



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:53 AM UTC

PDB ID : 5XXU / pdb_00005xxu
EMDB ID : EMD-6780
Title : Small subunit of Toxoplasma gondii ribosome
Authors : LI, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on : 2017-07-05
Resolution : 3.35 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

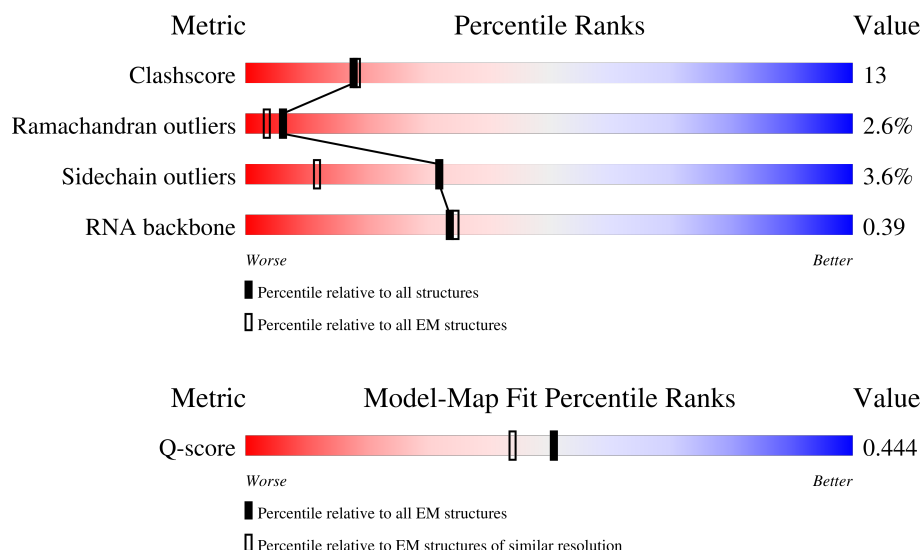
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.35 Å.

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



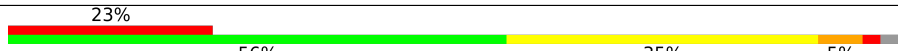
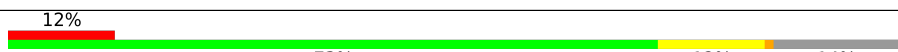
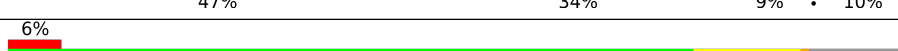
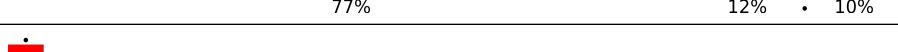
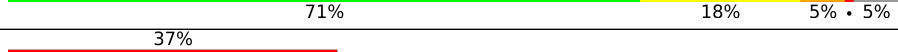
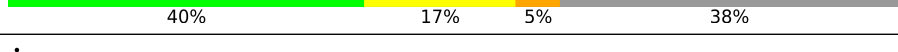
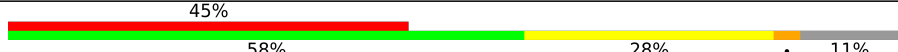
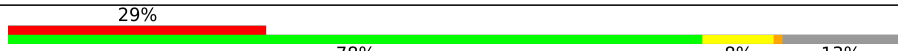
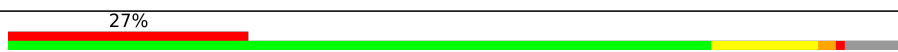
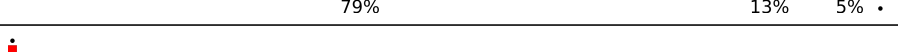
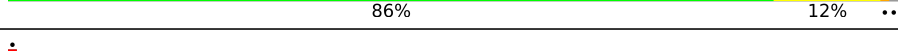
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

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

Mol	Chain	Length	Quality of chain
1	2	1791	
2	A	287	
3	B	259	

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Mol	Chain	Length	Quality of chain
4	C	269	
5	D	235	
6	E	263	
7	F	192	
8	G	256	
9	H	196	
10	I	205	
11	J	188	
12	K	152	
13	L	161	
14	M	142	
15	N	151	
16	O	156	
17	P	150	
18	Q	148	
19	R	132	
20	S	156	
21	T	160	
22	U	233	
23	V	82	
24	W	130	
25	X	143	
26	Y	135	
27	Z	161	
28	a	112	

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Mol	Chain	Length	Quality of chain
29	b	82	7% 77% 20%
30	c	68	24% 68% 15% 16%
31	d	54	17% 67% 20% 7% 6%
32	e	59	14% 81% 15%
33	f	154	29% 29% 71%
34	m	39	41% 41% 13%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 68955 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 RNA chain called 18S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1619	Total	C	N	O	P	0	0
			34513	15429	6130	11335	1619		

- Molecule 2 is a protein called Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	198	Total	C	N	O	S	0	0
			1565	1003	271	279	12		

- Molecule 3 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	212	Total	C	N	O	S	0	0
			1691	1070	301	303	17		

- Molecule 4 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	225	Total	C	N	O	S	0	0
			1750	1124	311	306	9		

- Molecule 5 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	200	Total	C	N	O	S	0	0
			1568	987	291	279	11		

- Molecule 6 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	259	Total	C	N	O	S	0	0
			2085	1325	400	346	14		

- Molecule 7 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	187	Total	C	N	O	S	0	0
			1475	921	280	263	11		

- Molecule 8 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	220	Total	C	N	O	S	0	0
			1782	1118	354	303	7		

- Molecule 9 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	177	Total	C	N	O	S	0	0
			1354	862	250	238	4		

- Molecule 10 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	185	Total	C	N	O	S	0	0
			1496	936	298	254	8		

- Molecule 11 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	178	Total	C	N	O	S	0	0
			1457	924	286	244	3		

- Molecule 12 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	94	Total	C	N	O	S	0	0
			675	433	118	122	2		

- Molecule 13 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	147	Total	C	N	O	S	0	0
			1206	766	231	203	6		

- Molecule 14 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	99	Total	C	N	O	0	0
			508	307	99	102		

- Molecule 15 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1204	773	225	204	2		

- Molecule 16 is a protein called Ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	129	Total	C	N	O	S	0	0
			966	591	194	177	4		

- Molecule 17 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	115	Total	C	N	O	S	0	0
			939	603	168	162	6		

- Molecule 18 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	138	Total	C	N	O	S	0	0
			1086	693	205	185	3		

- Molecule 19 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	117	Total	C	N	O	S	0	0
			947	590	182	171	4		

- Molecule 20 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1091	684	219	186	2		

- Molecule 21 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	151	Total	C	N	O	S	0	0
			1236	789	233	210	4		

- Molecule 22 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	103	Total	C	N	O	S	0	0
			823	517	153	151	2		

- Molecule 23 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	80	Total	C	N	O	S	0	0
			618	379	119	116	4		

- Molecule 24 is a protein called Ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1040	660	195	178	7		

- Molecule 25 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	135	Total	C	N	O	S	0	0
			1040	659	203	177	1		

- Molecule 26 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	128	Total	C	N	O	S	0	0
			1020	647	200	171	2		

- Molecule 27 is a protein called Ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	71	Total	C	N	O	S	0	0
			576	365	108	102	1		

- Molecule 28 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	99	Total	C	N	O	S	0	0
			794	480	171	137	6		

- Molecule 29 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	79	Total	C	N	O	S	0	0
			605	383	106	107	9		

- Molecule 30 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	57	Total	C	N	O	S	0	0
			448	279	91	77	1		

- Molecule 31 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	51	Total	C	N	O	S	0	0
			429	269	90	63	7		

- Molecule 32 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	50	Total	C	N	O	0	0
			391	242	85	64		

- Molecule 33 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	f	45	Total	C	N	O	0	0
			229	139	45	45		

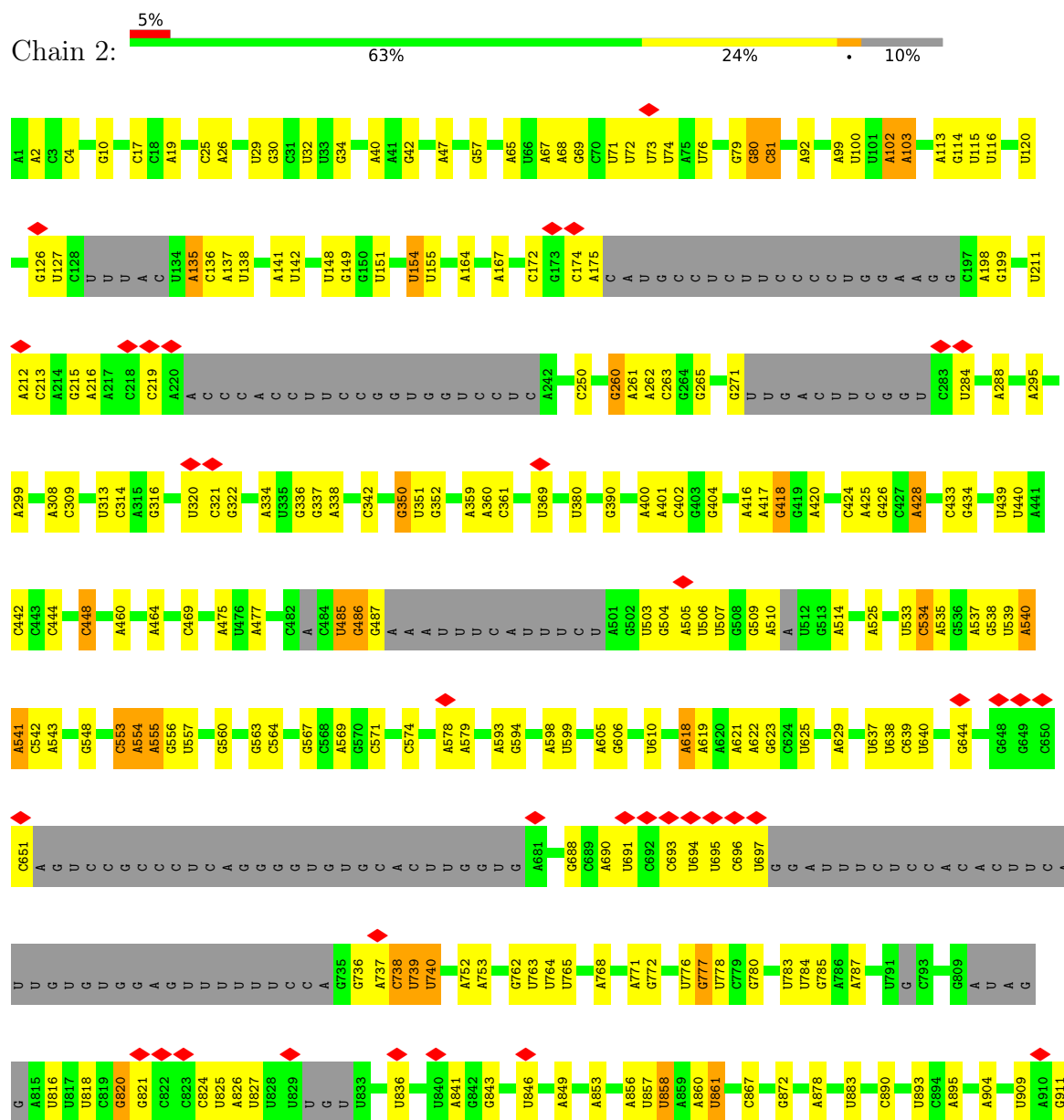
- Molecule 34 is a protein called Ribosomal protein eL41.

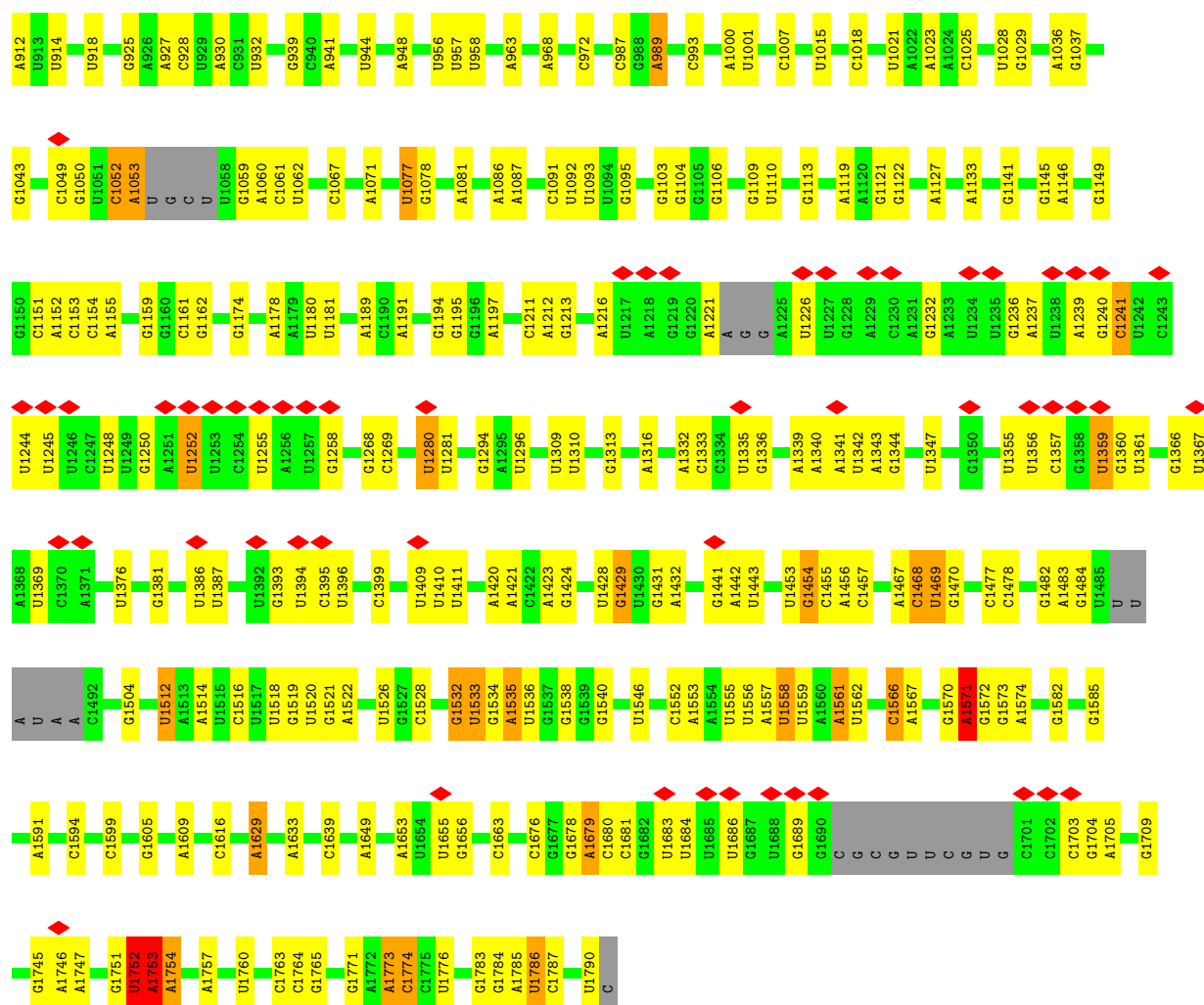
Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	38	Total	C	N	O	S	0	0
			348	213	89	44	2		

3 Residue-property plots

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

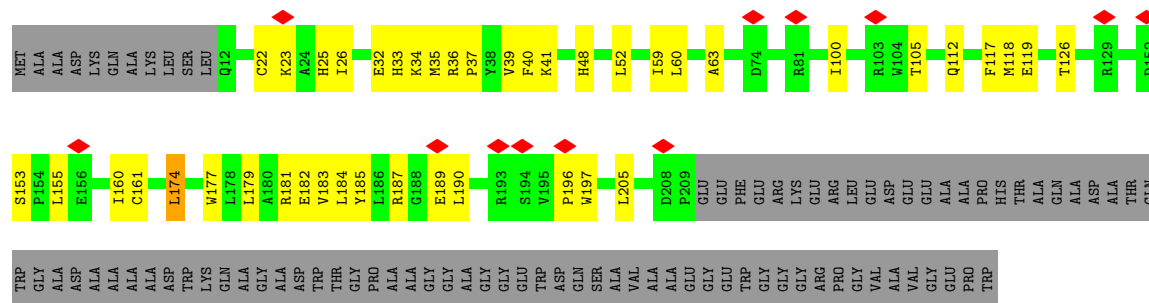
• Molecule 1: 18S RNA





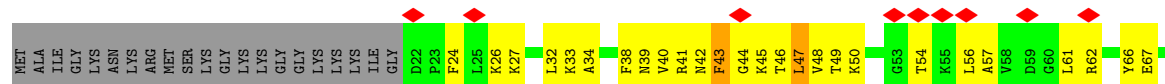
• Molecule 2: Ribosomal protein uS2

Chain A: 54% 15% 31%

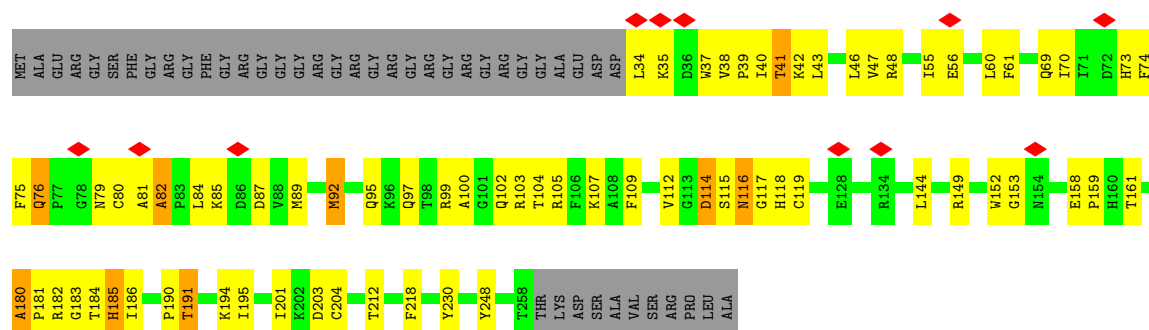


• Molecule 3: Ribosomal protein eS1

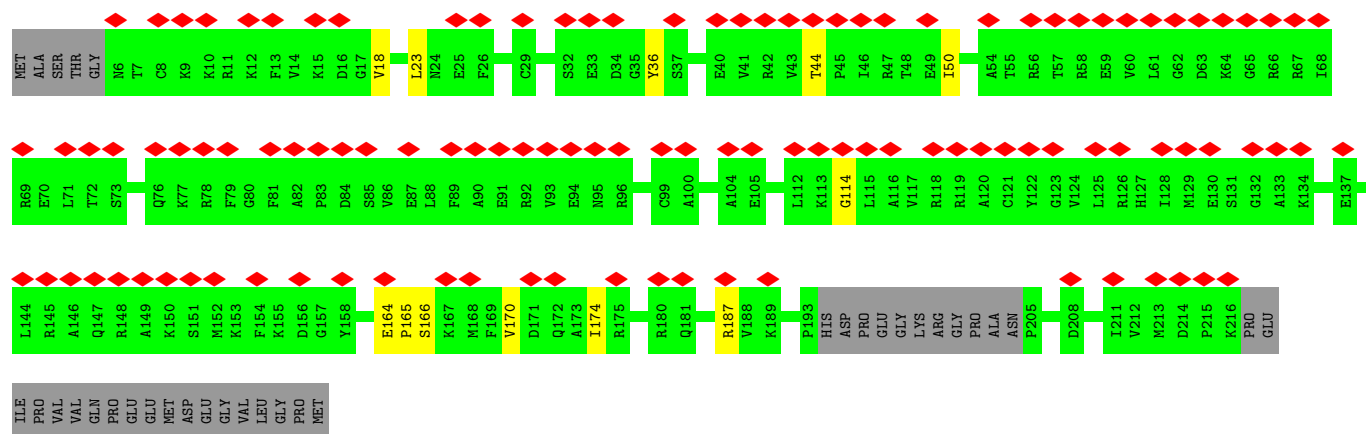
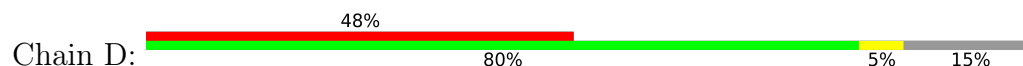
Chain B: 7% 44% 35% 18%



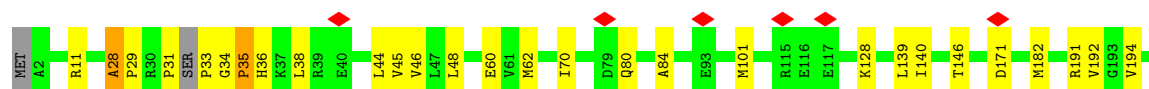
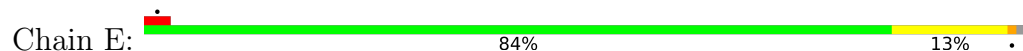
- Molecule 4: Ribosomal protein uS5

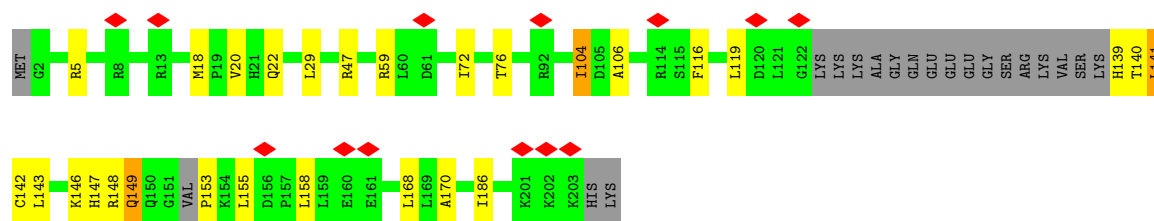


- Molecule 5: Ribosomal protein uS3



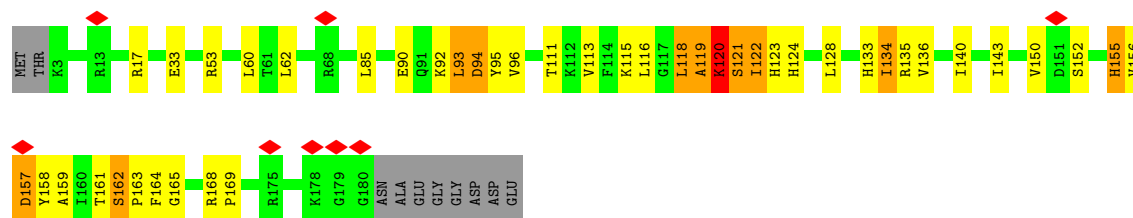
- Molecule 6: Ribosomal protein eS4





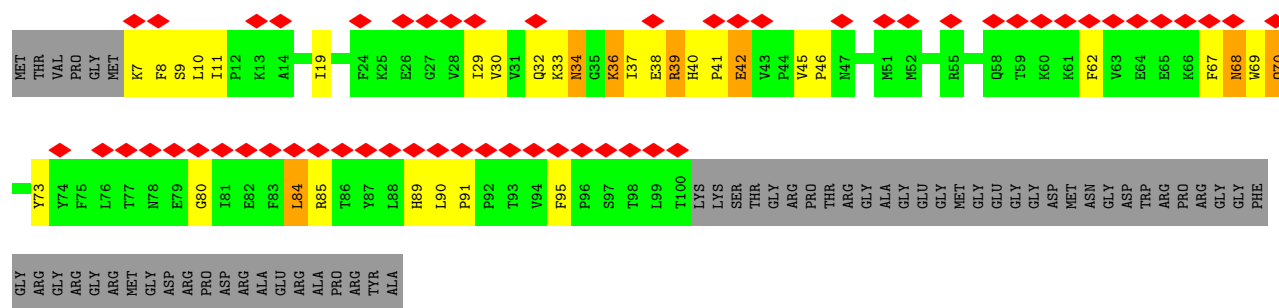
• Molecule 11: Ribosomal protein uS4

Chain J: 71% 18% 5% • 5%



• Molecule 12: Ribosomal protein eS10

Chain K: 37% 40% 17% 5% 38%



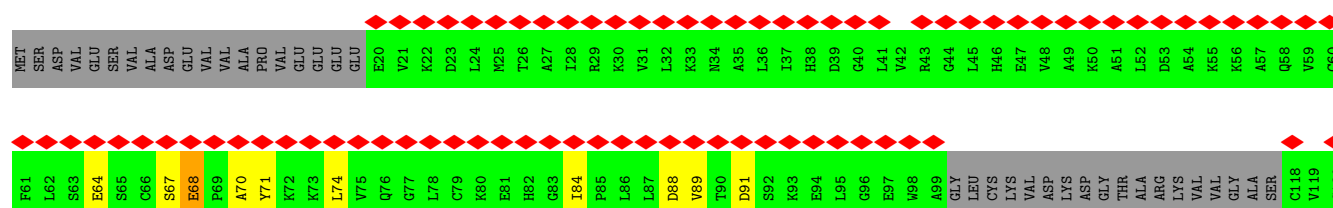
• Molecule 13: Ribosomal protein uS17

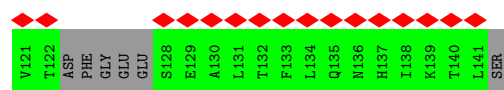
Chain L: 80% 11% • 9%



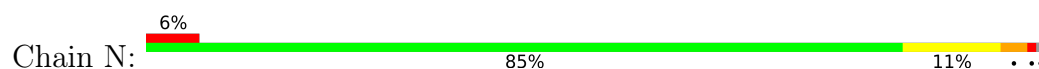
• Molecule 14: Ribosomal protein eS12

Chain M: 68% 63% 6% • 30%

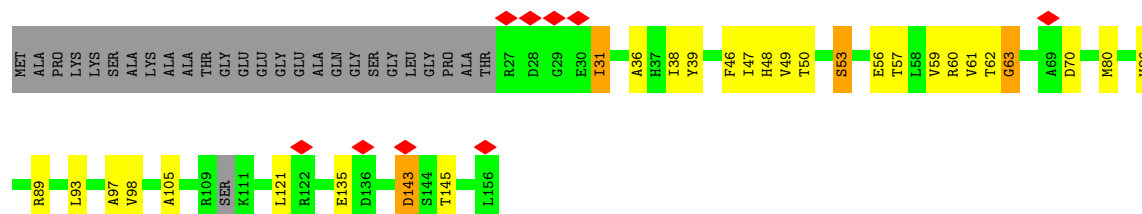




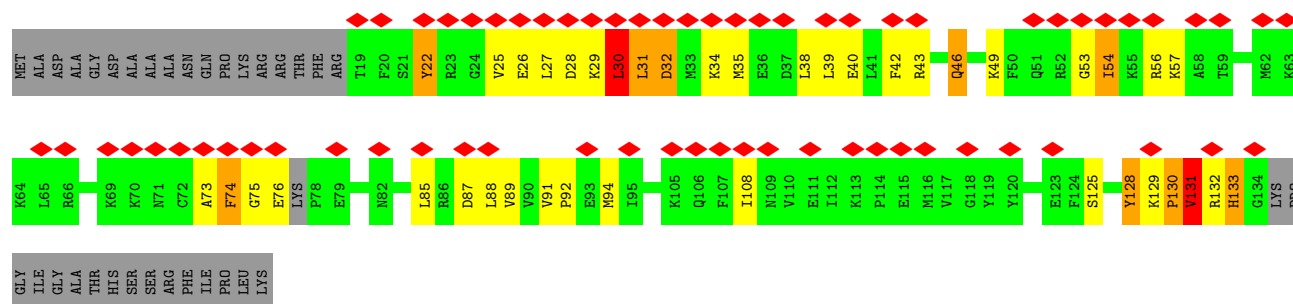
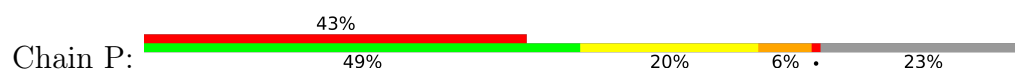
- Molecule 15: Ribosomal protein uS15



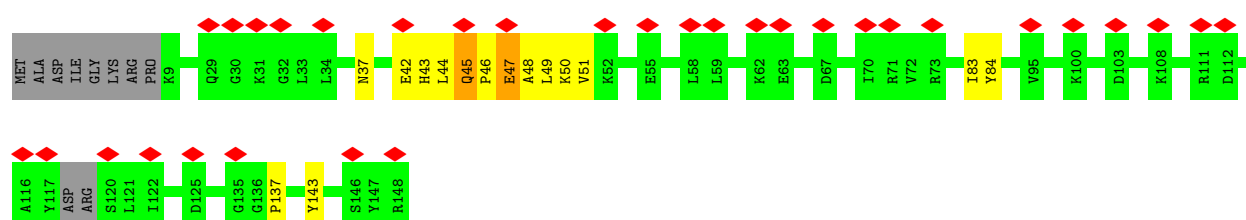
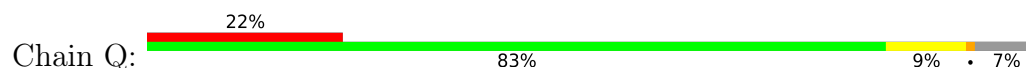
- Molecule 16: Ribosomal protein uS11



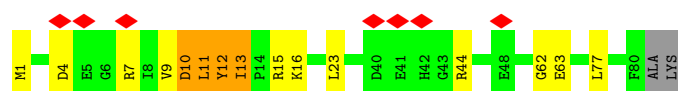
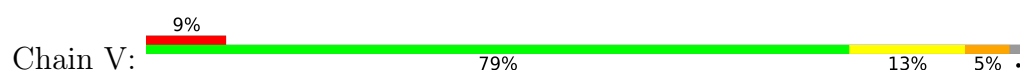
- Molecule 17: Ribosomal protein uS19



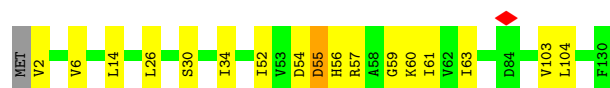
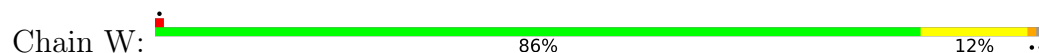
- Molecule 18: Ribosomal protein uS9



