ARG

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Mol	Chain	Res	Type
10	J	6	ARG
10	J	65	LEU
11	K	69	HIS
11	K	80	ASP
11	K	111	ASP
13	M	56	SER
13	M	61	THR
13	M	306	PHE
17	Q	158	HIS
18	R	149	LYS
18	R	174	ALA
18	R	226	ASP
19	S	154	THR
21	U	228	MET
21	U	250	MET
21	U	279	ARG
21	U	294	CYS
1	A	261	ARG
1	A	265	VAL
1	A	300	ALA
1	A	615	SER
1	A	1113	SER
2	B	118	LEU
2	B	226	GLU
2	B	839	GLY
2	B	1006	VAL
3	C	7	PRO
3	C	138	ASP
11	K	112	LYS
12	L	16	ILE
12	L	27	GLU
13	M	101	TYR
14	N	312	GLU
17	Q	126	SER
18	R	156	ASP
19	S	151	ARG
20	T	178	ALA
21	U	233	LEU
1	A	65	ILE
1	A	132	LYS
1	A	485	ASN
1	A	612	ASP

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Mol	Chain	Res	Type
1	A	817	PRO
1	A	935	GLN
1	A	1114	ALA
1	A	1274	GLU
2	B	290	TYR
2	B	460	HIS
2	B	521	GLY
2	B	1129	ASN
3	C	147	ASP
9	I	12	VAL
10	J	30	THR
13	M	41	VAL
13	M	60	ALA
18	R	139	PHE
19	S	160	ALA
1	A	650	GLY
1	A	726	GLU
1	A	729	PRO
2	B	1025	ASN
3	C	74	ILE
8	H	21	LYS
8	H	139	SER
9	I	67	GLN
1	A	687	ILE
2	B	253	GLY
3	C	218	ALA
9	I	68	ILE
12	L	20	GLY
1	A	621	ILE
1	A	622	SER
2	B	136	GLY
3	C	151	VAL
5	E	51	GLY
10	J	5	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1279/1748 (73%)	1228 (96%)	51 (4%)	38	73
2	B	1020/1028 (99%)	989 (97%)	31 (3%)	48	78
3	C	252/252 (100%)	246 (98%)	6 (2%)	57	82
4	D	119/126 (94%)	119 (100%)	0	100	100
5	E	192/192 (100%)	186 (97%)	6 (3%)	47	78
6	F	74/111 (67%)	73 (99%)	1 (1%)	74	89
7	G	152/153 (99%)	150 (99%)	2 (1%)	76	89
8	H	131/131 (100%)	127 (97%)	4 (3%)	47	78
9	I	112/112 (100%)	107 (96%)	5 (4%)	34	71
10	J	56/56 (100%)	54 (96%)	2 (4%)	42	76
11	K	106/106 (100%)	101 (95%)	5 (5%)	32	70
12	L	43/55 (78%)	41 (95%)	2 (5%)	32	70
13	M	263/268 (98%)	252 (96%)	11 (4%)	36	72
14	N	105/324 (32%)	104 (99%)	1 (1%)	82	91
15	O	90/98 (92%)	90 (100%)	0	100	100
16	P	159/293 (54%)	156 (98%)	3 (2%)	65	86
17	Q	164/373 (44%)	157 (96%)	7 (4%)	35	72
18	R	150/261 (58%)	144 (96%)	6 (4%)	38	73
19	S	121/448 (27%)	118 (98%)	3 (2%)	55	82
20	T	196/218 (90%)	189 (96%)	7 (4%)	42	76
21	U	148/266 (56%)	140 (95%)	8 (5%)	27	67
All	All	4932/6619 (74%)	4771 (97%)	161 (3%)	49	77

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	87	HIS
1	A	117	LEU
1	A	132	LYS
1	A	133	SER
1	A	181	HIS
1	A	204	HIS
1	A	205	VAL
1	A	212	LYS
1	A	213	LYS

