



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:14 PM UTC

PDB ID : 7QP7 / pdb_00007qp7
EMDB ID : EMD-14114
Title : Structure of the human 48S initiation complex in closed state (h48S AUG closed)
Authors : Yi, S.-H.; Petrychenko, V.; Schliep, J.E.; Goyal, A.; Linden, A.; Chari, A.; Urlaub, H.; Stark, H.; Rodnina, M.V.; Adio, S.; Fischer, N.
Deposited on : 2022-01-03
Resolution : 3.70 Å (reported)
Based on initial model : 6ZMW

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

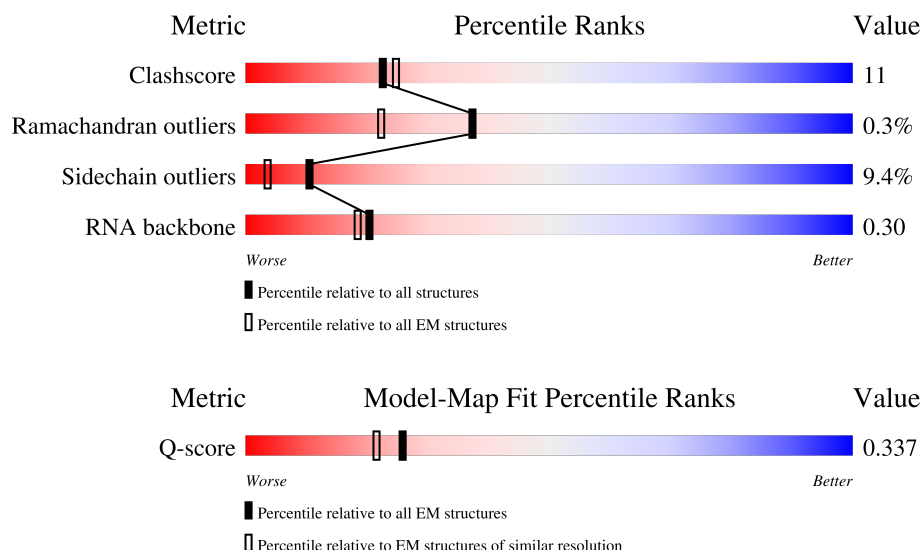
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	1	813	19% 47% 7% 45%
2	3	218	64% 89% 9%
3	4	357	15% 64% 8% 28%

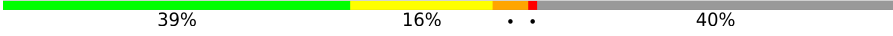
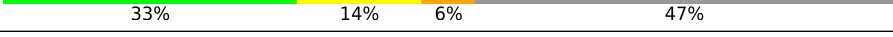
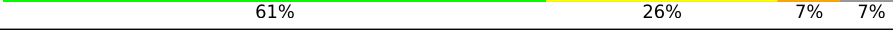
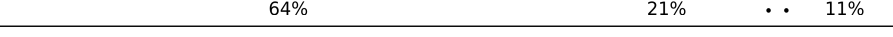
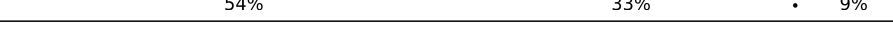
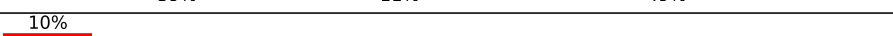
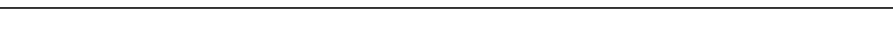
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Mol	Chain	Length	Quality of chain
4	5	564	
5	6	374	
6	7	255	
7	8	352	
8	9	25	
9	A	1869	
10	B	158	
11	C	263	
12	D	194	
13	E	143	
14	F	59	
15	G	194	
16	H	84	
17	I	151	
18	J	130	
19	K	83	
20	L	293	
21	M	135	
22	N	295	
23	O	264	
24	P	151	
25	Q	115	
26	R	208	
27	S	249	
28	T	133	

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Mol	Chain	Length	Quality of chain
29	V	204	
30	Y	146	
31	Z	243	
32	a	165	
33	b	145	
34	c	317	
35	d	145	
36	e	125	
37	f	152	
38	h	119	
39	i	56	
40	k	156	
41	m	132	
42	n	69	
43	o	320	
44	q	144	
45	r	315	
46	t	472	
47	u	1382	
48	v	445	
49	w	75	
50	x	548	
51	y	913	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 108194 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	447	Total	C	N	O	S	0	0
			2560	1570	492	493	5		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	21	Total	C	N	O	P	0	0
			441	199	78	144	20		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	8	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 8 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 9 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1719	Total	C	N	O	P	0	0
			36668	16378	6574	11998	1718		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 11 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 12 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 13 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 14 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	47	Total	C	N	O	S	0	0
			378	231	85	61	1		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 16 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 17 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 18 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 19 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 20 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 21 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	125	Total	C	N	O	S	0	0
			1015	639	185	187	4		

- Molecule 22 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 23 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 24 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 25 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 26 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 27 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 28 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 29 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 30 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 31 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 32 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 33 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	110	Total	C	N	O	S	0	0
			913	580	168	158	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 36 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

- Molecule 37 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 38 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 39 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 40 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	53	Total	C	N	O	S	0	0
			435	276	82	70	7		

- Molecule 41 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 42 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	77	Total	C	N	O		0	0
			616	389	111	116			

- Molecule 44 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	101	Total	C	N	O	S	0	0
			782	494	141	143	4		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	275	Total	C	N	O	S	0	0
			2215	1398	387	418	12		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	356	Total	C	N	O		0	0
			1750	1038	356	356			

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 49 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	421	Total	C	N	O	S	0	0
			2831	1746	521	555	9		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	642	Total	C	N	O	S	0	0
			5197	3274	925	963	35		

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	Q	1	Total	Zn	0
			1	1	
52	k	1	Total	Zn	0
			1	1	

THR
GLU
GLU
ILE
PRO
LEU
GLY
ASN
GLN

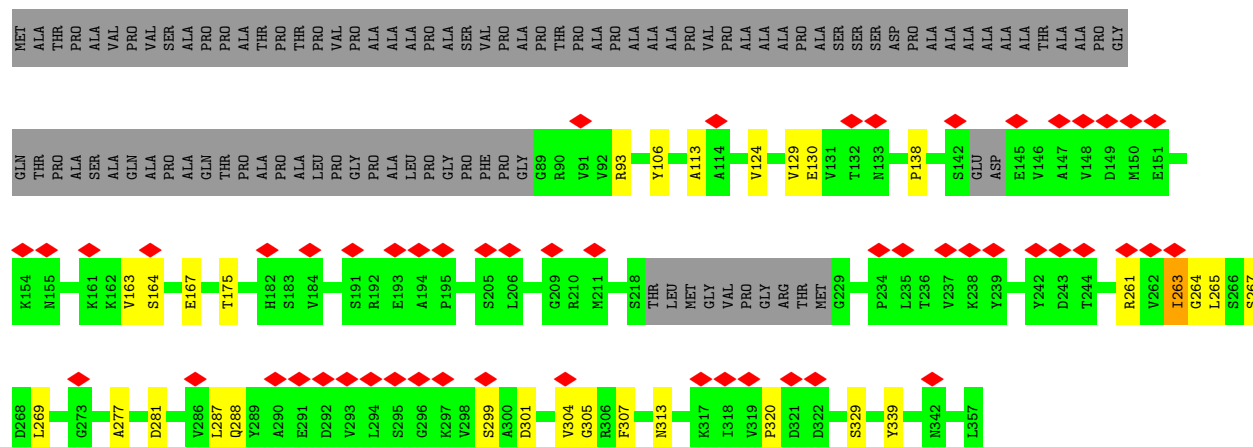
- Molecule 2: Eukaryotic translation initiation factor 3 subunit K

Chain 3: 



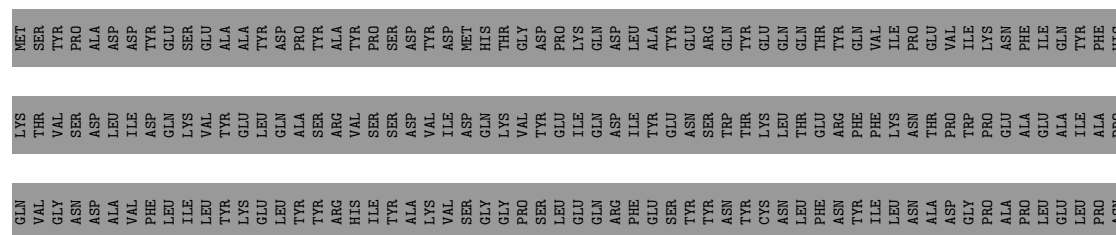
- Molecule 3: Eukaryotic translation initiation factor 3 subunit F

Chain 4: 

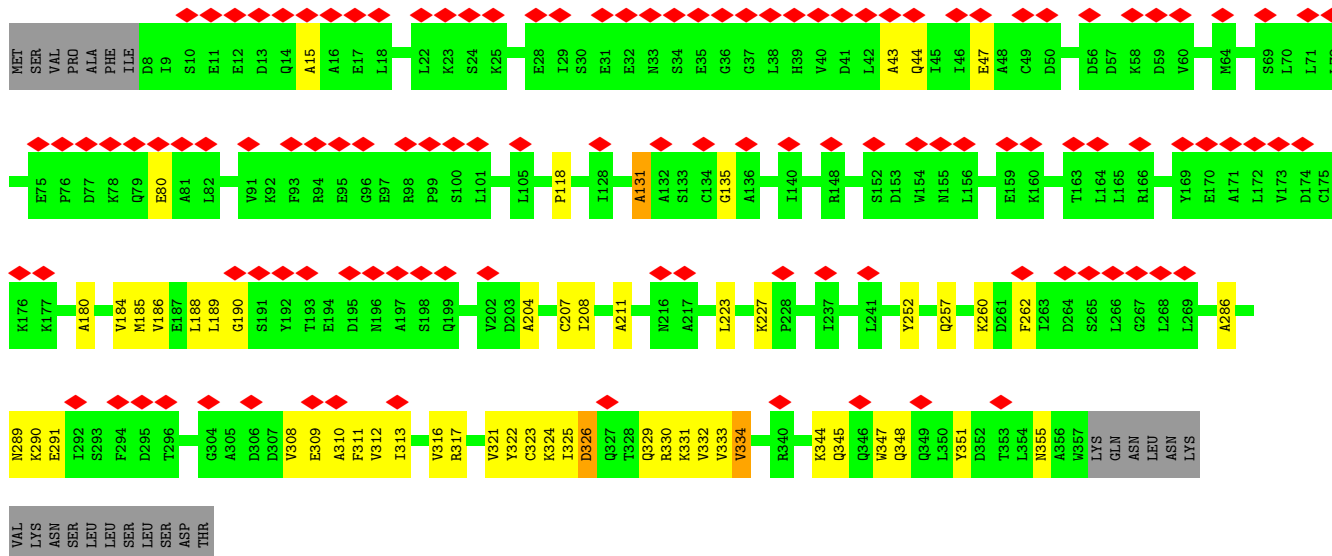
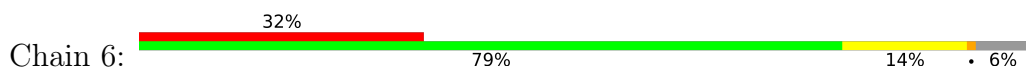


- Molecule 4: Eukaryotic translation initiation factor 3 subunit L

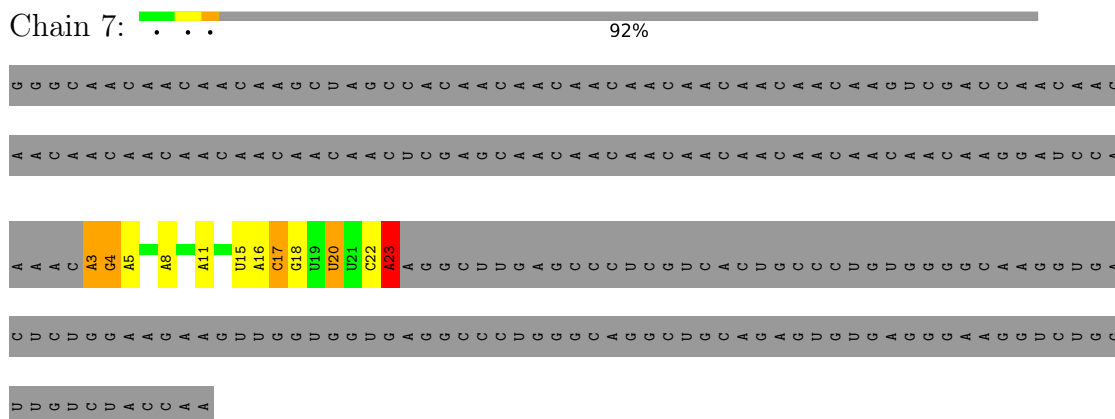
Chain 5: 



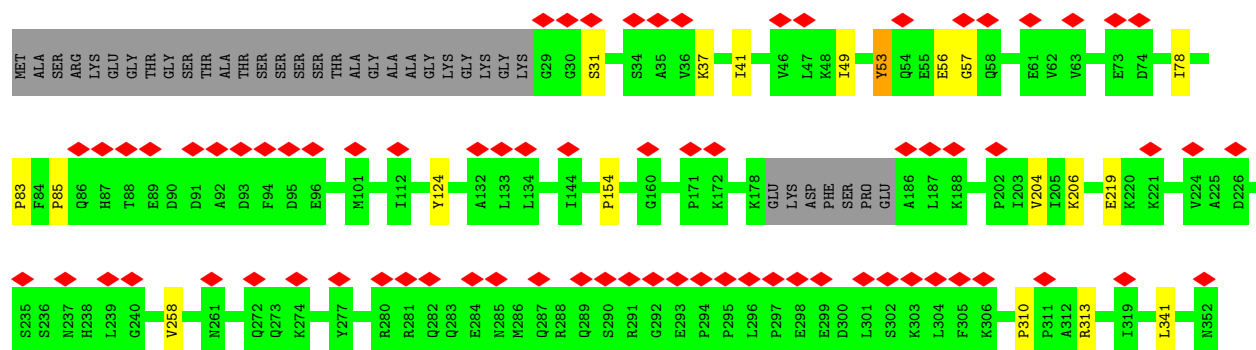
- Molecule 5: Eukaryotic translation initiation factor 3 subunit M



- Molecule 6: mRNA



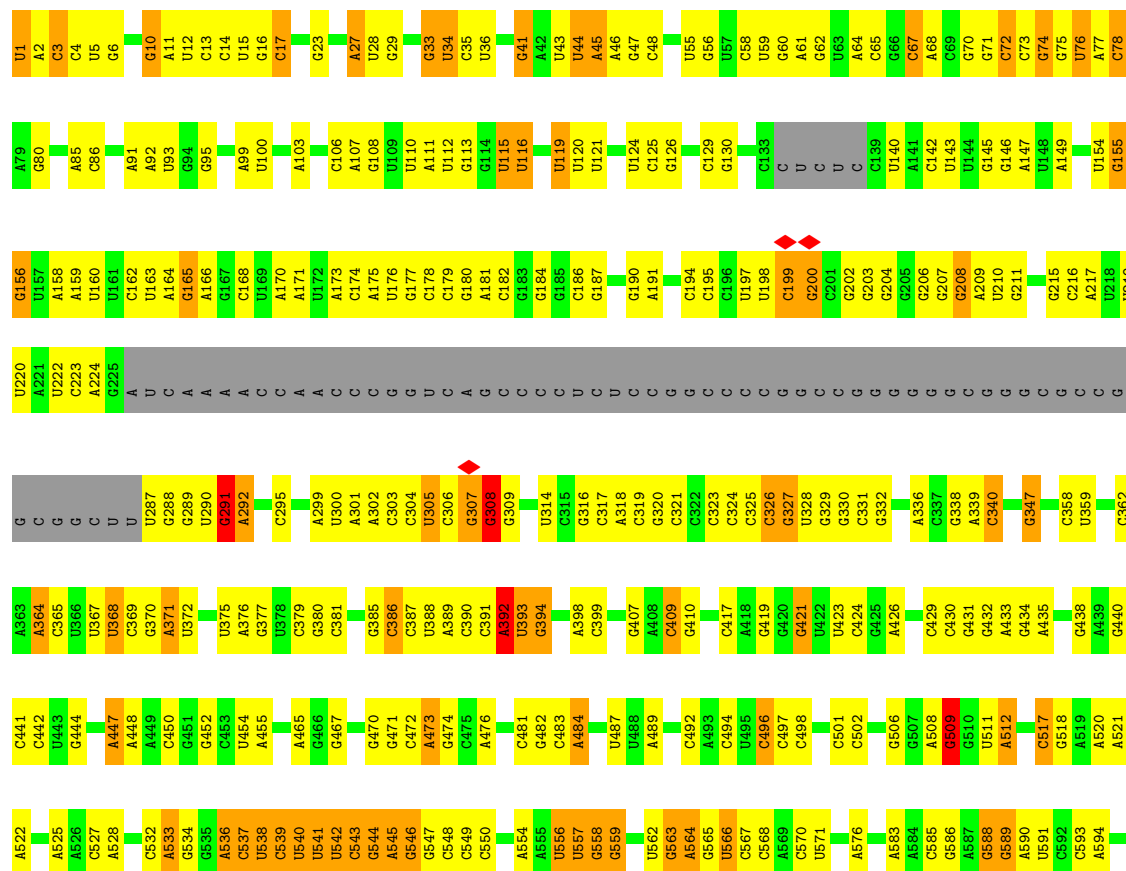
Chain 8: 21% 85% 5% 10%



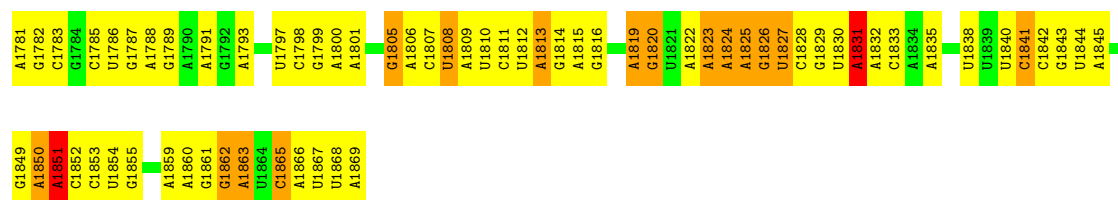
Chain 9: 68% 20% 8% .