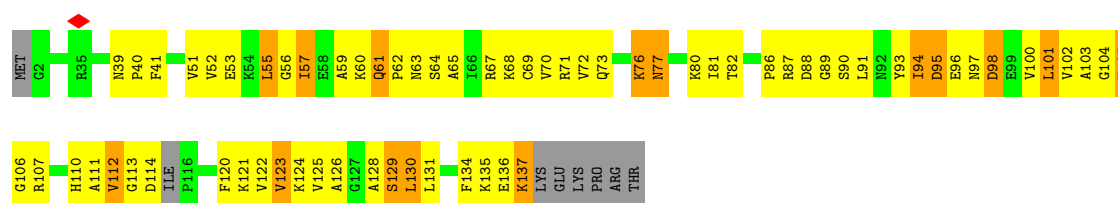
- Molecule 19: Ribosomal protein eS17



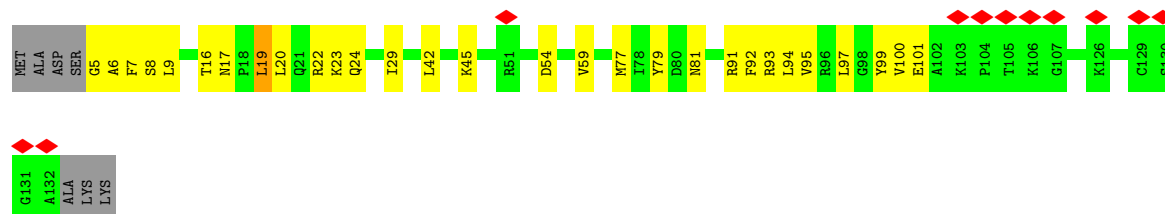
- Molecule 24: Ribosomal protein uS8



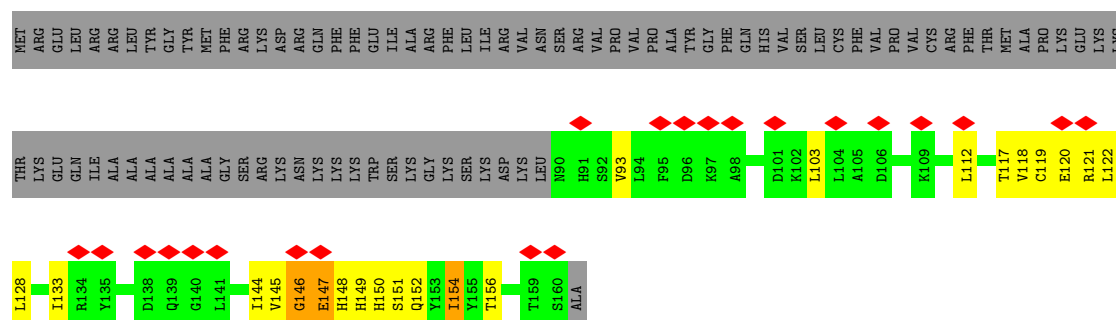
- Molecule 25: Ribosomal protein uS12



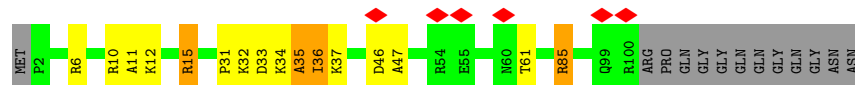
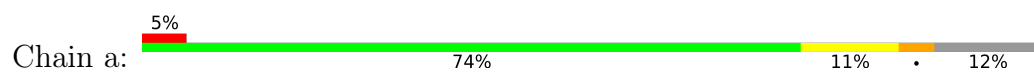
- Molecule 26: Ribosomal protein eS24



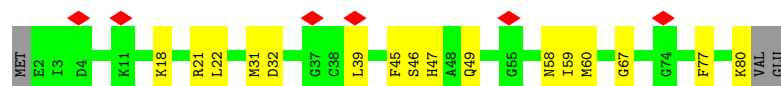
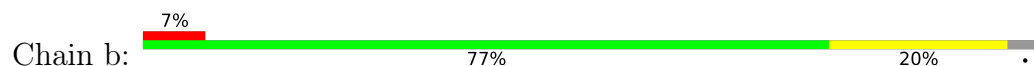
- Molecule 27: Ribosomal protein eS25



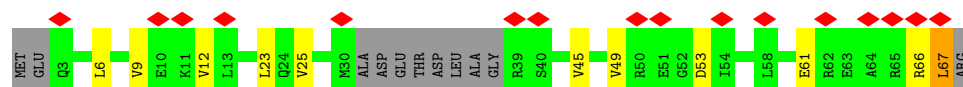
- Molecule 28: Ribosomal protein eS26



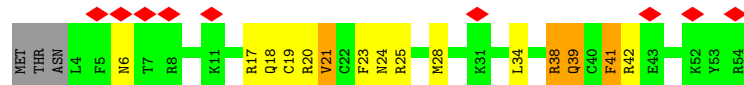
- Molecule 29: Ribosomal protein eS27



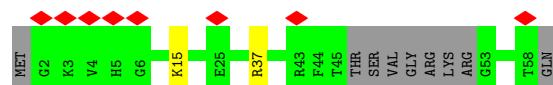
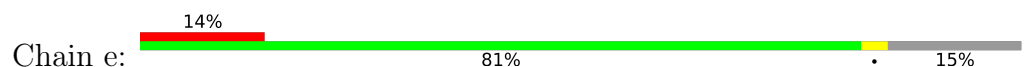
- Molecule 30: Ribosomal protein eS28



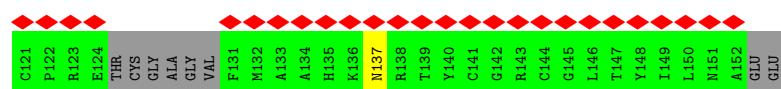
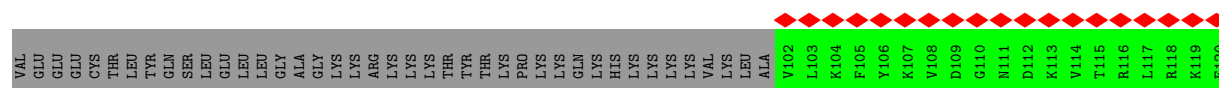
- Molecule 31: Ribosomal protein uS14



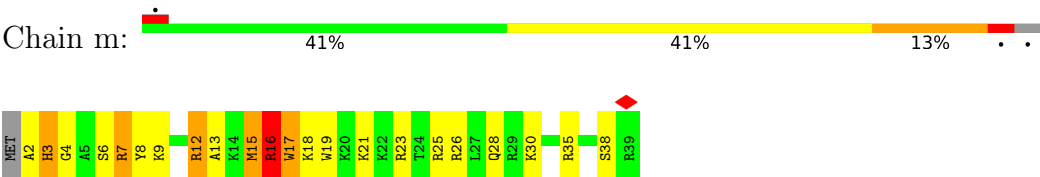
- Molecule 32: Ribosomal protein eS30



- Molecule 33: Ribosomal protein eS31



- Molecule 34: Ribosomal protein eL41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.37	0/38592	0.66	18/60102 (0.0%)
2	A	0.54	0/1600	0.77	0/2175
3	B	0.51	1/1716 (0.1%)	0.85	5/2297 (0.2%)
4	C	0.59	0/1792	0.94	11/2423 (0.5%)
5	D	0.54	0/1586	0.70	0/2121
6	E	0.53	0/2129	0.74	2/2860 (0.1%)
7	F	0.54	0/1495	0.99	7/2007 (0.3%)
8	G	0.51	0/1802	0.72	0/2390
9	H	0.53	1/1371 (0.1%)	1.03	10/1843 (0.5%)
10	I	0.52	0/1523	0.76	2/2031 (0.1%)
11	J	0.53	0/1481	0.92	3/1977 (0.2%)
12	K	0.73	1/691 (0.1%)	1.10	10/946 (1.1%)
13	L	0.46	0/1228	0.62	0/1639
14	M	0.72	0/507	0.94	1/703 (0.1%)
15	N	0.59	0/1230	0.90	5/1654 (0.3%)
16	O	0.53	0/977	0.82	2/1311 (0.2%)
17	P	0.54	0/955	0.93	7/1274 (0.5%)
18	Q	0.54	0/1102	0.78	1/1477 (0.1%)
19	R	0.56	0/956	0.90	1/1283 (0.1%)
20	S	0.54	0/1109	0.75	0/1489
21	T	0.56	0/1266	0.86	1/1706 (0.1%)
22	U	0.52	0/833	0.66	0/1126
23	V	0.51	0/627	0.82	0/842
24	W	0.49	0/1056	0.75	1/1412 (0.1%)
25	X	0.51	0/1057	1.01	4/1412 (0.3%)
26	Y	0.48	0/1036	0.76	0/1373
27	Z	0.52	0/587	0.88	1/793 (0.1%)
28	a	0.52	0/805	0.89	3/1076 (0.3%)
29	b	0.52	0/617	0.71	0/830
30	c	0.54	0/449	0.64	0/597
31	d	0.51	0/438	0.98	4/578 (0.7%)
32	e	0.49	0/396	0.67	0/522
33	f	0.61	0/228	0.72	0/315
34	m	0.41	0/353	0.81	1/457 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.46	3/73590 (0.0%)	0.74	100/107041 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	189	ILE	C-N	6.16	1.39	1.33
12	K	90	LEU	C-N	5.23	1.39	1.33
9	H	55	VAL	C-N	5.05	1.39	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	94	ILE	N-CA-C	10.00	120.02	110.42
28	a	35	ALA	N-CA-C	8.83	120.91	111.28
9	H	75	THR	N-CA-C	8.82	120.89	111.28
9	H	76	VAL	N-CA-C	8.44	121.99	113.47
31	d	41	PHE	N-CA-C	8.23	120.33	111.36
17	P	29	LYS	N-CA-C	8.22	120.32	111.36
7	F	39	HIS	N-CA-C	8.03	121.88	110.23
1	2	1077	U	C4'-C3'-O3'	7.94	121.31	109.40
9	H	115	VAL	N-CA-C	7.85	118.62	110.62
1	2	1566	C	C4'-C3'-O3'	7.66	120.89	109.40
15	N	22	PRO	C-N-CD	7.61	137.35	120.60
7	F	35	VAL	N-CA-C	7.38	118.45	108.11
1	2	1359	U	C4'-C3'-O3'	7.29	120.34	109.40
1	2	540	A	C4'-C3'-O3'	7.14	120.11	109.40
18	Q	45	GLN	C-N-CD	7.09	136.21	120.60
1	2	154	U	C2'-C3'-O3'	7.03	120.04	109.50
11	J	119	ALA	N-CA-C	6.93	118.84	111.28
1	2	1535	A	C2'-C3'-O3'	-6.90	103.35	113.70
14	M	64	GLU	N-CA-C	-6.86	103.74	111.14
25	X	61	GLN	C-N-CD	6.86	135.68	120.60
1	2	102	A	C2'-C3'-O3'	6.80	119.70	109.50
1	2	1752	U	C2'-C3'-O3'	6.76	119.65	109.50
11	J	155	HIS	N-CA-C	6.76	119.49	111.71
17	P	128	TYR	N-CA-C	6.73	119.95	109.52
1	2	1280	U	C2'-C3'-O3'	6.70	119.55	109.50
12	K	95	PHE	N-CA-C	6.59	120.54	108.94
1	2	350	G	C4'-C3'-O3'	6.57	119.25	109.40
3	B	80	GLY	N-CA-C	-6.44	105.00	112.73
9	H	132	ASP	N-CA-C	6.42	118.36	111.36
34	m	17	TRP	N-CA-C	6.28	118.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	26	TYR	N-CA-C	-6.21	104.59	111.36
4	C	180	ALA	CA-C-N	-6.15	114.31	120.21
4	C	180	ALA	C-N-CA	-6.15	114.31	120.21
12	K	90	LEU	CA-C-N	-6.08	114.12	120.38
12	K	90	LEU	C-N-CA	-6.08	114.12	120.38
31	d	21	VAL	N-CA-C	6.04	116.21	110.53
16	O	105	ALA	N-CA-C	-6.02	104.71	111.28
25	X	130	LEU	N-CA-C	6.02	117.92	111.36
25	X	123	VAL	N-CA-C	6.00	116.78	110.72
3	B	189	ILE	CB-CA-C	-5.92	108.08	114.35
4	C	114	ASP	N-CA-C	-5.86	99.35	108.90
7	F	27	ILE	N-CA-C	-5.83	102.04	109.80
24	W	55	ASP	N-CA-C	-5.77	102.91	110.53
1	2	1571	A	C2'-C3'-O3'	5.77	118.16	109.50
9	H	55	VAL	CA-C-N	-5.75	113.62	119.83
9	H	55	VAL	C-N-CA	-5.75	113.62	119.83
12	K	40	HIS	CA-C-N	-5.71	113.88	119.76
12	K	40	HIS	C-N-CA	-5.71	113.88	119.76
7	F	169	ALA	N-CA-C	-5.70	105.07	111.28
17	P	130	PRO	N-CA-C	5.67	124.16	112.47
28	a	37	LYS	N-CA-C	5.65	118.32	108.76
15	N	135	LEU	CA-C-N	-5.63	113.98	119.78
15	N	135	LEU	C-N-CA	-5.63	113.98	119.78
10	I	18	MET	CA-C-N	-5.62	114.14	119.76
10	I	18	MET	C-N-CA	-5.62	114.14	119.76
15	N	21	LYS	CA-C-N	-5.62	114.59	120.38
15	N	21	LYS	C-N-CA	-5.62	114.59	120.38
27	Z	146	GLY	N-CA-C	-5.61	102.95	111.14
9	H	191	PHE	CA-C-N	-5.60	113.99	119.76
9	H	191	PHE	C-N-CA	-5.60	113.99	119.76
3	B	189	ILE	CA-C-N	-5.56	114.16	120.89
3	B	189	ILE	C-N-CA	-5.56	114.16	120.89
4	C	38	VAL	CA-C-N	-5.55	114.05	119.76
4	C	38	VAL	C-N-CA	-5.55	114.05	119.76
4	C	76	GLN	CA-C-N	-5.52	114.07	119.76
4	C	76	GLN	C-N-CA	-5.52	114.07	119.76
9	H	133	ILE	N-CA-C	5.51	115.71	110.42
7	F	28	ALA	N-CA-C	5.50	119.69	112.92
12	K	91	PRO	CA-C-N	-5.50	114.09	119.76
12	K	91	PRO	C-N-CA	-5.50	114.09	119.76
19	R	37	GLU	N-CA-C	5.50	117.08	111.14
6	E	28	ALA	CA-C-N	-5.48	114.11	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	28	ALA	C-N-CA	-5.48	114.11	119.76
11	J	165	GLY	N-CA-C	5.48	119.30	112.73
12	K	11	ILE	CA-C-N	-5.46	114.08	119.92
12	K	11	ILE	C-N-CA	-5.46	114.08	119.92
7	F	20	ASP	N-CA-C	5.45	117.97	109.52
28	a	6	ARG	N-CA-C	-5.45	105.42	111.36
1	2	135	A	C2'-C3'-O3'	5.44	117.67	109.50
4	C	82	ALA	CA-C-N	-5.42	114.20	119.78
4	C	82	ALA	C-N-CA	-5.42	114.20	119.78
17	P	28	ASP	CA-C-N	5.42	127.98	120.29
17	P	28	ASP	C-N-CA	5.42	127.98	120.29
1	2	1753	A	C2'-C3'-O3'	-5.39	105.62	113.70
1	2	135	A	C4'-C3'-O3'	5.38	117.46	109.40
31	d	42	ARG	N-CA-C	5.37	117.14	111.28
1	2	541	A	C4'-C3'-O3'	5.37	117.45	109.40
12	K	34	ASN	N-CA-C	5.36	118.08	110.10
1	2	777	G	C2'-C3'-O3'	5.31	117.46	109.50
4	C	92	MET	CA-C-N	-5.25	114.20	120.13
4	C	92	MET	C-N-CA	-5.25	114.20	120.13
16	O	53	SER	N-CA-C	-5.23	105.58	111.28
1	2	260	G	C2'-C3'-O3'	5.15	121.43	113.70
1	2	541	A	C2'-C3'-O3'	5.14	117.20	109.50
17	P	131	VAL	N-CA-C	5.12	120.00	109.34
17	P	30	LEU	N-CA-C	5.12	116.86	111.28
21	T	127	GLU	N-CA-C	5.08	116.57	108.79
9	H	164	GLN	N-CA-C	5.06	117.12	108.67
3	B	189	ILE	O-C-N	5.04	123.65	120.07
31	d	38	ARG	N-CA-C	5.02	116.76	111.28

There are no chirality outliers.

There are no planarity outliers.

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	2	34513	0	17381	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1565	0	1602	58	0
3	B	1691	0	1746	165	0
4	C	1750	0	1806	106	0
5	D	1568	0	1657	11	0
6	E	2085	0	2183	24	0
7	F	1475	0	1519	213	0
8	G	1782	0	1927	42	0
9	H	1354	0	1378	174	0
10	I	1496	0	1553	21	0
11	J	1457	0	1553	79	0
12	K	675	0	591	48	0
13	L	1206	0	1257	8	0
14	M	508	0	277	2	0
15	N	1204	0	1289	39	0
16	O	966	0	994	33	0
17	P	939	0	982	70	0
18	Q	1086	0	1151	14	0
19	R	947	0	998	91	0
20	S	1091	0	1141	16	0
21	T	1236	0	1264	55	0
22	U	823	0	878	5	0
23	V	618	0	611	19	0
24	W	1040	0	1083	20	0
25	X	1040	0	1098	130	0
26	Y	1020	0	1087	37	0
27	Z	576	0	592	68	0
28	a	794	0	819	18	0
29	b	605	0	628	17	0
30	c	448	0	492	17	0
31	d	429	0	435	46	0
32	e	391	0	426	4	0
33	f	229	0	121	0	0
34	m	348	0	392	52	0
All	All	68955	0	52911	1635	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 13.