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Mol	Chain	Res	Type
1	A	220	ARG
1	A	231	GLU
1	A	261	ARG
1	A	264	VAL
1	A	277	THR
1	A	343	LEU
1	A	449	HIS
1	A	463	THR
1	A	477	LEU
1	A	500	GLU
1	A	508	SER
1	A	546	ARG
1	A	587	THR
1	A	595	ILE
1	A	611	ASP
1	A	619	LYS
1	A	625	ASP
1	A	666	ARG
1	A	839	HIS
1	A	849	ASP
1	A	908	THR
1	A	931	ARG
1	A	954	ARG
1	A	981	CYS
1	A	1036	ASN
1	A	1050	CYS
1	A	1066	ASP
1	A	1075	LYS
1	A	1115	LYS
1	A	1139	LEU
1	A	1192	TRP
1	A	1203	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1309	MET
1	A	1318	LYS
1	A	1319	LYS
1	A	1337	GLU
1	A	1339	ASP
1	A	1375	ARG
1	A	1420	ASN
2	B	73	HIS

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Mol	Chain	Res	Type
2	B	77	GLU
2	B	79	GLU
2	B	129	THR
2	B	133	ILE
2	B	146	LYS
2	B	161	CYS
2	B	168	ASP
2	B	225	LEU
2	B	250	SER
2	B	287	HIS
2	B	302	LYS
2	B	414	GLU
2	B	422	PHE
2	B	483	ARG
2	B	548	TRP
2	B	591	ARG
2	B	666	ASP
2	B	711	ILE
2	B	737	ILE
2	B	785	TYR
2	B	793	SER
2	B	853	LEU
2	B	880	LEU
2	B	881	GLU
2	B	895	PHE
2	B	896	LEU
2	B	897	ARG
2	B	957	THR
2	B	1054	MET
2	B	1069	ILE
3	C	5	ASN
3	C	63	PHE
3	C	114	HIS
3	C	137	ASN
3	C	195	THR
3	C	273	THR
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	64	HIS
5	E	127	LEU
5	E	172	ARG

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Mol	Chain	Res	Type
6	F	121	ASP
7	G	22	LEU
7	G	128	TYR
8	H	38	ASP
8	H	70	LEU
8	H	84	ARG
8	H	107	GLU
9	I	14	ILE
9	I	15	ARG
9	I	60	HIS
9	I	61	GLU
9	I	66	THR
10	J	36	ASP
10	J	47	ARG
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
11	K	111	ASP
11	K	112	LYS
12	L	19	CYS
12	L	27	GLU
13	M	10	LEU
13	M	14	THR
13	M	31	ASP
13	M	39	LEU
13	M	43	ASP
13	M	47	ASP
13	M	86	LYS
13	M	93	PHE
13	M	129	ASN
13	M	133	ASN
13	M	151	LEU
14	N	20	ASP
16	P	203	ARG
16	P	239	ARG
16	P	297	LYS
17	Q	16	ARG
17	Q	97	ARG
17	Q	103	VAL
17	Q	135	THR
17	Q	139	LEU
17	Q	177	LEU

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Mol	Chain	Res	Type
17	Q	202	GLU
18	R	108	HIS
18	R	177	ASN
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	209	GLN
19	S	35	ASP
19	S	166	ARG
19	S	177	MET
20	T	147	LYS
20	T	154	LYS
20	T	156	VAL
20	T	177	ARG
20	T	185	ASP
20	T	201	ASP
20	T	204	ASP
21	U	205	ASN
21	U	226	GLU
21	U	233	LEU
21	U	252	LYS
21	U	257	GLN
21	U	276	VAL
21	U	292	ASN
21	U	301	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	122	ASN
1	A	181	HIS
1	A	353	ASN
1	A	539	GLN
1	A	1034	GLN
1	A	1036	ASN
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	175	ASN
2	B	1021	HIS
3	C	137	ASN

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Mol	Chain	Res	Type
3	C	260	GLN
5	E	148	HIS
7	G	24	ASN
9	I	60	HIS
9	I	84	HIS
10	J	61	ASN
11	K	29	ASN
12	L	23	HIS
13	M	129	ASN
19	S	141	HIS
19	S	142	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.