Chain A: 39% 40% 12% 8%

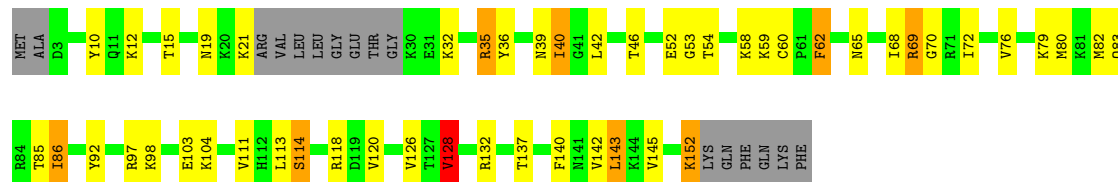


[illegible]



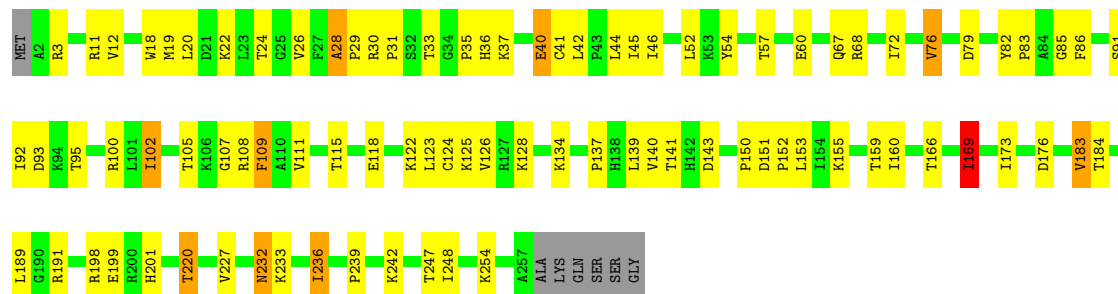
• Molecule 10: 40S ribosomal protein S11

Chain B: 58% 26% 5% • 10%



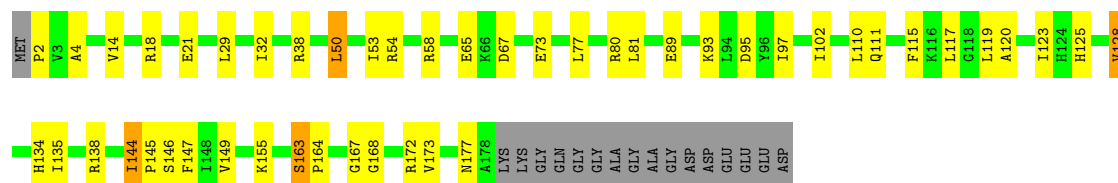
• Molecule 11: 40S ribosomal protein S4, X isoform

Chain C: 63% 30% • •



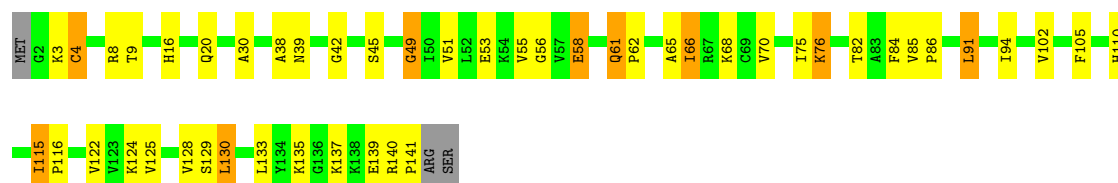
• Molecule 12: 40S ribosomal protein S9

Chain D: 66% 23% • 9%



• Molecule 13: 40S ribosomal protein S23

Chain E: 64% 27% 6% •



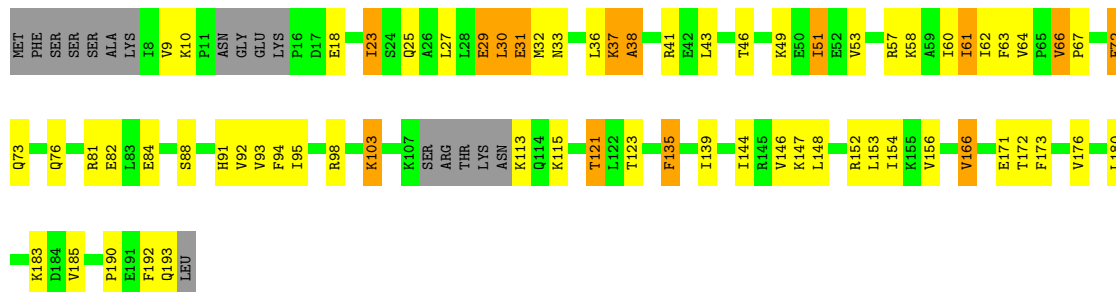
- Molecule 14: 40S ribosomal protein S30

Chain F: 



- Molecule 15: 40S ribosomal protein S7

Chain G: 



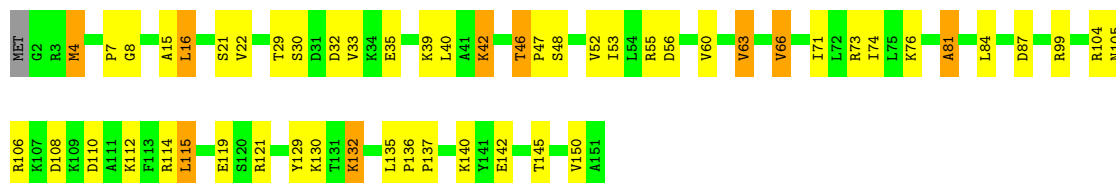
- Molecule 16: 40S ribosomal protein S27

Chain H: 



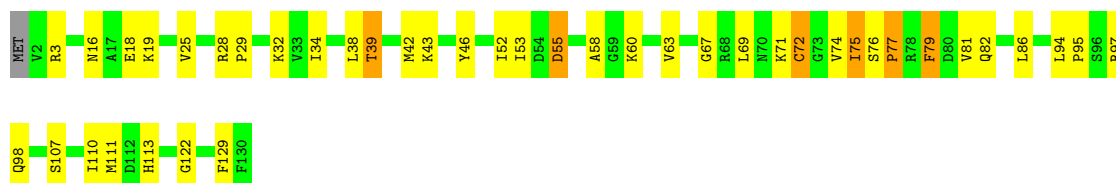
- Molecule 17: 40S ribosomal protein S13

Chain I: 



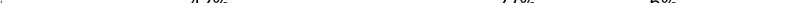
- Molecule 18: 40S ribosomal protein S15a

Chain J: 



- Molecule 19: 40S ribosomal protein S21

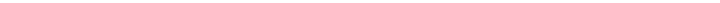
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- Chain L: 

[illegible]

- Chain M: 59% 28% 7%

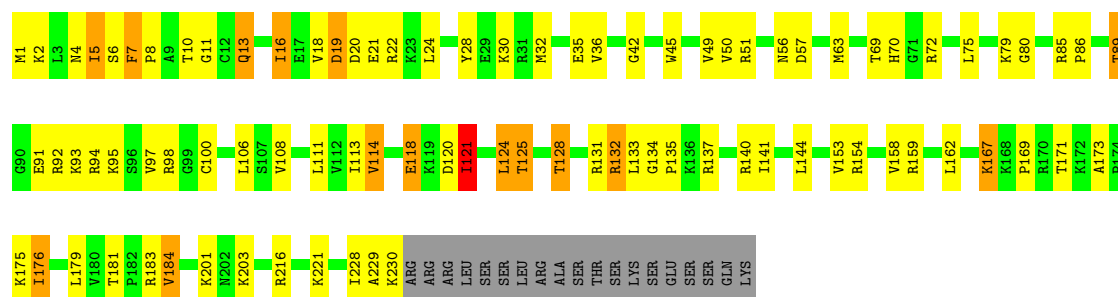
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ARG
VAL
ARG
THR
LYS
T8
V9
E18
K19
R23
K32
R33
V34
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I41
R47
N48
L57
N58
I61
G64
P65
V66
I69
S70
I71
K72
L73
Q74
E77
P86
S87
V88
S89
A90
L91
D92
Q93
E94
I95
D99
P100
D101
T102
L106
K107
L108
L109
D110
F111
S115
N116
T120
M127
F128
K132
GLY
PRO
VAL

- Chain N:  38% 25% 6% 30%

[illegible]

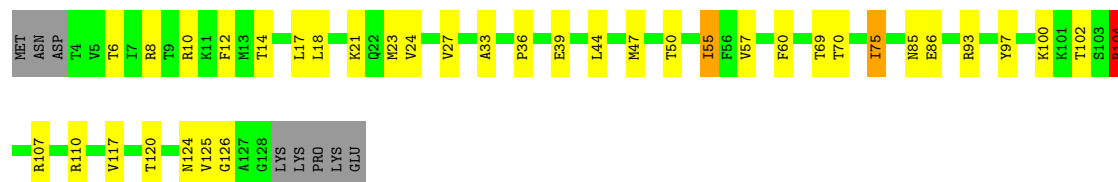
- 

Chain S: 



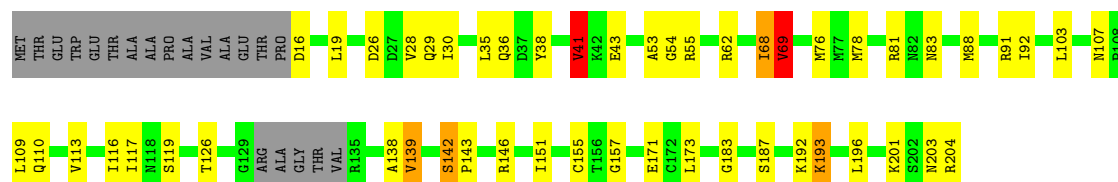
• Molecule 28: 40S ribosomal protein S24

Chain T: 



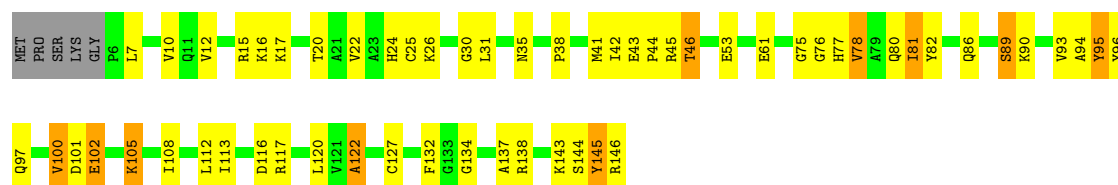
• Molecule 29: 40S ribosomal protein S5

Chain V: 



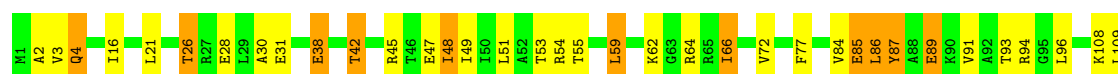
• Molecule 30: 40S ribosomal protein S16

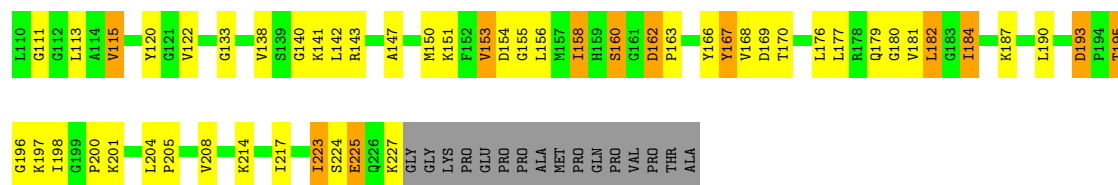
Chain Y: 



• Molecule 31: 40S ribosomal protein S3

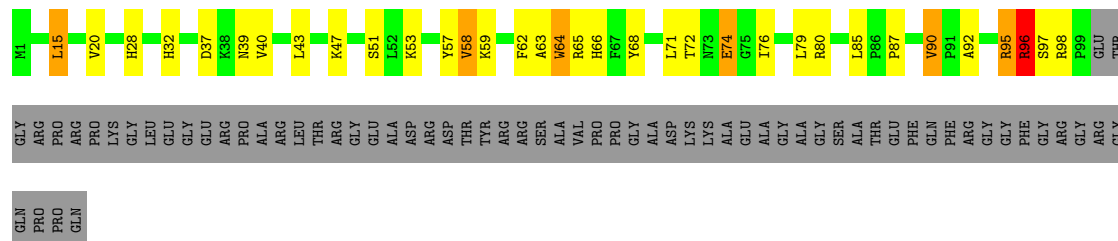
Chain Z: 





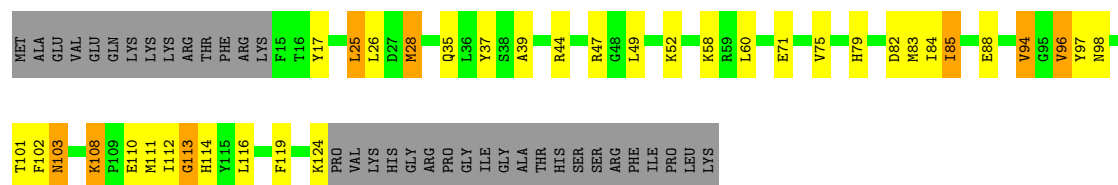
• Molecule 32: 40S ribosomal protein S10

Chain a: 39% 16% 40%



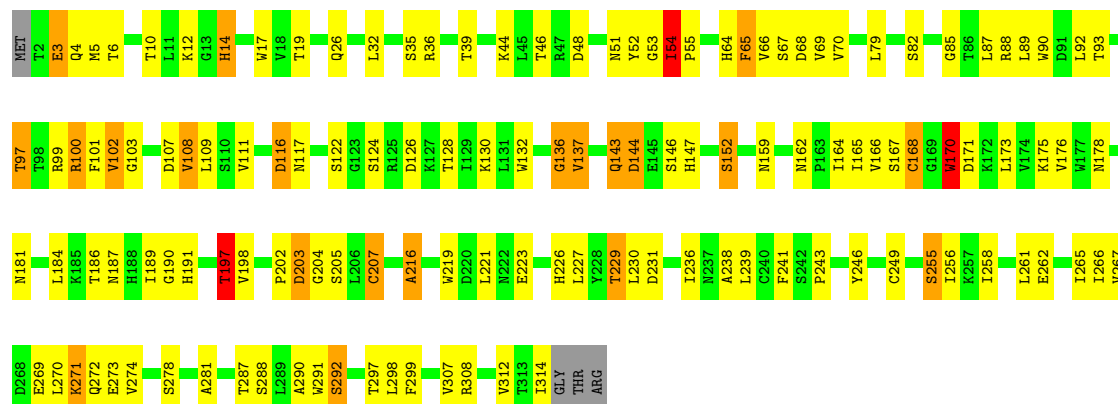
• Molecule 33: 40S ribosomal protein S15

Chain b: 50% 20% 6% 24%



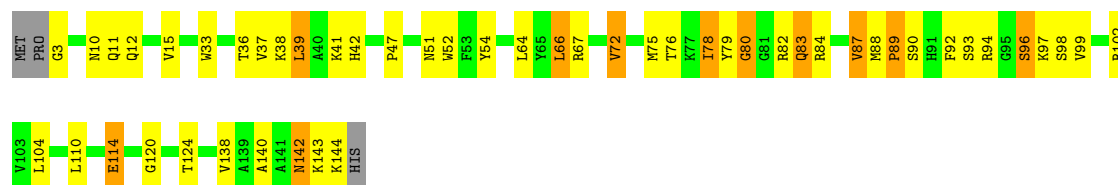
• Molecule 34: Receptor of activated protein C kinase 1

Chain c: 56% 35% 7%

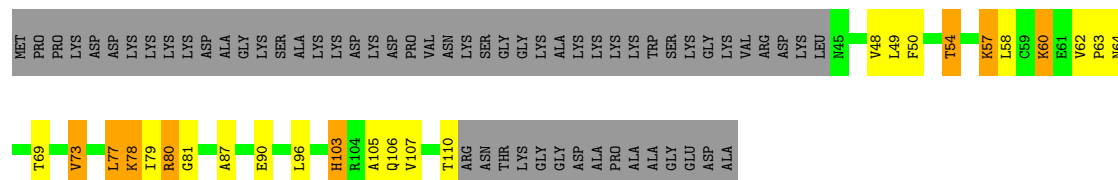
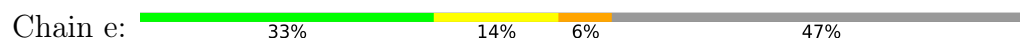


• Molecule 35: 40S ribosomal protein S19

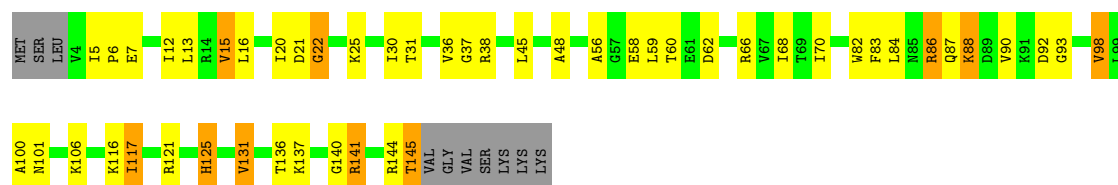
Chain d: 63% 27% 8%



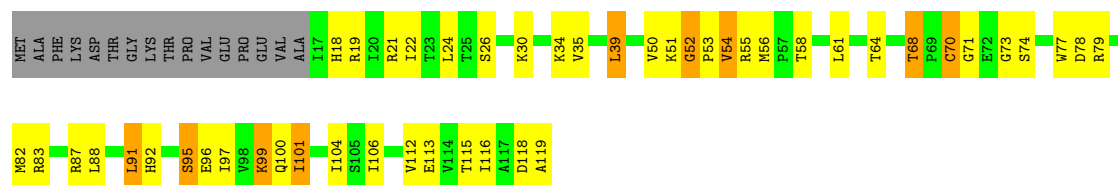
- Molecule 36: 40S ribosomal protein S25



- Molecule 37: 40S ribosomal protein S18



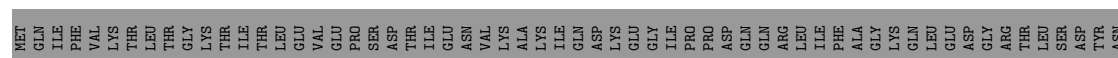
- Molecule 38: 40S ribosomal protein S20