All (1635) 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)
19:R:31:ASN:HA	19:R:34:ILE:CD1	1.41	1.48
7:F:6:LYS:N	7:F:36:PHE:CE1	1.78	1.44
25:X:59:ALA:CB	25:X:114:ASP:OD1	1.64	1.41
3:B:32:LEU:CB	3:B:44:GLY:HA3	1.51	1.41
1:2:1110:U:H5''	34:m:28:GLN:NE2	1.38	1.38
26:Y:17:ASN:OD1	26:Y:19:LEU:CD1	1.72	1.37
17:P:35:MET:O	17:P:39:LEU:CD1	1.70	1.37
12:K:39:ARG:CB	12:K:45:VAL:O	1.74	1.34
9:H:53:VAL:HG23	9:H:181:LYS:CD	1.55	1.34
25:X:100:VAL:CG1	25:X:122:VAL:HG13	1.55	1.34
25:X:55:LEU:HD22	25:X:69:CYS:SG	1.66	1.33
1:2:1533:U:N3	7:F:154:ILE:HG22	1.44	1.32
25:X:68:LYS:HG2	25:X:91:LEU:CD1	1.60	1.32
25:X:68:LYS:CB	25:X:91:LEU:HD11	1.60	1.30
25:X:100:VAL:CG1	25:X:122:VAL:CG1	2.09	1.30
25:X:68:LYS:CG	25:X:91:LEU:CD1	2.10	1.29
17:P:49:LYS:NZ	17:P:87:ASP:O	1.65	1.29
1:2:740:U:OP1	9:H:109:LYS:HG3	1.20	1.28
25:X:63:ASN:CB	25:X:114:ASP:OD2	1.82	1.28
3:B:26:LYS:O	3:B:50:LYS:HG2	1.18	1.28
4:C:181:PRO:O	4:C:184:THR:HG23	1.10	1.28
26:Y:17:ASN:OD1	26:Y:19:LEU:HD11	1.19	1.28
2:A:59:ILE:HG22	2:A:182:GLU:OE1	1.13	1.27
3:B:66:TYR:CE1	16:O:53:SER:OG	1.69	1.27
25:X:63:ASN:HB2	25:X:114:ASP:OD2	1.20	1.27
7:F:91:MET:CE	27:Z:112:LEU:HD11	1.63	1.26
11:J:155:HIS:O	11:J:157:ASP:OD1	1.53	1.26
7:F:7:LEU:CD2	7:F:13:TYR:OH	1.84	1.26
25:X:95:ASP:CB	25:X:98:ASP:OD2	1.84	1.25
25:X:68:LYS:CG	25:X:91:LEU:HD11	1.62	1.25
7:F:7:LEU:HD21	7:F:13:TYR:OH	1.19	1.24
7:F:6:LYS:O	7:F:36:PHE:HD1	1.18	1.24
9:H:139:ILE:HD13	9:H:156:VAL:CG1	1.68	1.23
15:N:23:PRO:HD2	15:N:26:LEU:CB	1.69	1.23
12:K:39:ARG:HB3	12:K:45:VAL:O	1.11	1.22
7:F:85:PHE:CD1	7:F:96:PRO:HB2	1.76	1.22
25:X:59:ALA:HB1	25:X:114:ASP:CG	1.61	1.21
25:X:95:ASP:HB2	25:X:98:ASP:OD2	1.05	1.21
25:X:95:ASP:O	25:X:98:ASP:CG	1.82	1.20
9:H:47:ILE:HD11	9:H:65:VAL:HG23	1.22	1.19
1:2:1252:U:O2'	12:K:10:LEU:CB	1.90	1.18
7:F:91:MET:HE3	27:Z:112:LEU:HD11	1.25	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:128:SER:HA	21:T:129:ASP:HB2	1.22	1.18
1:2:1469:U:C6	7:F:70:ASN:ND2	2.10	1.18
7:F:91:MET:CE	27:Z:112:LEU:CD1	2.22	1.17
3:B:66:TYR:CZ	16:O:53:SER:OG	1.97	1.17
1:2:10:G:O2'	4:C:102:GLN:NE2	1.75	1.16
9:H:53:VAL:HG23	9:H:181:LYS:HD2	1.22	1.16
3:B:32:LEU:HB2	3:B:44:GLY:CA	1.76	1.15
9:H:60:LYS:HE2	9:H:93:LYS:CA	1.77	1.15
25:X:68:LYS:HB3	25:X:91:LEU:HD11	1.19	1.15
7:F:6:LYS:O	7:F:36:PHE:CD1	1.99	1.15
9:H:72:TYR:HA	9:H:76:VAL:HG12	1.23	1.15
31:d:25:ARG:O	31:d:28:MET:HG3	1.45	1.15
4:C:181:PRO:O	4:C:184:THR:CG2	1.94	1.14
1:2:1765:G:N7	34:m:18:LYS:NZ	1.94	1.14
7:F:91:MET:HE3	27:Z:112:LEU:CD1	1.77	1.13
28:a:10:ARG:O	28:a:33:ASP:CG	1.90	1.13
3:B:26:LYS:O	3:B:50:LYS:CG	1.96	1.13
19:R:36:GLU:OE2	19:R:47:ARG:HD2	1.46	1.13
16:O:36:ALA:O	16:O:48:HIS:O	1.65	1.13
4:C:89:MET:HE3	4:C:195:ILE:CG2	1.79	1.13
19:R:31:ASN:HA	19:R:34:ILE:CG1	1.76	1.13
19:R:67:ARG:HA	19:R:67:ARG:HH21	1.12	1.12
25:X:95:ASP:O	25:X:98:ASP:OD1	1.66	1.12
1:2:739:U:C2	9:H:110:ARG:NH2	2.18	1.12
1:2:618:A:OP1	34:m:9:LYS:NZ	1.83	1.11
1:2:1533:U:C2	7:F:154:ILE:CG2	2.33	1.11
8:G:57:ASP:O	8:G:59:GLN:N	1.82	1.11
1:2:1469:U:C5	7:F:70:ASN:ND2	2.18	1.11
3:B:48:VAL:CG2	3:B:61:LEU:HD13	1.80	1.11
3:B:139:CYS:SG	3:B:172:MET:SD	2.48	1.11
12:K:7:LYS:N	12:K:46:PRO:HB3	1.63	1.11
7:F:6:LYS:HB3	7:F:11:TRP:O	1.51	1.11
2:A:117:PHE:CE2	4:C:41:THR:HG22	1.84	1.11
19:R:36:GLU:OE2	19:R:47:ARG:CD	1.99	1.10
10:I:140:THR:O	10:I:142:CYS:N	1.84	1.10
7:F:91:MET:HE3	27:Z:112:LEU:CG	1.82	1.10
19:R:31:ASN:CA	19:R:34:ILE:HD11	1.82	1.10
11:J:116:LEU:HD23	11:J:118:LEU:HD11	1.34	1.09
20:S:82:PRO:CD	21:T:49:TYR:HE1	1.65	1.09
9:H:60:LYS:HE2	9:H:93:LYS:HA	1.18	1.09
11:J:118:LEU:HD12	11:J:118:LEU:H	1.16	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:740:U:OP1	9:H:109:LYS:CG	1.99	1.09
9:H:55:VAL:HG13	9:H:58:GLY:HA3	1.33	1.09
9:H:67:VAL:HG13	9:H:68:PRO:HD2	1.35	1.09
19:R:36:GLU:OE2	19:R:47:ARG:CG	1.99	1.09
19:R:18:GLU:HA	19:R:71:LEU:HD23	1.30	1.09
20:S:82:PRO:HD3	21:T:49:TYR:HE1	1.11	1.09
25:X:134:PHE:CE1	32:e:15:LYS:HE3	1.88	1.08
27:Z:103:LEU:HD21	27:Z:122:LEU:HD11	1.16	1.08
4:C:103:ARG:CZ	4:C:105:ARG:NH2	2.16	1.08
25:X:68:LYS:HG2	25:X:91:LEU:HD12	1.23	1.08
4:C:89:MET:CE	4:C:195:ILE:HG23	1.84	1.08
28:a:10:ARG:O	28:a:33:ASP:OD2	1.71	1.08
3:B:61:LEU:HD23	3:B:91:ILE:HD13	1.17	1.08
19:R:31:ASN:HA	19:R:34:ILE:HD11	1.19	1.08
25:X:100:VAL:HG12	25:X:122:VAL:HG13	1.11	1.08
27:Z:144:ILE:CG1	27:Z:146:GLY:O	2.02	1.08
2:A:60:LEU:HA	2:A:182:GLU:OE2	1.54	1.07
26:Y:101:GLU:N	26:Y:101:GLU:OE1	1.88	1.07
31:d:34:LEU:HD21	31:d:41:PHE:HE1	1.14	1.07
2:A:59:ILE:CG2	2:A:182:GLU:OE1	2.02	1.07
2:A:185:TYR:CE2	2:A:190:LEU:HD12	1.90	1.06
11:J:60:LEU:CD1	11:J:93:LEU:HD11	1.84	1.06
1:2:1533:U:C6	7:F:154:ILE:HG23	1.91	1.06
7:F:16:VAL:O	7:F:17:ASN:ND2	1.88	1.06
7:F:8:PHE:CD1	7:F:82:ARG:HG3	1.90	1.06
27:Z:120:GLU:HB3	27:Z:121:ARG:NH1	1.70	1.06
9:H:139:ILE:HD13	9:H:156:VAL:HG13	1.12	1.06
1:2:1533:U:C5	7:F:152:ARG:O	2.09	1.06
7:F:62:ASN:OD1	7:F:74:LYS:NZ	1.88	1.06
11:J:60:LEU:HD13	11:J:93:LEU:CD1	1.85	1.06
19:R:74:GLN:O	19:R:78:ARG:N	1.86	1.05
9:H:47:ILE:HD11	9:H:65:VAL:CG2	1.84	1.05
25:X:100:VAL:HG11	25:X:122:VAL:HG11	1.39	1.05
26:Y:22:ARG:NH1	26:Y:24:GLN:OE1	1.88	1.05
1:2:1113:G:P	34:m:35:ARG:HH12	1.80	1.05
12:K:80:GLY:O	12:K:84:LEU:HD13	1.57	1.05
15:N:23:PRO:CD	15:N:26:LEU:CB	2.35	1.05
17:P:35:MET:O	17:P:39:LEU:HD12	1.53	1.05
19:R:19:LYS:HG3	19:R:20:TYR:HD2	1.22	1.04
1:2:1533:U:C2	7:F:154:ILE:HG22	1.93	1.04
7:F:85:PHE:HD1	7:F:96:PRO:HB2	0.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1533:U:N3	7:F:154:ILE:CG2	2.21	1.04
17:P:131:VAL:HG13	17:P:132:ARG:H	1.22	1.04
19:R:66:VAL:HG12	19:R:69:ILE:HD11	1.39	1.04
11:J:118:LEU:HD23	11:J:158:TYR:CE2	1.91	1.04
19:R:31:ASN:CA	19:R:34:ILE:CD1	2.33	1.04
7:F:21:LEU:HD22	30:c:6:LEU:HG	1.39	1.03
4:C:103:ARG:NH2	4:C:105:ARG:NH2	2.05	1.03
9:H:52:GLU:OE2	9:H:61:LYS:NZ	1.92	1.03
16:O:48:HIS:HD2	16:O:60:ARG:HG3	1.24	1.03
3:B:32:LEU:HB2	3:B:44:GLY:HA3	1.05	1.02
17:P:35:MET:O	17:P:39:LEU:HD13	1.59	1.02
3:B:141:ALA:CB	3:B:168:MET:HE1	1.90	1.02
4:C:95:GLN:HG2	4:C:104:THR:HG22	1.06	1.02
4:C:95:GLN:HG2	4:C:104:THR:CG2	1.89	1.02
7:F:62:ASN:OD1	7:F:74:LYS:CE	2.08	1.02
9:H:72:TYR:HA	9:H:76:VAL:CG1	1.88	1.02
1:2:740:U:OP1	9:H:109:LYS:HE3	1.59	1.01
7:F:91:MET:CE	27:Z:112:LEU:CG	2.37	1.01
19:R:19:LYS:HG3	19:R:20:TYR:CD2	1.94	1.01
20:S:82:PRO:HD3	21:T:49:TYR:CE1	1.95	1.01
30:c:66:ARG:O	30:c:67:LEU:HB2	1.57	1.01
1:2:1679:A:H1'	8:G:66:GLY:CA	1.90	1.01
25:X:55:LEU:CD2	25:X:69:CYS:SG	2.48	1.01
2:A:34:LYS:HB3	2:A:155:LEU:HD12	1.39	1.01
7:F:91:MET:HE1	27:Z:112:LEU:HD11	1.42	1.00
7:F:79:ARG:NH2	27:Z:149:HIS:NE2	2.09	1.00
15:N:23:PRO:HD2	15:N:26:LEU:HB3	1.05	1.00
25:X:100:VAL:HG11	25:X:122:VAL:CG1	1.84	1.00
1:2:740:U:P	9:H:109:LYS:HG3	2.00	1.00
3:B:38:PHE:CD1	3:B:73:LEU:HD12	1.94	1.00
11:J:116:LEU:CD2	11:J:118:LEU:HD11	1.92	1.00
23:V:11:LEU:HD12	23:V:11:LEU:H	1.27	1.00
1:2:1110:U:C5'	34:m:28:GLN:NE2	2.25	0.99
7:F:62:ASN:OD1	7:F:74:LYS:HE3	1.61	0.99
1:2:1533:U:C5	7:F:154:ILE:HG23	1.96	0.99
9:H:139:ILE:CD1	9:H:156:VAL:CG1	2.38	0.99
9:H:189:PHE:O	9:H:190:SER:HB3	1.62	0.99
3:B:32:LEU:HB3	3:B:44:GLY:HA3	1.41	0.99
7:F:94:LYS:HE3	7:F:99:VAL:CG2	1.93	0.99
7:F:5:ALA:HA	7:F:36:PHE:CZ	1.97	0.98
3:B:61:LEU:CD2	3:B:91:ILE:HD13	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:89:MET:CE	4:C:195:ILE:CG2	2.39	0.98
3:B:141:ALA:HB2	3:B:168:MET:HE1	1.46	0.98
1:2:1679:A:H1'	8:G:66:GLY:HA2	1.43	0.98
15:N:23:PRO:CD	15:N:26:LEU:HB3	1.91	0.98
25:X:51:VAL:HG13	25:X:70:VAL:CG1	1.94	0.97
31:d:34:LEU:CD2	31:d:41:PHE:CE1	2.47	0.97
3:B:61:LEU:HD23	3:B:91:ILE:CD1	1.93	0.97
7:F:85:PHE:HD1	7:F:96:PRO:CB	1.76	0.97
3:B:66:TYR:HE1	16:O:53:SER:HG	1.07	0.97
7:F:6:LYS:N	7:F:36:PHE:HE1	1.48	0.97
1:2:1533:U:C4	7:F:154:ILE:CG2	2.48	0.96
7:F:4:GLU:N	7:F:4:GLU:OE1	1.98	0.96
3:B:47:LEU:CD1	16:O:56:GLU:HG2	1.94	0.96
9:H:79:ILE:HG21	9:H:82:ARG:HD2	1.47	0.96
25:X:105:PHE:CD2	25:X:112:VAL:HG21	2.00	0.96
27:Z:144:ILE:HG13	27:Z:146:GLY:O	1.66	0.96
19:R:24:LEU:HB3	19:R:34:ILE:HD12	1.47	0.96
1:2:1561:A:H5'	21:T:54:HIS:NE2	1.81	0.96
9:H:67:VAL:CG1	9:H:68:PRO:HD2	1.95	0.95
27:Z:120:GLU:HB3	27:Z:121:ARG:HH11	1.31	0.95
1:2:1753:A:O2'	1:2:1754:A:O5'	1.85	0.95
34:m:15:MET:O	34:m:16:ARG:HB3	1.67	0.95
9:H:53:VAL:CG2	9:H:181:LYS:CD	2.44	0.95
31:d:34:LEU:HD21	31:d:41:PHE:CE1	2.00	0.95
1:2:893:U:O2	16:O:60:ARG:NH2	1.99	0.95
7:F:8:PHE:HE1	7:F:82:ARG:HB2	1.32	0.94
20:S:82:PRO:CD	21:T:49:TYR:CE1	2.49	0.94
17:P:39:LEU:HA	17:P:42:PHE:CD2	2.02	0.94
7:F:94:LYS:HE3	7:F:99:VAL:HG22	1.48	0.94
1:2:1109:G:C5	34:m:2:ALA:HB2	2.03	0.94
1:2:1533:U:C4	7:F:154:ILE:HG22	2.02	0.94
3:B:32:LEU:N	3:B:44:GLY:O	1.99	0.94
6:E:34:GLY:O	6:E:36:HIS:N	2.01	0.93
7:F:90:LEU:HD23	27:Z:112:LEU:HD23	1.50	0.93
7:F:150:ALA:HB2	7:F:160:CYS:SG	2.08	0.93
31:d:39:GLN:OE1	31:d:39:GLN:N	1.99	0.93
12:K:69:TRP:HZ3	31:d:21:VAL:HG22	1.33	0.93
11:J:33:GLU:O	11:J:122:ILE:HD13	1.68	0.93
1:2:1429:G:C8	31:d:39:GLN:HG2	2.03	0.93
7:F:173:SER:HA	7:F:178:ILE:CG2	1.99	0.93
11:J:116:LEU:CG	11:J:118:LEU:HD11	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:31:ASN:CG	19:R:34:ILE:HD11	1.94	0.93
26:Y:19:LEU:HD12	26:Y:20:LEU:H	1.32	0.93
7:F:6:LYS:CB	7:F:11:TRP:O	2.15	0.93
12:K:80:GLY:O	12:K:84:LEU:CD1	2.18	0.92
1:2:1752:U:O2'	1:2:1753:A:OP2	1.85	0.92
15:N:23:PRO:CD	15:N:26:LEU:HB2	1.97	0.92
7:F:167:ASN:HD21	7:F:175:ALA:H	1.15	0.92
11:J:133:HIS:CE1	11:J:164:PHE:CE2	2.58	0.92
7:F:91:MET:HE3	27:Z:112:LEU:CD2	1.98	0.92
34:m:12:ARG:HB3	34:m:12:ARG:NH1	1.85	0.92
27:Z:144:ILE:HG12	27:Z:146:GLY:O	1.70	0.92
1:2:1533:U:H5	7:F:152:ARG:O	1.51	0.92
8:G:57:ASP:OD2	8:G:98:ARG:HD3	1.70	0.92
9:H:130:LEU:HD21	9:H:179:TYR:CE1	2.04	0.92
1:2:1609:A:O2'	7:F:62:ASN:O	1.85	0.91
1:2:80:G:H2'	1:2:81:C:C6	2.05	0.91
31:d:34:LEU:CD2	31:d:41:PHE:HE1	1.82	0.91
1:2:1110:U:H5''	34:m:28:GLN:HE21	1.20	0.91
7:F:91:MET:CE	27:Z:112:LEU:HG	2.00	0.91
3:B:26:LYS:HA	3:B:50:LYS:HD2	1.52	0.91
12:K:70:GLN:HB2	31:d:23:PHE:HZ	1.32	0.91
25:X:95:ASP:HB2	25:X:98:ASP:CG	1.95	0.91
2:A:39:VAL:HG11	2:A:48:HIS:HB3	1.49	0.91
34:m:6:SER:O	34:m:8:TYR:N	2.03	0.91
9:H:68:PRO:HG2	9:H:71:VAL:HB	1.50	0.91
3:B:66:TYR:HE1	16:O:53:SER:OG	1.48	0.91
19:R:31:ASN:HA	19:R:34:ILE:HG12	1.52	0.90
27:Z:120:GLU:OE1	27:Z:121:ARG:NH1	2.04	0.90
3:B:26:LYS:CD	3:B:50:LYS:HD3	2.02	0.90
7:F:167:ASN:HD21	7:F:175:ALA:N	1.70	0.90
15:N:55:ARG:HH22	29:b:49:GLN:NE2	1.70	0.90
3:B:157:GLN:O	3:B:159:SER:N	2.05	0.90
7:F:91:MET:HE3	27:Z:112:LEU:HD21	1.53	0.90
3:B:38:PHE:CE1	3:B:73:LEU:HD12	2.07	0.89
19:R:70:SER:O	19:R:72:LYS:N	2.05	0.89
2:A:117:PHE:HE2	4:C:41:THR:HG22	1.28	0.89
7:F:90:LEU:HD23	27:Z:112:LEU:CD2	2.01	0.89
9:H:55:VAL:HG13	9:H:58:GLY:CA	2.01	0.89
25:X:55:LEU:HD22	25:X:69:CYS:HG	1.07	0.89
26:Y:17:ASN:OD1	26:Y:19:LEU:HD12	1.69	0.89
1:2:30:G:H5'	25:X:124:LYS:HE2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:64:MET:SD	7:F:80:ILE:HD11	2.12	0.89
7:F:94:LYS:CE	7:F:99:VAL:HG22	2.02	0.89
8:G:32:MET:HE2	8:G:63:MET:HG3	1.51	0.89
19:R:69:ILE:HG22	19:R:71:LEU:HG	1.52	0.89
25:X:100:VAL:CG1	25:X:122:VAL:HG11	1.92	0.89
1:2:30:G:OP1	25:X:124:LYS:NZ	2.04	0.89
19:R:31:ASN:CB	19:R:34:ILE:HD11	2.02	0.89
9:H:53:VAL:HG23	9:H:181:LYS:HD3	1.55	0.88
19:R:67:ARG:HD3	19:R:68:GLY:H	1.37	0.88
21:T:52:THR:HG21	21:T:69:ARG:NH2	1.86	0.88
9:H:164:GLN:HB3	9:H:165:LYS:HE3	1.55	0.88
9:H:79:ILE:HG13	9:H:80:GLN:H	1.39	0.88
1:2:1639:C:C2	1:2:1753:A:N6	2.42	0.88
3:B:47:LEU:HD13	16:O:56:GLU:HG2	1.53	0.88
4:C:95:GLN:CG	4:C:104:THR:HG22	2.00	0.88
25:X:59:ALA:HB1	25:X:114:ASP:OD1	0.70	0.88
25:X:68:LYS:HB3	25:X:91:LEU:CD1	2.03	0.87
19:R:73:LEU:HA	19:R:76:GLU:OE1	1.74	0.87
27:Z:117:THR:O	27:Z:121:ARG:HG2	1.75	0.87
7:F:90:LEU:HD11	27:Z:156:THR:HG22	1.57	0.87
11:J:161:THR:O	11:J:162:SER:OG	1.92	0.87
17:P:46:GLN:N	17:P:46:GLN:OE1	2.08	0.87
17:P:129:LYS:H	17:P:129:LYS:HD2	1.38	0.87
12:K:8:PHE:O	12:K:9:SER:OG	1.92	0.87
4:C:103:ARG:NH2	4:C:105:ARG:HH21	1.70	0.87
12:K:7:LYS:N	12:K:46:PRO:CB	2.37	0.87
22:U:183:PRO:O	31:d:38:ARG:NH2	2.07	0.86
1:2:1468:C:OP2	7:F:151:PHE:O	1.93	0.86
16:O:48:HIS:CD2	16:O:60:ARG:HG3	2.10	0.86
19:R:74:GLN:O	19:R:78:ARG:HG2	1.76	0.86
1:2:1773:A:OP1	34:m:23:ARG:NH2	2.08	0.86
7:F:94:LYS:HG3	7:F:95:ASN:H	1.40	0.86
9:H:79:ILE:HG22	9:H:82:ARG:CZ	2.06	0.86
11:J:93:LEU:O	11:J:96:VAL:HG22	1.76	0.86
6:E:84:ALA:HB1	6:E:101:MET:HE1	1.58	0.86
25:X:105:PHE:CG	25:X:112:VAL:HG21	2.10	0.86
1:2:71:U:O2	1:2:80:G:N1	2.08	0.86
9:H:45:LEU:HD13	9:H:46:VAL:N	1.90	0.86
19:R:67:ARG:HA	19:R:67:ARG:NH2	1.91	0.86
25:X:51:VAL:HG13	25:X:70:VAL:HG13	1.57	0.86
31:d:18:GLN:NE2	31:d:23:PHE:HD2	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:29:U:O3'	25:X:124:LYS:NZ	2.08	0.85
11:J:60:LEU:HD13	11:J:93:LEU:HD11	0.93	0.85
20:S:49:LYS:HE2	21:T:48:ASP:OD2	1.76	0.85
24:W:56:HIS:O	24:W:57:ARG:HG3	1.76	0.85
1:2:1774:C:OP2	34:m:15:MET:O	1.95	0.85
4:C:75:PHE:HA	4:C:80:CYS:SG	2.16	0.85
34:m:12:ARG:HB3	34:m:12:ARG:HH11	1.42	0.85
1:2:30:G:P	25:X:124:LYS:NZ	2.50	0.84
25:X:81:ILE:HG21	25:X:120:PHE:CD2	2.11	0.84
3:B:26:LYS:HD2	3:B:50:LYS:HD3	1.59	0.84
11:J:118:LEU:HD23	11:J:158:TYR:HE2	1.39	0.84
7:F:21:LEU:HD23	7:F:22:SER:N	1.91	0.84
9:H:42:VAL:O	9:H:45:LEU:N	2.11	0.84
1:2:1110:U:H5''	34:m:28:GLN:HE22	1.41	0.84
31:d:18:GLN:NE2	31:d:23:PHE:CD2	2.46	0.84
1:2:740:U:OP1	9:H:109:LYS:CE	2.25	0.84
7:F:8:PHE:CE1	7:F:82:ARG:HG3	2.12	0.84
1:2:1561:A:H4'	21:T:54:HIS:CD2	2.13	0.83
7:F:23:LEU:HD21	7:F:134:ARG:HE	1.43	0.83
12:K:69:TRP:CZ3	31:d:21:VAL:HG22	2.13	0.83
9:H:60:LYS:CE	9:H:93:LYS:H	1.91	0.83
1:2:1109:G:C5	34:m:2:ALA:CB	2.61	0.83
3:B:137:MET:HE1	3:B:184:LEU:HD21	1.59	0.83
31:d:38:ARG:HG3	31:d:39:GLN:OE1	1.78	0.83
4:C:230:TYR:OH	23:V:11:LEU:CD1	2.27	0.83
7:F:5:ALA:CA	7:F:36:PHE:CZ	2.62	0.83
16:O:38:ILE:HG12	16:O:47:ILE:CD1	2.09	0.83
1:2:1639:C:N1	1:2:1753:A:N6	2.27	0.83
11:J:156:VAL:C	11:J:157:ASP:OD1	2.22	0.82
24:W:55:ASP:OD1	24:W:59:GLY:HA2	1.79	0.82
4:C:99:ARG:HG3	4:C:100:ALA:H	1.44	0.82
9:H:79:ILE:CG2	9:H:82:ARG:HD2	2.09	0.82
1:2:1429:G:C4	31:d:39:GLN:HB3	2.15	0.82
3:B:175:GLU:HG2	3:B:193:ILE:CD1	2.10	0.82
2:A:34:LYS:HB3	2:A:155:LEU:CD1	2.09	0.82
7:F:91:MET:HE1	27:Z:112:LEU:CD1	1.97	0.82
3:B:187:LYS:O	3:B:190:PRO:HD2	1.79	0.82
15:N:20:ARG:O	15:N:21:LYS:HG2	1.80	0.82
17:P:27:LEU:HA	17:P:30:LEU:HD12	1.59	0.82
27:Z:120:GLU:CB	27:Z:121:ARG:NH1	2.42	0.82
1:2:618:A:P	34:m:9:LYS:HZ2	2.03	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:40:ILE:O	4:C:41:THR:OG1	1.96	0.82
25:X:95:ASP:CA	25:X:98:ASP:OD2	2.25	0.82
4:C:89:MET:HE3	4:C:195:ILE:HG23	1.45	0.82
4:C:181:PRO:HG2	4:C:184:THR:HG22	1.62	0.82
10:I:140:THR:O	10:I:143:LEU:N	2.13	0.82
17:P:130:PRO:HG2	20:S:129:TRP:CZ2	2.15	0.81
27:Z:147:GLU:N	27:Z:147:GLU:OE1	2.13	0.81
1:2:448:C:OP1	6:E:29:PRO:HD3	1.81	0.81
7:F:5:ALA:C	7:F:36:PHE:CE1	2.58	0.81
7:F:173:SER:HA	7:F:178:ILE:HG21	1.62	0.81
25:X:89:GLY:O	25:X:90:SER:OG	1.96	0.81
26:Y:19:LEU:HD12	26:Y:20:LEU:N	1.94	0.81
34:m:16:ARG:HG2	34:m:19:TRP:CD1	2.15	0.81
17:P:27:LEU:HA	17:P:30:LEU:CD1	2.10	0.81
21:T:51:LYS:HA	21:T:60:PRO:HD3	1.62	0.81
7:F:21:LEU:O	7:F:22:SER:OG	1.98	0.81
3:B:26:LYS:HA	3:B:50:LYS:CD	2.09	0.81
7:F:8:PHE:CE1	7:F:82:ARG:HB2	2.15	0.81
17:P:25:VAL:HG12	17:P:30:LEU:CD2	2.10	0.81
7:F:91:MET:HE2	27:Z:112:LEU:HG	1.62	0.81
26:Y:92:PHE:O	26:Y:95:VAL:HG12	1.81	0.81
7:F:21:LEU:HD22	30:c:6:LEU:CG	2.11	0.80
19:R:31:ASN:CA	19:R:34:ILE:HG12	2.11	0.80
7:F:16:VAL:HG22	7:F:98:GLN:OE1	1.80	0.80
21:T:50:VAL:HG12	21:T:52:THR:H	1.45	0.80
3:B:40:VAL:HG11	3:B:73:LEU:HA	1.62	0.80
11:J:116:LEU:HB3	11:J:118:LEU:CD1	2.12	0.80
1:2:534:C:P	11:J:168:ARG:HH12	2.04	0.80
25:X:55:LEU:HD21	25:X:57:ILE:HG23	1.64	0.80
3:B:90:ASP:OD1	3:B:91:ILE:N	2.14	0.80
30:c:66:ARG:O	30:c:67:LEU:CB	2.30	0.80
4:C:103:ARG:NH1	4:C:105:ARG:NE	2.30	0.80
1:2:548:G:N3	1:2:555:A:H2	1.80	0.80
7:F:8:PHE:CE1	7:F:82:ARG:CG	2.65	0.80
7:F:6:LYS:C	7:F:36:PHE:HD1	1.90	0.79
17:P:38:LEU:HG	17:P:42:PHE:HE2	1.45	0.79
17:P:53:GLY:C	17:P:54:ILE:HD12	2.07	0.79
19:R:24:LEU:O	19:R:24:LEU:HD12	1.82	0.79
3:B:168:MET:O	3:B:172:MET:HG3	1.82	0.79
3:B:175:GLU:HG2	3:B:193:ILE:HD12	1.64	0.79
1:2:927:A:P	28:a:32:LYS:HZ1	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:53:GLY:HA3	17:P:54:ILE:HG13	1.63	0.79
1:2:1113:G:P	34:m:35:ARG:NH1	2.55	0.79
2:A:32:GLU:OE1	2:A:153:SER:O	1.99	0.79
9:H:161:ARG:HG2	9:H:162:ASP:OD1	1.82	0.79
19:R:31:ASN:HA	19:R:34:ILE:HD13	1.60	0.79
2:A:60:LEU:CA	2:A:182:GLU:OE2	2.31	0.79
4:C:115:SER:O	4:C:116:ASN:HB2	1.80	0.79
17:P:31:LEU:HD22	17:P:92:PRO:O	1.83	0.79
1:2:30:G:P	25:X:124:LYS:HZ1	2.06	0.79
1:2:1639:C:O4'	1:2:1753:A:N1	2.15	0.79
2:A:184:LEU:HA	2:A:189:GLU:OE1	1.83	0.79
3:B:175:GLU:N	3:B:175:GLU:OE1	2.15	0.78
3:B:34:ALA:HB2	3:B:43:PHE:CE2	2.18	0.78
7:F:13:TYR:HB2	7:F:34:CYS:SG	2.22	0.78
1:2:1753:A:HO2'	1:2:1754:A:C5'	1.96	0.78
2:A:39:VAL:CG1	2:A:48:HIS:HB3	2.13	0.78
9:H:53:VAL:HG23	9:H:181:LYS:CG	2.12	0.78
19:R:36:GLU:OE2	19:R:47:ARG:HG3	1.83	0.78
30:c:67:LEU:HD13	30:c:67:LEU:O	1.83	0.78
3:B:141:ALA:HB3	3:B:168:MET:HE1	1.65	0.78
7:F:8:PHE:CD1	7:F:82:ARG:CG	2.67	0.78
1:2:554:A:O2'	1:2:555:A:O5'	2.02	0.78
9:H:47:ILE:CD1	9:H:65:VAL:CG2	2.62	0.78
21:T:127:GLU:N	21:T:127:GLU:OE1	2.16	0.78
25:X:100:VAL:HG13	25:X:122:VAL:CG1	2.13	0.78
2:A:187:ARG:HD2	2:A:189:GLU:CD	2.08	0.78
9:H:53:VAL:CG2	9:H:181:LYS:HD3	2.12	0.78
19:R:36:GLU:OE2	19:R:47:ARG:CB	2.32	0.78
9:H:168:ILE:HD11	9:H:191:PHE:HZ	1.49	0.77
26:Y:17:ASN:CG	26:Y:19:LEU:HD11	2.06	0.77
3:B:38:PHE:HZ	3:B:84:ILE:HG12	1.48	0.77
7:F:6:LYS:N	7:F:36:PHE:CD1	2.20	0.77
7:F:161:LEU:O	7:F:165:ILE:HG12	1.85	0.77
9:H:139:ILE:CD1	9:H:156:VAL:HG13	2.01	0.77
4:C:119:CYS:O	4:C:144:LEU:HD12	1.83	0.77
17:P:49:LYS:HZ2	17:P:89:VAL:HG23	1.49	0.77
25:X:68:LYS:HG3	25:X:91:LEU:CD1	2.13	0.77
3:B:141:ALA:HB2	3:B:168:MET:CE	2.15	0.77
7:F:13:TYR:CB	7:F:34:CYS:SG	2.72	0.77
9:H:60:LYS:CE	9:H:93:LYS:CA	2.62	0.77
9:H:60:LYS:CE	9:H:93:LYS:N	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:60:LYS:HE3	9:H:93:LYS:H	1.49	0.77
2:A:59:ILE:O	2:A:182:GLU:OE2	2.02	0.77
11:J:118:LEU:H	11:J:118:LEU:CD1	1.97	0.77
17:P:35:MET:O	17:P:39:LEU:HD11	1.84	0.77
17:P:25:VAL:HG12	17:P:30:LEU:HD23	1.66	0.76
9:H:135:SER:O	9:H:137:THR:N	2.18	0.76
3:B:38:PHE:CD1	3:B:73:LEU:CD1	2.68	0.76
7:F:167:ASN:ND2	7:F:175:ALA:HB2	2.00	0.76
25:X:137:LYS:HE2	25:X:137:LYS:C	2.10	0.76
3:B:48:VAL:HG21	3:B:61:LEU:HD13	1.66	0.76
7:F:8:PHE:CE1	7:F:82:ARG:CB	2.68	0.76
4:C:55:ILE:HD11	4:C:118:HIS:CE1	2.19	0.76
9:H:165:LYS:O	9:H:168:ILE:HG22	1.84	0.76
9:H:65:VAL:HG11	9:H:97:LEU:HD12	1.67	0.76
9:H:79:ILE:HG13	9:H:80:GLN:N	2.01	0.76
12:K:39:ARG:HB2	12:K:45:VAL:O	1.85	0.76
21:T:120:PHE:HB3	21:T:126:VAL:HG12	1.66	0.76
12:K:33:LYS:HD3	12:K:33:LYS:C	2.09	0.76
9:H:68:PRO:HG2	9:H:71:VAL:CB	2.16	0.75
17:P:54:ILE:HD12	17:P:54:ILE:N	2.01	0.75
17:P:129:LYS:HD2	17:P:129:LYS:N	2.00	0.75
19:R:31:ASN:C	19:R:34:ILE:HG12	2.11	0.75
25:X:128:ALA:O	25:X:129:SER:OG	2.01	0.75
26:Y:93:ARG:O	26:Y:97:LEU:CD1	2.35	0.75
4:C:103:ARG:CZ	4:C:105:ARG:HH21	1.99	0.75
6:E:31:PRO:HD2	6:E:38:LEU:CD1	2.17	0.75
1:2:151:U:H4'	8:G:58:LYS:O	1.87	0.75
11:J:116:LEU:HD23	11:J:118:LEU:CD1	2.13	0.75
1:2:1639:C:C6	1:2:1753:A:N6	2.55	0.74
12:K:39:ARG:N	12:K:39:ARG:HD2	2.02	0.74
19:R:69:ILE:HD12	19:R:69:ILE:N	2.02	0.74
19:R:66:VAL:CG1	19:R:69:ILE:HD11	2.16	0.74
19:R:36:GLU:CD	19:R:47:ARG:HD2	2.11	0.74
1:2:1639:C:C1'	1:2:1753:A:C6	2.71	0.74
4:C:75:PHE:HD1	4:C:80:CYS:SG	2.11	0.74
1:2:1109:G:C4	34:m:2:ALA:HB2	2.22	0.74
29:b:32:ASP:OD2	29:b:80:LYS:NZ	2.20	0.74
3:B:48:VAL:HG22	3:B:61:LEU:HD13	1.67	0.74
19:R:36:GLU:OE2	19:R:47:ARG:HB2	1.88	0.74
19:R:26:LEU:C	19:R:26:LEU:HD12	2.13	0.74
8:G:32:MET:CE	8:G:63:MET:HG3	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:49:LYS:CE	21:T:48:ASP:OD2	2.36	0.74
25:X:95:ASP:O	25:X:98:ASP:OD2	2.06	0.74
3:B:71:ALA:HB2	3:B:78:ASP:O	1.87	0.73
10:I:140:THR:O	10:I:141:LEU:C	2.31	0.73
19:R:67:ARG:HD3	19:R:68:GLY:N	2.02	0.73
1:2:1429:G:N9	31:d:39:GLN:HG2	2.03	0.73
1:2:927:A:OP1	28:a:32:LYS:NZ	2.15	0.73
3:B:190:PRO:O	3:B:191:GLU:HG2	1.87	0.73
9:H:55:VAL:CG1	9:H:58:GLY:HA3	2.14	0.73
25:X:112:VAL:HG12	25:X:113:GLY:N	2.03	0.73
20:S:82:PRO:HG3	21:T:49:TYR:CE1	2.22	0.73
1:2:618:A:P	34:m:9:LYS:NZ	2.60	0.73
1:2:1533:U:C4	7:F:154:ILE:HG23	2.19	0.73
4:C:89:MET:HE1	4:C:195:ILE:HG23	1.69	0.73
27:Z:103:LEU:HD21	27:Z:122:LEU:CD1	2.08	0.73
3:B:47:LEU:HD11	16:O:56:GLU:HG2	1.70	0.73
4:C:103:ARG:NH1	4:C:105:ARG:CZ	2.52	0.73
9:H:60:LYS:HE2	9:H:93:LYS:N	2.02	0.73
18:Q:47:GLU:O	18:Q:50:LYS:HB3	1.89	0.73
26:Y:22:ARG:CD	26:Y:77:MET:SD	2.77	0.73
30:c:66:ARG:HD3	30:c:66:ARG:C	2.14	0.73
4:C:99:ARG:HG3	4:C:100:ALA:N	2.03	0.73
17:P:25:VAL:CG1	17:P:30:LEU:HD23	2.18	0.73
25:X:63:ASN:HB3	25:X:114:ASP:OD2	1.87	0.73
3:B:48:VAL:HG21	3:B:61:LEU:HB2	1.71	0.73
23:V:11:LEU:HD12	23:V:11:LEU:N	2.04	0.73
3:B:61:LEU:HG	3:B:91:ILE:HD11	1.71	0.72
7:F:7:LEU:HD12	7:F:97:ILE:HD11	1.69	0.72
3:B:187:LYS:HE3	3:B:193:ILE:HD11	1.71	0.72
3:B:138:PHE:O	3:B:212:ILE:O	2.07	0.72
7:F:65:MET:O	7:F:66:MET:HG3	1.89	0.72
4:C:230:TYR:OH	23:V:11:LEU:HD12	1.90	0.72
11:J:93:LEU:C	11:J:93:LEU:HD12	2.14	0.72
18:Q:45:GLN:HA	18:Q:46:PRO:C	2.12	0.72
25:X:55:LEU:C	25:X:55:LEU:HD23	2.14	0.72
7:F:26:TYR:O	7:F:52:ALA:HB1	1.88	0.72
11:J:157:ASP:OD1	11:J:157:ASP:N	2.20	0.72
2:A:187:ARG:HD2	2:A:189:GLU:OE2	1.88	0.72
9:H:129:MET:O	9:H:133:ILE:HG23	1.89	0.72
17:P:38:LEU:HG	17:P:42:PHE:CE2	2.25	0.72
27:Z:149:HIS:CD2	27:Z:151:SER:H	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:26:LYS:CB	3:B:50:LYS:HD3	2.19	0.72
3:B:26:LYS:CA	3:B:50:LYS:CD	2.68	0.72
17:P:130:PRO:CG	20:S:129:TRP:CH2	2.73	0.72
24:W:30:SER:HB2	24:W:61:ILE:HG13	1.72	0.72
7:F:8:PHE:HE1	7:F:82:ARG:CB	2.01	0.71
7:F:94:LYS:CE	7:F:99:VAL:CG2	2.62	0.71
9:H:79:ILE:HB	9:H:82:ARG:HG2	1.72	0.71
2:A:190:LEU:HD11	2:A:197:TRP:CD1	2.25	0.71
7:F:90:LEU:CD2	27:Z:112:LEU:HD23	2.19	0.71
1:2:1639:C:C1'	1:2:1753:A:N1	2.54	0.71
7:F:173:SER:HA	7:F:178:ILE:HG23	1.71	0.71
16:O:36:ALA:C	16:O:48:HIS:O	2.32	0.71
27:Z:120:GLU:CB	27:Z:121:ARG:HH11	2.04	0.71
3:B:141:ALA:CB	3:B:168:MET:CE	2.68	0.71
9:H:140:VAL:CG2	9:H:159:ASP:HA	2.20	0.71
15:N:55:ARG:HH22	29:b:49:GLN:HE21	1.37	0.71
19:R:31:ASN:CA	19:R:34:ILE:CG1	2.61	0.71
21:T:49:TYR:O	21:T:50:VAL:HG23	1.90	0.71
3:B:32:LEU:HB2	3:B:44:GLY:C	2.15	0.71
7:F:79:ARG:HH21	27:Z:149:HIS:CE1	2.09	0.71
17:P:26:GLU:O	17:P:30:LEU:HG	1.90	0.71
17:P:31:LEU:CD2	17:P:92:PRO:O	2.39	0.70
17:P:131:VAL:HG13	17:P:132:ARG:N	2.03	0.70
18:Q:49:LEU:HB3	18:Q:83:ILE:HD13	1.73	0.70
7:F:24:VAL:O	7:F:25:ASP:HB3	1.91	0.70
20:S:82:PRO:CG	21:T:49:TYR:CE1	2.74	0.70
11:J:120:LYS:O	11:J:120:LYS:HG2	1.89	0.70
21:T:128:SER:CA	21:T:129:ASP:HB2	2.11	0.70
4:C:89:MET:HE3	4:C:195:ILE:HG21	1.73	0.70
19:R:69:ILE:HG22	19:R:71:LEU:CG	2.22	0.70
31:d:34:LEU:HD23	31:d:41:PHE:CD1	2.27	0.70
7:F:89:HIS:O	7:F:93:ASP:HB3	1.92	0.70
17:P:130:PRO:HG3	20:S:129:TRP:CH2	2.26	0.70
25:X:105:PHE:CD2	25:X:112:VAL:CG2	2.74	0.70
1:2:1110:U:C5'	34:m:28:GLN:HE21	1.97	0.70
2:A:41:LYS:NZ	19:R:104:ASP:HB2	2.06	0.70
11:J:133:HIS:CE1	11:J:164:PHE:CD2	2.79	0.70
2:A:36:ARG:NH1	2:A:36:ARG:HB2	2.07	0.70
21:T:49:TYR:C	21:T:50:VAL:HG23	2.17	0.69
27:Z:149:HIS:HD2	27:Z:151:SER:H	1.40	0.69
1:2:740:U:OP1	9:H:109:LYS:CD	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:128:THR:HG22	3:B:134:THR:HG22	1.74	0.69
4:C:103:ARG:NH1	4:C:105:ARG:NH2	2.40	0.69
6:E:31:PRO:HD2	6:E:38:LEU:HD11	1.73	0.69
19:R:66:VAL:HG12	19:R:69:ILE:CD1	2.20	0.69
19:R:67:ARG:HH21	19:R:67:ARG:CA	2.00	0.69
1:2:740:U:P	9:H:109:LYS:CG	2.76	0.69
1:2:1561:A:C5'	21:T:54:HIS:NE2	2.56	0.69
12:K:70:GLN:HB2	31:d:23:PHE:CZ	2.22	0.69
9:H:68:PRO:HG2	9:H:71:VAL:CG2	2.22	0.69
12:K:84:LEU:HD12	12:K:84:LEU:H	1.57	0.69
3:B:137:MET:CE	3:B:184:LEU:HD21	2.23	0.69
12:K:41:PRO:O	12:K:42:GLU:CB	2.40	0.69
16:O:39:TYR:HB3	16:O:46:PHE:HB2	1.75	0.69
3:B:168:MET:HG2	3:B:197:ILE:HG21	1.75	0.69
3:B:180:GLN:HE21	3:B:182:ARG:HB3	1.58	0.69
6:E:208:ILE:HD11	6:E:222:ILE:HG22	1.75	0.69
10:I:148:ARG:HG3	10:I:153:PRO:HG3	1.74	0.69
12:K:70:GLN:OE1	31:d:23:PHE:HE2	1.75	0.69
3:B:32:LEU:CB	3:B:44:GLY:CA	2.45	0.69
7:F:13:TYR:CG	7:F:34:CYS:SG	2.86	0.68
25:X:81:ILE:HG21	25:X:120:PHE:CE2	2.28	0.68
1:2:1639:C:N1	1:2:1753:A:C6	2.61	0.68
7:F:21:LEU:CD2	30:c:6:LEU:HG	2.19	0.68
9:H:45:LEU:HD13	9:H:45:LEU:C	2.18	0.68
1:2:19:A:H5'	25:X:107:ARG:NH1	2.09	0.68
6:E:48:LEU:HD21	6:E:70:ILE:HD11	1.75	0.68
7:F:6:LYS:O	7:F:36:PHE:HA	1.94	0.68
27:Z:124:VAL:HB	27:Z:128:LEU:HD12	1.75	0.68
1:2:1043:G:OP1	3:B:157:GLN:NE2	2.25	0.68
8:G:69:VAL:HG12	8:G:71:HIS:CD2	2.28	0.68
9:H:139:ILE:CD1	9:H:156:VAL:HG11	2.23	0.68
9:H:140:VAL:HG21	9:H:159:ASP:HA	1.74	0.68
11:J:158:TYR:CD1	11:J:164:PHE:HB2	2.29	0.68
2:A:34:LYS:CB	2:A:155:LEU:HD12	2.21	0.68
4:C:103:ARG:HH22	4:C:105:ARG:HH21	1.42	0.68
19:R:31:ASN:O	19:R:34:ILE:HG12	1.94	0.68
24:W:57:ARG:HG3	24:W:57:ARG:HH11	1.59	0.68
3:B:153:THR:OG1	3:B:154:CYS:N	2.25	0.68
7:F:15:ASP:O	7:F:16:VAL:HG12	1.93	0.68
25:X:81:ILE:CG2	25:X:120:PHE:CD2	2.77	0.68
1:2:1526:U:O2'	18:Q:45:GLN:OE1	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:11:ARG:HG3	6:E:28:ALA:HB2	1.76	0.67
8:G:32:MET:HE2	8:G:63:MET:CG	2.22	0.67
12:K:39:ARG:CG	12:K:45:VAL:O	2.42	0.67
26:Y:22:ARG:HD2	26:Y:77:MET:HG3	1.75	0.67
1:2:71:U:O2	1:2:80:G:C6	2.47	0.67
1:2:867:C:O2	29:b:49:GLN:OE1	2.12	0.67
25:X:73:GLN:HE21	25:X:80:LYS:HE3	1.60	0.67
9:H:79:ILE:HB	9:H:82:ARG:CD	2.24	0.67
21:T:46:TRP:O	21:T:49:TYR:HD2	1.78	0.67
2:A:63:ALA:HB2	2:A:182:GLU:CD	2.19	0.67
9:H:60:LYS:HE3	9:H:93:LYS:N	2.09	0.67
25:X:135:LYS:O	25:X:136:GLU:HB2	1.94	0.67
27:Z:120:GLU:CG	27:Z:121:ARG:NH1	2.58	0.67
3:B:34:ALA:N	3:B:43:PHE:HE2	1.91	0.67
17:P:49:LYS:HZ3	17:P:88:LEU:HA	1.59	0.67
12:K:84:LEU:HD12	12:K:84:LEU:N	2.09	0.67
1:2:1469:U:C4	7:F:70:ASN:ND2	2.63	0.67
1:2:858:U:H5'	15:N:20:ARG:HH12	1.59	0.67
1:2:1753:A:O2'	1:2:1754:A:C5'	2.41	0.67
4:C:181:PRO:HG2	4:C:184:THR:CG2	2.24	0.67
11:J:118:LEU:HD12	11:J:118:LEU:N	2.00	0.67
16:O:49:VAL:HB	16:O:59:VAL:HG12	1.77	0.67
25:X:76:LYS:HB2	25:X:77:ASN:OD1	1.95	0.67
7:F:167:ASN:ND2	7:F:175:ALA:N	2.42	0.66
13:L:88:ILE:HD12	13:L:126:VAL:HG13	1.75	0.66
1:2:80:G:H2'	1:2:81:C:C5	2.29	0.66
2:A:36:ARG:HB2	2:A:36:ARG:CZ	2.25	0.66
2:A:59:ILE:O	2:A:182:GLU:CD	2.38	0.66
25:X:103:ALA:HB2	25:X:123:VAL:HG21	1.77	0.66
1:2:80:G:C2'	1:2:81:C:C6	2.79	0.66
3:B:66:TYR:OH	16:O:53:SER:OG	2.12	0.66
4:C:103:ARG:CZ	4:C:105:ARG:CZ	2.73	0.66
7:F:94:LYS:HE3	7:F:99:VAL:HG23	1.74	0.66
1:2:1639:C:C2	1:2:1753:A:C6	2.83	0.66
7:F:5:ALA:HA	7:F:36:PHE:CE1	2.30	0.66
7:F:91:MET:O	7:F:92:THR:OG1	2.12	0.66
25:X:73:GLN:HE21	25:X:80:LYS:CE	2.08	0.66
7:F:7:LEU:HG	7:F:13:TYR:CZ	2.31	0.66
7:F:155:LYS:HG3	7:F:159:GLU:OE1	1.96	0.66
25:X:63:ASN:HB2	25:X:114:ASP:CG	2.17	0.66
5:D:18:VAL:HB	31:d:20:ARG:NH2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:35:MET:HA	17:P:38:LEU:HB3	1.78	0.66
31:d:18:GLN:HE21	31:d:23:PHE:HD2	1.44	0.66
10:I:119:LEU:HD12	10:I:153:PRO:HB2	1.76	0.66
1:2:1429:G:C4	31:d:39:GLN:CB	2.79	0.65
3:B:123:ALA:HB1	3:B:169:MET:HE3	1.78	0.65
21:T:49:TYR:O	21:T:50:VAL:CB	2.44	0.65
1:2:1533:U:N1	7:F:154:ILE:CG2	2.59	0.65
4:C:103:ARG:NH1	4:C:105:ARG:HE	1.94	0.65
9:H:155:LYS:HG2	9:H:188:VAL:HG13	1.78	0.65
19:R:32:LYS:HD3	19:R:48:ASN:OD1	1.96	0.65
34:m:12:ARG:HD2	34:m:12:ARG:C	2.21	0.65
1:2:739:U:O2	9:H:110:ARG:NH2	2.28	0.65
7:F:5:ALA:CA	7:F:36:PHE:CE1	2.79	0.65
12:K:70:GLN:OE1	31:d:23:PHE:CE2	2.50	0.65
1:2:10:G:C2'	4:C:102:GLN:HE22	2.09	0.65
7:F:39:HIS:CD2	7:F:74:LYS:HD3	2.32	0.65
19:R:72:LYS:O	19:R:76:GLU:HG3	1.96	0.65
28:a:34:LYS:O	28:a:34:LYS:HG2	1.96	0.65
1:2:1533:U:N1	7:F:154:ILE:HG23	2.11	0.65
4:C:191:THR:HG23	4:C:218:PHE:HE2	1.62	0.65
7:F:21:LEU:HD23	7:F:21:LEU:C	2.21	0.65
12:K:69:TRP:HZ3	31:d:21:VAL:CG2	2.09	0.65
1:2:1752:U:HO2'	1:2:1753:A:P	2.16	0.64
9:H:142:LYS:O	24:W:54:ASP:HB3	1.97	0.64
9:H:168:ILE:CD1	9:H:191:PHE:HZ	2.10	0.64
19:R:69:ILE:CG2	19:R:71:LEU:HG	2.26	0.64
3:B:61:LEU:CD2	3:B:91:ILE:CD1	2.64	0.64
7:F:39:HIS:HE1	18:Q:84:TYR:OH	1.78	0.64
17:P:73:ALA:O	17:P:74:PHE:HB3	1.95	0.64
25:X:40:PRO:HB2	25:X:81:ILE:HD11	1.78	0.64
25:X:51:VAL:CG1	25:X:70:VAL:HG13	2.27	0.64
9:H:137:THR:O	9:H:138:GLU:HB2	1.97	0.64
11:J:116:LEU:HD22	11:J:156:VAL:HG23	1.79	0.64
1:2:944:U:P	3:B:165:ARG:HH11	2.20	0.64
9:H:79:ILE:HD12	9:H:82:ARG:HG3	1.79	0.64
1:2:418:G:O2'	8:G:59:GLN:NE2	2.31	0.64
4:C:181:PRO:CD	4:C:184:THR:HG21	2.28	0.64
6:E:34:GLY:O	6:E:35:PRO:C	2.40	0.64
17:P:39:LEU:HD12	17:P:39:LEU:N	2.12	0.64
19:R:73:LEU:C	19:R:73:LEU:HD23	2.22	0.64
2:A:100:ILE:HD11	2:A:118:MET:HE1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:163:ALA:O	3:B:167:LYS:HG2	1.98	0.64
4:C:183:GLY:O	4:C:185:HIS:HD2	1.81	0.64
11:J:135:ARG:N	11:J:157:ASP:O	2.31	0.64
8:G:68:LEU:C	8:G:69:VAL:HG23	2.23	0.64
12:K:84:LEU:CD1	12:K:84:LEU:H	2.10	0.64
21:T:128:SER:HA	21:T:129:ASP:CB	2.09	0.64
17:P:129:LYS:H	17:P:129:LYS:CD	2.09	0.64
28:a:12:LYS:HG3	28:a:15:ARG:HG3	1.80	0.64
3:B:48:VAL:HG12	3:B:48:VAL:O	1.96	0.63
9:H:67:VAL:CG1	9:H:72:TYR:HB2	2.28	0.63
1:2:1679:A:H1'	8:G:66:GLY:HA3	1.76	0.63
4:C:184:THR:HG22	11:J:53:ARG:HH21	1.62	0.63
9:H:139:ILE:HD11	9:H:156:VAL:HG11	1.80	0.63
3:B:33:LYS:HZ2	3:B:41:ARG:HG3	1.62	0.63
4:C:184:THR:O	4:C:185:HIS:HB2	1.99	0.63
7:F:7:LEU:CD2	7:F:13:TYR:HH	2.10	0.63
1:2:1639:C:H1'	1:2:1753:A:C6	2.33	0.63
3:B:165:ARG:O	3:B:169:MET:HG2	1.98	0.63
7:F:6:LYS:CA	7:F:36:PHE:CD1	2.81	0.63
24:W:56:HIS:O	24:W:57:ARG:NH1	2.31	0.63
12:K:69:TRP:CZ3	31:d:21:VAL:HG13	2.32	0.63
3:B:32:LEU:H	3:B:44:GLY:C	2.04	0.63
7:F:27:ILE:HG23	7:F:56:ILE:HD12	1.81	0.63
7:F:6:LYS:CA	7:F:36:PHE:CE1	2.79	0.63
11:J:94:ASP:OD1	11:J:94:ASP:N	2.30	0.63
21:T:50:VAL:HG12	21:T:52:THR:N	2.13	0.63
1:2:1585:G:O2'	7:F:71:ASN:ND2	2.31	0.63
4:C:185:HIS:O	4:C:203:ASP:HA	1.98	0.63
25:X:59:ALA:CB	25:X:114:ASP:CG	2.43	0.63
25:X:96:GLU:O	25:X:97:ASN:HB2	1.98	0.63
9:H:79:ILE:HB	9:H:82:ARG:CG	2.28	0.63
3:B:34:ALA:CA	3:B:43:PHE:HE2	2.11	0.62
7:F:90:LEU:CD1	27:Z:156:THR:HG22	2.29	0.62
19:R:74:GLN:C	19:R:78:ARG:HG2	2.24	0.62
2:A:59:ILE:C	2:A:182:GLU:OE2	2.42	0.62
7:F:6:LYS:C	7:F:36:PHE:CD1	2.71	0.62
9:H:63:PHE:HE2	9:H:93:LYS:CD	2.13	0.62
3:B:38:PHE:CZ	3:B:84:ILE:HG12	2.32	0.62
19:R:69:ILE:HG21	19:R:71:LEU:HD21	1.82	0.62
25:X:68:LYS:HG3	25:X:91:LEU:HD11	1.71	0.62
3:B:26:LYS:HB3	3:B:50:LYS:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:13:TYR:HB2	7:F:34:CYS:HG	1.63	0.62
26:Y:22:ARG:NE	26:Y:77:MET:SD	2.73	0.62
1:2:1429:G:H4'	31:d:24:ASN:HD22	1.65	0.62
25:X:55:LEU:HD23	25:X:56:GLY:N	2.13	0.62
28:a:35:ALA:O	28:a:36:ILE:HB	2.00	0.62
1:2:569:A:N1	25:X:114:ASP:HB2	2.14	0.62
1:2:1252:U:C2'	12:K:10:LEU:CB	2.77	0.62
1:2:1561:A:H4'	21:T:54:HIS:NE2	2.14	0.62
4:C:117:GLY:H	4:C:149:ARG:HH22	1.47	0.62
9:H:72:TYR:CA	9:H:76:VAL:HG12	2.14	0.62
21:T:46:TRP:O	21:T:49:TYR:CD2	2.52	0.62
24:W:52:ILE:HG23	24:W:52:ILE:O	2.00	0.62
25:X:51:VAL:CG1	25:X:70:VAL:CG1	2.75	0.62
27:Z:118:VAL:CG1	27:Z:122:LEU:HD12	2.29	0.62
28:a:11:ALA:C	28:a:33:ASP:OD2	2.43	0.62
3:B:45:LYS:O	3:B:46:THR:CG2	2.46	0.62
11:J:118:LEU:CD2	11:J:158:TYR:CE2	2.77	0.62
11:J:136:VAL:HG22	11:J:156:VAL:HG12	1.82	0.62
12:K:36:LYS:NZ	12:K:36:LYS:HB3	2.15	0.62
21:T:49:TYR:O	21:T:50:VAL:CG2	2.48	0.62
27:Z:147:GLU:O	27:Z:148:HIS:HB2	2.00	0.62
3:B:42:ASN:O	3:B:43:PHE:HB3	1.99	0.62
11:J:120:LYS:O	11:J:121:SER:HB3	1.98	0.62
17:P:25:VAL:HG12	17:P:30:LEU:HD21	1.81	0.62
7:F:7:LEU:C	7:F:8:PHE:HD2	2.08	0.61
4:C:42:LYS:HG3	4:C:248:TYR:HE1	1.65	0.61
11:J:158:TYR:CD1	11:J:164:PHE:CB	2.83	0.61
11:J:116:LEU:HG	11:J:118:LEU:HD11	1.82	0.61
7:F:27:ILE:HG23	7:F:56:ILE:CD1	2.30	0.61
19:R:18:GLU:HA	19:R:71:LEU:CD2	2.18	0.61
27:Z:103:LEU:CD2	27:Z:122:LEU:HD11	2.11	0.61
1:2:30:G:H5'	25:X:124:LYS:CE	2.30	0.61
1:2:1571:A:H61	7:F:69:ARG:NH2	1.99	0.61
3:B:186:LYS:O	3:B:190:PRO:HD3	2.00	0.61
7:F:39:HIS:HD2	7:F:74:LYS:HD3	1.64	0.61
9:H:134:VAL:HG23	9:H:158:LEU:HD21	1.82	0.61
25:X:68:LYS:CB	25:X:91:LEU:CD1	2.49	0.61
3:B:40:VAL:CG1	3:B:73:LEU:HA	2.29	0.61
4:C:47:VAL:HG21	4:C:70:ILE:HG23	1.83	0.61
27:Z:119:CYS:O	27:Z:122:LEU:O	2.18	0.61
7:F:39:HIS:CE1	18:Q:84:TYR:OH	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:69:ILE:CG2	19:R:71:LEU:HD21	2.31	0.61
29:b:31:MET:HE2	29:b:46:SER:HA	1.81	0.61
7:F:36:PHE:O	7:F:37:VAL:HG12	2.01	0.61
9:H:57:GLN:O	9:H:57:GLN:HG3	1.99	0.61
1:2:30:G:P	25:X:124:LYS:HZ3	2.17	0.61
21:T:50:VAL:O	21:T:51:LYS:HG2	2.00	0.61
3:B:137:MET:HE2	3:B:188:PHE:HZ	1.66	0.60
9:H:65:VAL:HG13	9:H:97:LEU:HG	1.82	0.60
11:J:116:LEU:CB	11:J:118:LEU:HD11	2.30	0.60
25:X:105:PHE:CG	25:X:112:VAL:CG2	2.82	0.60
1:2:534:C:OP2	11:J:168:ARG:NH1	2.34	0.60
3:B:187:LYS:C	3:B:190:PRO:HD2	2.25	0.60
11:J:116:LEU:HB3	11:J:118:LEU:HD11	1.84	0.60
3:B:81:PHE:O	3:B:82:ARG:HB3	2.01	0.60
18:Q:49:LEU:CB	18:Q:83:ILE:HD13	2.31	0.60
25:X:103:ALA:HB2	25:X:123:VAL:CG2	2.32	0.60
2:A:41:LYS:O	2:A:41:LYS:HG2	2.01	0.60
7:F:27:ILE:HG12	7:F:56:ILE:HD11	1.84	0.60
9:H:172:LEU:HD11	9:H:190:SER:HA	1.84	0.60
1:2:1109:G:C6	34:m:2:ALA:HB2	2.37	0.60
4:C:42:LYS:HG3	4:C:248:TYR:CE1	2.36	0.60
7:F:13:TYR:CG	7:F:34:CYS:HB2	2.37	0.60
7:F:156:THR:OG1	7:F:159:GLU:HG3	2.02	0.60
1:2:1469:U:N3	7:F:157:ILE:HD12	2.17	0.60
4:C:180:ALA:HB1	4:C:184:THR:HG21	1.84	0.60
21:T:49:TYR:O	21:T:50:VAL:HB	2.01	0.60
10:I:140:THR:C	10:I:142:CYS:N	2.56	0.60
19:R:74:GLN:O	19:R:78:ARG:CG	2.50	0.60
3:B:184:LEU:O	3:B:184:LEU:HD12	2.02	0.60
8:G:67:VAL:HG23	8:G:68:LEU:N	2.16	0.60
9:H:67:VAL:N	9:H:98:VAL:O	2.35	0.60
9:H:79:ILE:CG2	9:H:82:ARG:CD	2.79	0.60
9:H:105:PRO:HB2	9:H:107:ASP:OD1	2.01	0.60
9:H:107:ASP:O	9:H:109:LYS:N	2.35	0.60
1:2:80:G:H2'	1:2:81:C:H6	1.64	0.59
3:B:74:ASN:HB3	3:B:76:ASP:OD1	2.02	0.59
19:R:69:ILE:HD12	19:R:69:ILE:H	1.66	0.59
25:X:89:GLY:C	25:X:90:SER:HG	2.05	0.59
1:2:1751:G:C2'	1:2:1752:U:H5'	2.32	0.59
9:H:103:MET:HE3	9:H:122:LEU:HD13	1.84	0.59
23:V:12:TYR:HD1	23:V:13:ILE:N	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:98:ASP:OD1	25:X:98:ASP:N	2.32	0.59
3:B:48:VAL:O	3:B:49:THR:HB	2.01	0.59
7:F:5:ALA:N	7:F:36:PHE:CZ	2.71	0.59
8:G:67:VAL:O	8:G:68:LEU:HB2	2.01	0.59
9:H:110:ARG:O	9:H:111:LYS:HB2	2.02	0.59
9:H:155:LYS:HG2	9:H:188:VAL:CG1	2.33	0.59
1:2:10:G:H1'	4:C:102:GLN:NE2	2.17	0.59
11:J:133:HIS:ND1	11:J:164:PHE:CD2	2.71	0.59
15:N:138:THR:HG22	15:N:138:THR:O	2.01	0.59
4:C:75:PHE:CD1	4:C:80:CYS:SG	2.94	0.59
17:P:25:VAL:CG1	17:P:30:LEU:CD2	2.80	0.59
3:B:26:LYS:C	3:B:50:LYS:HG2	2.18	0.59
7:F:23:LEU:HD21	7:F:134:ARG:NE	2.15	0.59
25:X:95:ASP:C	25:X:98:ASP:OD2	2.45	0.59
8:G:58:LYS:NZ	8:G:58:LYS:HB3	2.18	0.59
9:H:130:LEU:HD21	9:H:179:TYR:CD1	2.36	0.59
2:A:179:LEU:O	2:A:183:VAL:HG23	2.03	0.59
7:F:172:SER:O	7:F:173:SER:HB3	2.03	0.59
9:H:41:ASP:OD1	9:H:41:ASP:N	2.33	0.59
9:H:189:PHE:O	9:H:190:SER:CB	2.41	0.59
2:A:117:PHE:CE2	4:C:41:THR:CG2	2.75	0.59
8:G:69:VAL:CG1	8:G:71:HIS:CD2	2.86	0.59
9:H:46:VAL:CG1	9:H:71:VAL:HG21	2.33	0.59
15:N:136:PRO:HG2	15:N:139:TRP:HB2	1.85	0.59
21:T:50:VAL:HG11	21:T:65:TRP:CH2	2.37	0.59
7:F:21:LEU:HD22	30:c:6:LEU:CD1	2.32	0.58
9:H:76:VAL:HG22	9:H:76:VAL:O	2.02	0.58
9:H:193:GLN:O	9:H:193:GLN:HG3	2.03	0.58
12:K:70:GLN:CB	31:d:23:PHE:HZ	2.09	0.58
21:T:50:VAL:HG12	21:T:51:LYS:N	2.18	0.58
1:2:1110:U:C5'	34:m:28:GLN:HE22	2.06	0.58
3:B:45:LYS:C	3:B:46:THR:HG23	2.28	0.58
3:B:86:LEU:HD23	3:B:100:PHE:HB2	1.83	0.58
4:C:73:HIS:O	4:C:76:GLN:HG3	2.02	0.58
27:Z:93:VAL:O	27:Z:128:LEU:HD21	2.03	0.58
1:2:1753:A:HO2'	1:2:1754:A:P	2.26	0.58
9:H:53:VAL:CB	9:H:181:LYS:HD3	2.33	0.58
12:K:8:PHE:C	12:K:9:SER:HG	1.99	0.58
16:O:47:ILE:HG22	16:O:61:VAL:HB	1.84	0.58
17:P:49:LYS:HZ1	17:P:87:ASP:C	1.91	0.58
30:c:67:LEU:HD13	30:c:67:LEU:C	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:33:LYS:NZ	3:B:41:ARG:HG3	2.19	0.58
7:F:6:LYS:CA	7:F:11:TRP:O	2.50	0.58
21:T:52:THR:CG2	21:T:69:ARG:NH2	2.62	0.58
7:F:13:TYR:CG	7:F:34:CYS:CB	2.87	0.58
15:N:23:PRO:CG	15:N:25:TRP:CE2	2.86	0.58
21:T:51:LYS:HE2	21:T:53:ALA:O	2.03	0.58
24:W:60:LYS:NZ	29:b:21:ARG:O	2.36	0.58
4:C:37:TRP:H	4:C:37:TRP:CD1	2.22	0.58
4:C:55:ILE:CG2	4:C:74:PHE:CD2	2.86	0.58
7:F:7:LEU:HD23	7:F:13:TYR:OH	1.97	0.58
8:G:52:ILE:HD11	8:G:109:LEU:HD22	1.85	0.58
9:H:79:ILE:CG1	9:H:80:GLN:H	2.15	0.58
17:P:34:LYS:O	17:P:38:LEU:HB2	2.03	0.58
19:R:17:VAL:O	19:R:71:LEU:CD2	2.52	0.58
19:R:27:ASP:OD1	19:R:28:PHE:N	2.36	0.58
27:Z:120:GLU:CD	27:Z:121:ARG:HH12	2.08	0.58
7:F:7:LEU:HD21	7:F:13:TYR:HH	1.58	0.58
12:K:38:GLU:HA	12:K:38:GLU:OE1	2.02	0.58
25:X:41:PHE:HZ	25:X:102:VAL:HG12	1.68	0.58
1:2:1109:G:C5	34:m:2:ALA:HB1	2.39	0.58
19:R:19:LYS:HG3	19:R:20:TYR:CE2	2.39	0.58
17:P:32:ASP:OD1	17:P:32:ASP:N	2.37	0.58
25:X:87:ARG:NH1	25:X:131:LEU:HD21	2.19	0.58
1:2:533:U:H5'	11:J:168:ARG:HH22	1.67	0.57
3:B:166:LYS:O	3:B:170:THR:HG22	2.04	0.57
5:D:44:THR:HG22	22:U:220:ILE:HG21	1.86	0.57
10:I:142:CYS:O	10:I:146:LYS:HG3	2.04	0.57
16:O:47:ILE:CG2	16:O:61:VAL:HB	2.34	0.57
1:2:1113:G:OP2	34:m:35:ARG:NH1	2.37	0.57
3:B:191:GLU:O	3:B:191:GLU:HG3	2.04	0.57
11:J:119:ALA:O	11:J:120:LYS:HD3	2.04	0.57
31:d:38:ARG:CZ	31:d:39:GLN:HE22	2.18	0.57
4:C:39:PRO:HD3	4:C:48:ARG:HE	1.69	0.57
1:2:1533:U:C2	7:F:154:ILE:HG21	2.37	0.57
4:C:117:GLY:N	4:C:149:ARG:HH22	2.02	0.57
7:F:23:LEU:HD21	7:F:134:ARG:HH11	1.69	0.57
31:d:25:ARG:O	31:d:28:MET:CG	2.37	0.57
15:N:23:PRO:CG	15:N:26:LEU:HB2	2.33	0.57
17:P:74:PHE:CD2	17:P:75:GLY:N	2.73	0.57
25:X:95:ASP:C	25:X:98:ASP:OD1	2.44	0.57
7:F:167:ASN:ND2	7:F:175:ALA:H	1.96	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:140:VAL:HG23	9:H:159:ASP:CA	2.35	0.57
1:2:1109:G:N7	34:m:2:ALA:HB1	2.20	0.57
7:F:16:VAL:CG2	7:F:98:GLN:HB2	2.35	0.57
19:R:69:ILE:HG22	19:R:71:LEU:CD2	2.35	0.57
25:X:112:VAL:HG12	25:X:113:GLY:H	1.68	0.57
31:d:34:LEU:CD2	31:d:41:PHE:CD1	2.84	0.57
34:m:12:ARG:HH11	34:m:12:ARG:CB	2.14	0.57
25:X:95:ASP:C	25:X:98:ASP:CG	2.68	0.57
27:Z:118:VAL:HG13	27:Z:122:LEU:HD12	1.87	0.57
3:B:26:LYS:CA	3:B:50:LYS:HD2	2.27	0.57
9:H:45:LEU:HD23	9:H:76:VAL:CG2	2.35	0.57
25:X:77:ASN:OD1	25:X:77:ASN:N	2.38	0.57
29:b:32:ASP:OD2	29:b:80:LYS:CE	2.53	0.57
1:2:618:A:O5'	34:m:9:LYS:NZ	2.38	0.56
2:A:59:ILE:HG22	2:A:182:GLU:CD	2.17	0.56
7:F:23:LEU:CD2	7:F:134:ARG:HH11	2.18	0.56
9:H:53:VAL:CG2	9:H:181:LYS:HD2	2.15	0.56
24:W:57:ARG:HG3	24:W:57:ARG:NH1	2.18	0.56
34:m:15:MET:O	34:m:16:ARG:CB	2.49	0.56
15:N:129:TYR:HB3	15:N:135:LEU:HG	1.86	0.56
18:Q:43:HIS:CG	18:Q:44:LEU:N	2.71	0.56
27:Z:148:HIS:CG	27:Z:149:HIS:N	2.73	0.56
1:2:554:A:C6	1:2:555:A:N6	2.73	0.56
1:2:1469:U:OP2	7:F:156:THR:HA	2.06	0.56
3:B:61:LEU:CG	3:B:91:ILE:HD11	2.34	0.56
3:B:100:PHE:CE2	3:B:185:VAL:CG2	2.89	0.56
4:C:76:GLN:HE21	4:C:79:ASN:HD22	1.52	0.56
26:Y:97:LEU:HD22	26:Y:99:TYR:CE2	2.40	0.56
34:m:4:GLY:O	34:m:7:ARG:HB2	2.04	0.56
10:I:76:THR:HG21	10:I:104:ILE:HG23	1.86	0.56
19:R:36:GLU:CD	19:R:47:ARG:HB2	2.30	0.56
21:T:51:LYS:HD2	21:T:56:LYS:O	2.04	0.56
2:A:63:ALA:CB	2:A:182:GLU:HG2	2.36	0.56
4:C:85:LYS:O	4:C:112:VAL:HG23	2.06	0.56
21:T:128:SER:HB2	21:T:129:ASP:C	2.30	0.56
9:H:53:VAL:HG12	9:H:62:ALA:O	2.06	0.56
1:2:1241:C:O4'	1:2:1241:C:O2	2.24	0.56
19:R:20:TYR:CE1	19:R:38:VAL:HB	2.41	0.56
19:R:66:VAL:O	19:R:69:ILE:HD13	2.06	0.56
27:Z:120:GLU:CD	27:Z:121:ARG:NH1	2.64	0.56
7:F:10:ARG:HD2	21:T:6:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:79:ARG:NH2	27:Z:149:HIS:CE1	2.71	0.56
9:H:65:VAL:HG13	9:H:65:VAL:O	2.05	0.56
12:K:70:GLN:CB	31:d:23:PHE:CZ	2.88	0.56
1:2:599:U:OP2	25:X:106:GLY:HA2	2.05	0.56
4:C:42:LYS:O	4:C:46:LEU:HG	2.06	0.56
1:2:10:G:C1'	4:C:102:GLN:HE22	2.19	0.55
3:B:48:VAL:HG21	3:B:61:LEU:CD1	2.34	0.55
7:F:64:MET:SD	7:F:80:ILE:CD1	2.92	0.55
12:K:33:LYS:N	12:K:70:GLN:O	2.39	0.55
18:Q:43:HIS:CG	18:Q:44:LEU:H	2.22	0.55
7:F:79:ARG:HE	27:Z:149:HIS:HE1	1.54	0.55
7:F:155:LYS:NZ	7:F:159:GLU:HB3	2.21	0.55
17:P:39:LEU:CD1	17:P:39:LEU:H	2.19	0.55
3:B:124:PHE:HB3	3:B:138:PHE:CD1	2.41	0.55
4:C:181:PRO:HD2	4:C:184:THR:HG21	1.87	0.55
15:N:23:PRO:HD3	15:N:26:LEU:CD2	2.36	0.55
19:R:73:LEU:HD23	19:R:73:LEU:O	2.06	0.55
2:A:33:HIS:O	2:A:36:ARG:HG2	2.05	0.55
3:B:61:LEU:CG	3:B:91:ILE:CD1	2.85	0.55
11:J:124:HIS:HD2	11:J:128:LEU:CD1	2.19	0.55
25:X:90:SER:HA	25:X:93:TYR:CD2	2.41	0.55
26:Y:22:ARG:HD2	26:Y:77:MET:CG	2.37	0.55
26:Y:93:ARG:O	26:Y:97:LEU:HD13	2.06	0.55
17:P:130:PRO:HG2	20:S:129:TRP:CH2	2.38	0.55
6:E:31:PRO:HD2	6:E:38:LEU:HD12	1.86	0.55
26:Y:5:GLY:O	26:Y:6:ALA:HB3	2.06	0.55
26:Y:97:LEU:HD23	26:Y:99:TYR:OH	2.07	0.55
27:Z:149:HIS:CD2	27:Z:151:SER:N	2.75	0.55
34:m:19:TRP:HE3	34:m:19:TRP:HA	1.71	0.55
9:H:53:VAL:HG23	9:H:181:LYS:HG3	1.89	0.55
11:J:124:HIS:CD2	11:J:128:LEU:HD11	2.41	0.55
11:J:133:HIS:CE1	11:J:164:PHE:HE2	2.23	0.55
25:X:86:PRO:HG2	25:X:130:LEU:HD12	1.88	0.55
26:Y:22:ARG:HD2	26:Y:77:MET:SD	2.47	0.55
4:C:92:MET:HE3	4:C:107:LYS:HE3	1.89	0.55
6:E:194:VAL:O	6:E:210:LEU:HB2	2.07	0.55
8:G:57:ASP:HB3	8:G:106:LEU:CB	2.36	0.55
12:K:33:LYS:HD3	12:K:33:LYS:O	2.07	0.55
2:A:34:LYS:HD2	23:V:62:GLY:O	2.07	0.54
3:B:67:GLU:OE1	3:B:83:LYS:NZ	2.37	0.54
11:J:93:LEU:HD12	11:J:94:ASP:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:69:ILE:CG2	19:R:71:LEU:CD2	2.86	0.54
22:U:165:ALA:HB3	22:U:204:ASP:HB2	1.89	0.54
25:X:61:GLN:HA	25:X:62:PRO:C	2.32	0.54
3:B:26:LYS:CA	3:B:50:LYS:HD3	2.37	0.54
9:H:104:LEU:CD2	9:H:108:PHE:HB2	2.36	0.54
1:2:1113:G:OP1	34:m:35:ARG:NH1	2.41	0.54
9:H:42:VAL:O	9:H:43:ARG:C	2.51	0.54
15:N:139:TRP:CE3	15:N:139:TRP:C	2.86	0.54
17:P:75:GLY:O	17:P:76:GLU:HB2	2.07	0.54
1:2:1753:A:P	1:2:1753:A:H3'	2.47	0.54
2:A:117:PHE:CZ	4:C:41:THR:HG22	2.37	0.54
6:E:191:ARG:NH2	6:E:218:PHE:CD2	2.65	0.54
7:F:7:LEU:C	7:F:8:PHE:CD2	2.86	0.54
11:J:90:GLU:OE1	11:J:90:GLU:N	2.40	0.54
19:R:26:LEU:HD12	19:R:27:ASP:N	2.23	0.54
34:m:19:TRP:HA	34:m:19:TRP:CE3	2.42	0.54
2:A:187:ARG:HB3	2:A:189:GLU:OE1	2.07	0.54
15:N:139:TRP:O	15:N:139:TRP:HE3	1.90	0.54
23:V:12:TYR:CD1	23:V:13:ILE:N	2.75	0.54
3:B:48:VAL:HG21	3:B:61:LEU:HD22	1.88	0.54
16:O:62:THR:O	16:O:63:GLY:C	2.51	0.54
19:R:71:LEU:O	19:R:72:LYS:HB3	2.07	0.54
23:V:12:TYR:CD1	23:V:12:TYR:C	2.85	0.54
3:B:26:LYS:O	3:B:50:LYS:CB	2.55	0.54
8:G:64:MET:HG3	8:G:67:VAL:CG1	2.38	0.54
9:H:114:LYS:HG3	9:H:115:VAL:HG23	1.89	0.54
2:A:23:LYS:HB3	2:A:26:ILE:HD12	1.90	0.54
9:H:132:ASP:N	9:H:132:ASP:OD1	2.41	0.54
20:S:85:PHE:CE2	21:T:49:TYR:HD1	2.25	0.54
1:2:1533:U:C5	7:F:154:ILE:N	2.76	0.54
9:H:68:PRO:CG	9:H:71:VAL:CG2	2.86	0.54
9:H:79:ILE:HG22	9:H:82:ARG:NH1	2.22	0.54
9:H:116:ARG:O	9:H:117:PRO:C	2.49	0.54
14:M:70:ALA:O	14:M:74:LEU:N	2.37	0.54
16:O:38:ILE:HG12	16:O:47:ILE:HD12	1.85	0.54
25:X:55:LEU:CD2	25:X:69:CYS:HG	1.99	0.54
1:2:1469:U:N1	7:F:70:ASN:ND2	2.49	0.54
3:B:45:LYS:O	3:B:46:THR:HG23	2.07	0.54
8:G:62:PRO:HG2	8:G:83:CYS:SG	2.47	0.54
15:N:23:PRO:HB2	15:N:25:TRP:CD1	2.43	0.54
19:R:21:TYR:C	19:R:21:TYR:CD2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:41:PHE:C	31:d:41:PHE:CD2	2.85	0.54
1:2:30:G:C5'	25:X:124:LYS:HE2	2.30	0.53
1:2:927:A:P	28:a:32:LYS:NZ	2.79	0.53
3:B:82:ARG:HA	3:B:105:MET:HA	1.91	0.53
3:B:128:THR:HG22	3:B:134:THR:CG2	2.37	0.53
17:P:39:LEU:O	17:P:42:PHE:HB2	2.07	0.53
19:R:67:ARG:C	19:R:69:ILE:HD12	2.33	0.53
1:2:1764:C:OP1	34:m:17:TRP:HB3	2.09	0.53
9:H:107:ASP:OD1	9:H:107:ASP:N	2.40	0.53
20:S:85:PHE:HE2	21:T:49:TYR:HD1	1.56	0.53
31:d:19:CYS:HB3	31:d:24:ASN:H	1.73	0.53
9:H:112:GLY:O	9:H:113:LEU:HB3	2.09	0.53
11:J:118:LEU:HD23	11:J:158:TYR:CD2	2.41	0.53
17:P:31:LEU:HD23	17:P:31:LEU:N	2.23	0.53
24:W:14:LEU:HD13	24:W:63:ILE:HD11	1.90	0.53
1:2:1571:A:H61	7:F:69:ARG:HH22	1.56	0.53
9:H:61:LYS:O	9:H:93:LYS:HB3	2.09	0.53
15:N:23:PRO:HD3	15:N:26:LEU:HD22	1.89	0.53
19:R:18:GLU:CA	19:R:71:LEU:HD23	2.21	0.53
25:X:81:ILE:CG2	25:X:120:PHE:CE2	2.92	0.53
26:Y:16:THR:HG22	26:Y:23:LYS:HE3	1.91	0.53
1:2:448:C:OP1	6:E:29:PRO:CD	2.54	0.53
3:B:137:MET:CE	3:B:188:PHE:HZ	2.21	0.53
4:C:115:SER:O	4:C:116:ASN:CB	2.56	0.53
19:R:30:ILE:O	19:R:34:ILE:HG23	2.08	0.53
1:2:1751:G:H2'	1:2:1752:U:H5'	1.91	0.53
7:F:167:ASN:ND2	7:F:175:ALA:CB	2.71	0.53
9:H:83:LEU:O	9:H:83:LEU:HD23	2.09	0.53
11:J:124:HIS:CD2	11:J:128:LEU:CD1	2.92	0.53
25:X:105:PHE:CE2	25:X:112:VAL:HG21	2.42	0.53
26:Y:92:PHE:C	26:Y:95:VAL:HG12	2.34	0.53
28:a:12:LYS:CG	28:a:15:ARG:HG3	2.39	0.53
29:b:47:HIS:HD2	29:b:67:GLY:C	2.16	0.53
34:m:21:LYS:O	34:m:25:ARG:HG2	2.08	0.53
4:C:55:ILE:HG23	4:C:74:PHE:CD2	2.44	0.53
9:H:79:ILE:CG2	9:H:82:ARG:CZ	2.85	0.53
10:I:139:HIS:C	10:I:139:HIS:CD2	2.86	0.53
18:Q:48:ALA:O	18:Q:51:VAL:HG12	2.08	0.53
25:X:103:ALA:CB	25:X:123:VAL:CG2	2.86	0.53
1:2:738:C:O2	9:H:110:ARG:HD3	2.09	0.53
3:B:199:ASN:HA	3:B:202:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:64:MET:HG3	8:G:67:VAL:HG13	1.90	0.53
9:H:63:PHE:CE2	9:H:93:LYS:CD	2.92	0.53
25:X:64:SER:O	25:X:65:ALA:HB2	2.09	0.53
25:X:124:LYS:HA	25:X:129:SER:HA	1.89	0.53
26:Y:7:PHE:CE1	26:Y:45:LYS:HD3	2.44	0.53
1:2:944:U:P	3:B:165:ARG:NH1	2.82	0.52
4:C:75:PHE:CA	4:C:80:CYS:SG	2.94	0.52
8:G:73:VAL:HG12	8:G:74:ARG:N	2.23	0.52
12:K:32:GLN:CD	12:K:34:ASN:OD1	2.52	0.52
7:F:86:GLU:HG2	27:Z:145:VAL:HG11	1.90	0.52
19:R:69:ILE:CG2	19:R:71:LEU:CG	2.86	0.52
1:2:1753:A:O2'	1:2:1754:A:P	2.67	0.52
4:C:182:ARG:O	11:J:53:ARG:NH2	2.40	0.52
5:D:18:VAL:CG2	31:d:20:ARG:HH22	2.23	0.52
21:T:120:PHE:CB	21:T:126:VAL:HG12	2.37	0.52
25:X:63:ASN:CG	25:X:114:ASP:OD2	2.52	0.52
1:2:80:G:C2'	1:2:81:C:H6	2.19	0.52
7:F:13:TYR:CD1	7:F:34:CYS:HB2	2.45	0.52
9:H:114:LYS:HG3	9:H:115:VAL:N	2.25	0.52
3:B:103:MET:HE1	3:B:188:PHE:HB3	1.90	0.52
5:D:18:VAL:HG21	31:d:20:ARG:HH22	1.74	0.52
9:H:56:PRO:O	9:H:57:GLN:HG2	2.10	0.52
9:H:168:ILE:CD1	9:H:191:PHE:CZ	2.92	0.52
31:d:38:ARG:CZ	31:d:39:GLN:NE2	2.73	0.52
3:B:48:VAL:HG11	3:B:57:ALA:O	2.09	0.52
7:F:154:ILE:O	7:F:154:ILE:HG13	2.10	0.52
21:T:51:LYS:HE3	21:T:56:LYS:O	2.10	0.52
2:A:36:ARG:NH1	2:A:36:ARG:CB	2.73	0.52
9:H:140:VAL:CG2	9:H:159:ASP:CA	2.88	0.52
12:K:36:LYS:NZ	12:K:36:LYS:CB	2.73	0.52
2:A:40:PHE:CD1	2:A:41:LYS:N	2.78	0.52
3:B:48:VAL:HG21	3:B:61:LEU:CG	2.40	0.52
7:F:64:MET:HG3	7:F:64:MET:O	2.10	0.52
8:G:57:ASP:C	8:G:59:GLN:N	2.64	0.52
8:G:69:VAL:CG1	8:G:71:HIS:NE2	2.73	0.52
17:P:39:LEU:CD1	17:P:39:LEU:N	2.73	0.52
1:2:861:U:O2	1:2:861:U:O4'	2.28	0.51
1:2:1512:U:O2	1:2:1512:U:O4'	2.27	0.51
4:C:89:MET:HE1	4:C:194:LYS:HB2	1.91	0.51
4:C:182:ARG:O	11:J:53:ARG:NH1	2.39	0.51
9:H:45:LEU:HD23	9:H:76:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:67:VAL:HG12	9:H:72:TYR:HB2	1.92	0.51
15:N:21:LYS:N	15:N:22:PRO:CD	2.73	0.51
7:F:7:LEU:O	7:F:8:PHE:HB2	2.10	0.51
1:2:533:U:C5'	11:J:168:ARG:HH22	2.23	0.51
3:B:48:VAL:HG21	3:B:61:LEU:CB	2.38	0.51
7:F:5:ALA:CB	7:F:34:CYS:SG	2.98	0.51
7:F:5:ALA:H	7:F:36:PHE:HZ	1.59	0.51
8:G:57:ASP:HA	8:G:107:ALA:H	1.74	0.51
21:T:51:LYS:HA	21:T:60:PRO:CD	2.37	0.51
21:T:52:THR:O	21:T:52:THR:HG22	2.09	0.51
28:a:10:ARG:NH2	28:a:31:PRO:HG2	2.26	0.51
2:A:184:LEU:HD12	2:A:189:GLU:OE1	2.10	0.51
3:B:82:ARG:NH1	3:B:103:MET:SD	2.83	0.51
13:L:73:ILE:HD12	13:L:140:PHE:CE1	2.44	0.51
1:2:10:G:H1'	4:C:102:GLN:HE22	1.75	0.51
17:P:128:TYR:CD1	17:P:128:TYR:C	2.88	0.51
24:W:6:VAL:HG12	24:W:34:ILE:HD11	1.92	0.51
28:a:10:ARG:HB2	28:a:10:ARG:NH1	2.25	0.51
1:2:1061:C:O3'	3:B:149:GLN:HG3	2.10	0.51
3:B:49:THR:HG22	3:B:50:LYS:N	2.24	0.51
7:F:158:ALA:CB	27:Z:152:GLN:OE1	2.59	0.51
9:H:67:VAL:HG12	9:H:68:PRO:O	2.10	0.51
12:K:34:ASN:ND2	12:K:37:ILE:CB	2.73	0.51
15:N:23:PRO:HD3	15:N:26:LEU:CB	2.34	0.51
19:R:75:GLU:HA	19:R:78:ARG:HB2	1.93	0.51
27:Z:148:HIS:CG	27:Z:149:HIS:H	2.29	0.51
29:b:32:ASP:CG	29:b:80:LYS:NZ	2.68	0.51
17:P:53:GLY:CA	17:P:54:ILE:HG13	2.39	0.51
2:A:59:ILE:O	2:A:182:GLU:OE1	2.28	0.51
3:B:48:VAL:O	3:B:48:VAL:CG1	2.58	0.51
4:C:61:PHE:HA	23:V:15:ARG:CZ	2.41	0.51
9:H:114:LYS:HG3	9:H:115:VAL:H	1.75	0.51
21:T:51:LYS:O	21:T:52:THR:HB	2.11	0.51
24:W:55:ASP:OD1	24:W:55:ASP:N	2.40	0.51
1:2:1429:G:H4'	31:d:24:ASN:ND2	2.25	0.51
3:B:187:LYS:CE	3:B:193:ILE:HD11	2.40	0.51
4:C:55:ILE:HG22	4:C:74:PHE:CE2	2.46	0.51
4:C:76:GLN:O	4:C:80:CYS:HB2	2.11	0.51
4:C:81:ALA:N	4:C:82:ALA:HA	2.26	0.51
9:H:79:ILE:CB	9:H:82:ARG:CD	2.88	0.51
9:H:140:VAL:HG23	9:H:159:ASP:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:168:LEU:HB3	10:I:186:ILE:HD11	1.93	0.51
26:Y:93:ARG:O	26:Y:97:LEU:HD12	2.11	0.51
34:m:6:SER:O	34:m:9:LYS:N	2.44	0.51
4:C:119:CYS:C	4:C:144:LEU:HD12	2.36	0.50
15:N:23:PRO:HG3	15:N:25:TRP:CE2	2.46	0.50
17:P:128:TYR:HD1	17:P:129:LYS:O	1.94	0.50
3:B:66:TYR:CE1	16:O:53:SER:CB	2.86	0.50
4:C:212:THR:HG23	4:C:218:PHE:CD1	2.47	0.50