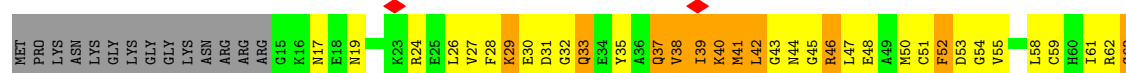


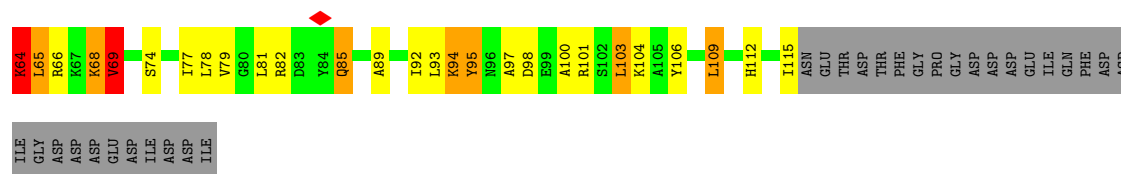
- Molecule 39: 40S ribosomal protein S29



- Molecule 40: Ubiquitin-40S ribosomal protein S27a

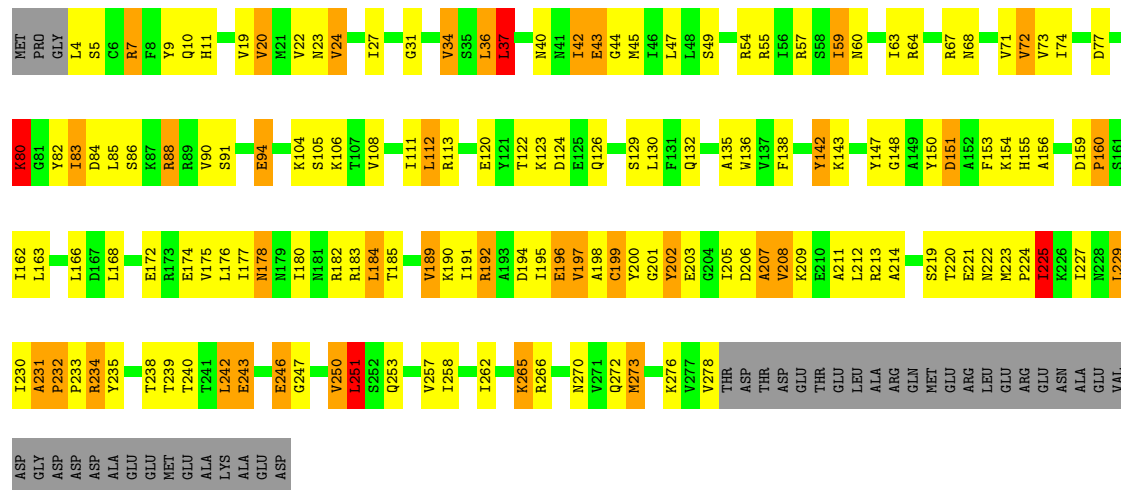






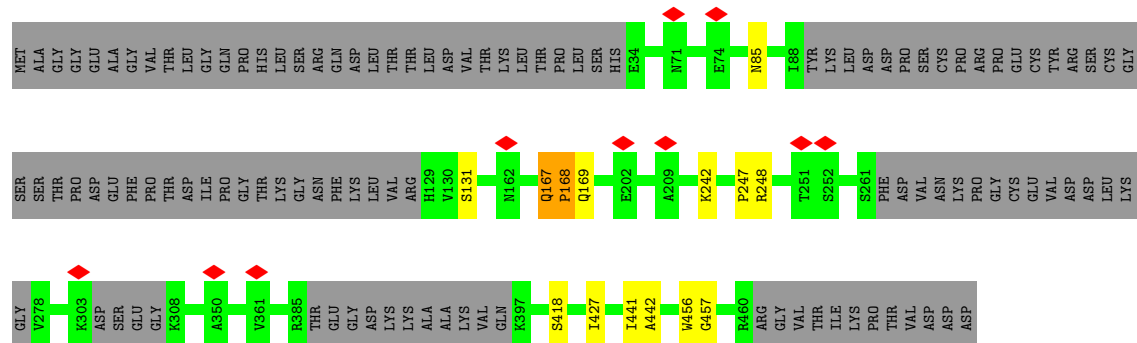
• Molecule 45: Eukaryotic translation initiation factor 2 subunit 1

Chain r: 40% 35% 11% 13%



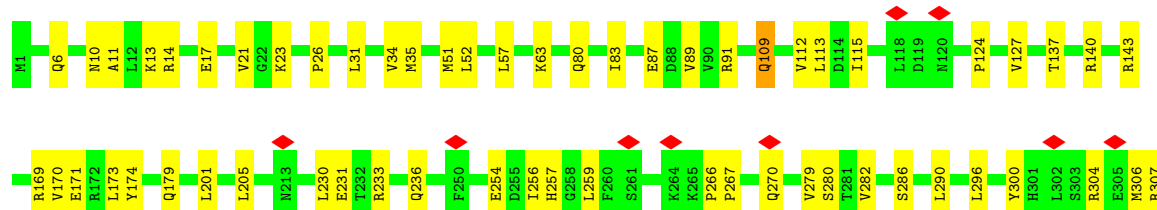
• Molecule 46: Eukaryotic translation initiation factor 2 subunit 3

Chain t: 72% 25%

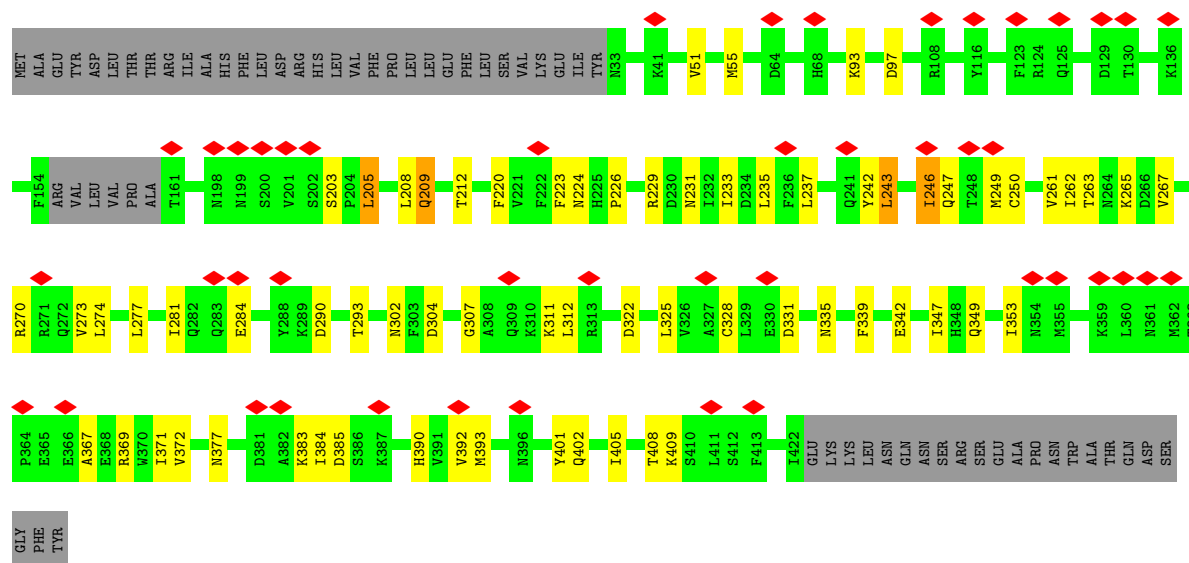


• Molecule 47: Eukaryotic translation initiation factor 3 subunit A

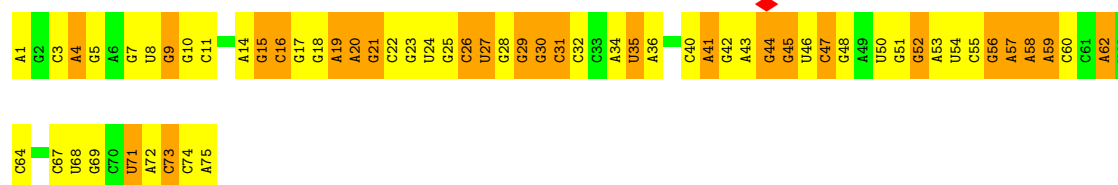
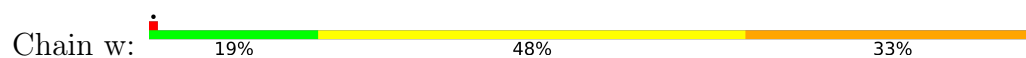
Chain u: 10% 39% 11% 49%



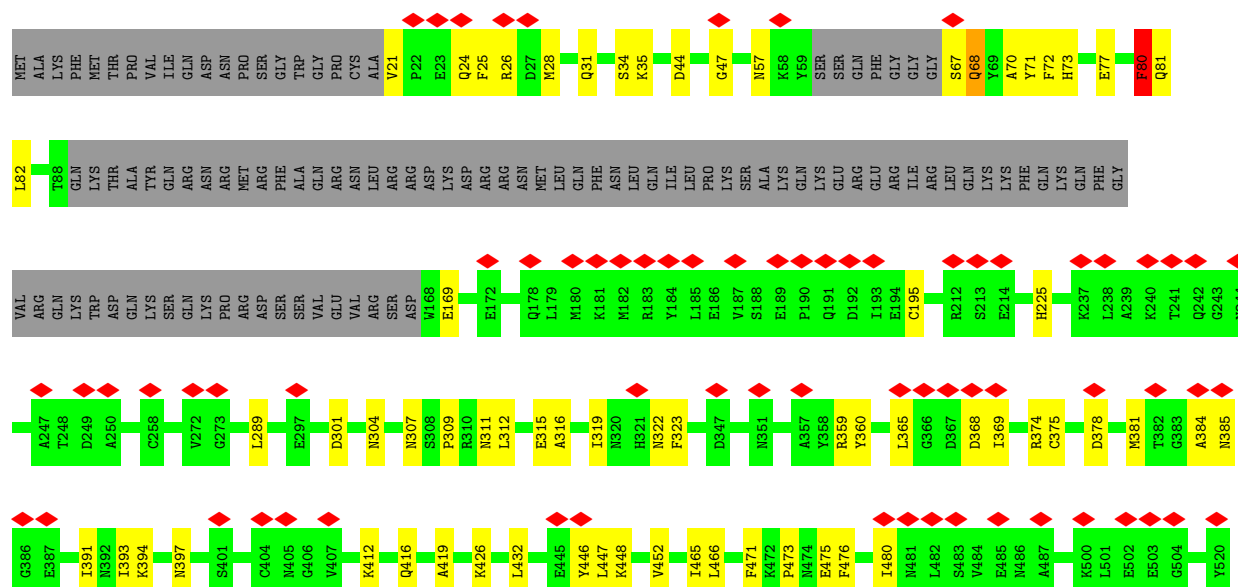
- Molecule 48: Eukaryotic translation initiation factor 3 subunit E

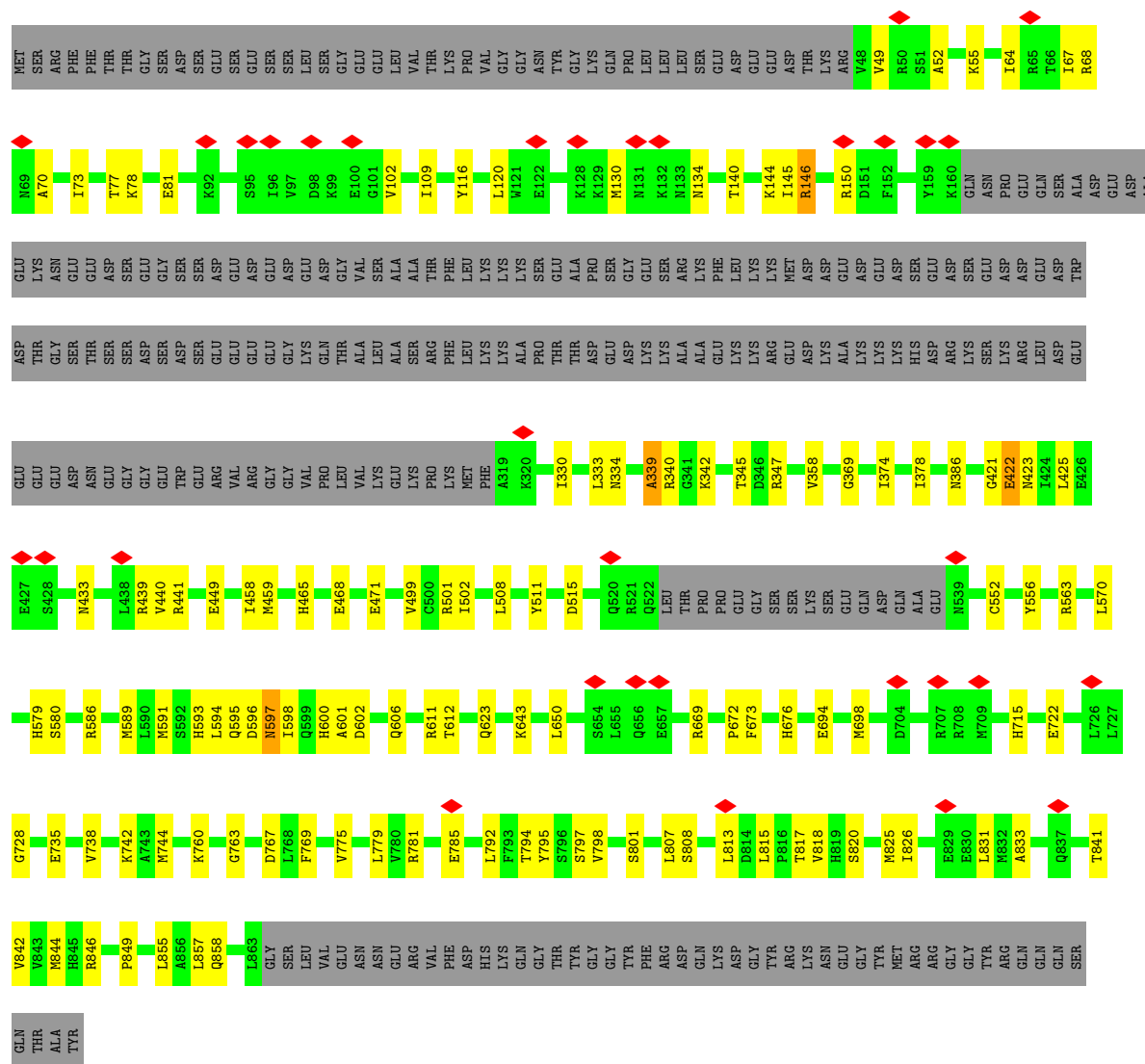


• Molecule 49: Initiator Met-tRNA-i



• Molecule 50: Eukaryotic translation initiation factor 3 subunit D





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	364950	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	24.271	Depositor
Minimum map value	-11.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.15	Depositor
Map size (Å)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 5MC, OMU, 5MU, A2M, UR3, OMC, PSU, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.61	0/2581	1.01	7/3561 (0.2%)
2	3	0.55	0/1055	0.98	1/1469 (0.1%)
3	4	0.70	0/1269	1.03	3/1762 (0.2%)
4	5	0.54	0/1575	0.93	3/2187 (0.1%)
5	6	0.62	0/1926	1.04	9/2669 (0.3%)
6	7	0.68	2/492 (0.4%)	0.96	1/764 (0.1%)
7	8	0.67	0/1569	1.08	6/2183 (0.3%)
8	9	1.60	1/231 (0.4%)	1.19	2/294 (0.7%)
9	A	0.44	0/40362	0.72	39/62905 (0.1%)
10	B	1.34	3/1186 (0.3%)	1.37	16/1585 (1.0%)
11	C	1.33	3/2077 (0.1%)	1.25	23/2796 (0.8%)
12	D	1.39	6/1502 (0.4%)	1.28	20/2008 (1.0%)
13	E	1.56	4/1105 (0.4%)	1.50	21/1476 (1.4%)
14	F	1.35	0/380	1.42	6/496 (1.2%)
15	G	1.23	1/1451 (0.1%)	1.37	22/1942 (1.1%)
16	H	1.30	2/644 (0.3%)	1.30	9/864 (1.0%)
17	I	1.38	2/1232 (0.2%)	1.36	25/1656 (1.5%)
18	J	1.67	3/1051 (0.3%)	1.56	23/1406 (1.6%)
19	K	1.48	0/623	1.45	14/833 (1.7%)
20	L	1.62	8/1743 (0.5%)	1.37	20/2354 (0.8%)
21	M	1.33	2/1029 (0.2%)	1.30	8/1383 (0.6%)
22	N	1.53	7/1670 (0.4%)	1.51	36/2271 (1.6%)
23	O	0.39	0/1742	0.70	0/2330
24	P	1.59	8/1010 (0.8%)	1.65	24/1353 (1.8%)
25	Q	1.43	4/805 (0.5%)	1.51	13/1079 (1.2%)
26	R	1.12	2/1654 (0.1%)	1.26	23/2203 (1.0%)
27	S	1.01	0/1885	1.28	19/2510 (0.8%)
28	T	1.30	2/1032 (0.2%)	1.21	6/1371 (0.4%)
29	V	1.54	3/1481 (0.2%)	1.36	20/1988 (1.0%)
30	Y	1.46	3/1142 (0.3%)	1.40	15/1528 (1.0%)
31	Z	1.43	1/1793 (0.1%)	1.44	25/2414 (1.0%)
32	a	1.27	2/859 (0.2%)	1.29	11/1159 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	1.17	2/929 (0.2%)	1.29	12/1241 (1.0%)
34	c	1.15	4/2493 (0.2%)	1.36	30/3394 (0.9%)
35	d	1.42	2/1123 (0.2%)	1.29	10/1504 (0.7%)
36	e	1.29	0/529	1.44	9/712 (1.3%)
37	f	1.29	1/1194 (0.1%)	1.39	20/1599 (1.3%)
38	h	1.40	2/827 (0.2%)	1.43	10/1110 (0.9%)
39	i	1.40	1/429 (0.2%)	1.35	5/568 (0.9%)
40	k	0.92	0/444	1.48	11/588 (1.9%)
41	m	0.53	0/960	0.92	1/1286 (0.1%)
42	n	1.36	0/500	1.39	5/669 (0.7%)
43	o	0.56	0/628	0.89	0/846
44	q	1.02	2/792 (0.3%)	1.63	24/1062 (2.3%)
45	r	0.94	0/2247	1.35	31/3029 (1.0%)
46	t	0.58	0/1745	0.98	2/2417 (0.1%)
47	u	0.55	0/5475	0.89	8/7432 (0.1%)
48	v	0.59	0/2672	0.94	2/3647 (0.1%)
49	w	0.40	0/1795	0.71	1/2798 (0.0%)
50	x	0.56	0/2874	0.90	4/3925 (0.1%)
51	y	0.51	0/5284	0.84	8/7123 (0.1%)
All	All	0.88	83/113096 (0.1%)	1.03	663/161749 (0.4%)