7:F:7:LEU:CG	7:F:13:TYR:OH	2.54	0.50
8:G:58:LYS:HB3	8:G:58:LYS:HZ3	1.75	0.50
15:N:18:TRP:CE2	24:W:56:HIS:CE1	3.00	0.50
21:T:129:ASP:N	21:T:130:PRO:HD3	2.26	0.50
3:B:149:GLN:HE21	3:B:151:LYS:HB3	1.76	0.50
8:G:58:LYS:NZ	8:G:58:LYS:CB	2.73	0.50
19:R:22:ALA:C	19:R:23:LYS:HG3	2.36	0.50
12:K:30:VAL:HG11	12:K:73:TYR:HD1	1.76	0.50
17:P:35:MET:O	17:P:38:LEU:HB3	2.11	0.50
17:P:39:LEU:HD12	17:P:39:LEU:H	1.75	0.50
25:X:59:ALA:HB2	25:X:67:ARG:HE	1.76	0.50
9:H:116:ARG:O	9:H:116:ARG:HG2	2.10	0.50
5:D:18:VAL:HB	31:d:20:ARG:HH22	1.76	0.50
6:E:192:VAL:CG2	6:E:242:LYS:O	2.59	0.50
7:F:7:LEU:CD2	7:F:13:TYR:CZ	2.88	0.50
9:H:53:VAL:CG2	9:H:181:LYS:CG	2.86	0.50
2:A:177:TRP:CZ3	2:A:181:ARG:NH1	2.80	0.50
4:C:114:ASP:OD2	4:C:118:HIS:HB2	2.12	0.50
4:C:184:THR:OG1	4:C:203:ASP:HB3	2.12	0.50
7:F:13:TYR:CD2	7:F:34:CYS:HB2	2.47	0.50
7:F:66:MET:O	7:F:70:ASN:HB3	2.11	0.50
9:H:172:LEU:HD11	9:H:190:SER:H	1.77	0.50
11:J:113:VAL:CG1	11:J:119:ALA:HB2	2.41	0.50
14:M:68:GLU:CB	14:M:71:TYR:CB	2.90	0.50
17:P:131:VAL:HG22	17:P:132:ARG:N	2.26	0.50
4:C:60:LEU:O	23:V:15:ARG:NE	2.43	0.50
7:F:13:TYR:CD2	7:F:34:CYS:SG	3.05	0.50
26:Y:19:LEU:CD1	26:Y:20:LEU:N	2.73	0.50
1:2:1533:U:O4	7:F:154:ILE:HA	2.11	0.49
3:B:26:LYS:HA	3:B:50:LYS:HD3	1.92	0.49
3:B:120:LEU:HG	3:B:142:PHE:HE1	1.76	0.49
5:D:18:VAL:CB	31:d:20:ARG:HH22	2.25	0.49
10:I:149:GLN:N	10:I:149:GLN:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:16:LYS:HG3	23:V:23:LEU:HD23	1.92	0.49
26:Y:94:LEU:HD22	26:Y:99:TYR:HD2	1.77	0.49
1:2:1532:G:H2'	27:Z:125:ASN:HB2	1.94	0.49
10:I:5:ARG:NE	10:I:29:LEU:O	2.41	0.49
10:I:170:ALA:HB2	10:I:186:ILE:HD12	1.94	0.49
12:K:7:LYS:N	12:K:46:PRO:CG	2.75	0.49
12:K:34:ASN:CG	12:K:37:ILE:CB	2.85	0.49
24:W:60:LYS:HZ2	29:b:22:LEU:C	2.20	0.49
3:B:89:GLU:OE1	3:B:223:PHE:HD1	1.94	0.49
9:H:165:LYS:HD3	9:H:165:LYS:N	2.27	0.49
11:J:113:VAL:HG12	11:J:119:ALA:HB2	1.94	0.49
13:L:88:ILE:HD12	13:L:126:VAL:CG1	2.41	0.49
26:Y:22:ARG:HB3	26:Y:79:TYR:CD1	2.47	0.49
9:H:45:LEU:C	9:H:45:LEU:CD1	2.85	0.49
18:Q:43:HIS:ND1	18:Q:44:LEU:N	2.59	0.49
19:R:31:ASN:O	19:R:34:ILE:CG1	2.59	0.49
4:C:181:PRO:N	4:C:184:THR:HG21	2.27	0.49
9:H:134:VAL:HG13	9:H:135:SER:N	2.27	0.49
12:K:32:GLN:CG	12:K:34:ASN:OD1	2.60	0.49
15:N:22:PRO:HD2	15:N:65:SER:HB3	1.95	0.49
25:X:134:PHE:HE1	32:e:15:LYS:HE3	1.63	0.49
1:2:80:G:O2'	1:2:81:C:H6	1.95	0.49
1:2:989:A:O2'	1:2:1776:U:O2	2.27	0.49
9:H:133:ILE:HG13	9:H:134:VAL:N	2.26	0.49
11:J:158:TYR:HD1	11:J:164:PHE:HB2	1.72	0.49
25:X:110:HIS:ND1	25:X:111:ALA:N	2.60	0.49
26:Y:8:SER:O	26:Y:29:ILE:HA	2.13	0.49
30:c:12:VAL:HG23	30:c:23:LEU:HD21	1.94	0.49
31:d:34:LEU:HD23	31:d:41:PHE:HD1	1.76	0.49
1:2:1469:U:C5	7:F:70:ASN:HD21	1.70	0.49
3:B:24:PHE:CD2	16:O:93:LEU:HD22	2.46	0.49
7:F:8:PHE:CD1	7:F:82:ARG:CD	2.95	0.49
1:2:1786:U:O4	28:a:34:LYS:HE3	2.13	0.49
3:B:84:ILE:HD11	3:B:100:PHE:CD1	2.47	0.49
4:C:190:PRO:HD3	11:J:17:ARG:HH22	1.78	0.49
9:H:172:LEU:HD11	9:H:190:SER:CA	2.43	0.49
17:P:39:LEU:CA	17:P:42:PHE:CD2	2.86	0.49
3:B:120:LEU:HG	3:B:142:PHE:CE1	2.47	0.49
7:F:16:VAL:HG21	7:F:98:GLN:HB2	1.94	0.49
9:H:47:ILE:CD1	9:H:65:VAL:HG21	2.41	0.49
11:J:116:LEU:HB3	11:J:118:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:155:HIS:C	11:J:157:ASP:OD1	2.47	0.49
1:2:1558:U:O2	1:2:1558:U:O4'	2.30	0.48
1:2:1653:A:H5'	34:m:38:SER:OG	2.13	0.48
3:B:34:ALA:N	3:B:43:PHE:CE2	2.79	0.48
6:E:60:GLU:OE1	26:Y:22:ARG:NH2	2.45	0.48
8:G:57:ASP:O	8:G:58:LYS:C	2.50	0.48
9:H:79:ILE:CB	9:H:82:ARG:HD2	2.43	0.48
1:2:1629:A:C2	34:m:13:ALA:N	2.80	0.48
7:F:8:PHE:HD1	7:F:82:ARG:CD	2.25	0.48
7:F:21:LEU:CD2	7:F:21:LEU:C	2.86	0.48
8:G:31:ARG:HH22	8:G:68:LEU:HD11	1.78	0.48
9:H:53:VAL:HB	9:H:181:LYS:HD3	1.94	0.48
6:E:45:VAL:HG23	6:E:46:VAL:HG13	1.95	0.48
19:R:17:VAL:O	19:R:71:LEU:HD22	2.12	0.48
30:c:67:LEU:C	30:c:67:LEU:CD1	2.86	0.48
3:B:186:LYS:O	3:B:186:LYS:HD2	2.13	0.48
7:F:5:ALA:HB1	7:F:34:CYS:SG	2.54	0.48
9:H:53:VAL:CG2	9:H:181:LYS:HG3	2.44	0.48
34:m:8:TYR:HD1	34:m:8:TYR:O	1.96	0.48
25:X:72:VAL:O	25:X:80:LYS:HA	2.13	0.48
4:C:230:TYR:OH	23:V:11:LEU:HD13	2.13	0.48
8:G:67:VAL:CG2	8:G:68:LEU:N	2.77	0.48
10:I:119:LEU:HD21	10:I:148:ARG:HH21	1.79	0.48
15:N:23:PRO:HG2	15:N:26:LEU:H	1.79	0.48
18:Q:42:GLU:OE1	21:T:14:THR:HG21	2.13	0.48
27:Z:145:VAL:HG22	27:Z:156:THR:HG23	1.95	0.48
1:2:1533:U:C4	7:F:154:ILE:HA	2.49	0.48
3:B:175:GLU:CG	3:B:193:ILE:CD1	2.90	0.48
7:F:64:MET:HE1	7:F:161:LEU:HD22	1.94	0.48
7:F:142:ILE:HD12	7:F:165:ILE:HD13	1.95	0.48
19:R:67:ARG:O	19:R:69:ILE:HD12	2.14	0.48
2:A:63:ALA:CB	2:A:182:GLU:CD	2.86	0.48
4:C:37:TRP:CE2	4:C:69:GLN:HB3	2.48	0.48
4:C:99:ARG:CG	4:C:100:ALA:H	2.12	0.48
9:H:142:LYS:C	9:H:143:ARG:HG3	2.38	0.48
19:R:75:GLU:O	19:R:79:GLU:HG2	2.14	0.48
1:2:1122:G:OP1	34:m:25:ARG:NH2	2.47	0.48
9:H:63:PHE:CE2	9:H:93:LYS:HD3	2.49	0.48
12:K:32:GLN:HG2	12:K:34:ASN:OD1	2.14	0.48
1:2:1161:C:OP1	7:F:67:HIS:HA	2.13	0.48
1:2:1679:A:C8	8:G:66:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:84:ILE:HD12	3:B:102:GLY:O	2.14	0.48
7:F:6:LYS:HA	7:F:11:TRP:O	2.13	0.48
21:T:46:TRP:O	21:T:48:ASP:N	2.47	0.48
1:2:1533:U:C5	7:F:153:ASN:C	2.92	0.47
4:C:89:MET:CE	4:C:195:ILE:HG22	2.38	0.47
9:H:186:ASP:N	9:H:186:ASP:OD1	2.45	0.47
19:R:26:LEU:C	19:R:26:LEU:CD1	2.85	0.47
1:2:765:U:C2	11:J:143:ILE:HD13	2.49	0.47
1:2:1429:G:N3	31:d:39:GLN:HB3	2.29	0.47
3:B:45:LYS:C	3:B:46:THR:CG2	2.87	0.47
15:N:20:ARG:HH21	24:W:56:HIS:CD2	2.31	0.47
25:X:95:ASP:CB	25:X:98:ASP:CG	2.70	0.47
1:2:10:G:C2'	4:C:102:GLN:NE2	2.72	0.47
2:A:60:LEU:N	2:A:182:GLU:OE2	2.47	0.47
3:B:40:VAL:O	3:B:40:VAL:HG13	2.15	0.47
11:J:152:SER:HA	11:J:155:HIS:HD2	1.78	0.47
17:P:35:MET:HA	17:P:38:LEU:CB	2.43	0.47
25:X:137:LYS:C	25:X:137:LYS:CE	2.86	0.47
3:B:62:ARG:NH2	3:B:89:GLU:O	2.47	0.47
3:B:78:ASP:HB3	3:B:79:GLN:OE1	2.14	0.47
10:I:20:VAL:O	10:I:20:VAL:HG13	2.14	0.47
13:L:73:ILE:HD12	13:L:140:PHE:CZ	2.48	0.47
4:C:191:THR:HG23	4:C:218:PHE:CE2	2.46	0.47
7:F:38:PRO:HB3	7:F:57:VAL:HG12	1.97	0.47
19:R:67:ARG:O	19:R:69:ILE:CD1	2.62	0.47
3:B:74:ASN:O	3:B:75:ASN:HB3	2.15	0.47
7:F:94:LYS:HG3	7:F:95:ASN:N	2.18	0.47
9:H:79:ILE:CG2	9:H:82:ARG:NE	2.77	0.47
9:H:105:PRO:O	9:H:108:PHE:HB3	2.14	0.47
15:N:20:ARG:O	15:N:21:LYS:CG	2.56	0.47
15:N:23:PRO:HD3	15:N:26:LEU:HB2	1.91	0.47
24:W:60:LYS:HZ2	29:b:22:LEU:HA	1.80	0.47
25:X:55:LEU:CD2	25:X:55:LEU:C	2.85	0.47
1:2:120:U:H1'	6:E:33:PRO:O	2.14	0.47
1:2:574:C:H41	25:X:63:ASN:ND2	2.13	0.47
1:2:598:A:H4'	25:X:104:GLY:O	2.15	0.47
1:2:1533:U:C4	7:F:154:ILE:CA	2.97	0.47
4:C:34:LEU:HD12	4:C:35:LYS:HD2	1.96	0.47
4:C:103:ARG:NH1	4:C:105:ARG:HH21	2.07	0.47
9:H:53:VAL:HG13	9:H:53:VAL:O	2.15	0.47
9:H:63:PHE:HE2	9:H:93:LYS:HD3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:23:PRO:HG2	15:N:25:TRP:CD2	2.50	0.47
19:R:38:VAL:HG23	19:R:39:ALA:N	2.29	0.47
25:X:73:GLN:HE21	25:X:80:LYS:HE2	1.79	0.47
7:F:26:TYR:OH	30:c:53:ASP:CG	2.58	0.47
8:G:65:GLN:H	8:G:65:GLN:CD	2.23	0.47
11:J:90:GLU:N	11:J:90:GLU:CD	2.73	0.47
11:J:93:LEU:CD1	11:J:93:LEU:C	2.85	0.47
12:K:32:GLN:CD	12:K:34:ASN:HD21	2.23	0.47
27:Z:144:ILE:CG2	27:Z:146:GLY:O	2.63	0.47
1:2:872:G:P	3:B:158:THR:OG1	2.73	0.47
3:B:82:ARG:HG2	3:B:83:LYS:N	2.29	0.47
7:F:7:LEU:CG	7:F:13:TYR:CZ	2.97	0.47
26:Y:59:VAL:HA	26:Y:97:LEU:HD21	1.96	0.47
1:2:872:G:OP1	3:B:158:THR:OG1	2.32	0.47
2:A:25:HIS:HB3	2:A:52:LEU:HD21	1.96	0.47
12:K:39:ARG:HD2	12:K:39:ARG:O	2.15	0.47
1:2:548:G:O2'	1:2:555:A:N1	2.44	0.46
1:2:739:U:H4'	9:H:109:LYS:HB2	1.98	0.46
1:2:1561:A:C4'	21:T:54:HIS:NE2	2.79	0.46
2:A:190:LEU:CD1	2:A:197:TRP:CD1	2.95	0.46
3:B:34:ALA:CB	3:B:43:PHE:HE2	2.27	0.46
12:K:19:ILE:HD11	12:K:45:VAL:HG21	1.98	0.46
9:H:45:LEU:HD23	9:H:76:VAL:HG21	1.97	0.46
11:J:116:LEU:CB	11:J:118:LEU:CD1	2.86	0.46
17:P:25:VAL:HG11	17:P:30:LEU:HD23	1.97	0.46
28:a:10:ARG:HH22	28:a:31:PRO:CG	2.29	0.46
34:m:26:ARG:O	34:m:30:LYS:HG3	2.15	0.46
1:2:554:A:H2'	1:2:555:A:C8	2.50	0.46
9:H:134:VAL:CG2	9:H:158:LEU:HD21	2.45	0.46
29:b:77:PHE:CD1	29:b:77:PHE:C	2.93	0.46
1:2:548:G:C2	1:2:555:A:H2	2.33	0.46
3:B:169:MET:HE2	3:B:169:MET:HB3	1.80	0.46
4:C:92:MET:HE2	4:C:109:PHE:HE2	1.80	0.46
9:H:103:MET:CE	9:H:122:LEU:HD13	2.45	0.46
11:J:133:HIS:ND1	11:J:164:PHE:HD2	2.12	0.46
3:B:26:LYS:HB3	3:B:50:LYS:CD	2.45	0.46
6:E:182:MET:HB2	6:E:228:ILE:HD11	1.97	0.46
1:2:32:U:OP1	25:X:137:LYS:HD2	2.16	0.46
3:B:26:LYS:CB	3:B:50:LYS:CD	2.90	0.46
2:A:119:GLU:OE1	4:C:42:LYS:HG2	2.16	0.46
3:B:49:THR:CG2	3:B:50:LYS:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:89:GLU:OE1	3:B:223:PHE:CD1	2.68	0.46
7:F:65:MET:HE2	7:F:74:LYS:HA	1.97	0.46
11:J:111:THR:O	11:J:115:LYS:N	2.36	0.46
11:J:140:ILE:HG21	11:J:159:ALA:CB	2.46	0.46
25:X:68:LYS:HG3	25:X:91:LEU:HD13	1.97	0.46
27:Z:118:VAL:HG12	27:Z:122:LEU:HD12	1.97	0.46
6:E:208:ILE:HD12	6:E:225:VAL:HG21	1.97	0.46
9:H:55:VAL:HG23	9:H:56:PRO:HD2	1.96	0.46
20:S:132:LYS:HD2	20:S:138:THR:HG22	1.97	0.46
27:Z:120:GLU:CB	27:Z:121:ARG:HH12	2.23	0.46
1:2:740:U:P	9:H:109:LYS:HE3	2.54	0.46
6:E:62:MET:HE2	6:E:80:GLN:HE22	1.82	0.45
9:H:67:VAL:CG1	9:H:68:PRO:CD	2.81	0.45
1:2:485:U:O2	1:2:485:U:O4'	2.34	0.45
1:2:1178:A:OP1	17:P:129:LYS:HE2	2.17	0.45
4:C:181:PRO:CG	4:C:184:THR:CG2	2.93	0.45
10:I:119:LEU:CD1	10:I:153:PRO:HB2	2.42	0.45
11:J:140:ILE:HG21	11:J:159:ALA:HB1	1.97	0.45
12:K:32:GLN:CD	12:K:34:ASN:ND2	2.75	0.45
19:R:21:TYR:HE1	19:R:61:ILE:HG21	1.81	0.45
19:R:67:ARG:CD	19:R:68:GLY:N	2.76	0.45
25:X:81:ILE:CG2	25:X:120:PHE:HD2	2.25	0.45
30:c:9:VAL:HG13	30:c:25:VAL:HG13	1.97	0.45
1:2:79:G:C6	1:2:80:G:N7	2.84	0.45
1:2:1454:G:N3	1:2:1454:G:H2'	2.31	0.45
2:A:34:LYS:CD	23:V:62:GLY:O	2.64	0.45
5:D:23:LEU:HD21	5:D:50:ILE:HD11	1.99	0.45
6:E:34:GLY:C	6:E:36:HIS:N	2.74	0.45
7:F:156:THR:N	7:F:159:GLU:OE1	2.49	0.45
9:H:79:ILE:HD12	9:H:82:ARG:CG	2.44	0.45
11:J:92:LYS:HB2	11:J:95:TYR:HD2	1.80	0.45
19:R:31:ASN:CG	19:R:34:ILE:CD1	2.79	0.45
23:V:1:MET:O	23:V:9:VAL:HG12	2.16	0.45
1:2:553:C:H5''	1:2:554:A:OP1	2.16	0.45
4:C:103:ARG:HH12	4:C:105:ARG:HE	1.61	0.45
7:F:8:PHE:CD1	7:F:82:ARG:HD2	2.52	0.45
7:F:91:MET:CE	27:Z:112:LEU:HD21	2.37	0.45
9:H:79:ILE:HG22	9:H:82:ARG:NE	2.31	0.45
12:K:33:LYS:HB2	12:K:70:GLN:O	2.17	0.45
20:S:49:LYS:HE3	21:T:48:ASP:OD2	2.14	0.45
21:T:51:LYS:HB2	21:T:58:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:60:LYS:NZ	29:b:22:LEU:HA	2.31	0.45
25:X:71:ARG:HD3	25:X:80:LYS:HD3	1.97	0.45
34:m:19:TRP:CE3	34:m:19:TRP:CA	2.99	0.45
4:C:186:ILE:HD11	4:C:201:ILE:O	2.17	0.45
31:d:17:ARG:O	31:d:25:ARG:HG2	2.16	0.45
34:m:12:ARG:O	34:m:13:ALA:C	2.59	0.45
1:2:533:U:H5'	11:J:168:ARG:NH2	2.31	0.45
3:B:78:ASP:OD1	3:B:79:GLN:N	2.46	0.45
7:F:65:MET:CE	7:F:74:LYS:HG3	2.47	0.45
17:P:49:LYS:HZ3	17:P:88:LEU:CA	2.29	0.45
19:R:28:PHE:HA	19:R:55:THR:HG21	1.98	0.45
1:2:599:U:P	25:X:106:GLY:HA2	2.56	0.45
3:B:26:LYS:O	3:B:50:LYS:CD	2.63	0.45
17:P:49:LYS:HZ3	17:P:89:VAL:H	1.65	0.45
19:R:17:VAL:O	19:R:21:TYR:HB2	2.16	0.45
26:Y:97:LEU:HD12	26:Y:97:LEU:H	1.82	0.45
27:Z:145:VAL:HG21	27:Z:154:ILE:HG22	1.99	0.45
2:A:187:ARG:CD	2:A:189:GLU:CD	2.87	0.45
7:F:23:LEU:HD21	7:F:134:ARG:NH1	2.32	0.45
9:H:72:TYR:O	9:H:72:TYR:CD2	2.70	0.45
22:U:182:SER:O	31:d:38:ARG:NH1	2.38	0.45
1:2:1052:C:H3'	1:2:1053:A:H5''	1.99	0.45
1:2:1763:C:H3'	34:m:16:ARG:NH1	2.32	0.45
2:A:22:CYS:SG	2:A:174:LEU:HD13	2.57	0.45
2:A:35:MET:HE3	2:A:35:MET:HB3	1.84	0.45
4:C:181:PRO:CD	4:C:184:THR:CG2	2.94	0.45
7:F:150:ALA:CB	7:F:160:CYS:SG	2.94	0.45
7:F:156:THR:HG21	27:Z:152:GLN:HG2	1.99	0.45
11:J:163:PRO:HG3	11:J:169:PRO:HA	1.99	0.45
29:b:77:PHE:CD1	29:b:77:PHE:O	2.70	0.45
1:2:1533:U:O4	7:F:153:ASN:O	2.35	0.45
4:C:159:PRO:HD3	23:V:9:VAL:HG21	1.98	0.45
10:I:116:PHE:CZ	10:I:147:HIS:ND1	2.85	0.45
12:K:85:ARG:O	12:K:89:HIS:N	2.44	0.45
31:d:34:LEU:HD23	31:d:41:PHE:CE1	2.36	0.45
1:2:80:G:O2'	1:2:81:C:O4'	2.34	0.44
2:A:40:PHE:CE1	2:A:41:LYS:HB2	2.52	0.44
3:B:86:LEU:HD23	3:B:100:PHE:CB	2.47	0.44
4:C:184:THR:HG22	11:J:53:ARG:NH2	2.30	0.44
9:H:46:VAL:HG22	9:H:47:ILE:N	2.30	0.44
9:H:79:ILE:HB	9:H:82:ARG:NE	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:23:PRO:HG2	15:N:25:TRP:CE2	2.51	0.44
17:P:53:GLY:C	17:P:54:ILE:CD1	2.87	0.44
23:V:11:LEU:O	23:V:12:TYR:CD2	2.70	0.44
25:X:86:PRO:O	25:X:87:ARG:HB2	2.16	0.44
1:2:1561:A:H4'	21:T:54:HIS:HD2	1.76	0.44
3:B:26:LYS:HD3	3:B:50:LYS:HD3	1.93	0.44
5:D:174:ILE:HD13	5:D:187:ARG:HG2	1.97	0.44
10:I:116:PHE:CE2	10:I:147:HIS:HB3	2.52	0.44
25:X:59:ALA:CA	25:X:114:ASP:OD1	2.55	0.44
29:b:45:PHE:CD2	29:b:47:HIS:O	2.70	0.44
1:2:19:A:H5'	25:X:107:ARG:HH11	1.82	0.44
2:A:63:ALA:HB2	2:A:182:GLU:CG	2.47	0.44
4:C:39:PRO:HD2	4:C:48:ARG:HH11	1.81	0.44
8:G:76:LEU:HD21	8:G:92:LYS:HB3	1.98	0.44
9:H:172:LEU:HD11	9:H:190:SER:N	2.33	0.44
25:X:72:VAL:HG12	25:X:73:GLN:N	2.32	0.44
27:Z:148:HIS:CE1	27:Z:149:HIS:O	2.70	0.44
3:B:33:LYS:NZ	3:B:41:ARG:CG	2.80	0.44
4:C:76:GLN:NE2	4:C:79:ASN:HD22	2.14	0.44
8:G:57:ASP:HB3	8:G:106:LEU:HB3	1.98	0.44
8:G:69:VAL:HG12	8:G:70:ASN:N	2.32	0.44
15:N:23:PRO:HG3	15:N:25:TRP:CZ2	2.52	0.44
28:a:11:ALA:HB3	28:a:33:ASP:OD1	2.17	0.44
3:B:45:LYS:O	3:B:46:THR:HG22	2.15	0.44
11:J:161:THR:C	11:J:162:SER:HG	2.05	0.44
30:c:66:ARG:HD3	30:c:67:LEU:N	2.33	0.44
1:2:103:A:OP2	1:2:308:A:N6	2.50	0.44
1:2:428:A:N3	1:2:440:U:O2'	2.49	0.44
19:R:24:LEU:HB2	19:R:31:ASN:OD1	2.17	0.44
25:X:88:ASP:OD1	25:X:89:GLY:N	2.50	0.44
1:2:1469:U:C4	7:F:157:ILE:CD1	3.01	0.44
1:2:1469:U:OP2	7:F:157:ILE:N	2.47	0.44
3:B:34:ALA:CB	3:B:43:PHE:CE2	2.94	0.44
16:O:47:ILE:HG23	16:O:86:VAL:HG21	2.00	0.44
25:X:134:PHE:CZ	32:e:15:LYS:HE3	2.44	0.44
1:2:19:A:C5'	25:X:107:ARG:HH11	2.30	0.44
1:2:820:G:H2'	1:2:820:G:N3	2.33	0.44
4:C:43:LEU:HA	4:C:43:LEU:HD23	1.74	0.44
19:R:22:ALA:O	19:R:23:LYS:HG3	2.17	0.44
25:X:40:PRO:CB	25:X:81:ILE:HD11	2.47	0.44
26:Y:9:LEU:HD23	26:Y:29:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:21:LEU:C	7:F:22:SER:HG	2.10	0.44
7:F:21:LEU:HD13	30:c:6:LEU:HG	2.00	0.44
7:F:143:CYS:SG	7:F:147:ARG:NH2	2.91	0.44
8:G:69:VAL:HG11	8:G:71:HIS:NE2	2.33	0.44
3:B:127:VAL:HG21	3:B:176:ALA:HB3	1.99	0.43
6:E:44:LEU:HD21	6:E:70:ILE:HG21	2.00	0.43
17:P:49:LYS:NZ	17:P:88:LEU:HA	2.31	0.43
21:T:53:ALA:HB3	21:T:56:LYS:HG2	1.99	0.43
25:X:121:LYS:HE2	25:X:121:LYS:HB3	1.79	0.43
27:Z:120:GLU:CG	27:Z:121:ARG:HH11	2.29	0.43
1:2:764:U:O4'	1:2:764:U:O2	2.35	0.43
1:2:827:U:O2	1:2:827:U:O4'	2.35	0.43
4:C:117:GLY:N	4:C:149:ARG:HH12	2.17	0.43
7:F:11:TRP:CE2	7:F:96:PRO:HG3	2.53	0.43
9:H:31:GLU:CB	9:H:43:ARG:HH22	2.30	0.43
17:P:39:LEU:HA	17:P:42:PHE:CE2	2.48	0.43
7:F:5:ALA:N	7:F:36:PHE:HZ	2.14	0.43
8:G:76:LEU:CD2	8:G:92:LYS:HB3	2.49	0.43
7:F:35:VAL:HG12	7:F:36:PHE:O	2.18	0.43
7:F:151:PHE:CD2	7:F:151:PHE:C	2.96	0.43
16:O:38:ILE:HG12	16:O:47:ILE:HD11	1.95	0.43
17:P:38:LEU:O	17:P:42:PHE:CE2	2.70	0.43
17:P:91:VAL:HG12	17:P:94:MET:HE2	2.00	0.43
25:X:61:GLN:HB3	25:X:62:PRO:HA	1.99	0.43
34:m:3:HIS:HB3	34:m:7:ARG:HA	1.99	0.43
34:m:8:TYR:O	34:m:8:TYR:CD1	2.71	0.43
1:2:548:G:N3	1:2:555:A:C2	2.71	0.43
2:A:184:LEU:HG	2:A:189:GLU:OE1	2.18	0.43
4:C:60:LEU:CD1	23:V:13:ILE:O	2.67	0.43
6:E:128:LYS:HG2	6:E:140:ILE:HD11	1.99	0.43
9:H:179:TYR:CD2	9:H:187:ALA:HB2	2.54	0.43
27:Z:148:HIS:NE2	27:Z:149:HIS:O	2.52	0.43
16:O:47:ILE:CG2	16:O:86:VAL:HG21	2.49	0.43
16:O:50:THR:HG22	16:O:57:THR:HA	1.99	0.43
26:Y:7:PHE:CE1	26:Y:45:LYS:CD	3.01	0.43
2:A:41:LYS:HZ3	19:R:104:ASP:HB2	1.82	0.43
9:H:38:LEU:O	9:H:42:VAL:HG23	2.19	0.43
9:H:45:LEU:HD23	9:H:76:VAL:CB	2.49	0.43
18:Q:49:LEU:HD23	18:Q:49:LEU:HA	1.81	0.43
1:2:740:U:P	9:H:109:LYS:CD	3.06	0.43
1:2:1570:G:H2'	1:2:1570:G:N3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:47:LEU:HD12	3:B:47:LEU:H	1.84	0.43
17:P:57:LYS:HE2	17:P:85:LEU:HD21	2.00	0.43
17:P:108:ILE:HD11	17:P:125:SER:CB	2.49	0.43
17:P:132:ARG:O	17:P:133:HIS:O	2.37	0.43
25:X:51:VAL:HG23	25:X:98:ASP:O	2.19	0.43
1:2:1151:C:O2	1:2:1151:C:O4'	2.36	0.43
9:H:63:PHE:HE2	9:H:93:LYS:CE	2.32	0.43
10:I:140:THR:C	10:I:142:CYS:H	2.24	0.43
21:T:49:TYR:C	21:T:50:VAL:CG2	2.85	0.43
26:Y:17:ASN:OD1	26:Y:19:LEU:CG	2.59	0.43
6:E:192:VAL:O	6:E:192:VAL:HG23	2.19	0.42
7:F:155:LYS:HZ2	7:F:159:GLU:HB3	1.82	0.42
27:Z:119:CYS:C	27:Z:122:LEU:O	2.62	0.42
7:F:13:TYR:CB	7:F:34:CYS:HG	2.26	0.42
7:F:167:ASN:ND2	7:F:175:ALA:CA	2.83	0.42
23:V:9:VAL:HG22	23:V:10:ASP:N	2.34	0.42
31:d:19:CYS:O	31:d:23:PHE:N	2.49	0.42
8:G:32:MET:HE2	8:G:63:MET:SD	2.59	0.42
8:G:69:VAL:HG12	8:G:70:ASN:H	1.84	0.42
9:H:142:LYS:O	9:H:143:ARG:HG3	2.19	0.42
13:L:75:GLY:N	13:L:88:ILE:HD11	2.34	0.42
25:X:94:ILE:HD13	25:X:125:VAL:HG21	2.01	0.42
1:2:1639:C:H1'	1:2:1753:A:N1	2.31	0.42
2:A:34:LYS:O	2:A:37:PRO:HD2	2.19	0.42
15:N:18:TRP:CZ2	24:W:56:HIS:HE1	2.35	0.42
16:O:47:ILE:HG23	16:O:47:ILE:O	2.19	0.42
28:a:10:ARG:HB2	28:a:10:ARG:CZ	2.48	0.42
3:B:27:LYS:HA	3:B:49:THR:HA	2.01	0.42
9:H:65:VAL:HG11	9:H:97:LEU:CD1	2.43	0.42
10:I:143:LEU:HD23	10:I:143:LEU:HA	1.83	0.42
24:W:60:LYS:HZ2	29:b:22:LEU:CA	2.32	0.42
8:G:75:LEU:O	8:G:94:ARG:HA	2.20	0.42
15:N:139:TRP:CE3	15:N:139:TRP:O	2.72	0.42
16:O:31:ILE:HG23	16:O:97:ALA:HB2	2.01	0.42
22:U:146:ILE:HG21	22:U:201:ARG:HD2	2.01	0.42
25:X:107:ARG:NH2	25:X:110:HIS:CE1	2.87	0.42
26:Y:22:ARG:CD	26:Y:77:MET:CG	2.98	0.42
29:b:32:ASP:OD1	29:b:80:LYS:NZ	2.52	0.42
3:B:34:ALA:HB2	3:B:43:PHE:CD2	2.55	0.42
3:B:47:LEU:HD12	3:B:47:LEU:O	2.18	0.42
27:Z:117:THR:HG22	27:Z:121:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:858:U:H5'	15:N:20:ARG:NH1	2.30	0.42
2:A:190:LEU:HD21	2:A:197:TRP:HE1	1.85	0.42
3:B:184:LEU:HG	3:B:188:PHE:CE2	2.55	0.42
7:F:79:ARG:HE	27:Z:149:HIS:CE1	2.37	0.42
17:P:38:LEU:O	17:P:42:PHE:CD2	2.73	0.42
19:R:24:LEU:HB3	19:R:34:ILE:CD1	2.34	0.42
34:m:21:LYS:HE2	34:m:25:ARG:NH2	2.35	0.42
1:2:485:U:H3'	1:2:486:G:H5''	2.02	0.42
3:B:48:VAL:HG21	3:B:61:LEU:CD2	2.50	0.42
3:B:100:PHE:CE2	3:B:185:VAL:HG22	2.54	0.42
7:F:6:LYS:CB	7:F:36:PHE:HE1	2.32	0.42
7:F:24:VAL:O	7:F:24:VAL:HG13	2.19	0.42
9:H:130:LEU:CD2	9:H:179:TYR:CE1	2.90	0.42
28:a:11:ALA:O	28:a:33:ASP:OD2	2.38	0.42
3:B:83:LYS:HD2	16:O:135:GLU:OE2	2.20	0.42
7:F:62:ASN:CG	7:F:74:LYS:NZ	2.72	0.42
9:H:42:VAL:HG13	9:H:45:LEU:HB3	2.02	0.42
17:P:34:LYS:HA	17:P:34:LYS:HD2	1.78	0.42
28:a:10:ARG:HH22	28:a:31:PRO:HG2	1.85	0.42
9:H:104:LEU:CD2	9:H:108:PHE:CB	2.98	0.41
9:H:168:ILE:HG23	9:H:169:GLU:N	2.35	0.41
9:H:189:PHE:CD1	9:H:189:PHE:N	2.88	0.41
25:X:68:LYS:CG	25:X:91:LEU:HD13	2.32	0.41
30:c:45:VAL:HG21	30:c:49:VAL:HG21	2.01	0.41
2:A:185:TYR:HE2	2:A:190:LEU:HD12	1.68	0.41
16:O:46:PHE:CD1	16:O:62:THR:HG22	2.55	0.41
25:X:125:VAL:O	25:X:126:ALA:HB3	2.20	0.41
5:D:23:LEU:HD21	5:D:50:ILE:CD1	2.50	0.41
7:F:94:LYS:HE2	7:F:99:VAL:CG2	2.49	0.41
18:Q:50:LYS:HB3	18:Q:50:LYS:HE2	1.80	0.41
19:R:32:LYS:O	19:R:36:GLU:HG2	2.20	0.41
3:B:172:MET:HE2	3:B:172:MET:HB3	1.91	0.41
5:D:164:GLU:N	5:D:165:PRO:CD	2.83	0.41
8:G:68:LEU:O	8:G:69:VAL:HG23	2.19	0.41
9:H:54:GLU:O	9:H:54:GLU:HG3	2.19	0.41
12:K:69:TRP:HZ3	31:d:21:VAL:HG13	1.81	0.41
16:O:89:ARG:CZ	16:O:93:LEU:HD21	2.51	0.41
17:P:49:LYS:HZ3	17:P:89:VAL:N	2.18	0.41
34:m:6:SER:O	34:m:7:ARG:C	2.62	0.41
1:2:958:U:H5''	15:N:71:ILE:HD12	2.02	0.41
3:B:141:ALA:HB3	3:B:168:MET:CE	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:144:LYS:O	3:B:144:LYS:HG3	2.20	0.41
3:B:153:THR:O	3:B:154:CYS:SG	2.79	0.41
7:F:158:ALA:HB3	27:Z:152:GLN:OE1	2.19	0.41
13:L:126:VAL:HG23	13:L:145:VAL:HG12	2.02	0.41
15:N:18:TRP:CZ2	24:W:56:HIS:CE1	3.09	0.41
25:X:55:LEU:O	25:X:69:CYS:O	2.38	0.41
1:2:1469:U:C4	7:F:157:ILE:HD12	2.55	0.41
7:F:5:ALA:HB3	7:F:34:CYS:SG	2.60	0.41
25:X:80:LYS:C	25:X:81:ILE:HG13	2.46	0.41
25:X:101:LEU:HD23	25:X:101:LEU:HA	1.78	0.41
1:2:1109:G:C4	34:m:2:ALA:CB	2.96	0.41
1:2:1528:C:OP2	27:Z:150:HIS:HB3	2.20	0.41
2:A:155:LEU:HD22	2:A:161:CYS:SG	2.61	0.41
3:B:89:GLU:HB3	3:B:223:PHE:HE1	1.86	0.41
7:F:7:LEU:O	7:F:11:TRP:HE3	2.04	0.41
7:F:90:LEU:CD1	27:Z:156:THR:CG2	2.98	0.41
11:J:134:ILE:HA	11:J:157:ASP:O	2.20	0.41
12:K:38:GLU:O	12:K:39:ARG:C	2.64	0.41
15:N:21:LYS:HE2	15:N:21:LYS:HB3	1.62	0.41
26:Y:9:LEU:HD23	26:Y:29:ILE:CG2	2.50	0.41
1:2:1062:U:H5"	3:B:150:VAL:HG22	2.02	0.41
3:B:38:PHE:O	3:B:39:ASN:CB	2.69	0.41
5:D:166:SER:O	5:D:170:VAL:HG22	2.21	0.41
11:J:123:HIS:CE1	32:e:37:ARG:HD2	2.55	0.41
11:J:161:THR:O	11:J:162:SER:CB	2.69	0.41
13:L:82:MET:HG3	13:L:85:ALA:HB3	2.02	0.41
15:N:4:MET:HE3	15:N:124:ARG:NH2	2.36	0.41
16:O:36:ALA:HB2	16:O:98:VAL:HG13	2.02	0.41
16:O:48:HIS:CE1	16:O:50:THR:CG2	3.04	0.41
17:P:35:MET:CA	17:P:38:LEU:HB3	2.48	0.41
21:T:46:TRP:O	21:T:47:ILE:C	2.64	0.41
25:X:57:ILE:CD1	25:X:69:CYS:SG	3.09	0.41
25:X:73:GLN:HG2	25:X:80:LYS:HG2	2.03	0.41
27:Z:149:HIS:HD2	27:Z:151:SER:N	2.10	0.41
34:m:7:ARG:CG	34:m:17:TRP:CE2	3.04	0.41
34:m:8:TYR:CD1	34:m:8:TYR:C	2.99	0.41
3:B:26:LYS:O	3:B:50:LYS:N	2.48	0.41
3:B:86:LEU:CD2	3:B:100:PHE:HB2	2.51	0.41
9:H:134:VAL:HG22	9:H:137:THR:OG1	2.21	0.41
11:J:92:LYS:N	11:J:92:LYS:HD2	2.35	0.41
17:P:30:LEU:HG	17:P:30:LEU:H	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:22:ALA:O	19:R:23:LYS:CB	2.69	0.41
19:R:66:VAL:C	19:R:69:ILE:HD13	2.45	0.41
23:V:11:LEU:CD1	23:V:11:LEU:N	2.73	0.41
1:2:554:A:O2'	1:2:555:A:P	2.79	0.40
7:F:13:TYR:CD1	7:F:34:CYS:CB	3.04	0.40
7:F:26:TYR:CZ	7:F:131:PRO:HG2	2.56	0.40
9:H:42:VAL:O	9:H:45:LEU:HB3	2.22	0.40
9:H:80:GLN:HA	9:H:80:GLN:HE21	1.86	0.40
25:X:52:VAL:HG13	25:X:53:GLU:N	2.35	0.40
26:Y:9:LEU:HD21	26:Y:42:LEU:HD11	2.03	0.40
4:C:40:ILE:O	4:C:41:THR:CB	2.70	0.40
4:C:190:PRO:HD3	11:J:17:ARG:NH2	2.36	0.40
7:F:21:LEU:O	7:F:22:SER:CB	2.69	0.40
8:G:59:GLN:HA	8:G:59:GLN:OE1	2.20	0.40
11:J:158:TYR:CD1	11:J:164:PHE:HB3	2.56	0.40
21:T:52:THR:CG2	21:T:69:ARG:CZ	3.00	0.40
9:H:112:GLY:O	9:H:113:LEU:CB	2.70	0.40
10:I:106:ALA:HB2	10:I:168:LEU:HG	2.03	0.40
15:N:23:PRO:HD2	15:N:23:PRO:O	2.21	0.40
19:R:66:VAL:CG1	19:R:69:ILE:CD1	2.91	0.40
19:R:74:GLN:O	19:R:78:ARG:CB	2.69	0.40
26:Y:91:ARG:NH2	26:Y:100:VAL:CG1	2.85	0.40
2:A:63:ALA:CB	2:A:182:GLU:CG	2.99	0.40
9:H:36:SER:CB	9:H:39:LYS:CB	2.99	0.40
9:H:72:TYR:O	9:H:72:TYR:CG	2.74	0.40
11:J:158:TYR:CE1	11:J:164:PHE:HB3	2.56	0.40
4:C:76:GLN:O	4:C:80:CYS:CB	2.70	0.40
4:C:84:LEU:HD12	4:C:114:ASP:HB3	2.03	0.40
11:J:113:VAL:O	11:J:116:LEU:HB3	2.22	0.40
11:J:116:LEU:HD12	11:J:116:LEU:HA	1.95	0.40
13:L:126:VAL:CG2	13:L:142:VAL:HG23	2.51	0.40
21:T:129:ASP:OD2	21:T:134:GLY:O	2.40	0.40
25:X:81:ILE:HG22	25:X:82:THR:N	2.37	0.40
25:X:105:PHE:CD1	25:X:112:VAL:HG21	2.56	0.40
30:c:66:ARG:C	30:c:66:ARG:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	196/287 (68%)	186 (95%)	6 (3%)	4 (2%)	6	24
3	B	210/259 (81%)	188 (90%)	14 (7%)	8 (4%)	2	14
4	C	223/269 (83%)	207 (93%)	11 (5%)	5 (2%)	5	23
5	D	196/235 (83%)	182 (93%)	13 (7%)	1 (0%)	24	52
6	E	255/263 (97%)	226 (89%)	27 (11%)	2 (1%)	16	44
7	F	183/192 (95%)	168 (92%)	8 (4%)	7 (4%)	2	14
8	G	216/256 (84%)	199 (92%)	12 (6%)	5 (2%)	5	22
9	H	173/196 (88%)	149 (86%)	17 (10%)	7 (4%)	2	14
10	I	179/205 (87%)	168 (94%)	8 (4%)	3 (2%)	7	27
11	J	176/188 (94%)	162 (92%)	9 (5%)	5 (3%)	4	19
12	K	92/152 (60%)	83 (90%)	4 (4%)	5 (5%)	1	9
13	L	143/161 (89%)	132 (92%)	10 (7%)	1 (1%)	18	46
14	M	93/142 (66%)	73 (78%)	14 (15%)	6 (6%)	1	6
15	N	148/151 (98%)	135 (91%)	9 (6%)	4 (3%)	4	20
16	O	125/156 (80%)	106 (85%)	15 (12%)	4 (3%)	3	17
17	P	111/150 (74%)	99 (89%)	6 (5%)	6 (5%)	1	9
18	Q	134/148 (90%)	120 (90%)	11 (8%)	3 (2%)	5	23
19	R	115/132 (87%)	103 (90%)	7 (6%)	5 (4%)	2	13
20	S	133/156 (85%)	122 (92%)	6 (4%)	5 (4%)	2	14
21	T	149/160 (93%)	134 (90%)	11 (7%)	4 (3%)	4	20
22	U	101/233 (43%)	97 (96%)	4 (4%)	0	100	100
23	V	78/82 (95%)	67 (86%)	8 (10%)	3 (4%)	2	14
24	W	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
25	X	131/143 (92%)	116 (88%)	11 (8%)	4 (3%)	3	17
26	Y	126/135 (93%)	114 (90%)	10 (8%)	2 (2%)	7	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	69/161 (43%)	59 (86%)	9 (13%)	1 (1%)	9	30
28	a	97/112 (87%)	85 (88%)	7 (7%)	5 (5%)	1	9
29	b	77/82 (94%)	67 (87%)	7 (9%)	3 (4%)	2	14
30	c	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
31	d	49/54 (91%)	47 (96%)	2 (4%)	0	100	100
32	e	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
33	f	41/154 (27%)	36 (88%)	4 (10%)	1 (2%)	4	21
34	m	36/39 (92%)	31 (86%)	2 (6%)	3 (8%)	0	4
All	All	4281/5310 (81%)	3871 (90%)	298 (7%)	112 (3%)	6	20