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	2	ARG	CA-C	-6.93	1.44	1.52
20	L	172	ASN	CA-C	-6.45	1.44	1.52
20	L	170	TRP	CA-C	-6.23	1.45	1.52
34	c	168	CYS	CA-C	-6.23	1.45	1.52
20	L	229	CYS	CA-C	-6.22	1.45	1.52
21	M	47	ARG	CA-C	-6.19	1.45	1.52
12	D	163	SER	CA-C	-6.19	1.46	1.53
24	P	138	ASP	CA-C	-6.17	1.46	1.53
22	N	161	ILE	CA-C	-6.05	1.46	1.52
21	M	41	ILE	CA-C	-6.00	1.47	1.52
30	Y	144	SER	CA-C	-5.94	1.45	1.52
11	C	30	ARG	CA-C	-5.89	1.45	1.52
24	P	133	THR	CA-C	-5.88	1.47	1.53
17	I	136	PRO	CA-C	-5.87	1.48	1.52
24	P	135	ILE	CA-C	-5.83	1.46	1.52
44	q	41	MET	CA-C	-5.78	1.47	1.53
20	L	207	ALA	CA-C	-5.75	1.45	1.53
38	h	26	SER	CA-C	-5.75	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	21	GLU	CA-C	-5.74	1.45	1.52
20	L	194	ARG	CA-C	-5.73	1.45	1.52
13	E	45	SER	CA-C	-5.68	1.45	1.52
30	Y	145	TYR	CA-C	-5.67	1.45	1.53
6	7	23	A	C1'-N9	-5.64	1.39	1.48
17	I	48	SER	CA-C	-5.61	1.45	1.52
24	P	62	VAL	CA-C	-5.57	1.45	1.52
28	T	33	ALA	CA-C	-5.55	1.45	1.53
12	D	18	ARG	CA-C	-5.54	1.46	1.52
37	f	86	ARG	CA-C	-5.53	1.46	1.52
13	E	53	GLU	CA-C	-5.53	1.46	1.52
26	R	178	ARG	CA-C	-5.52	1.45	1.52
12	D	144	ILE	CA-C	-5.51	1.48	1.53
31	Z	54	ARG	CA-C	-5.50	1.46	1.53
6	7	20	U	C1'-N1	5.48	1.55	1.47
39	i	26	ASN	CA-C	-5.48	1.46	1.52
10	B	114	SER	CA-C	-5.47	1.46	1.53
25	Q	97	PRO	CA-C	-5.45	1.48	1.52
20	L	226	ALA	CA-C	-5.44	1.46	1.52
11	C	199	GLU	CA-C	-5.38	1.46	1.52
22	N	90	PHE	CA-C	-5.37	1.45	1.52
18	J	79	PHE	CA-C	-5.37	1.45	1.53
30	Y	143	LYS	CA-C	-5.34	1.46	1.52
34	c	216	ALA	CA-C	-5.32	1.46	1.52
28	T	27	VAL	CA-C	-5.31	1.46	1.52
24	P	63	LYS	N-CA	-5.30	1.39	1.46
18	J	75	ILE	CA-C	-5.29	1.46	1.52
16	H	11	SER	CA-C	-5.29	1.47	1.53
22	N	103	PHE	CA-C	-5.28	1.46	1.52
18	J	94	LEU	CA-C	-5.28	1.47	1.53
12	D	4	ALA	CA-C	-5.28	1.47	1.53
24	P	36	SER	CA-C	-5.28	1.46	1.52
20	L	163	VAL	CA-C	-5.27	1.49	1.52
25	Q	28	ARG	CA-C	-5.27	1.45	1.52
13	E	84	PHE	CA-C	-5.26	1.46	1.52
22	N	168	ALA	CA-C	-5.25	1.46	1.52
35	d	83	GLN	CA-C	-5.24	1.46	1.52
22	N	91	ALA	CA-C	-5.24	1.46	1.52
29	V	142	SER	CA-CB	-5.22	1.46	1.53
29	V	193	LYS	CA-C	-5.22	1.46	1.52
33	b	44	ARG	CA-C	-5.21	1.46	1.52
34	c	124	SER	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	102	VAL	CA-C	-5.18	1.46	1.52
20	L	142	LYS	CA-C	-5.17	1.46	1.52
29	V	36	GLN	CA-C	-5.17	1.46	1.52
11	C	76	VAL	CA-C	-5.17	1.46	1.52
16	H	48	SER	CA-C	-5.17	1.46	1.52
15	G	153	LEU	CA-C	-5.15	1.46	1.52
25	Q	96	THR	CA-C	-5.15	1.47	1.52
10	B	69	ARG	CA-C	-5.15	1.46	1.52
32	a	32	HIS	CA-C	-5.13	1.48	1.53
33	b	35	GLN	C-O	-5.13	1.18	1.24
22	N	111	GLN	CA-C	-5.12	1.46	1.52
12	D	73	GLU	CA-C	-5.11	1.46	1.52
13	E	58	GLU	CA-C	-5.10	1.46	1.53
35	d	89	PRO	CA-C	-5.10	1.46	1.52
24	P	98	ARG	CA-C	-5.09	1.46	1.52
38	h	83	ARG	CA-C	-5.09	1.46	1.52
44	q	42	LEU	N-CA	-5.08	1.39	1.46
32	a	62	PHE	CA-C	-5.08	1.46	1.52
10	B	92	TYR	CA-C	-5.08	1.46	1.52
34	c	236	ILE	CA-C	-5.07	1.48	1.53
25	Q	35	ALA	CA-C	-5.06	1.46	1.52
22	N	104	THR	CA-C	-5.04	1.46	1.52
24	P	70	SER	CA-C	-5.01	1.46	1.53

All (663) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	7	VAL	N-CA-C	-19.27	77.15	108.95
10	B	53	GLY	N-CA-C	18.38	136.07	112.54
37	f	100	ALA	N-CA-C	15.19	127.32	111.07
44	q	45	GLY	N-CA-C	-14.93	94.82	112.73
44	q	42	LEU	N-CA-C	-14.18	86.14	109.24
34	c	190	GLY	N-CA-C	13.37	128.78	112.73
20	L	135	GLY	N-CA-C	13.02	133.29	115.32
27	S	121	ILE	N-CA-C	-12.02	97.85	109.02
27	S	124	LEU	N-CA-C	11.91	124.34	111.36
32	a	96	ARG	N-CA-C	-11.68	92.10	109.62
18	J	76	SER	CA-C-N	-11.67	107.38	119.99
18	J	76	SER	C-N-CA	-11.67	107.38	119.99
30	Y	43	GLU	N-CA-C	11.65	129.71	113.16
18	J	76	SER	N-CA-C	11.49	127.74	112.35
13	E	76	LYS	N-CA-C	11.47	123.53	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	192	GLU	N-CA-C	11.37	123.75	111.36
34	c	278	SER	N-CA-C	-11.35	90.61	109.46
36	e	103	HIS	N-CA-C	-11.27	92.14	108.60
45	r	84	ASP	N-CA-C	-11.27	91.30	108.99
40	k	136	PHE	N-CA-C	-11.02	99.27	111.28
22	N	3	GLY	N-CA-C	-10.94	99.24	112.48
24	P	140	THR	N-CA-C	-10.90	92.62	109.95
27	S	19	ASP	N-CA-C	10.72	123.05	111.36
24	P	66	ARG	N-CA-C	-10.69	99.42	111.82
12	D	89	GLU	N-CA-C	10.57	122.80	111.28
31	Z	87	TYR	N-CA-C	10.56	125.81	111.24
24	P	104	ARG	N-CA-C	10.54	122.35	111.07
40	k	130	VAL	N-CA-C	-10.51	96.16	109.30
30	Y	95	TYR	N-CA-C	-10.31	100.04	111.28
18	J	55	ASP	N-CA-C	-10.28	95.25	110.46
18	J	75	ILE	N-CA-C	-10.16	93.07	107.80
18	J	77	PRO	N-CA-C	-10.15	93.96	111.32
33	b	47	ARG	N-CA-C	-10.13	93.66	109.76
34	c	92	LEU	N-CA-C	9.94	122.11	111.28
51	y	422	GLU	N-CA-C	-9.88	95.06	109.59
18	J	72	CYS	N-CA-C	-9.86	93.95	109.23
44	q	52	PHE	N-CA-C	-9.79	100.45	111.71
26	R	146	GLN	N-CA-C	9.73	122.91	111.71
31	Z	111	GLY	N-CA-C	-9.69	94.09	111.15
29	V	107	ASN	N-CA-C	-9.69	95.53	109.48
38	h	104	ILE	N-CA-C	-9.60	89.37	109.34
48	v	209	GLN	CA-CB-CG	-9.57	94.95	114.10
29	V	119	SER	N-CA-C	9.47	121.68	111.36
21	M	41	ILE	N-CA-C	-9.47	97.57	107.89
39	i	13	LYS	N-CA-C	-9.39	99.53	113.61
35	d	78	ILE	CB-CA-C	-9.25	99.65	112.14
17	I	81	ALA	N-CA-C	9.25	121.39	109.64
13	E	56	GLY	N-CA-C	-9.22	96.35	111.38
22	N	35	GLU	N-CA-C	-9.18	102.46	114.31
17	I	8	GLY	N-CA-C	9.17	122.48	111.93
38	h	52	GLY	CA-C-N	-9.16	110.13	119.93
38	h	52	GLY	C-N-CA	-9.16	110.13	119.93
45	r	202	TYR	N-CA-C	-9.10	101.36	111.28
40	k	132	MET	N-CA-C	-9.08	96.34	109.96
31	Z	197	LYS	N-CA-C	-9.05	101.32	111.82
36	e	60	LYS	N-CA-C	9.00	120.86	111.14
18	J	28	ARG	N-CA-C	8.92	124.30	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	170	TRP	N-CA-C	-8.91	102.11	113.16
45	r	43	GLU	N-CA-C	8.90	122.27	110.53
22	N	158	ASP	N-CA-C	8.85	121.01	111.36
13	E	42	GLY	N-CA-C	-8.77	96.89	112.77
37	f	15	VAL	N-CA-C	8.76	118.76	110.53
26	R	79	ILE	N-CA-C	8.75	118.75	110.53
36	e	77	LEU	N-CA-C	-8.63	94.46	108.52
44	q	19	ASN	N-CA-C	8.58	122.53	109.23
28	T	85	ASN	N-CA-C	8.49	120.61	111.36
11	C	24	THR	N-CA-C	8.48	120.14	111.07
45	r	231	ALA	N-CA-C	-8.48	97.52	110.32
7	8	56	GLU	N-CA-C	-8.47	100.95	113.40
26	R	30	GLY	N-CA-C	-8.46	98.75	111.10
30	Y	127	CYS	N-CA-C	8.44	122.47	110.23
13	E	66	ILE	N-CA-C	8.43	121.13	108.23
15	G	66	VAL	CB-CA-C	-8.37	105.48	114.35
16	H	29	ASN	N-CA-C	-8.35	102.87	113.72
20	L	175	GLY	N-CA-C	8.34	126.54	111.02
42	n	66	ARG	N-CA-C	8.30	119.95	111.07
34	c	52	TYR	N-CA-C	-8.28	103.16	113.18
34	c	102	VAL	N-CA-C	8.23	121.08	113.10
15	G	9	VAL	N-CA-C	8.17	120.12	109.58
12	D	38	ARG	N-CA-C	8.16	120.25	111.36
22	N	90	PHE	N-CA-C	-8.16	102.39	111.28
39	i	9	SER	N-CA-C	-8.13	102.42	111.28
42	n	36	ASP	N-CA-C	8.12	120.21	111.36
19	K	31	SER	N-CA-C	8.12	122.00	110.23
34	c	204	GLY	N-CA-C	-8.07	104.43	114.92
45	r	230	ILE	N-CA-C	-8.06	104.88	111.81
9	A	1604	G	C2'-C3'-O3'	-8.02	101.67	113.70
25	Q	96	THR	CA-C-N	-7.99	113.90	119.66
25	Q	96	THR	C-N-CA	-7.99	113.90	119.66
17	I	84	LEU	N-CA-C	-7.99	99.94	110.40
24	P	138	ASP	CB-CA-C	-7.99	104.42	114.40
24	P	111	GLY	N-CA-C	7.98	122.31	112.73
22	N	202	TYR	N-CA-C	7.97	120.05	111.36
35	d	37	VAL	N-CA-C	7.96	119.32	108.17
45	r	185	THR	N-CA-C	7.96	124.47	113.16
25	Q	92	ARG	N-CA-C	-7.95	102.69	111.36
31	Z	198	ILE	N-CA-C	7.95	118.73	110.62
14	F	81	ALA	N-CA-C	7.95	120.03	111.36
21	M	115	SER	N-CA-C	7.93	119.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	32	LYS	N-CA-C	-7.89	95.65	108.52
33	b	113	GLY	N-CA-C	7.88	122.86	112.77
26	R	180	GLY	N-CA-C	7.88	122.03	112.49
24	P	23	GLU	N-CA-C	-7.86	102.19	112.41
31	Z	160	SER	N-CA-C	7.85	122.35	109.24
37	f	92	ASP	N-CA-C	7.85	119.91	111.36
12	D	119	LEU	N-CA-C	-7.82	103.32	113.17
45	r	265	LYS	N-CA-C	-7.79	100.24	110.53
10	B	97	ARG	N-CA-C	7.78	119.84	111.36
19	K	3	ASN	N-CA-C	-7.75	100.30	110.53
29	V	53	ALA	N-CA-C	-7.74	99.00	110.23
24	P	63	LYS	N-CA-C	7.74	122.42	108.48
44	q	29	LYS	N-CA-C	7.72	121.38	110.50
33	b	98	ASN	N-CA-C	-7.71	103.43	112.92
15	G	88	SER	N-CA-C	7.70	119.31	111.07
1	1	328	SER	N-CA-C	7.68	121.97	109.76
32	a	74	GLU	N-CA-C	-7.66	102.93	111.28
13	E	110	HIS	N-CA-C	-7.61	97.55	109.72
20	L	203	GLY	N-CA-C	-7.61	103.10	112.68
5	6	334	VAL	N-CA-C	7.59	118.62	111.48
9	A	368	U	C2'-C3'-O3'	7.59	120.89	109.50
17	I	66	VAL	N-CA-C	7.59	118.38	110.72
13	E	91	LEU	N-CA-C	-7.57	103.31	112.54
40	k	138	ARG	N-CA-C	7.56	120.63	110.35
19	K	28	ASP	N-CA-C	-7.55	91.88	107.67
20	L	76	LYS	N-CA-C	7.53	119.28	111.14
24	P	135	ILE	CA-C-N	-7.50	110.46	119.84
24	P	135	ILE	C-N-CA	-7.50	110.46	119.84
15	G	103	LYS	CA-C-N	-7.50	112.28	119.85
15	G	103	LYS	C-N-CA	-7.50	112.28	119.85
22	N	28	THR	N-CA-C	7.49	119.45	111.28
24	P	94	HIS	N-CA-C	-7.49	98.81	110.42
37	f	84	LEU	N-CA-C	7.49	120.53	110.35
34	c	44	LYS	N-CA-C	-7.48	96.54	108.73
10	B	39	ASN	N-CA-C	-7.46	98.99	110.10
26	R	67	TRP	N-CA-C	-7.44	97.14	108.67
27	S	7	PHE	N-CA-C	-7.43	98.04	109.64
44	q	50	MET	N-CA-C	-7.41	96.44	108.52
45	r	192	ARG	N-CA-C	7.41	120.59	108.52
18	J	28	ARG	CA-C-N	-7.39	110.60	119.84
18	J	28	ARG	C-N-CA	-7.39	110.60	119.84
44	q	43	GLY	N-CA-C	-7.38	95.68	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	70	ASN	N-CA-C	-7.35	100.80	110.07
33	b	39	ALA	N-CA-C	7.33	119.27	111.28
26	R	41	ARG	N-CA-C	7.31	120.99	110.10
34	c	281	ALA	N-CA-C	7.30	120.50	109.41
32	a	32	HIS	N-CA-C	-7.26	100.42	109.64
20	L	66	LEU	N-CA-C	-7.26	103.37	111.28
34	c	255	SER	N-CA-C	7.25	121.22	109.40
24	P	68	GLU	N-CA-C	-7.25	103.38	111.28
30	Y	134	GLY	N-CA-C	7.25	127.12	112.34
45	r	106	LYS	N-CA-C	-7.23	103.40	111.28
35	d	66	LEU	N-CA-C	-7.22	99.83	110.52
38	h	74	SER	N-CA-C	-7.21	103.03	112.41
45	r	160	PRO	N-CA-C	-7.18	106.38	114.92
44	q	17	ASN	N-CA-C	7.17	118.88	111.14
26	R	45	THR	N-CA-C	7.16	121.28	111.39
37	f	22	GLY	N-CA-C	-7.15	101.34	112.85
10	B	54	THR	N-CA-C	7.14	119.15	111.36
31	Z	86	LEU	N-CA-C	7.14	119.06	111.28
44	q	97	ALA	N-CA-C	7.12	119.04	111.28
16	H	79	PHE	N-CA-C	7.11	121.10	109.72
38	h	106	ILE	N-CA-C	-7.11	98.19	108.36
45	r	251	LEU	N-CA-C	-7.09	103.55	111.28
13	E	61	GLN	N-CA-C	7.09	123.22	113.16
35	d	36	THR	N-CA-C	7.06	121.91	113.16
25	Q	13	LYS	N-CA-C	-7.05	96.85	108.76
45	r	184	LEU	N-CA-C	7.04	121.87	112.30
29	V	55	ARG	N-CA-C	-7.03	103.24	112.24
17	I	84	LEU	CA-C-N	-7.03	112.75	119.85
17	I	84	LEU	C-N-CA	-7.03	112.75	119.85
29	V	38	TYR	N-CA-C	7.02	119.02	111.36
15	G	66	VAL	CA-C-N	-7.02	111.26	119.05
15	G	66	VAL	C-N-CA	-7.02	111.26	119.05
33	b	28	MET	N-CA-C	7.00	120.39	110.23
31	Z	21	LEU	N-CA-C	-6.99	103.66	111.28
22	N	109	THR	N-CA-C	6.99	121.97	113.17
36	e	105	ALA	N-CA-C	6.99	118.69	111.14
38	h	54	VAL	N-CA-C	-6.95	98.46	108.53
27	S	132	ARG	N-CA-C	6.92	118.83	111.28
31	Z	113	LEU	N-CA-C	-6.92	98.20	108.79
45	r	5	SER	N-CA-C	6.92	119.69	109.24
11	C	93	ASP	N-CA-C	6.92	118.90	111.36
26	R	139	LYS	N-CA-C	6.90	120.65	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	52	THR	N-CA-C	6.89	120.48	110.28
9	A	1268	C	C1'-C2'-O2'	-6.86	98.11	108.40
29	V	157	GLY	N-CA-C	-6.86	104.50	112.73
15	G	33	ASN	N-CA-C	-6.86	99.27	109.15
15	G	121	THR	N-CA-C	6.86	119.95	110.35
29	V	78	MET	N-CA-C	6.86	117.64	108.38
17	I	7	PRO	N-CA-C	6.86	123.06	113.53
34	c	103	GLY	N-CA-C	6.86	120.96	112.73
26	R	122	GLY	N-CA-C	-6.85	103.48	113.48
45	r	203	GLU	N-CA-C	-6.85	96.48	108.20
51	y	49	VAL	CB-CA-C	-6.85	104.88	112.68
33	b	26	LEU	N-CA-C	-6.84	103.82	111.28
24	P	64	ALA	N-CA-C	-6.84	103.08	113.89
3	4	167	GLU	N-CA-C	6.84	120.66	109.85
34	c	231	ASP	N-CA-C	6.82	120.01	108.90
27	S	125	THR	N-CA-C	6.81	123.83	113.61
31	Z	48	ILE	N-CA-C	-6.81	100.16	109.55
1	1	564	THR	N-CA-C	6.80	120.62	111.24
11	C	22	LYS	N-CA-C	6.79	118.69	111.28
15	G	10	LYS	N-CA-C	-6.78	97.83	109.15
31	Z	96	LEU	N-CA-C	6.77	118.66	111.28
31	Z	166	TYR	N-CA-C	6.75	118.72	111.36
35	d	90	SER	N-CA-C	6.75	119.44	110.53
17	I	115	LEU	N-CA-C	-6.75	103.92	111.28
44	q	32	GLY	N-CA-C	-6.75	106.44	115.21
18	J	60	LYS	N-CA-C	-6.73	98.50	108.79
15	G	37	LYS	N-CA-C	6.72	118.60	111.28
45	r	122	THR	N-CA-C	-6.72	104.66	112.92
20	L	264	SER	CA-C-N	-6.71	111.60	119.05
20	L	264	SER	C-N-CA	-6.71	111.60	119.05
27	S	94	ARG	N-CA-C	-6.69	99.75	109.59
15	G	135	PHE	CA-C-N	-6.69	111.62	119.05
15	G	135	PHE	C-N-CA	-6.69	111.62	119.05
45	r	142	TYR	N-CA-C	6.69	118.65	111.36
24	P	80	ASP	N-CA-C	6.67	118.63	111.36
42	n	18	LEU	N-CA-C	6.67	118.34	111.14
18	J	82	GLN	N-CA-C	-6.65	101.58	110.55
9	A	1831	A	C2'-C3'-O3'	6.63	123.65	113.70
21	M	90	ALA	N-CA-C	-6.63	104.94	113.16
22	N	103	PHE	N-CA-C	-6.62	97.93	108.73
10	B	70	GLY	N-CA-C	6.62	123.33	111.02
22	N	206	ASP	CA-C-N	-6.60	111.79	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	206	ASP	C-N-CA	-6.60	111.79	119.32
37	f	90	VAL	CB-CA-C	-6.60	103.52	111.97
20	L	99	GLY	N-CA-C	6.60	120.65	112.73
38	h	95	SER	N-CA-C	6.59	118.46	111.28
34	c	152	SER	N-CA-C	6.59	118.46	111.28
29	V	43	GLU	CB-CA-C	-6.58	108.99	116.63
27	S	42	GLY	N-CA-C	6.58	120.74	111.00
39	i	31	ILE	CB-CA-C	-6.58	102.90	111.25
10	B	62	PHE	N-CA-C	6.57	118.52	111.36
12	D	117	LEU	N-CA-C	-6.57	105.14	113.02
22	N	80	ARG	N-CA-C	-6.56	100.57	110.28
33	b	114	HIS	N-CA-C	6.56	118.48	110.41
14	F	94	ALA	N-CA-C	6.55	119.92	109.24
15	G	18	GLU	N-CA-C	6.55	118.42	111.28
9	A	1638	G	C2'-C3'-O3'	-6.54	103.90	113.70
27	S	20	ASP	N-CA-C	6.53	120.17	109.72
22	N	201	LEU	N-CA-C	-6.53	104.16	111.28
26	R	142	SER	N-CA-C	-6.53	100.76	110.23
10	B	60	CYS	CA-C-N	-6.53	112.18	118.97
10	B	60	CYS	C-N-CA	-6.53	112.18	118.97
31	Z	162	ASP	CA-C-N	-6.53	112.90	119.56
31	Z	162	ASP	C-N-CA	-6.53	112.90	119.56
26	R	156	ALA	N-CA-C	6.51	121.28	112.88
34	c	162	ASN	CA-C-N	-6.51	113.06	119.76
34	c	162	ASN	C-N-CA	-6.51	113.06	119.76
34	c	312	VAL	CB-CA-C	-6.49	105.29	112.68
45	r	154	LYS	N-CA-C	-6.47	104.22	111.28
36	e	62	VAL	CA-C-N	-6.47	112.96	119.56
36	e	62	VAL	C-N-CA	-6.47	112.96	119.56
32	a	43	LEU	N-CA-C	-6.46	104.23	111.28
9	A	291	G	C2'-C3'-O3'	6.46	123.38	113.70
47	u	351	LYS	N-CA-C	-6.45	105.16	113.16
21	M	116	ASN	N-CA-C	6.45	121.20	112.88
22	N	146	ALA	N-CA-C	6.43	119.75	108.75
9	A	1825	A	C2'-C3'-O3'	-6.43	104.06	113.70
37	f	90	VAL	N-CA-C	6.42	116.59	110.42
9	A	1542	C	C4'-C3'-O3'	6.42	122.62	113.00
20	L	223	TYR	N-CA-C	-6.41	98.95	109.40
29	V	54	GLY	N-CA-C	6.40	128.34	113.18
12	D	172	ARG	N-CA-C	6.38	118.23	111.28
48	v	312	LEU	N-CA-C	-6.38	104.19	112.23
51	y	146	ARG	NE-CZ-NH2	-6.38	113.46	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	169	ILE	CB-CA-C	-6.37	105.05	111.80
12	D	50	LEU	N-CA-C	-6.36	104.34	111.28
15	G	94	PHE	N-CA-C	6.36	118.98	108.49
26	R	145	ILE	N-CA-C	6.36	117.14	110.72
45	r	273	MET	N-CA-C	6.35	117.88	108.60
13	E	49	GLY	N-CA-C	6.35	122.57	111.14
21	M	101	ASP	N-CA-C	6.34	118.19	111.28
30	Y	145	TYR	N-CA-C	-6.34	100.53	110.36
21	M	19	LYS	N-CA-C	-6.33	98.88	109.07
13	E	61	GLN	CA-C-N	-6.33	112.03	119.05
13	E	61	GLN	C-N-CA	-6.33	112.03	119.05
17	I	136	PRO	N-CA-C	-6.33	103.81	110.58
45	r	147	TYR	N-CA-C	6.32	118.17	111.28
27	S	114	VAL	N-CA-C	6.32	116.47	110.53
44	q	95	TYR	N-CA-C	6.32	119.55	109.24
15	G	38	ALA	N-CA-C	-6.32	104.31	111.07
20	L	61	MET	N-CA-C	-6.32	100.45	109.24
28	T	86	GLU	N-CA-C	6.32	118.80	110.08
32	a	15	LEU	N-CA-C	-6.32	104.40	111.28
9	A	1542	C	C2'-C3'-O3'	-6.31	104.23	113.70
31	Z	2	ALA	N-CA-C	-6.31	104.40	111.28
25	Q	10	ARG	N-CA-C	-6.30	100.87	110.14
11	C	76	VAL	CB-CA-C	-6.30	103.71	111.08
30	Y	75	GLY	N-CA-C	6.30	123.96	112.37
24	P	133	THR	CA-C-N	-6.27	113.31	119.90
24	P	133	THR	C-N-CA	-6.27	113.31	119.90
45	r	40	ASN	N-CA-C	6.27	120.27	112.24
19	K	22	ARG	N-CA-C	-6.26	99.81	109.52
45	r	80	LYS	N-CA-C	6.26	119.43	110.10
31	Z	28	GLU	N-CA-C	6.25	118.17	111.36
37	f	21	ASP	N-CA-C	6.25	119.12	109.07
27	S	167	LYS	N-CA-C	6.24	118.55	109.07
16	H	22	LYS	N-CA-C	6.23	121.02	113.17
9	A	1533	A	C4'-C3'-O3'	-6.22	103.67	113.00
7	8	53	TYR	N-CA-C	-6.21	104.13	111.03
29	V	183	GLY	N-CA-C	-6.21	106.57	115.64
44	q	26	LEU	N-CA-C	6.21	118.73	110.53
31	Z	204	LEU	N-CA-C	-6.21	101.21	109.84
25	Q	72	HIS	N-CA-C	-6.21	98.40	108.52
47	u	501	THR	N-CA-C	-6.21	103.81	112.25
19	K	67	ASP	N-CA-C	-6.20	104.52	111.28
47	u	6	GLN	N-CA-C	-6.20	104.52	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	38	ALA	N-CA-C	6.20	120.98	113.17
24	P	27	VAL	N-CA-C	-6.19	99.50	108.36
9	A	606	G	C4'-C3'-O3'	6.19	118.68	109.40
1	1	319	PHE	N-CA-C	6.18	119.10	109.52
34	c	136	GLY	N-CA-C	-6.18	106.55	115.27
35	d	10	ASN	N-CA-C	-6.17	99.81	109.25
14	F	107	LYS	N-CA-C	-6.16	104.56	111.28
40	k	131	PHE	N-CA-C	6.16	118.73	108.20
19	K	24	ILE	N-CA-C	-6.15	101.61	109.30
22	N	104	THR	CA-C-N	-6.14	113.43	119.76
22	N	104	THR	C-N-CA	-6.14	113.43	119.76
38	h	99	LYS	N-CA-C	-6.14	104.50	111.07
12	D	134	HIS	N-CA-C	6.13	118.05	111.36
25	Q	63	VAL	N-CA-C	-6.13	99.59	108.36
5	6	15	ALA	N-CA-C	6.13	119.55	111.28
45	r	205	ILE	N-CA-C	6.13	116.87	110.62
35	d	94	ARG	N-CA-C	6.12	118.42	110.53
10	B	52	GLU	N-CA-C	6.12	118.03	111.36
31	Z	168	VAL	N-CA-C	6.12	117.10	108.36
15	G	31	GLU	N-CA-C	-6.11	104.62	111.28
13	E	115	ILE	CA-C-N	-6.11	112.20	119.84
13	E	115	ILE	C-N-CA	-6.11	112.20	119.84
40	k	121	CYS	N-CA-C	6.10	118.50	110.08