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	158	THR
4	C	116	ASN
6	E	35	PRO
7	F	16	VAL
8	G	58	LYS
8	G	69	VAL
8	G	153	VAL
9	H	108	PHE
10	I	141	LEU
12	K	42	GLU
12	K	68	ASN
14	M	67	SER
17	P	43	ARG
17	P	131	VAL
17	P	133	HIS
19	R	23	LYS
19	R	71	LEU
20	S	14	ILE
21	T	50	VAL
29	b	18	LYS
34	m	7	ARG
2	A	196	PRO
3	B	43	PHE
3	B	154	CYS
7	F	94	LYS
9	H	34	SER

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Mol	Chain	Res	Type
9	H	150	ASN
10	I	155	LEU
13	L	57	ASP
14	M	89	VAL
15	N	4	MET
16	O	70	ASP
16	O	143	ASP
18	Q	37	ASN
18	Q	143	TYR
20	S	60	GLU
21	T	41	PHE
21	T	129	ASP
23	V	10	ASP
25	X	112	VAL
28	a	47	ALA
29	b	58	ASN
29	b	59	ILE
34	m	16	ARG
3	B	54	THR
4	C	185	HIS
7	F	5	ALA
9	H	36	SER
10	I	59	ARG
11	J	120	LYS
12	K	62	PHE
14	M	88	ASP
17	P	22	TYR
17	P	56	ARG
17	P	74	PHE
20	S	61	LEU
20	S	90	LYS
23	V	4	ASP
25	X	95	ASP
28	a	85	ARG
2	A	126	THR
3	B	209	ASN
3	B	220	LYS
3	B	221	PRO
4	C	41	THR
4	C	158	GLU
6	E	232	GLU
7	F	37	VAL