2	3	149	THR	N-CA-C	6.10	120.89	113.38
14	F	118	ASN	N-CA-C	6.10	117.93	111.28
20	L	191	VAL	CB-CA-C	-6.09	102.63	110.98
18	J	110	ILE	N-CA-C	-6.08	98.24	107.73
18	J	39	THR	N-CA-C	-6.08	104.65	111.28
44	q	93	LEU	N-CA-C	6.08	118.21	110.61
18	J	63	VAL	CB-CA-C	-6.08	102.08	110.96
27	S	228	ILE	N-CA-C	6.08	116.86	110.72
5	6	44	GLN	N-CA-C	-6.08	104.37	112.94
13	E	4	CYS	N-CA-C	-6.07	101.05	110.10
40	k	106	TYR	N-CA-C	-6.06	99.02	108.90
13	E	58	GLU	N-CA-C	6.06	118.35	110.53
25	Q	60	ASP	N-CA-C	-6.06	102.71	110.53
31	Z	77	PHE	N-CA-C	-6.05	105.48	112.92
30	Y	46	THR	N-CA-C	-6.00	104.81	111.71
16	H	4	ALA	N-CA-C	6.00	119.84	111.74
9	A	392	A	C1'-C2'-O2'	5.99	117.39	108.40
17	I	4	MET	N-CA-C	5.99	117.48	111.07
17	I	119	GLU	N-CA-C	-5.98	104.76	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1521	C	C4'-C3'-O3'	5.98	118.36	109.40
22	N	93	ALA	N-CA-C	5.96	117.58	111.14
34	c	236	ILE	CB-CA-C	-5.96	105.89	112.68
37	f	48	ALA	N-CA-C	-5.96	102.85	110.53
50	x	480	ILE	N-CA-C	-5.96	106.61	111.91
9	A	1240	A	C4'-C3'-O3'	-5.95	104.07	113.00
9	A	1823	A	C2'-C3'-O3'	-5.95	104.77	113.70
16	H	5	LYS	N-CA-C	-5.95	99.96	109.96
9	A	1269	G	C3'-C2'-O2'	5.95	119.62	110.70
22	N	31	ASP	N-CA-C	-5.94	100.81	110.20
42	n	26	GLN	N-CA-C	5.93	117.74	111.28
37	f	137	LYS	N-CA-C	5.92	117.81	111.36
44	q	40	LYS	N-CA-C	-5.92	100.89	109.59
11	C	67	GLN	N-CA-C	-5.92	106.11	113.15
16	H	30	SER	N-CA-C	5.91	118.53	110.55
22	N	60	LEU	N-CA-C	-5.91	104.84	111.28
12	D	144	ILE	CB-CA-C	-5.91	104.06	110.85
44	q	58	LEU	N-CA-C	-5.89	99.57	107.88
9	A	1520	G	C2'-C3'-O3'	-5.89	104.87	113.70
45	r	206	ASP	N-CA-C	5.89	117.70	111.28
29	V	69	VAL	CB-CA-C	-5.88	104.20	112.14
13	E	39	ASN	N-CA-C	-5.88	100.86	109.50
40	k	123	SER	N-CA-C	-5.88	101.71	110.23
15	G	61	ILE	CB-CA-C	-5.88	104.30	111.88
37	f	140	GLY	N-CA-C	-5.88	107.13	115.30
17	I	108	ASP	N-CA-C	-5.87	101.35	110.10
25	Q	36	ILE	N-CA-C	-5.87	102.00	109.58
29	V	116	ILE	N-CA-C	-5.87	104.63	110.62
29	V	193	LYS	N-CA-C	-5.87	104.79	111.07
47	u	508	GLY	N-CA-C	5.87	124.31	112.34
17	I	112	LYS	N-CA-C	-5.86	104.89	111.28
5	6	223	LEU	N-CA-C	-5.86	104.34	112.30
7	8	206	LYS	N-CA-C	5.85	117.66	111.28
20	L	60	TRP	N-CA-C	-5.84	99.61	108.67
45	r	129	SER	N-CA-C	-5.84	104.91	111.28
22	N	152	SER	N-CA-C	5.84	118.60	110.20
24	P	70	SER	CA-C-N	-5.84	112.57	119.05
24	P	70	SER	C-N-CA	-5.84	112.57	119.05
17	I	132	LYS	N-CA-C	-5.83	106.14	113.20
45	r	130	LEU	N-CA-C	-5.83	104.92	111.28
11	C	247	THR	N-CA-C	-5.82	102.84	110.53
20	L	78	LEU	N-CA-C	-5.82	105.02	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	104	THR	N-CA-C	-5.82	98.90	109.44
9	A	1522	A	C2'-C3'-O3'	-5.82	104.97	113.70
24	P	109	GLY	N-CA-C	5.82	119.27	112.23
11	C	28	ALA	CA-C-N	-5.81	113.78	119.76
11	C	28	ALA	C-N-CA	-5.81	113.78	119.76
30	Y	122	ALA	N-CA-C	5.81	118.25	110.35
32	a	58	VAL	N-CA-C	5.81	117.11	108.46
34	c	126	ASP	N-CA-C	-5.81	106.17	113.20
40	k	119	ARG	N-CA-C	5.80	118.19	110.53
22	N	52	LYS	N-CA-C	-5.80	104.96	111.28
26	R	51	GLY	N-CA-C	-5.79	107.66	115.36
4	5	405	ASP	N-CA-C	5.79	122.60	109.81
6	7	17	C	C4'-C3'-O3'	5.78	118.08	109.40
17	I	60	VAL	CB-CA-C	-5.78	104.42	111.88
40	k	128	ALA	N-CA-C	5.78	119.08	111.28
26	R	192	GLY	N-CA-C	5.77	122.99	112.37
17	I	104	ARG	N-CA-C	5.77	117.38	111.14
20	L	219	ILE	N-CA-C	-5.77	101.58	109.37
34	c	3	GLU	N-CA-C	-5.77	105.34	112.38
7	8	124	TYR	N-CA-C	5.77	117.99	110.43
12	D	135	ILE	N-CA-C	5.77	116.61	108.36
22	N	148	CYS	N-CA-C	5.77	118.51	108.76
22	N	5	LEU	N-CA-C	5.77	120.31	113.28
11	C	37	LYS	N-CA-C	5.76	118.19	110.35
29	V	151	ILE	N-CA-C	-5.76	104.75	110.62
9	A	1591	C	C4'-C3'-O3'	-5.75	104.37	113.00
5	6	227	LYS	N-CA-C	-5.74	96.25	108.66
19	K	68	SER	N-CA-C	5.74	117.62	111.36
44	q	41	MET	CA-C-N	-5.74	114.80	122.72
44	q	41	MET	C-N-CA	-5.74	114.80	122.72
31	Z	182	LEU	N-CA-C	-5.74	100.54	109.72
38	h	51	LYS	N-CA-C	-5.73	101.80	110.28
5	6	334	VAL	N-CA-CB	-5.73	105.90	111.57
19	K	19	ALA	N-CA-C	5.72	117.60	111.36
20	L	104	ASP	N-CA-C	5.72	118.23	108.90
9	A	1532	C	C5'-C4'-C3'	-5.72	107.42	116.00
17	I	30	SER	N-CA-C	-5.72	105.05	111.28
27	S	85	ARG	N-CA-C	-5.72	100.25	109.40
22	N	88	LEU	N-CA-C	-5.71	105.05	111.28
27	S	85	ARG	CA-C-N	-5.71	112.71	119.84
27	S	85	ARG	C-N-CA	-5.71	112.71	119.84
37	f	93	GLY	N-CA-C	-5.70	106.30	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	120	GLY	N-CA-C	-5.70	102.81	110.56
36	e	57	LYS	N-CA-C	-5.70	105.07	111.28
19	K	33	GLN	N-CA-C	-5.70	99.12	108.41
37	f	48	ALA	CA-C-N	-5.70	114.93	122.85
37	f	48	ALA	C-N-CA	-5.70	114.93	122.85
44	q	101	ARG	N-CA-C	-5.68	105.09	111.28
31	Z	4	GLN	N-CA-C	-5.68	100.43	109.23
34	c	271	LYS	N-CA-C	-5.68	102.00	110.23
46	t	242	LYS	N-CA-C	5.68	117.55	111.36
19	K	13	VAL	N-CA-C	-5.67	101.27	107.73
44	q	39	ILE	N-CA-C	-5.67	104.84	110.62
28	T	93	ARG	N-CA-C	-5.66	105.11	111.28
35	d	80	GLY	N-CA-C	5.66	119.79	112.54
19	K	29	HIS	N-CA-C	-5.65	106.09	112.87
51	y	339	ALA	N-CA-C	-5.64	105.14	113.61
9	A	1667	U	C2'-C3'-O3'	-5.64	105.24	113.70
12	D	97	ILE	CB-CA-C	-5.64	104.53	112.14
26	R	82	VAL	N-CA-C	5.64	116.41	110.72
12	D	168	GLY	N-CA-C	5.63	118.60	112.29
13	E	9	THR	CB-CA-C	-5.63	101.65	110.94
44	q	69	VAL	N-CA-C	5.63	121.05	109.34
32	a	57	TYR	N-CA-C	5.62	117.49	111.36
15	G	91	HIS	N-CA-C	-5.62	100.81	109.52
5	6	131	ALA	N-CA-C	5.62	117.95	110.53
22	N	69	GLU	N-CA-C	5.62	117.20	111.14
30	Y	137	ALA	N-CA-C	5.62	117.40	111.28
12	D	29	LEU	N-CA-C	-5.61	105.16	111.28
29	V	173	LEU	N-CA-C	-5.60	105.07	111.07
18	J	52	ILE	N-CA-C	5.59	115.31	107.37
13	E	30	ALA	N-CA-C	5.59	117.38	111.28
22	N	161	ILE	CA-C-N	-5.59	113.80	119.83
22	N	161	ILE	C-N-CA	-5.59	113.80	119.83
25	Q	16	GLY	N-CA-C	5.59	119.25	112.49
12	D	67	ASP	CA-C-N	-5.58	112.85	119.05
12	D	67	ASP	C-N-CA	-5.58	112.85	119.05
34	c	168	CYS	N-CA-C	-5.58	100.86	109.52
45	r	207	ALA	N-CA-C	5.58	117.04	111.07
17	I	56	ASP	N-CA-C	5.57	117.43	111.36
9	A	1379	A	C2'-C3'-O3'	-5.57	105.34	113.70
11	C	109	PHE	N-CA-C	-5.57	102.16	110.23
9	A	1841	C	C2'-C3'-O3'	-5.56	105.36	113.70
22	N	72	ALA	N-CA-C	5.55	118.10	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R	161	LEU	N-CA-C	-5.55	105.14	111.07
18	J	52	ILE	CB-CA-C	-5.54	105.92	111.80
39	i	23	VAL	CB-CA-C	-5.54	104.66	111.92
19	K	9	VAL	N-CA-C	5.54	118.22	112.90
31	Z	167	TYR	N-CA-C	5.54	117.39	111.36
26	R	81	VAL	CB-CA-C	-5.53	104.24	111.81
36	e	64	ASN	N-CA-C	5.53	117.38	111.36
24	P	148	GLY	N-CA-C	5.52	122.25	112.53
18	J	97	ARG	N-CA-C	-5.52	105.26	111.28
26	R	184	ARG	N-CA-C	5.52	118.28	110.50
11	C	191	ARG	N-CA-C	-5.52	100.71	109.59
44	q	98	ASP	N-CA-C	-5.51	105.27	111.28
51	y	669	ARG	N-CA-C	-5.51	105.25	112.41
22	N	132	GLN	CA-C-N	-5.50	112.94	119.05
22	N	132	GLN	C-N-CA	-5.50	112.94	119.05
34	c	67	SER	N-CA-C	5.50	117.36	111.36
37	f	131	VAL	N-CA-C	5.50	117.46	112.29
9	A	1533	A	C5'-C4'-O4'	5.50	118.04	109.80
14	F	98	LYS	N-CA-C	5.49	117.54	109.24
17	I	42	LYS	N-CA-C	-5.49	105.29	111.28
34	c	307	VAL	N-CA-C	-5.49	102.50	109.58
9	A	1207	G	C2'-C3'-O3'	-5.49	105.47	113.70
9	A	1533	A	C2'-C3'-O3'	-5.48	105.48	113.70
20	L	151	ILE	CB-CA-C	-5.48	104.96	111.97
18	J	19	LYS	N-CA-C	-5.47	105.31	111.28
11	C	201	HIS	N-CA-C	-5.47	98.65	109.10
30	Y	78	VAL	CB-CA-C	-5.46	104.76	112.14
34	c	197	THR	N-CA-C	5.46	117.37	109.07
25	Q	12	LYS	N-CA-C	-5.46	99.51	108.41
9	A	838	G	C4'-C3'-O3'	5.45	117.57	109.40
12	D	93	LYS	N-CA-C	-5.45	100.89	109.50
11	C	95	THR	N-CA-C	-5.44	106.64	113.28
31	Z	153	VAL	CB-CA-C	-5.43	102.60	110.63
16	H	27	SER	CA-C-N	-5.42	113.06	119.84
16	H	27	SER	C-N-CA	-5.42	113.06	119.84
37	f	45	LEU	N-CA-C	-5.42	105.37	111.28
20	L	165	VAL	CB-CA-C	-5.42	102.75	110.83
13	E	85	VAL	N-CA-C	-5.42	103.06	108.96
32	a	28	HIS	N-CA-C	5.41	119.50	113.01
10	B	132	ARG	CA-C-N	-5.40	113.09	119.84
10	B	132	ARG	C-N-CA	-5.40	113.09	119.84
5	6	333	VAL	N-CA-C	5.40	120.56	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	9	VAL	N-CA-CB	-5.40	105.30	112.26
1	l	485	GLU	N-CA-C	5.39	118.13	110.10
40	k	133	ALA	N-CA-C	5.39	117.68	108.90
51	y	744	MET	N-CA-C	-5.39	106.39	113.12
5	6	291	GLU	N-CA-C	5.38	120.52	113.30
37	f	125	HIS	N-CA-C	-5.38	105.42	111.28
17	I	21	SER	N-CA-C	5.38	117.66	110.35
29	V	196	LEU	N-CA-C	-5.38	105.42	111.28
41	m	79	VAL	N-CA-C	-5.38	108.60	113.71
20	L	133	TYR	N-CA-C	-5.37	99.35	110.80
9	A	540	U	C2'-C3'-O3'	-5.37	105.65	113.70
11	C	85	GLY	N-CA-C	5.36	120.80	112.60
25	Q	97	PRO	N-CA-C	-5.36	104.84	110.58
27	S	80	GLY	N-CA-C	-5.36	108.25	115.21
13	E	128	VAL	N-CA-C	-5.35	100.53	108.45
35	d	72	VAL	CB-CA-C	-5.35	104.92	112.14
9	A	1233	G	C2'-C3'-O3'	-5.35	105.68	113.70
30	Y	53	GLU	CA-C-N	-5.34	113.41	118.97
30	Y	53	GLU	C-N-CA	-5.34	113.41	118.97
29	V	41	VAL	CB-CA-C	-5.34	105.06	110.93
26	R	107	THR	CA-C-N	-5.34	113.12	119.05
26	R	107	THR	C-N-CA	-5.34	113.12	119.05
17	I	74	ILE	N-CA-C	-5.33	105.18	110.62
32	a	64	TRP	CB-CA-C	-5.33	103.88	112.09
33	b	44	ARG	N-CA-C	-5.33	105.47	111.28
49	w	31	C	C2'-C3'-O3'	-5.33	105.71	113.70
33	b	52	LYS	N-CA-C	-5.32	105.49	111.28
18	J	58	ALA	N-CA-C	5.31	116.75	111.07
7	8	57	GLY	N-CA-C	-5.31	100.61	113.18
9	A	588	G	C2'-C3'-O3'	-5.31	101.54	109.50
34	c	269	GLU	N-CA-C	-5.30	99.89	108.52
47	u	661	LEU	N-CA-C	5.29	117.13	111.36
30	Y	117	ARG	N-CA-C	-5.29	105.51	111.28
9	A	1466	G	C2'-C3'-O3'	-5.29	105.77	113.70
26	R	199	LEU	N-CA-C	-5.29	105.51	111.28
12	D	167	GLY	N-CA-C	-5.29	101.62	111.14
17	I	53	ILE	N-CA-C	-5.29	105.23	110.62
21	M	58	MET	N-CA-C	-5.28	105.52	111.28
20	L	159	LYS	N-CA-C	-5.28	105.53	111.28
31	Z	153	VAL	N-CA-C	5.27	115.49	108.11
8	9	13	LEU	N-CA-C	-5.27	105.54	111.28
46	t	168	PRO	N-CA-C	5.27	123.32	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	f	66	ARG	N-CA-C	-5.26	105.54	111.28
28	T	104	ARG	N-CA-C	-5.26	105.55	111.28
11	C	184	THR	N-CA-C	5.26	117.09	111.36
37	f	36	VAL	N-CA-C	-5.25	100.91	108.53
32	a	39	ASN	N-CA-C	5.25	118.64	111.39
34	c	108	VAL	CB-CA-C	-5.24	105.12	111.88
45	r	10	GLN	N-CA-C	5.24	116.99	111.28
45	r	225	ILE	N-CA-C	-5.24	98.45	109.34
47	u	643	ILE	N-CA-C	-5.24	99.56	107.73
27	S	92	ARG	N-CA-C	-5.23	100.87	109.40
12	D	21	GLU	N-CA-C	-5.23	99.76	108.34
24	P	69	SER	N-CA-C	5.23	119.63	112.88
31	Z	180	GLY	N-CA-C	-5.22	103.75	110.69
10	B	143	LEU	N-CA-C	5.21	117.04	111.36
11	C	42	LEU	N-CA-C	-5.21	100.45	109.15
24	P	112	ALA	N-CA-C	5.21	116.96	111.28
15	G	23	ILE	N-CA-C	5.21	115.93	110.62
27	S	11	GLY	N-CA-C	-5.21	108.06	115.30
22	N	68	ILE	N-CA-C	-5.20	101.91	108.93
12	D	18	ARG	CA-C-N	-5.20	113.28	119.05
12	D	18	ARG	C-N-CA	-5.20	113.28	119.05
33	b	71	GLU	N-CA-C	-5.20	99.97	108.76
4	5	388	LEU	N-CA-C	5.20	116.95	111.28
51	y	423	ASN	N-CA-C	5.20	118.01	110.42
12	D	80	ARG	N-CA-C	-5.20	105.62	111.28
9	A	308	G	C2'-C3'-O3'	5.19	117.28	109.50
10	B	128	VAL	CB-CA-C	-5.18	105.89	111.59
13	E	122	VAL	CB-CA-C	-5.18	103.88	110.98
47	u	507	ILE	N-CA-C	-5.18	102.17	109.63
17	I	46	THR	CA-C-N	-5.18	113.30	119.05
17	I	46	THR	C-N-CA	-5.18	113.30	119.05
27	S	91	GLU	N-CA-C	-5.18	100.74	109.07
28	T	120	THR	N-CA-C	-5.18	106.22	112.54
11	C	151	ASP	N-CA-C	-5.17	103.07	109.64
18	J	16	ASN	N-CA-C	-5.17	105.64	111.28
8	9	8	LYS	N-CA-C	-5.16	105.66	111.28
3	4	138	PRO	N-CA-C	-5.15	103.10	111.19
22	N	178	LEU	N-CA-C	-5.15	105.67	111.28
39	i	16	GLN	N-CA-C	-5.15	105.79	111.71
7	8	313	ARG	N-CA-C	5.14	118.34	111.24
36	e	80	ARG	N-CA-C	-5.14	103.36	110.35
45	r	175	VAL	N-CA-C	-5.14	105.38	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	40	GLU	N-CA-C	5.14	118.58	112.72
20	L	94	ILE	N-CA-C	-5.14	105.38	110.62
1	1	719	GLN	CB-CA-C	-5.13	110.67	116.63
29	V	142	SER	CA-C-N	-5.13	113.35	119.05
29	V	142	SER	C-N-CA	-5.13	113.35	119.05
30	Y	30	GLY	N-CA-C	5.13	122.99	113.76
34	c	54	ILE	CA-C-N	-5.13	114.63	119.76
34	c	54	ILE	C-N-CA	-5.13	114.63	119.76
17	I	110	ASP	N-CA-C	-5.12	105.69	111.28
44	q	24	ARG	N-CA-C	5.12	117.25	108.90
11	C	242	LYS	N-CA-C	5.11	118.49	111.54
15	G	64	VAL	CA-C-N	-5.11	114.69	119.90
15	G	64	VAL	C-N-CA	-5.11	114.69	119.90
24	P	36	SER	N-CA-C	-5.11	101.60	109.52
31	Z	184	ILE	CB-CA-C	-5.11	103.22	110.83
44	q	28	PHE	N-CA-C	5.10	117.17	109.41
26	R	20	PRO	N-CA-C	5.10	119.10	111.14
9	A	170	A	C2'-C3'-O3'	-5.10	106.05	113.70
11	C	54	TYR	N-CA-C	5.09	116.91	111.36
28	T	75	ILE	CB-CA-C	-5.09	104.18	111.31
38	h	73	GLY	N-CA-C	5.09	117.07	110.45
30	Y	102	GLU	N-CA-C	5.09	116.83	111.28
37	f	101	ASN	N-CA-C	-5.09	105.81	111.36
50	x	80	PHE	N-CA-C	5.09	116.83	111.28
29	V	62	ARG	N-CA-C	-5.08	107.08	113.28
3	4	175	THR	N-CA-C	-5.08	103.98	110.53
24	P	33	ILE	CB-CA-C	-5.08	104.80	111.25
47	u	378	ASN	N-CA-C	5.07	117.57	109.96
9	A	1362	U	C2'-C3'-O3'	-5.07	101.90	109.50
4	5	206	LYS	N-CA-C	5.07	116.61	111.14
34	c	292	SER	N-CA-C	-5.06	103.84	110.53
26	R	154	LYS	N-CA-C	-5.06	105.76	111.28
10	B	65	ASN	N-CA-C	5.06	117.44	109.39
21	M	64	GLY	N-CA-C	5.06	122.66	112.34
9	A	1269	G	C1'-C2'-O2'	-5.04	100.83	108.40
9	A	1268	C	C2'-C3'-O3'	-5.04	106.13	113.70
45	r	232	PRO	N-CA-C	5.04	116.85	110.70
1	1	318	ILE	N-CA-C	-5.04	101.22	108.53
44	q	74	SER	N-CA-C	5.04	118.54	111.74
51	y	808	SER	N-CA-C	-5.04	107.17	113.72
9	A	1544	C	C2'-C3'-O3'	-5.04	106.15	113.70
16	H	18	LYS	N-CA-C	5.03	116.60	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	82	ASP	N-CA-C	5.03	118.52	112.38
1	1	582	GLY	N-CA-C	5.03	120.25	112.45
11	C	232	ASN	N-CA-C	-5.03	106.45	112.59
9	A	307	G	C2'-C3'-O3'	5.03	117.04	109.50
9	A	1240	A	C2'-C3'-O3'	-5.02	106.16	113.70
10	B	76	VAL	CB-CA-C	-5.02	103.63	110.96
18	J	32	LYS	N-CA-C	-5.02	105.81	111.28
32	a	62	PHE	CB-CA-C	-5.02	100.62	109.70
45	r	37	LEU	N-CA-C	5.02	116.44	111.07
14	F	82	ARG	N-CA-C	5.01	119.03	113.02
25	Q	26	CYS	CB-CA-C	-5.01	102.33	110.85
18	J	98	GLN	N-CA-C	5.01	119.26	113.20
33	b	102	PHE	N-CA-C	-5.01	103.44	110.50
11	C	86	PHE	N-CA-C	-5.01	102.64	110.10
22	N	140	VAL	N-CA-C	5.00	116.36	111.91
42	n	46	VAL	CB-CA-C	-5.00	103.23	110.63
50	x	21	VAL	CA-C-N	-5.00	115.63	120.98
50	x	21	VAL	C-N-CA	-5.00	115.63	120.98