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Mol	Chain	Res	Type
8	G	172	LYS
9	H	113	LEU
9	H	117	PRO
11	J	62	LEU
11	J	121	SER
14	M	68	GLU
14	M	84	ILE
14	M	91	ASP
15	N	28	ILE
15	N	60	VAL
19	R	94	ALA
20	S	83	THR
28	a	36	ILE
33	f	137	ASN
34	m	3	HIS
2	A	105	THR
3	B	224	ASP
7	F	15	ASP
7	F	119	ALA
8	G	146	ASN
9	H	190	SER
11	J	162	SER
12	K	67	PHE
15	N	21	LYS
19	R	87	GLU
19	R	111	ILE
25	X	129	SER
28	a	46	ASP
4	C	153	GLY
7	F	22	SER
11	J	134	ILE
23	V	7	ARG
26	Y	54	ASP
27	Z	154	ILE
28	a	61	THR
2	A	160	ILE
18	Q	137	PRO
25	X	39	ASN
16	O	31	ILE
16	O	63	GLY
5	D	114	GLY
26	Y	81	ASN

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Mol	Chain	Res	Type
12	K	29	ILE
21	T	47	ILE

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	
2	A	171/225 (76%)	168 (98%)	3 (2%)	51	66
3	B	188/225 (84%)	180 (96%)	8 (4%)	26	52
4	C	187/213 (88%)	180 (96%)	7 (4%)	30	55
5	D	171/199 (86%)	170 (99%)	1 (1%)	78	79
6	E	225/229 (98%)	220 (98%)	5 (2%)	45	63
7	F	158/162 (98%)	151 (96%)	7 (4%)	25	51
8	G	189/212 (89%)	185 (98%)	4 (2%)	47	64
9	H	139/181 (77%)	129 (93%)	10 (7%)	13	39
10	I	159/176 (90%)	153 (96%)	6 (4%)	29	55
11	J	154/161 (96%)	146 (95%)	8 (5%)	21	48
12	K	60/128 (47%)	55 (92%)	5 (8%)	10	35
13	L	133/144 (92%)	124 (93%)	9 (7%)	14	41
14	M	8/120 (7%)	8 (100%)	0	100	100
15	N	128/129 (99%)	125 (98%)	3 (2%)	44	62
16	O	98/114 (86%)	94 (96%)	4 (4%)	27	53
17	P	103/129 (80%)	96 (93%)	7 (7%)	14	41
18	Q	111/119 (93%)	110 (99%)	1 (1%)	70	75
19	R	104/118 (88%)	101 (97%)	3 (3%)	37	60
20	S	116/134 (87%)	113 (97%)	3 (3%)	40	61
21	T	128/135 (95%)	126 (98%)	2 (2%)	55	67
22	U	96/211 (46%)	96 (100%)	0	100	100
23	V	64/65 (98%)	58 (91%)	6 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	113/114 (99%)	109 (96%)	4 (4%)	32	57
25	X	106/115 (92%)	97 (92%)	9 (8%)	10	33
26	Y	106/111 (96%)	105 (99%)	1 (1%)	70	75
27	Z	63/139 (45%)	61 (97%)	2 (3%)	34	58
28	a	88/97 (91%)	86 (98%)	2 (2%)	44	62
29	b	72/75 (96%)	70 (97%)	2 (3%)	38	60
30	c	48/56 (86%)	46 (96%)	2 (4%)	26	52
31	d	45/48 (94%)	43 (96%)	2 (4%)	25	51
32	e	40/48 (83%)	40 (100%)	0	100	100
33	f	3/130 (2%)	3 (100%)	0	100	100
34	m	33/34 (97%)	30 (91%)	3 (9%)	9	30
All	All	3607/4496 (80%)	3478 (96%)	129 (4%)	32	56

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	112	GLN
2	A	174	LEU
2	A	205	LEU
3	B	47	LEU
3	B	56	LEU
3	B	125	VAL
3	B	139	CYS
3	B	140	ILE
3	B	158	THR
3	B	169	MET
3	B	175	GLU
4	C	56	GLU
4	C	87	ASP
4	C	97	GLN
4	C	152	TRP
4	C	161	THR
4	C	191	THR
4	C	204	CYS
5	D	36	TYR
6	E	139	LEU
6	E	146	THR
6	E	171	ASP

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Mol	Chain	Res	Type
6	E	210	LEU
6	E	233	LYS
7	F	4	GLU
7	F	15	ASP
7	F	16	VAL
7	F	25	ASP
7	F	37	VAL
7	F	58	GLU
7	F	95	ASN
8	G	49	ILE
8	G	128	GLU
8	G	163	GLU
8	G	210	LEU
9	H	41	ASP
9	H	46	VAL
9	H	55	VAL
9	H	103	MET
9	H	104	LEU
9	H	106	LEU
9	H	107	ASP
9	H	132	ASP
9	H	186	ASP
9	H	188	VAL
10	I	22	GLN
10	I	47	ARG
10	I	72	ILE
10	I	104	ILE
10	I	149	GLN
10	I	158	LEU
11	J	85	LEU
11	J	93	LEU
11	J	94	ASP
11	J	118	LEU
11	J	120	LYS
11	J	122	ILE
11	J	150	VAL
11	J	157	ASP
12	K	36	LYS
12	K	39	ARG
12	K	68	ASN
12	K	70	GLN
12	K	84	LEU

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Mol	Chain	Res	Type
13	L	9	GLU
13	L	49	LEU
13	L	66	VAL
13	L	72	VAL
13	L	87	VAL
13	L	88	ILE
13	L	110	THR
13	L	113	LEU
13	L	146	GLU
15	N	60	VAL
15	N	84	LEU
15	N	121	ARG
16	O	80	MET
16	O	121	LEU
16	O	143	ASP
16	O	145	THR
17	P	22	TYR
17	P	30	LEU
17	P	31	LEU
17	P	32	ASP
17	P	40	GLU
17	P	46	GLN
17	P	54	ILE
18	Q	47	GLU
19	R	67	ARG
19	R	69	ILE
19	R	85	VAL
20	S	14	ILE
20	S	15	LEU
20	S	92	VAL
21	T	49	TYR
21	T	127	GLU
23	V	11	LEU
23	V	12	TYR
23	V	13	ILE
23	V	44	ARG
23	V	63	GLU
23	V	77	LEU
24	W	2	VAL
24	W	26	LEU
24	W	103	VAL
24	W	104	LEU

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Mol	Chain	Res	Type
25	X	55	LEU
25	X	57	ILE
25	X	60	LYS
25	X	76	LYS
25	X	77	ASN
25	X	98	ASP
25	X	101	LEU
25	X	105	PHE
25	X	137	LYS
26	Y	19	LEU
27	Z	133	ILE
27	Z	147	GLU
28	a	15	ARG
28	a	85	ARG
29	b	39	LEU
29	b	60	MET
30	c	61	GLU
30	c	67	LEU
31	d	6	ASN
31	d	39	GLN
34	m	12	ARG
34	m	15	MET
34	m	16	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	12	GLN
2	A	51	ASN
2	A	98	GLN
2	A	112	GLN
2	A	133	GLN
3	B	74	ASN
3	B	95	ASN
3	B	180	GLN
3	B	232	HIS
4	C	76	GLN
4	C	102	GLN
4	C	118	HIS
4	C	185	HIS
4	C	249	GLN
6	E	36	HIS

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Mol	Chain	Res	Type
6	E	80	GLN
7	F	17	ASN
7	F	39	HIS
7	F	71	ASN
7	F	95	ASN
7	F	125	GLN
7	F	136	ASN
7	F	167	ASN
8	G	59	GLN
8	G	192	GLN
9	H	80	GLN
10	I	11	HIS
10	I	139	HIS
10	I	178	GLN
11	J	72	GLN
11	J	110	GLN
11	J	139	HIS
11	J	155	HIS
12	K	47	ASN
12	K	72	ASN
13	L	108	ASN
13	L	130	GLN
13	L	157	GLN
15	N	105	ASN
15	N	134	GLN
16	O	37	HIS
16	O	48	HIS
16	O	118	GLN
17	P	71	ASN
17	P	109	ASN
19	R	31	ASN
20	S	77	GLN
20	S	87	ASN
20	S	97	HIS
21	T	34	HIS
21	T	96	GLN
21	T	142	GLN
22	U	132	HIS
23	V	38	GLN
23	V	60	GLN
24	W	56	HIS
24	W	113	HIS

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Mol	Chain	Res	Type
25	X	5	ASN
25	X	63	ASN
25	X	73	GLN
27	Z	158	ASN
28	a	97	ASN
29	b	17	HIS
29	b	47	HIS
29	b	49	GLN
31	d	18	GLN
31	d	26	HIS
34	m	3	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1602/1791 (89%)	433 (27%)	48 (2%)

All (433) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	40	A
1	2	42	G
1	2	47	A
1	2	57	G
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	U
1	2	73	U
1	2	74	U
1	2	76	U
1	2	81	C
1	2	92	A
1	2	99	A

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Mol	Chain	Res	Type
1	2	100	U
1	2	103	A
1	2	113	A
1	2	114	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	127	U
1	2	135	A
1	2	136	C
1	2	137	A
1	2	138	U
1	2	141	A
1	2	142	U
1	2	148	U
1	2	149	G
1	2	154	U
1	2	155	U
1	2	164	A
1	2	167	A
1	2	172	C
1	2	174	C
1	2	175	A
1	2	199	G
1	2	211	U
1	2	212	A
1	2	213	C
1	2	215	G
1	2	216	A
1	2	219	C
1	2	250	C
1	2	260	G
1	2	261	A
1	2	262	A
1	2	263	C
1	2	265	G
1	2	271	G
1	2	284	U
1	2	288	A
1	2	295	A
1	2	299	A
1	2	309	C

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Mol	Chain	Res	Type
1	2	313	U
1	2	314	C
1	2	316	G
1	2	320	U
1	2	321	C
1	2	322	G
1	2	334	A
1	2	336	G
1	2	337	G
1	2	338	A
1	2	342	C
1	2	350	G
1	2	351	U
1	2	352	G
1	2	359	A
1	2	360	A
1	2	361	C
1	2	369	U
1	2	380	U
1	2	390	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	417	A
1	2	418	G
1	2	420	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	433	C
1	2	434	G
1	2	439	U
1	2	442	C
1	2	444	C
1	2	448	C
1	2	460	A
1	2	464	A
1	2	469	C
1	2	475	A

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Mol	Chain	Res	Type
1	2	477	A
1	2	485	U
1	2	486	G
1	2	487	G
1	2	503	U
1	2	504	G
1	2	505	A
1	2	506	U
1	2	507	U
1	2	509	G
1	2	510	A
1	2	514	A
1	2	525	A
1	2	534	C
1	2	535	A
1	2	537	A
1	2	538	G
1	2	539	U
1	2	540	A
1	2	541	A
1	2	542	C
1	2	543	A
1	2	553	C
1	2	554	A
1	2	555	A
1	2	556	G
1	2	557	U
1	2	560	G
1	2	563	G
1	2	564	C
1	2	567	G
1	2	571	C
1	2	578	A
1	2	579	A
1	2	593	A
1	2	594	G
1	2	605	A
1	2	610	U
1	2	618	A
1	2	619	A
1	2	621	A
1	2	622	A

Continued on next page...

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Mol	Chain	Res	Type
1	2	623	G
1	2	625	U
1	2	629	A
1	2	637	U
1	2	638	U
1	2	639	C
1	2	640	U
1	2	644	G
1	2	651	C
1	2	688	G
1	2	690	A
1	2	691	U
1	2	693	C
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	U
1	2	736	G
1	2	737	A
1	2	738	C
1	2	739	U
1	2	740	U
1	2	752	A
1	2	753	A
1	2	762	G
1	2	763	U
1	2	768	A
1	2	771	A
1	2	772	G
1	2	776	U
1	2	777	G
1	2	778	U
1	2	780	G
1	2	783	U
1	2	784	U
1	2	785	G
1	2	787	A
1	2	816	U
1	2	818	U
1	2	820	G
1	2	821	G
1	2	824	C

Continued on next page...

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Mol	Chain	Res	Type
1	2	825	U
1	2	826	A
1	2	836	U
1	2	841	A
1	2	843	G
1	2	846	U
1	2	849	A
1	2	853	A
1	2	856	A
1	2	857	U
1	2	858	U
1	2	860	A
1	2	861	U
1	2	878	A
1	2	883	U
1	2	890	C
1	2	895	A
1	2	904	A
1	2	909	U
1	2	911	G
1	2	912	A
1	2	914	U
1	2	918	U
1	2	925	G
1	2	928	C
1	2	930	A
1	2	932	U
1	2	939	G
1	2	941	A
1	2	948	A
1	2	956	U
1	2	957	U
1	2	963	A
1	2	968	A
1	2	972	C
1	2	987	C
1	2	989	A
1	2	993	C
1	2	1000	A
1	2	1001	U
1	2	1007	C
1	2	1015	U

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Mol	Chain	Res	Type
1	2	1018	C
1	2	1021	U
1	2	1023	A
1	2	1025	C
1	2	1028	U
1	2	1029	G
1	2	1036	A
1	2	1037	G
1	2	1049	C
1	2	1050	G
1	2	1052	C
1	2	1053	A
1	2	1060	A
1	2	1067	C
1	2	1071	A
1	2	1077	U
1	2	1078	G
1	2	1081	A
1	2	1086	A
1	2	1087	A
1	2	1091	C
1	2	1092	U
1	2	1093	U
1	2	1095	G
1	2	1103	G
1	2	1104	G
1	2	1106	G
1	2	1119	A
1	2	1121	G
1	2	1127	A
1	2	1133	A
1	2	1141	G
1	2	1145	G
1	2	1146	A
1	2	1149	G
1	2	1152	A
1	2	1153	C
1	2	1154	C
1	2	1155	A
1	2	1159	G
1	2	1162	G
1	2	1174	G

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Mol	Chain	Res	Type
1	2	1180	U
1	2	1181	U
1	2	1189	A
1	2	1191	A
1	2	1194	G
1	2	1195	G
1	2	1197	A
1	2	1212	A
1	2	1213	G
1	2	1216	A
1	2	1221	A
1	2	1226	U
1	2	1232	G
1	2	1236	G
1	2	1237	A
1	2	1239	A
1	2	1240	G
1	2	1241	C
1	2	1244	U
1	2	1245	U
1	2	1248	U
1	2	1250	G
1	2	1252	U
1	2	1255	U
1	2	1258	G
1	2	1269	C
1	2	1280	U
1	2	1281	U
1	2	1294	G
1	2	1296	U
1	2	1309	U
1	2	1310	U
1	2	1313	G
1	2	1316	A
1	2	1332	A
1	2	1333	C
1	2	1335	U
1	2	1336	G
1	2	1340	A
1	2	1341	A
1	2	1342	U
1	2	1343	A

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Mol	Chain	Res	Type
1	2	1344	G
1	2	1347	U
1	2	1355	U
1	2	1356	U
1	2	1357	C
1	2	1359	U
1	2	1360	G
1	2	1361	U
1	2	1366	G
1	2	1367	U
1	2	1369	U
1	2	1376	U
1	2	1381	G
1	2	1386	U
1	2	1387	U
1	2	1393	G
1	2	1394	U
1	2	1395	C
1	2	1396	U
1	2	1399	C
1	2	1409	U
1	2	1411	U
1	2	1420	A
1	2	1421	A
1	2	1423	A
1	2	1424	G
1	2	1428	U
1	2	1429	G
1	2	1431	G
1	2	1432	A
1	2	1441	G
1	2	1442	A
1	2	1443	U
1	2	1453	U
1	2	1454	G
1	2	1455	C
1	2	1456	A
1	2	1457	C
1	2	1467	A
1	2	1468	C
1	2	1469	U
1	2	1470	G

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Mol	Chain	Res	Type
1	2	1478	C
1	2	1482	G
1	2	1483	A
1	2	1484	G
1	2	1504	G
1	2	1512	U
1	2	1514	A
1	2	1516	C
1	2	1518	U
1	2	1519	G
1	2	1520	U
1	2	1521	G
1	2	1522	A
1	2	1533	U
1	2	1534	G
1	2	1535	A
1	2	1536	U
1	2	1538	G
1	2	1540	G
1	2	1546	U
1	2	1552	C
1	2	1553	A
1	2	1555	U
1	2	1556	U
1	2	1557	A
1	2	1558	U
1	2	1559	U
1	2	1561	A
1	2	1562	U
1	2	1566	C
1	2	1567	A
1	2	1571	A
1	2	1572	G
1	2	1573	G
1	2	1574	A
1	2	1582	G
1	2	1591	A
1	2	1594	C
1	2	1599	C
1	2	1605	G
1	2	1616	C
1	2	1629	A

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Mol	Chain	Res	Type
1	2	1633	A
1	2	1649	A
1	2	1655	U
1	2	1656	G
1	2	1663	C
1	2	1676	C
1	2	1679	A
1	2	1680	C
1	2	1681	C
1	2	1683	U
1	2	1684	U
1	2	1686	U
1	2	1689	G
1	2	1703	C
1	2	1704	G
1	2	1705	A
1	2	1709	G
1	2	1745	G
1	2	1746	A
1	2	1747	A
1	2	1752	U
1	2	1753	A
1	2	1754	A
1	2	1757	A
1	2	1760	U
1	2	1771	G
1	2	1773	A
1	2	1774	C
1	2	1783	G
1	2	1784	G
1	2	1785	A
1	2	1786	U
1	2	1787	C
1	2	1790	U

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	68	A
1	2	80	G
1	2	102	A
1	2	135	A

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Mol	Chain	Res	Type
1	2	154	U
1	2	198	A
1	2	211	U
1	2	213	C
1	2	260	G
1	2	261	A
1	2	350	G
1	2	400	A
1	2	417	A
1	2	425	A
1	2	540	A
1	2	541	A
1	2	553	C
1	2	554	A
1	2	555	A
1	2	606	G
1	2	637	U
1	2	739	U
1	2	777	G
1	2	956	U
1	2	1001	U
1	2	1059	G
1	2	1077	U
1	2	1103	G
1	2	1152	A
1	2	1211	C
1	2	1268	G
1	2	1280	U
1	2	1339	A
1	2	1359	U
1	2	1393	G
1	2	1410	U
1	2	1453	U
1	2	1468	C
1	2	1469	U
1	2	1477	C
1	2	1532	G
1	2	1535	A
1	2	1556	U
1	2	1566	C
1	2	1571	A
1	2	1678	G

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Mol	Chain	Res	Type
1	2	1752	U
1	2	1753	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

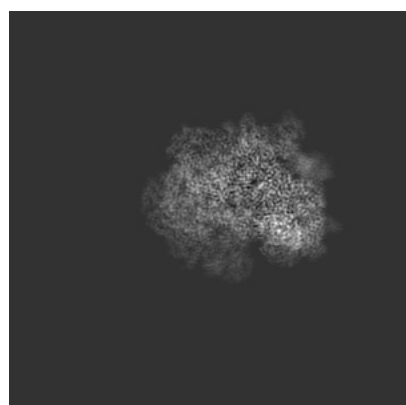
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6780. These allow visual inspection of the internal detail of the map and identification of artifacts.

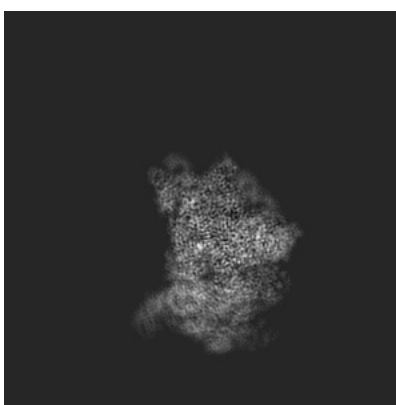
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

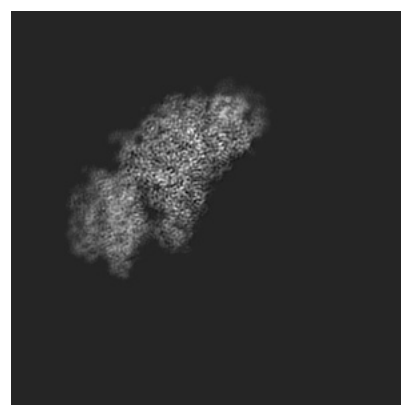
6.1.1 Primary map



X



Y

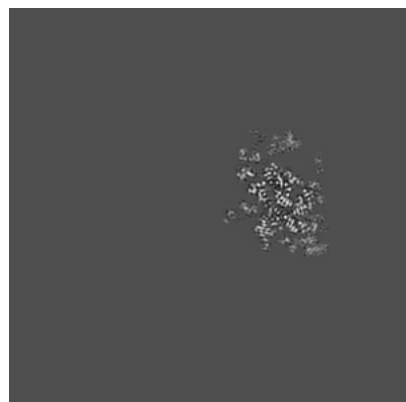


Z

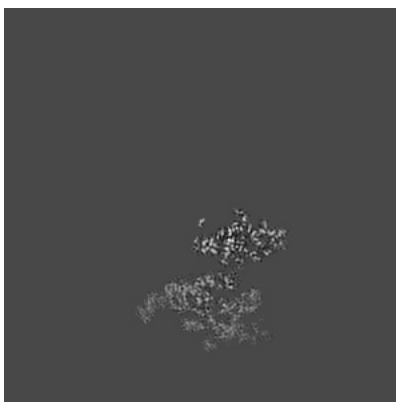
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

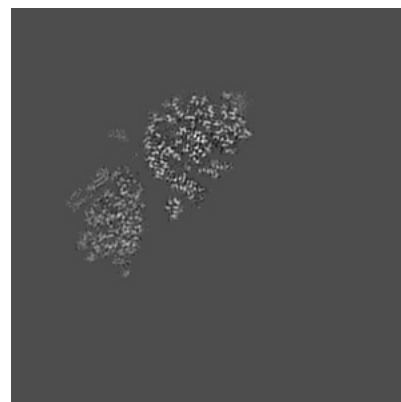
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

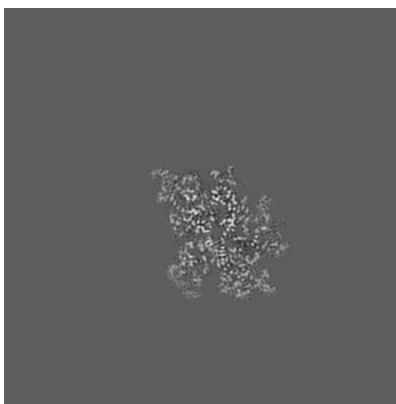
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

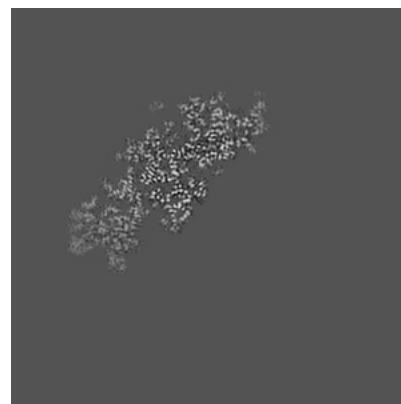
6.3.1 Primary map



X Index: 130



Y Index: 209

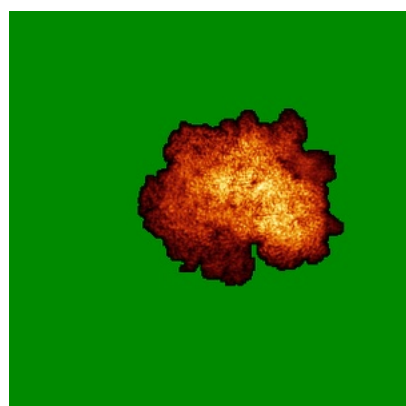


Z Index: 179

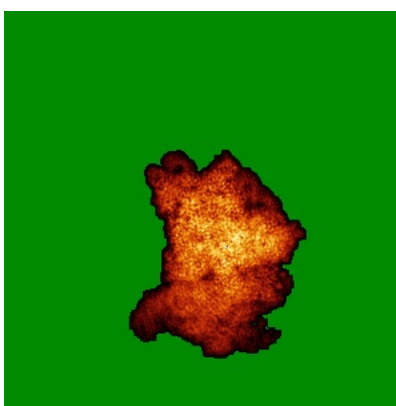
The images above show the largest variance slices of the map in three orthogonal directions.