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	1	2560	0	1609	29	0
2	3	1057	0	475	9	0
3	4	1272	0	564	26	0
4	5	1581	0	689	8	0
5	6	1917	0	1096	56	0
6	7	441	0	228	14	0
7	8	1571	0	683	12	0
8	9	230	0	276	5	0
9	A	36668	0	18551	747	0
10	B	1166	0	1233	60	0
11	C	2035	0	2138	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	1477	0	1589	15	0
13	E	1087	0	1154	16	0
14	F	378	0	417	4	0
15	G	1430	0	1520	27	0
16	H	631	0	657	13	0
17	I	1208	0	1294	21	0
18	J	1034	0	1080	20	0
19	K	617	0	622	9	0
20	L	1707	0	1794	46	0
21	M	1015	0	1060	26	0
22	N	1633	0	1640	50	0
23	O	1715	0	1785	32	0
24	P	997	0	1021	37	0
25	Q	792	0	841	33	0
26	R	1627	0	1706	39	0
27	S	1862	0	2018	81	0
28	T	1015	0	1086	21	0
29	V	1461	0	1511	26	0
30	Y	1124	0	1193	37	0
31	Z	1765	0	1865	65	0
32	a	834	0	861	21	0
33	b	913	0	952	17	0
34	c	2436	0	2393	61	0
35	d	1105	0	1138	37	0
36	e	523	0	573	12	0
37	f	1176	0	1233	20	0
38	h	817	0	882	29	0
39	i	419	0	415	13	0
40	k	435	0	434	22	0
41	m	950	0	987	28	0
42	n	498	0	525	12	0
43	o	616	0	600	29	0
44	q	782	0	773	43	0
45	r	2215	0	2266	120	0
46	t	1750	0	806	5	0
47	u	5383	0	5085	140	0
48	v	2635	0	2207	58	0
49	w	1604	0	816	48	0
50	x	2831	0	2199	45	0
51	y	5197	0	5201	91	0
52	Q	1	0	0	0	0
52	k	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	108194	0	83741	2158	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 11.