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

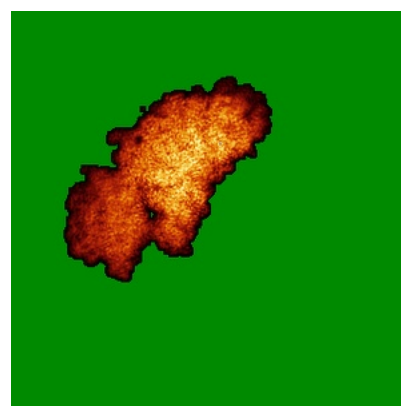
6.4.1 Primary map



X



Y



Z

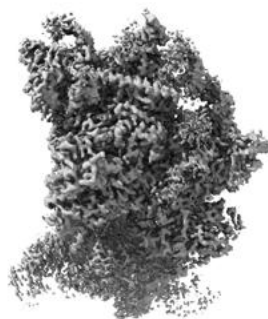
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

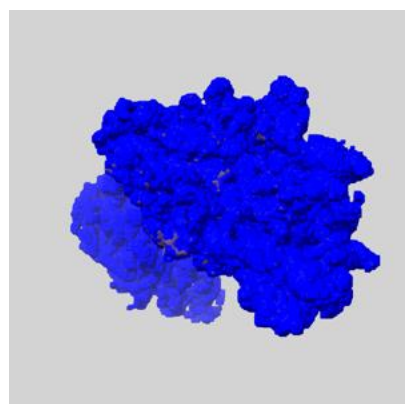
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

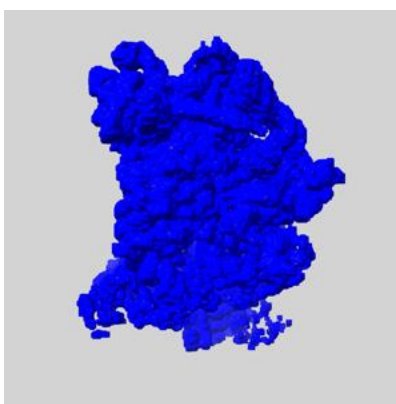
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

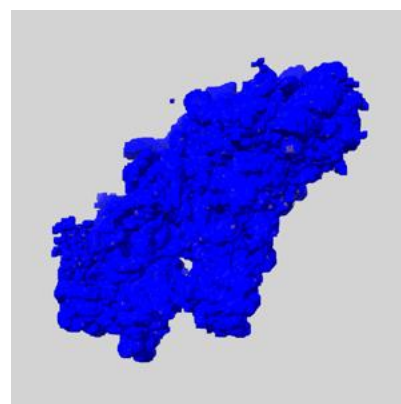
6.6.1 emd_6780_msk_1.map [i](#)



X



Y

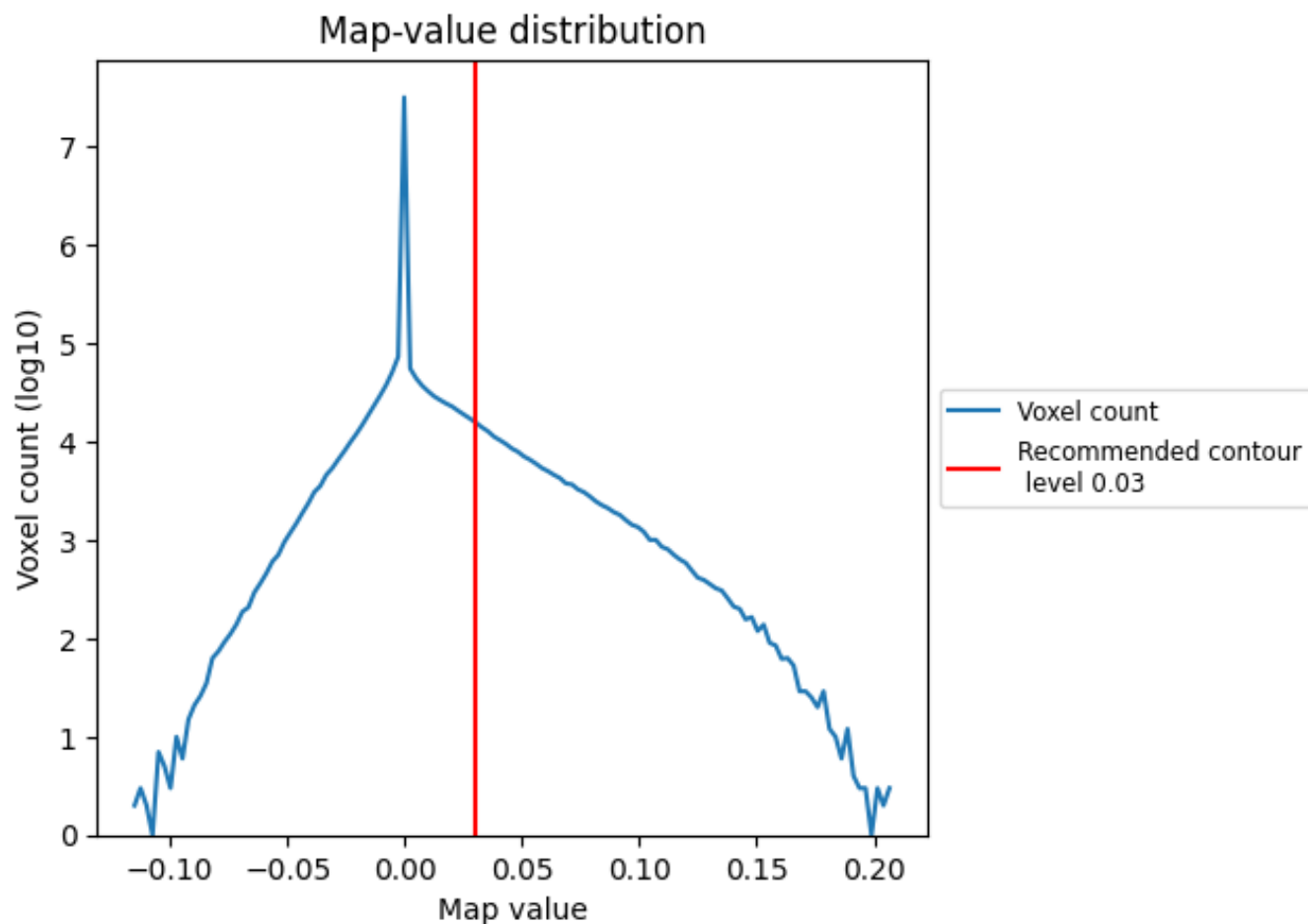


Z

7 Map analysis [i](#)

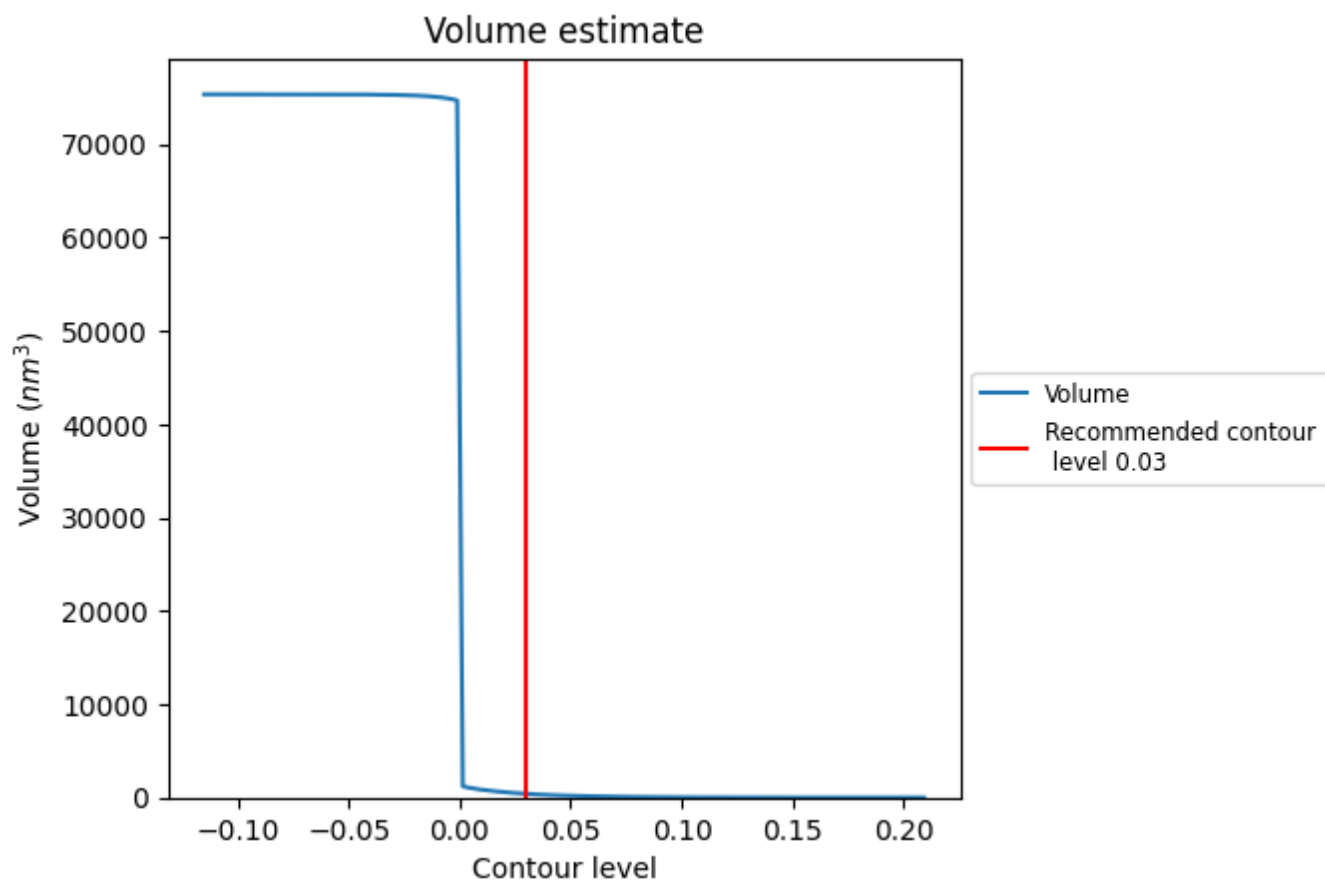
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

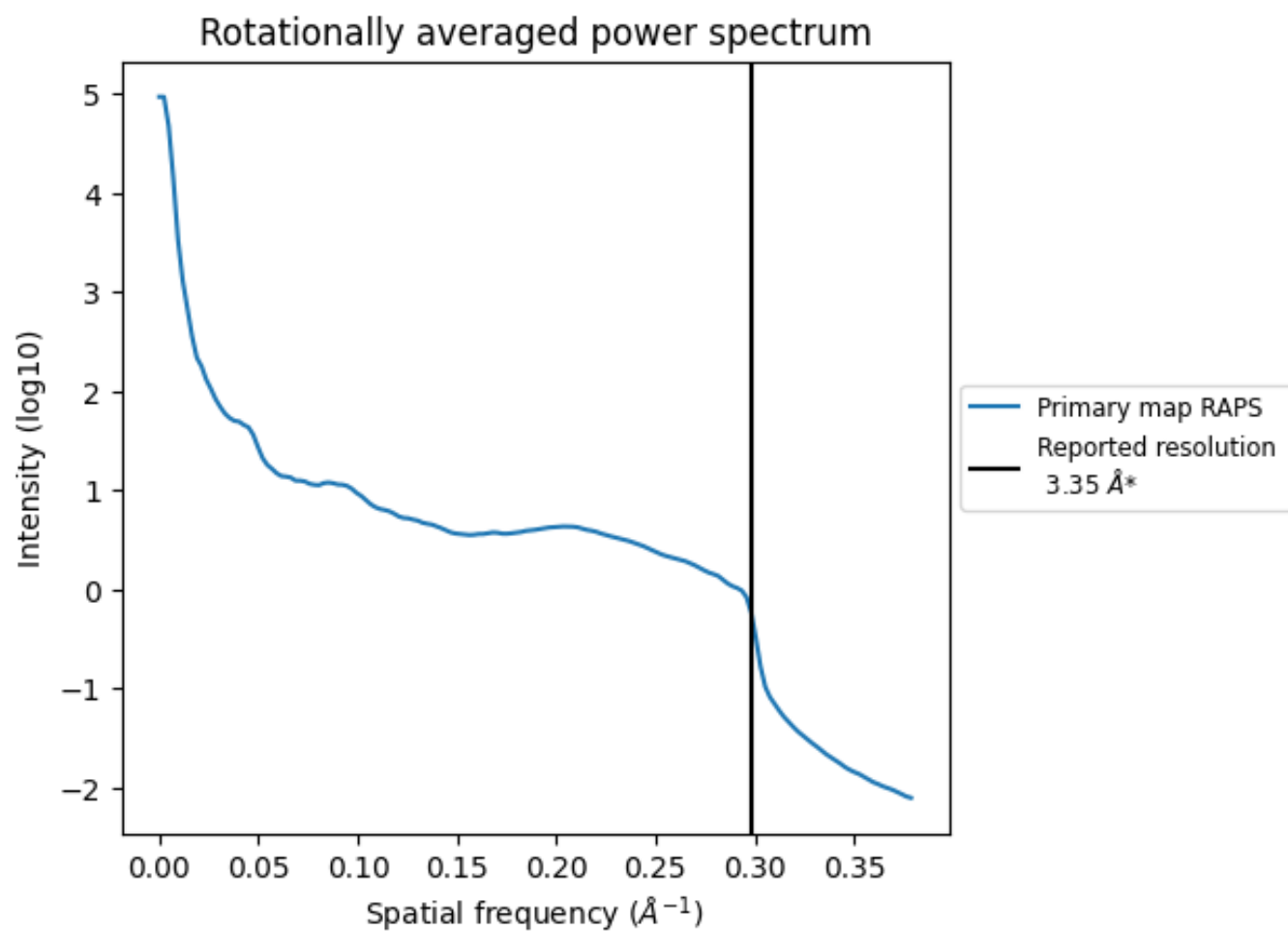
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm³; this corresponds to an approximate mass of 362 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

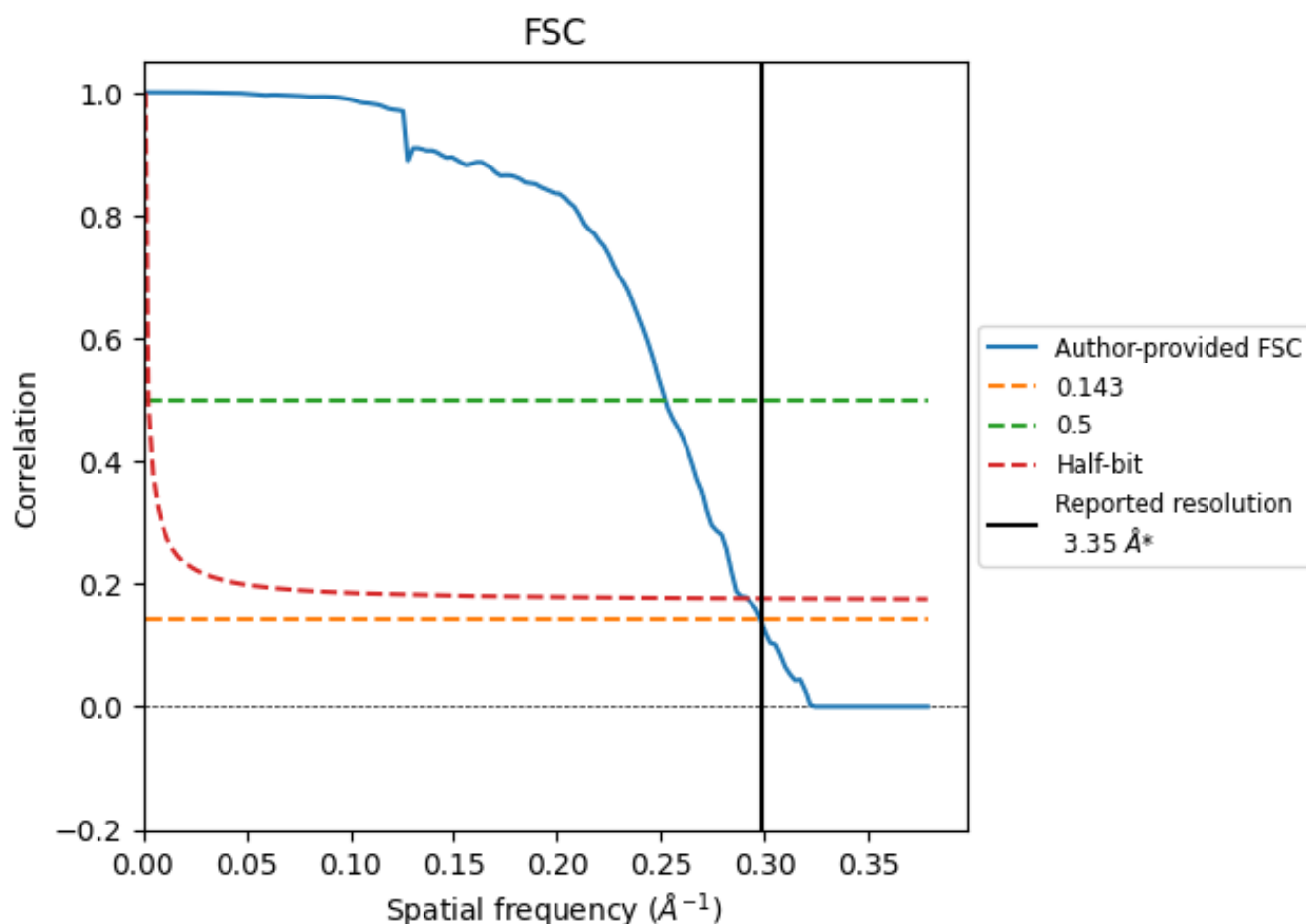


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

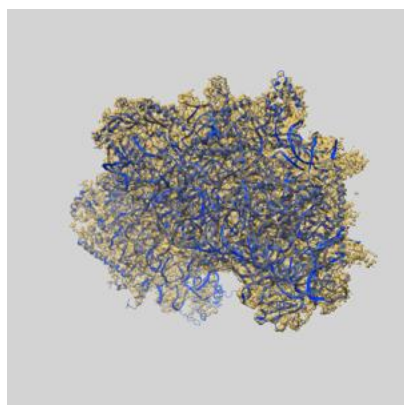
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.97	3.43
Unmasked-calculated*	-	-	-

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

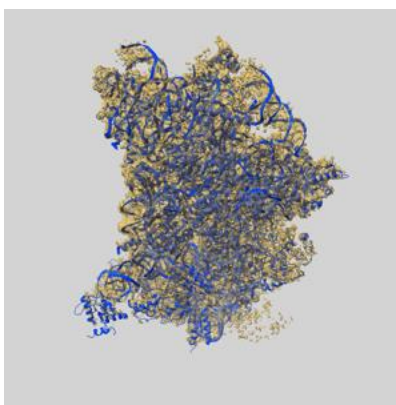
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6780 and PDB model 5XXU. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

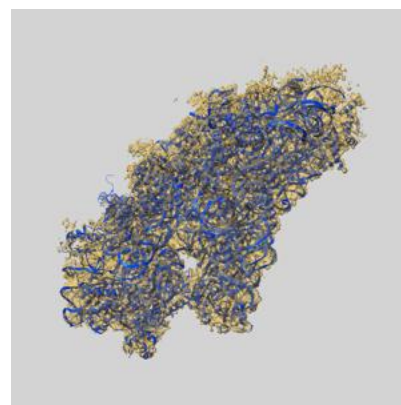
9.1 Map-model overlay [i](#)



X



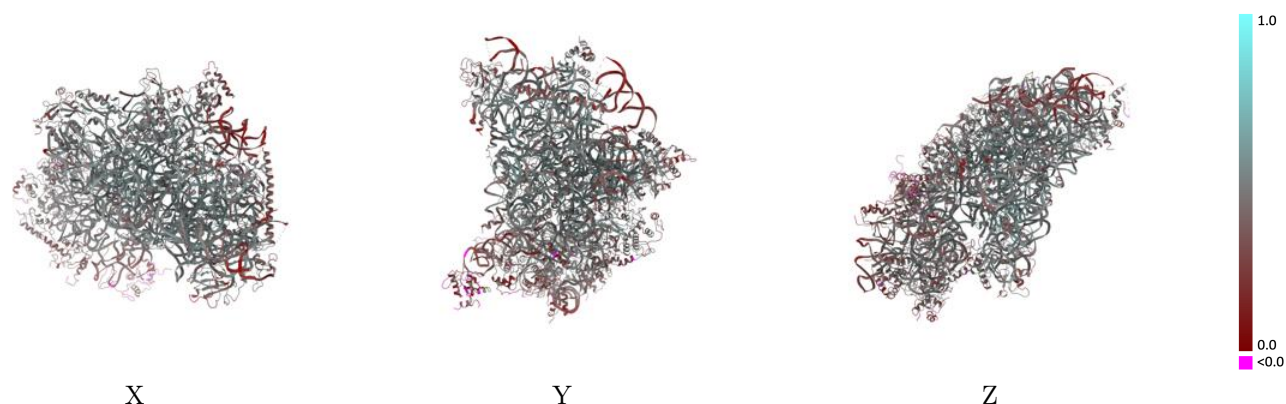
Y



Z

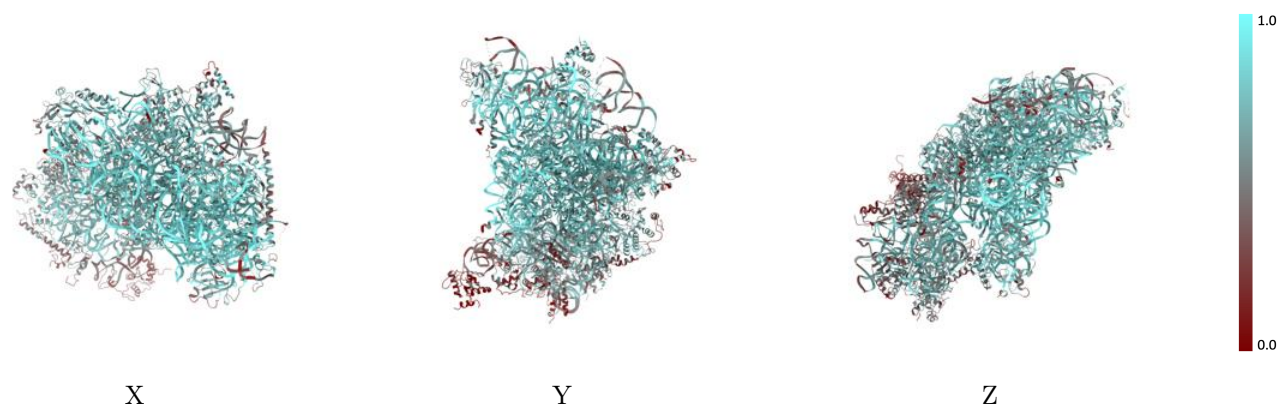
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



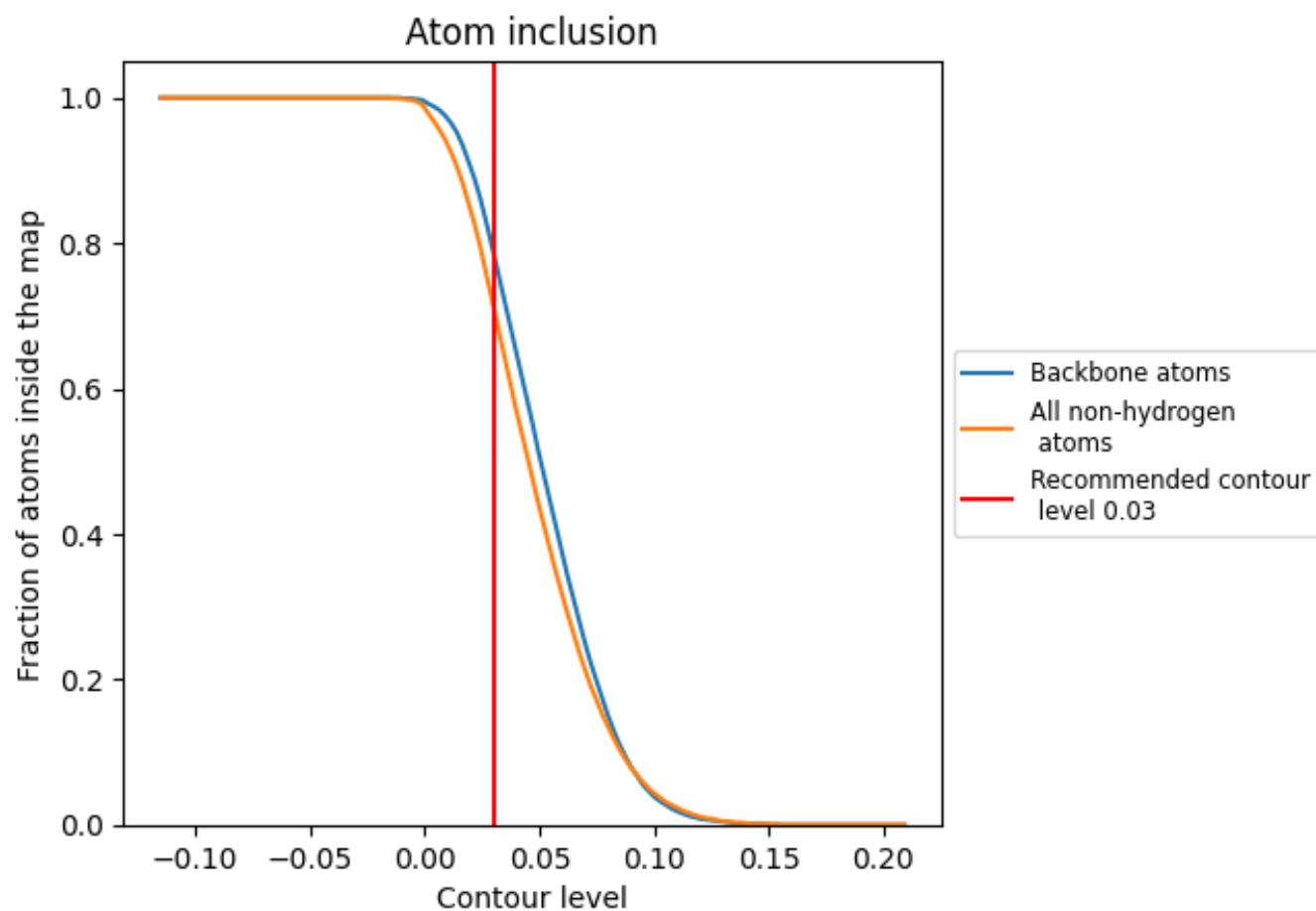
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.4440
2	 0.8150	 0.4650
A	 0.6630	 0.4400
B	 0.6760	 0.4540
C	 0.7290	 0.4750
D	 0.3740	 0.3360
E	 0.7250	 0.4760
F	 0.5530	 0.4100
G	 0.6190	 0.4090
H	 0.5900	 0.4250
I	 0.7360	 0.4860
J	 0.7200	 0.4570
K	 0.3500	 0.3020
L	 0.7470	 0.4960
M	 0.0890	 0.1730
N	 0.6960	 0.4690
O	 0.6730	 0.4710
P	 0.3730	 0.3120
Q	 0.5450	 0.4110
R	 0.3860	 0.3370
S	 0.5040	 0.3630
T	 0.5180	 0.3760
U	 0.3920	 0.3460
V	 0.6570	 0.4420
W	 0.7280	 0.4990
X	 0.7520	 0.5030
Y	 0.7080	 0.4590
Z	 0.5110	 0.3400
a	 0.7280	 0.4680
b	 0.7010	 0.4640
c	 0.5440	 0.4160
d	 0.6090	 0.4210
e	 0.6430	 0.4230
f	 0.1180	 0.1380
m	 0.7660	 0.5120