All (2158) 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)
10:B:86:ILE:HD11	10:B:113:LEU:CB	1.58	1.32
6:7:23:A:C2	31:Z:108:LYS:NZ	1.98	1.30
10:B:86:ILE:CD1	10:B:113:LEU:HB2	1.61	1.29
10:B:86:ILE:CD1	10:B:113:LEU:HD13	1.63	1.27
10:B:80:MET:HG2	10:B:86:ILE:CG2	1.68	1.24
27:S:7:PHE:CD1	27:S:8:PRO:HD2	1.73	1.22
10:B:80:MET:HG2	10:B:86:ILE:HG22	1.22	1.22
10:B:82:MET:HE1	10:B:85:THR:CG2	1.72	1.20
10:B:82:MET:CE	10:B:85:THR:HB	1.71	1.19
9:A:1349:G:C5	9:A:1350:U:C4	2.33	1.17
6:7:23:A:C2	31:Z:108:LYS:CE	2.27	1.17
45:r:192:ARG:HG3	45:r:278:VAL:HG13	1.27	1.16
9:A:76:U:C5	27:S:159:ARG:NH1	2.15	1.14
6:7:23:A:N1	31:Z:108:LYS:HE2	1.59	1.14
27:S:49:VAL:HB	27:S:114:VAL:HG13	1.16	1.12
48:v:208:LEU:HD23	48:v:209:GLN:HE21	1.12	1.11
27:S:49:VAL:CG1	27:S:114:VAL:HG11	1.79	1.11
48:v:205:LEU:O	48:v:209:GLN:HG2	1.46	1.10
27:S:49:VAL:HB	27:S:114:VAL:CG1	1.80	1.10
31:Z:55:THR:HG21	43:o:245:ASN:HD21	1.02	1.08
27:S:49:VAL:CG1	27:S:114:VAL:CG1	2.31	1.07
9:A:1231:C:N4	9:A:1232:U:O4	1.87	1.07
9:A:1349:G:C6	9:A:1350:U:C4	2.41	1.07
27:S:98:ARG:HD2	27:S:106:LEU:HD21	1.36	1.06
9:A:113:G:H22	9:A:292:A:H2'	1.13	1.06
10:B:86:ILE:HD11	10:B:113:LEU:CD1	1.84	1.06
27:S:10:THR:O	27:S:128:THR:HB	1.56	1.05
9:A:1859:A:N1	9:A:1860:A:C6	2.23	1.05
9:A:1859:A:C6	9:A:1860:A:N6	2.24	1.05
45:r:63:ILE:O	45:r:63:ILE:HD12	1.57	1.04
24:P:64:ALA:HB3	24:P:67:ASP:HB2	1.39	1.04
10:B:82:MET:HE3	10:B:85:THR:HB	1.08	1.04
27:S:49:VAL:CB	27:S:114:VAL:CG1	2.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:86:ILE:CD1	10:B:113:LEU:CD1	2.36	1.04
38:h:54:VAL:HG12	38:h:56:MET:CE	1.87	1.04
10:B:86:ILE:HD12	10:B:113:LEU:HD13	1.40	1.03
9:A:695:C:H2'	9:A:696:G:C8	1.94	1.02
10:B:82:MET:CE	10:B:85:THR:CB	2.38	1.02
6:7:23:A:N1	31:Z:108:LYS:CE	2.22	1.01
44:q:40:LYS:HB3	44:q:48:GLU:HB3	1.39	1.01
48:v:208:LEU:HD23	48:v:209:GLN:NE2	1.75	1.01
9:A:1231:C:C4	9:A:1232:U:C4	2.49	1.00
27:S:7:PHE:HD1	27:S:8:PRO:HD2	0.87	1.00
27:S:49:VAL:HG12	27:S:114:VAL:CG1	1.90	1.00
10:B:82:MET:HE1	10:B:85:THR:HG22	1.40	1.00
45:r:192:ARG:HG3	45:r:278:VAL:CG1	1.92	1.00
9:A:392:A:H3'	9:A:393:U:H5''	1.42	1.00
9:A:545:A:H2'	9:A:546:G:C8	1.97	1.00
9:A:1315:U:C2	9:A:1316:C:C6	2.51	0.99
27:S:7:PHE:HD1	27:S:8:PRO:CD	1.74	0.99
38:h:54:VAL:HG12	38:h:56:MET:HE2	1.45	0.98
9:A:1315:U:C2	9:A:1316:C:C5	2.51	0.98
9:A:113:G:N2	9:A:292:A:H2'	1.78	0.98
38:h:96:GLU:O	38:h:100:GLN:HG2	1.64	0.98
9:A:695:C:H2'	9:A:696:G:H8	1.25	0.96
6:7:3:A:C2	6:7:4:G:N2	2.32	0.96
45:r:42:ILE:HG22	45:r:82:TYR:OH	1.64	0.96
9:A:1859:A:C2	9:A:1860:A:C5	2.54	0.95
9:A:1349:G:C5	9:A:1350:U:C5	2.54	0.95
10:B:82:MET:HE3	10:B:85:THR:CB	1.95	0.95
9:A:1351:G:C2	9:A:1379:A:C5	2.54	0.95
9:A:1859:A:N6	9:A:1860:A:N6	2.15	0.95
6:7:23:A:H2	31:Z:108:LYS:HD3	1.32	0.94
20:L:179:THR:HG21	20:L:198:ALA:H	1.32	0.94
9:A:896:U:H2'	9:A:897:U:H5''	1.50	0.94
9:A:1754:G:O2'	9:A:1755:C:OP1	1.85	0.94
5:6:317:ARG:HG2	47:u:398:PHE:HE1	1.32	0.93
48:v:208:LEU:CD2	48:v:209:GLN:HE21	1.79	0.93
38:h:97:ILE:O	38:h:100:GLN:HG3	1.70	0.92
45:r:223:MET:HB3	45:r:250:VAL:HG21	1.51	0.92
9:A:1144:A:H2'	9:A:1145:A:C8	2.04	0.91
9:A:1255:G:OP1	9:A:1256:G:O2'	1.89	0.91
48:v:209:GLN:HE22	48:v:246:ILE:HD12	1.34	0.91
10:B:80:MET:CG	10:B:86:ILE:HG22	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:86:ILE:HD11	10:B:113:LEU:CG	1.99	0.90
27:S:134:GLY:HA3	27:S:158:VAL:HG11	1.51	0.90
6:7:23:A:C2	31:Z:108:LYS:HD3	2.07	0.89
45:r:132:GLN:HA	45:r:136:TRP:HB2	1.54	0.89
31:Z:55:THR:HG21	43:o:245:ASN:ND2	1.88	0.89
10:B:128:VAL:HG23	10:B:140:PHE:HD2	1.36	0.88
45:r:212:LEU:CD2	45:r:229:LEU:HD22	2.03	0.88
44:q:37:GLN:CG	44:q:39:ILE:HG13	2.03	0.88
9:A:1351:G:C6	9:A:1379:A:N6	2.41	0.88
37:f:22:GLY:HA2	37:f:56:ALA:HB3	1.55	0.88
9:A:545:A:O2'	9:A:546:G:O4'	1.91	0.87
44:q:37:GLN:HG2	44:q:39:ILE:HG13	1.53	0.87
10:B:86:ILE:HD11	10:B:113:LEU:HB2	0.87	0.86
45:r:273:MET:SD	45:r:276:LYS:NZ	2.49	0.86
10:B:82:MET:CE	10:B:85:THR:CG2	2.54	0.86
45:r:4:LEU:N	45:r:113:ARG:HH12	1.72	0.86
9:A:410:G:C6	9:A:431:G:C6	2.63	0.85
5:6:310:ALA:HB2	47:u:401:LEU:HD13	1.57	0.85
6:7:23:A:C2	31:Z:108:LYS:CD	2.58	0.85
27:S:176:ILE:N	27:S:176:ILE:HD12	1.91	0.85
10:B:82:MET:HE2	10:B:85:THR:O	1.76	0.85
9:A:77:A:H1'	27:S:176:ILE:HD13	1.57	0.85
9:A:1457:U:H2'	9:A:1458:G:H8	1.39	0.85
12:D:58:ARG:HE	20:L:199:PRO:HG3	1.43	0.84
9:A:1275:G:O4'	9:A:1506:A:N6	2.12	0.83
9:A:33:G:H2'	9:A:34:U:H5'	1.61	0.83
10:B:86:ILE:CD1	10:B:113:LEU:CB	2.36	0.83
45:r:192:ARG:HB2	45:r:278:VAL:HG11	1.60	0.83
9:A:536:A:O5'	9:A:537:C:H5''	1.78	0.83
9:A:410:G:O6	9:A:431:G:C6	2.31	0.83
9:A:1542:C:H5''	9:A:1542:C:H6	1.44	0.83
30:Y:97:GLN:HB2	30:Y:105:LYS:HD3	1.59	0.83
9:A:1483:A:H4'	31:Z:160:SER:HB2	1.59	0.82
38:h:54:VAL:CG1	38:h:56:MET:CE	2.57	0.82
48:v:205:LEU:O	48:v:209:GLN:CG	2.28	0.82
27:S:49:VAL:C	27:S:114:VAL:HG12	2.04	0.82
48:v:208:LEU:CD2	48:v:209:GLN:NE2	2.40	0.82
6:7:23:A:H2	31:Z:108:LYS:CD	1.91	0.82
45:r:192:ARG:CG	45:r:278:VAL:CG1	2.58	0.82
9:A:1315:U:N3	9:A:1316:C:C5	2.48	0.82
10:B:128:VAL:CG2	10:B:140:PHE:CD2	2.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:33:G:C2'	9:A:34:U:H5'	2.10	0.81
9:A:155:G:C6	9:A:164:A:N6	2.48	0.81
9:A:1351:G:N2	9:A:1379:A:C8	2.49	0.81
27:S:49:VAL:HG12	27:S:114:VAL:HG12	1.62	0.81
27:S:134:GLY:HA3	27:S:158:VAL:CG1	2.09	0.81
45:r:224:PRO:HD2	45:r:239:THR:HG23	1.61	0.81
9:A:1225:U:H2'	9:A:1226:G:H5'	1.61	0.81
10:B:128:VAL:HG23	10:B:140:PHE:CD2	2.16	0.81
9:A:1225:U:C2'	9:A:1226:G:H5'	2.10	0.81
9:A:489:A:C2	9:A:512:A:C2	2.68	0.80
9:A:1092:G:C6	9:A:1158:G:O6	2.34	0.80
9:A:1859:A:H2'	9:A:1860:A:C8	2.17	0.80
9:A:155:G:O2'	9:A:156:G:H5'	1.80	0.80
9:A:1415:C:H2'	9:A:1416:C:C6	2.16	0.80
10:B:82:MET:HE1	10:B:85:THR:CB	2.06	0.80
9:A:1349:G:C6	9:A:1350:U:O4	2.34	0.80
35:d:143:LYS:O	35:d:144:LYS:HB2	1.82	0.80
3:4:339:TYR:CB	48:v:409:LYS:HE2	2.12	0.80
9:A:940:U:H2'	9:A:941:C:C6	2.17	0.80
31:Z:59:LEU:HD22	43:o:308:LEU:HD12	1.64	0.80
27:S:7:PHE:CE1	27:S:113:ILE:O	2.35	0.79
28:T:12:PHE:HZ	28:T:21:LYS:HD3	1.47	0.79
45:r:212:LEU:CD2	45:r:229:LEU:CD2	2.59	0.79
3:4:113:ALA:O	47:u:569:LEU:HD13	1.82	0.79
5:6:317:ARG:HG2	47:u:398:PHE:CE1	2.17	0.79
9:A:223:C:H2'	9:A:224:A:H8	1.47	0.79
27:S:98:ARG:CD	27:S:106:LEU:HD21	2.11	0.79
35:d:143:LYS:O	35:d:144:LYS:CB	2.28	0.79
5:6:324:LYS:HB2	47:u:447:TYR:HA	1.63	0.78
49:w:58:A:H3'	49:w:59:A:H8	1.46	0.78
9:A:27:A2M:HM'1	9:A:483:C:H1'	1.64	0.78
9:A:12:U:H2'	9:A:13:C:C6	2.18	0.78
9:A:1452:A:O2'	9:A:1475:G:N2	2.16	0.78
9:A:410:G:C6	9:A:431:G:N1	2.52	0.78
9:A:1386:A:C6	9:A:1387:G:C4	2.72	0.78
16:H:56:CYS:HB3	16:H:60:SER:HB2	1.65	0.78
41:m:93:LYS:NZ	41:m:102:LYS:HD3	1.99	0.78
45:r:197:VAL:HG11	45:r:212:LEU:HD12	1.66	0.77
34:c:290:ALA:HB3	34:c:299:PHE:HB2	1.65	0.77
9:A:1542:C:H5''	9:A:1542:C:C6	2.19	0.77
9:A:497:C:C2	9:A:498:C:C5	2.73	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:199:C:H2'	9:A:200:G:H21	1.50	0.77
27:S:49:VAL:HG12	27:S:114:VAL:HG11	1.52	0.77
9:A:896:U:C2'	9:A:897:U:H5''	2.14	0.77
45:r:227:ILE:HD12	45:r:235:TYR:HD2	1.48	0.77
9:A:1859:A:N6	9:A:1860:A:H62	1.82	0.77
9:A:961:G:H21	45:r:55:ARG:HH21	1.30	0.76
27:S:10:THR:O	27:S:128:THR:CB	2.32	0.76
45:r:212:LEU:HD21	45:r:229:LEU:HD22	1.66	0.76
9:A:1593:C:H4'	30:Y:45:ARG:NH1	2.00	0.76
19:K:34:MET:HE3	22:N:143:PRO:HB2	1.68	0.76
10:B:80:MET:HG2	10:B:86:ILE:HG21	1.68	0.76
5:6:323:CYS:HB3	47:u:448:GLN:HB3	1.65	0.76
9:A:423:U:O2'	9:A:424:C:H5'	1.85	0.76
9:A:1859:A:N1	9:A:1860:A:N6	2.32	0.76
32:a:74:GLU:N	32:a:74:GLU:OE1	2.18	0.76
9:A:74:G:H5'	9:A:74:G:N3	1.99	0.76
27:S:49:VAL:HG11	27:S:114:VAL:HG11	1.65	0.76
27:S:50:VAL:HA	27:S:113:ILE:HA	1.68	0.76
42:n:51:ARG:HG3	50:x:416:GLN:HE22	1.51	0.76
9:A:1231:C:C4	9:A:1232:U:O4	2.38	0.76
45:r:77:ASP:H	45:r:82:TYR:HA	1.48	0.76
9:A:1457:U:H2'	9:A:1458:G:C8	2.19	0.75
9:A:155:G:H2'	9:A:156:G:C8	2.19	0.75
45:r:67:ARG:HH12	49:w:21:G:H4'	1.50	0.75
45:r:43:GLU:O	45:r:82:TYR:CE1	2.39	0.75
21:M:111:PHE:HE1	22:N:12:GLU:HA	1.51	0.75
34:c:87:LEU:HD21	34:c:122:SER:HB3	1.68	0.75
49:w:22:C:H2'	49:w:23:G:C8	2.21	0.75
9:A:1351:G:N1	9:A:1379:A:C6	2.55	0.74
49:w:47:C:H2'	49:w:58:A:H1'	1.69	0.74
9:A:223:C:H2'	9:A:224:A:C8	2.22	0.74
9:A:1349:G:C8	9:A:1350:U:C5	2.75	0.74
9:A:219:U:H1'	26:R:184:ARG:HD2	1.69	0.74
9:A:393:U:H5'	51:y:146:ARG:NH2	2.02	0.74
9:A:1231:C:N4	9:A:1232:U:C4	2.54	0.74
50:x:359:ARG:H	50:x:375:CYS:HB2	1.52	0.74
5:6:308:VAL:HA	5:6:311:PHE:HB3	1.70	0.74
17:I:142:GLU:HB2	17:I:145:THR:HG22	1.68	0.74
38:h:54:VAL:CG1	38:h:56:MET:HE1	2.16	0.74
49:w:22:C:H2'	49:w:23:G:H8	1.53	0.74
45:r:192:ARG:CG	45:r:278:VAL:HG13	2.11	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:59:LEU:CD1	43:o:308:LEU:HG	2.19	0.73
48:v:347:ILE:HG23	51:y:826:ILE:HD12	1.70	0.73
10:B:86:ILE:CG1	10:B:113:LEU:HB2	2.18	0.73
7:8:258:VAL:HA	51:y:857:LEU:HD13	1.70	0.73
27:S:7:PHE:HB3	27:S:10:THR:HG23	1.71	0.73
31:Z:59:LEU:HD13	43:o:308:LEU:HG	1.70	0.73
9:A:1728:U:H2'	9:A:1729:U:O4'	1.88	0.73
9:A:1349:G:N7	9:A:1350:U:C5	2.57	0.72
15:G:31:GLU:O	15:G:37:LYS:HB2	1.89	0.72
51:y:831:LEU:HG	51:y:844:MET:HB2	1.70	0.72
10:B:120:VAL:HG12	10:B:145:VAL:HG11	1.69	0.72
9:A:1859:A:C2	9:A:1860:A:C6	2.76	0.72
10:B:82:MET:CE	10:B:85:THR:O	2.38	0.72
9:A:1349:G:C4	9:A:1350:U:C5	2.78	0.72
9:A:1310:U:H5''	40:k:130:VAL:HG13	1.72	0.72
10:B:82:MET:CE	10:B:85:THR:HG22	2.17	0.72
22:N:77:ILE:HG12	22:N:99:ILE:HB	1.72	0.72
35:d:142:ASN:C	35:d:142:ASN:OD1	2.32	0.72
45:r:198:ALA:HB2	45:r:270:ASN:HB2	1.70	0.72
45:r:214:ALA:HB1	45:r:257:VAL:HG12	1.72	0.72
38:h:61:LEU:HD12	38:h:82:MET:HE2	1.72	0.71
41:m:79:VAL:HG21	41:m:85:LEU:HB2	1.72	0.71
9:A:1859:A:C6	9:A:1860:A:C6	2.74	0.71
24:P:31:CYS:HB2	24:P:93:LEU:HD23	1.72	0.71
27:S:98:ARG:HD2	27:S:106:LEU:CD2	2.18	0.71
21:M:41:ILE:HG12	31:Z:208:VAL:HG13	1.72	0.71
9:A:489:A:C6	9:A:512:A:N1	2.58	0.71
24:P:125:LYS:HB3	25:Q:58:VAL:HG12	1.73	0.71
28:T:57:VAL:HB	28:T:60:PHE:HE1	1.55	0.71
34:c:128:THR:HB	34:c:143:GLN:HB3	1.72	0.71
9:A:429:C:C2	9:A:430:C:C5	2.79	0.71
34:c:197:THR:HG21	34:c:238:ALA:HA	1.72	0.71
49:w:19:A:H2'	49:w:20:A:H4'	1.72	0.71
29:V:142:SER:HB2	42:n:50:VAL:HG22	1.73	0.71
27:S:49:VAL:O	27:S:114:VAL:N	2.24	0.70
42:n:38:THR:HA	50:x:426:LYS:HE2	1.73	0.70
9:A:909:G:C6	9:A:910:G:C5	2.79	0.70
11:C:137:PRO:HB2	11:C:150:PRO:HD2	1.72	0.70
27:S:176:ILE:HD12	27:S:176:ILE:H	1.56	0.70
44:q:61:ILE:HD11	44:q:65:LEU:HB2	1.72	0.70
29:V:35:LEU:HD21	29:V:146:ARG:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:288:GLN:CB	5:6:348:GLN:HE21	2.04	0.70
44:q:51:CYS:HB3	44:q:54:GLY:H	1.55	0.70
45:r:231:ALA:HB2	49:w:73:C:N3	2.06	0.70
9:A:1092:G:O2'	9:A:1093:A:H5'	1.90	0.70
28:T:117:VAL:HG21	28:T:125:VAL:HG21	1.74	0.70
24:P:97:LEU:HD11	24:P:112:ALA:HB1	1.74	0.70
45:r:227:ILE:HG23	45:r:235:TYR:HB2	1.73	0.69
9:A:570:C:C5	9:A:571:U:C5	2.80	0.69
45:r:42:ILE:HG22	45:r:82:TYR:CZ	2.25	0.69
9:A:410:G:O6	9:A:431:G:O6	2.10	0.69
21:M:111:PHE:CE1	22:N:12:GLU:HA	2.28	0.69
27:S:176:ILE:H	27:S:176:ILE:CD1	2.05	0.69
9:A:155:G:C2	9:A:164:A:C5	2.81	0.69
9:A:497:C:H2'	9:A:498:C:H6	1.56	0.69
9:A:1351:G:C6	9:A:1379:A:C6	2.80	0.69
27:S:49:VAL:CB	27:S:114:VAL:HG13	2.02	0.69
34:c:36:ARG:HA	34:c:65:PHE:HB3	1.74	0.69
51:y:421:GLY:HA2	51:y:440:VAL:HA	1.75	0.69
5:6:290:LYS:HA	5:6:331:LYS:H	1.57	0.69
27:S:45:TRP:CH2	27:S:121:ILE:HG12	2.28	0.69
25:Q:21:ILE:HG12	25:Q:32:LYS:HA	1.73	0.69
48:v:290:ASP:HB3	48:v:293:THR:HB	1.75	0.69
9:A:1351:G:N2	9:A:1379:A:C5	2.61	0.68
9:A:1805:G:C6	9:A:1806:A:C5	2.81	0.68
17:I:99:ARG:HE	17:I:115:LEU:HD21	1.59	0.68
31:Z:42:THR:HG22	31:Z:45:ARG:H	1.59	0.68
3:4:304:VAL:C	47:u:538:LYS:HG2	2.18	0.68
9:A:797:C:H4'	9:A:798:G:OP2	1.94	0.68
20:L:102:LEU:HD12	20:L:132:ASP:HB3	1.74	0.68
44:q:37:GLN:HG3	44:q:39:ILE:CG1	2.23	0.68
9:A:1124:C:H5''	23:O:150:ILE:HG12	1.75	0.68
9:A:1144:A:H2'	9:A:1145:A:H8	1.59	0.68
45:r:4:LEU:N	45:r:113:ARG:NH1	2.40	0.68
44:q:40:LYS:CB	44:q:48:GLU:HB3	2.19	0.68
30:Y:38:PRO:HB2	30:Y:41:MET:HG2	1.75	0.68
51:y:64:ILE:HG12	51:y:109:ILE:HD11	1.74	0.68
9:A:695:C:C2'	9:A:696:G:H8	2.04	0.68
9:A:1315:U:C4	9:A:1316:C:C4	2.82	0.68
9:A:585:C:O2'	9:A:586:G:H5'	1.94	0.68
45:r:197:VAL:HG11	45:r:212:LEU:CD1	2.24	0.68
45:r:231:ALA:HB2	49:w:73:C:C4	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1315:U:O2	9:A:1316:C:C6	2.46	0.68
10:B:128:VAL:HG21	10:B:140:PHE:CD2	2.28	0.68
25:Q:58:VAL:CG2	25:Q:59:PHE:N	2.56	0.68
49:w:1:A:H2	49:w:72:A:H1'	1.58	0.67
9:A:570:C:C4	9:A:571:U:C5	2.82	0.67
9:A:1315:U:N3	9:A:1316:C:C4	2.62	0.67
40:k:119:ARG:HD3	40:k:132:MET:HE3	1.76	0.67
41:m:93:LYS:HZ1	41:m:102:LYS:HD3	1.57	0.67
5:6:324:LYS:H	47:u:448:GLN:H	1.42	0.67
41:m:81:ASP:HB3	41:m:84:LYS:HB2	1.76	0.67
47:u:405:GLU:HA	47:u:408:THR:HG22	1.77	0.67
9:A:3:C:H5'	20:L:205:VAL:HG12	1.76	0.67
9:A:1349:G:C5	9:A:1350:U:O4	2.47	0.67
27:S:176:ILE:N	27:S:176:ILE:CD1	2.57	0.67
45:r:192:ARG:HB2	45:r:278:VAL:CG1	2.24	0.67
9:A:1829:G:H1'	9:A:1850:MA6:H2	1.76	0.67
11:C:139:LEU:HD23	11:C:150:PRO:HB3	1.76	0.67
1:1:565:ILE:HD11	1:1:579:VAL:HB	1.75	0.66
5:6:317:ARG:NH1	47:u:399:ASN:OD1	2.27	0.66
9:A:223:C:C2	9:A:299:A:C2	2.82	0.66
9:A:928:G:H1	9:A:1013:U:H3	1.43	0.66
24:P:64:ALA:HB3	24:P:67:ASP:CB	2.22	0.66
34:c:255:SER:HB3	34:c:271:LYS:HA	1.76	0.66
9:A:186:C:H2'	9:A:187:G:C8	2.30	0.66
29:V:143:PRO:HG3	42:n:54:ASP:HB3	1.77	0.66
9:A:829:C:H4'	9:A:830:A:OP1	1.94	0.66
27:S:79:LYS:HB2	27:S:86:PRO:HG3	1.77	0.66
9:A:1:U:C2	9:A:3:C:C5	2.84	0.66
9:A:393:U:H5'	51:y:146:ARG:HH22	1.60	0.66
34:c:68:ASP:HB3	34:c:111:VAL:HG22	1.78	0.66
5:6:324:LYS:O	47:u:448:GLN:HG3	1.94	0.66
11:C:20:LEU:HD21	11:C:46:ILE:HD12	1.78	0.66
50:x:31:GLN:NE2	50:x:67:SER:N	2.43	0.66
9:A:1208:A:N1	9:A:1209:A:C5	2.64	0.66
5:6:309:GLU:HB3	47:u:447:TYR:OH	1.96	0.66
9:A:926:A:H61	9:A:1015:U:H3	1.42	0.66
9:A:1232:U:H2'	9:A:1233:G:C8	2.30	0.66
9:A:1474:A:H2'	9:A:1475:G:C8	2.31	0.66
30:Y:102:GLU:HG2	34:c:55:PRO:HB2	1.78	0.66
40:k:138:ARG:HB3	40:k:149:CYS:HA	1.77	0.65
9:A:1859:A:H2'	9:A:1860:A:H8	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:12:PHE:CZ	28:T:21:LYS:HD3	2.31	0.65
5:6:321:VAL:HB	47:u:514:MET:CE	2.26	0.65
31:Z:49:ILE:HD12	43:o:309:ILE:HD11	1.77	0.65
45:r:183:ARG:HH12	49:w:54:U:H4'	1.62	0.65
49:w:9:G:C5	49:w:20:A:H1'	2.31	0.65
5:6:321:VAL:HB	47:u:514:MET:SD	2.37	0.65
9:A:155:G:H2'	9:A:156:G:H8	1.61	0.65
43:o:269:TYR:HB3	43:o:284:PHE:HB2	1.77	0.65
45:r:194:ASP:HB3	45:r:272:GLN:HB3	1.78	0.65
9:A:392:A:C3'	9:A:393:U:H5''	2.24	0.65
49:w:72:A:H2'	49:w:73:C:H2'	1.78	0.65
9:A:545:A:C2'	9:A:546:G:C8	2.77	0.65
22:N:124:VAL:HG23	22:N:146:ALA:HB2	1.78	0.65
9:A:1283:C:O2'	9:A:1313:A:N1	2.27	0.65
47:u:329:ILE:HB	47:u:367:ARG:HH11	1.61	0.65
9:A:429:C:N3	9:A:430:C:C5	2.65	0.65
9:A:1351:G:C2	9:A:1379:A:C6	2.84	0.65
9:A:1859:A:C4	9:A:1860:A:N7	2.64	0.65
9:A:367:U:H3	51:y:144:LYS:HE3	1.60	0.65
9:A:398:A:O2'	9:A:1027:A:C2	2.48	0.65
45:r:108:VAL:HG13	45:r:153:PHE:HE2	1.62	0.65
27:S:7:PHE:CD1	27:S:113:ILE:O	2.49	0.64
9:A:392:A:H3'	9:A:393:U:C5'	2.24	0.64
9:A:1786:U:H2'	9:A:1787:G:C8	2.32	0.64
24:P:92:ALA:HB2	24:P:125:LYS:HB2	1.78	0.64
30:Y:132:PHE:HD2	38:h:79:ARG:HH12	1.43	0.64
38:h:22:ILE:HD11	38:h:91:LEU:HD11	1.78	0.64
47:u:482:VAL:O	51:y:798:VAL:HG23	1.98	0.64
38:h:52:GLY:O	38:h:53:PRO:C	2.32	0.64
49:w:68:U:H2'	49:w:69:G:C8	2.31	0.64
9:A:1588:A:H2'	9:A:1589:A:C8	2.32	0.64
11:C:35:PRO:HD2	11:C:83:PRO:HG2	1.80	0.64
23:O:78:GLU:OE1	47:u:10:ASN:ND2	2.30	0.64
9:A:909:G:C4	9:A:910:G:C8	2.86	0.64
9:A:1181:A:H2'	9:A:1182:A:C8	2.33	0.64
9:A:1349:G:C6	9:A:1350:U:N3	2.65	0.64
9:A:1543:U:H6	9:A:1543:U:H5''	1.61	0.64
11:C:183:VAL:HG11	11:C:220:THR:HG21	1.80	0.64
9:A:145:G:H2'	9:A:146:G:C8	2.32	0.64
9:A:751:G:H22	9:A:789:G:H5''	1.63	0.64
9:A:1283:C:H42	41:m:102:LYS:HE3	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1208:A:N6	9:A:1209:A:N6	2.46	0.64
9:A:1228:A:H2'	9:A:1229:G:C8	2.32	0.64
31:Z:55:THR:CG2	43:o:245:ASN:HD21	1.94	0.64
38:h:115:THR:HG23	38:h:119:ALA:OXT	1.98	0.64
50:x:391:ILE:HG22	50:x:446:TYR:HB2	1.80	0.64
9:A:896:U:C3'	9:A:897:U:H5''	2.28	0.63
9:A:1351:G:N2	9:A:1379:A:N7	2.46	0.63
9:A:1593:C:H4'	30:Y:45:ARG:HH11	1.63	0.63
9:A:113:G:C2	9:A:292:A:C4	2.85	0.63
50:x:378:ASP:HB2	50:x:393:ILE:H	1.63	0.63
9:A:497:C:N3	9:A:498:C:C5	2.65	0.63
9:A:1386:A:N6	9:A:1387:G:C6	2.67	0.63
47:u:296:LEU:HB3	47:u:322:VAL:HG23	1.79	0.63
9:A:925:G:H1	9:A:1017:U:H3	1.45	0.63
34:c:85:GLY:HA2	34:c:108:VAL:HG23	1.79	0.63
48:v:246:ILE:HD13	50:x:24:GLN:HG3	1.79	0.63
9:A:543:C:H5''	9:A:544:G:N7	2.13	0.63
9:A:981:A:H2'	9:A:982:G:C8	2.34	0.63
9:A:1453:C:C5	9:A:1455:A:H1'	2.32	0.63
9:A:1587:G:C5	35:d:67:ARG:HG2	2.33	0.63
9:A:1859:A:N1	9:A:1860:A:C5	2.63	0.63
9:A:1139:C:H2'	9:A:1140:G:O4'	1.99	0.63
9:A:1416:C:C2	9:A:1425:G:C2	2.87	0.63
50:x:289:LEU:HD23	50:x:316:ALA:HB1	1.81	0.63
9:A:326:C:H3'	9:A:327:G:H5''	1.80	0.63
9:A:880:G:H2'	9:A:881:G:O4'	1.99	0.63
9:A:1337:C:H2'	9:A:1338:G:C8	2.33	0.63
9:A:1349:G:O6	9:A:1350:U:O4	2.16	0.62
10:B:86:ILE:CD1	10:B:113:LEU:CG	2.68	0.62
45:r:199:CYS:HB2	45:r:207:ALA:HB1	1.81	0.62
9:A:545:A:H2'	9:A:546:G:N7	2.13	0.62
45:r:212:LEU:HD23	45:r:229:LEU:CD2	2.28	0.62
46:t:418:SER:H	46:t:427:ILE:HA	1.63	0.62
49:w:9:G:H1'	49:w:45:G:C8	2.34	0.62
5:6:323:CYS:CB	47:u:448:GLN:HB3	2.28	0.62
3:4:313:ASN:O	5:6:334:VAL:HG13	1.99	0.62
9:A:444:G:O6	26:R:26:LYS:HE2	1.99	0.62
9:A:924:G:H5'	17:I:4:MET:HE3	1.81	0.62
9:A:1690:U:H2'	9:A:1691:U:C6	2.35	0.62
27:S:57:ASP:HA	27:S:106:LEU:HD23	1.80	0.62
35:d:41:LYS:HE3	35:d:93:SER:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1208:A:C2	9:A:1209:A:C5	2.88	0.62
9:A:1349:G:N7	9:A:1350:U:C4	2.67	0.62
9:A:1351:G:N1	9:A:1379:A:C5	2.67	0.62
49:w:15:G:H2'	49:w:16:C:C2	2.35	0.62
49:w:56:G:H2'	49:w:57:A:C8	2.35	0.62
9:A:1397:U:O4	30:Y:12:VAL:HG13	1.98	0.62
50:x:452:VAL:HG22	50:x:465:ILE:HG22	1.80	0.62
1:1:659:TRP:HA	1:1:666:VAL:HA	1.80	0.62
35:d:80:GLY:HA3	35:d:92:PHE:HE1	1.64	0.62
9:A:222:U:O2'	9:A:223:C:H5'	2.00	0.62
21:M:99:ASP:HA	21:M:120:THR:HG22	1.82	0.62
45:r:60:ASN:HD22	49:w:40:C:H5''	1.64	0.62
1:1:546:ILE:HB	1:1:557:ASP:HB2	1.81	0.62
9:A:497:C:H2'	9:A:498:C:C6	2.35	0.62
9:A:1283:C:H42	41:m:102:LYS:HB3	1.63	0.61
24:P:129:ILE:O	25:Q:65:PRO:HG3	1.99	0.61
25:Q:39:PHE:HD1	25:Q:70:LYS:HD3	1.65	0.61
5:6:325:ILE:HA	47:u:449:SER:OG	2.00	0.61
9:A:1720:U:O4	9:A:1814:G:N2	2.33	0.61
33:b:49:LEU:HD13	33:b:83:MET:HE1	1.83	0.61
48:v:247:GLN:HG2	48:v:250:CYS:HB2	1.82	0.61
9:A:10:G:H21	20:L:114:LYS:HA	1.64	0.61
9:A:223:C:O2'	9:A:224:A:H5'	1.99	0.61
9:A:887:U:H2'	9:A:888:U:H2'	1.82	0.61
17:I:29:THR:HB	17:I:32:ASP:H	1.65	0.61
9:A:489:A:N1	9:A:512:A:C6	2.69	0.61
9:A:1386:A:N7	9:A:1387:G:N7	2.48	0.61
9:A:1452:A:C4	9:A:1476:A:C2	2.89	0.61
9:A:1499:U:H4'	31:Z:176:LEU:HD13	1.82	0.61
23:O:175:GLU:O	23:O:179:ASN:ND2	2.34	0.61
48:v:209:GLN:NE2	48:v:246:ILE:HD12	2.10	0.61
3:4:304:VAL:O	47:u:538:LYS:HG2	2.00	0.61
27:S:7:PHE:HB3	27:S:10:THR:CG2	2.28	0.61
28:T:36:PRO:HB2	28:T:39:GLU:HG2	1.82	0.61
9:A:984:C:O2	24:P:138:ASP:HB3	2.01	0.61
22:N:148:CYS:SG	22:N:152:SER:HB2	2.40	0.61
49:w:40:C:H2'	49:w:41:A:C8	2.35	0.61
9:A:1386:A:C5	9:A:1387:G:C5	2.88	0.61
9:A:1680:G:H4'	42:n:20:ARG:HD3	1.81	0.61
45:r:192:ARG:CB	45:r:278:VAL:HG11	2.30	0.61
44:q:37:GLN:CG	44:q:39:ILE:CG1	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1305:C:H5'	40:k:93:HIS:NE2	2.15	0.61
9:A:1786:U:H2'	9:A:1787:G:H8	1.66	0.61
32:a:65:ARG:HD2	39:i:25:SER:HB3	1.82	0.61
9:A:833:C:H2'	9:A:834:C:C6	2.35	0.60
9:A:896:U:H2'	9:A:897:U:C5'	2.30	0.60
20:L:165:VAL:HG21	20:L:217:ALA:HB1	1.83	0.60
29:V:138:ALA:HB2	29:V:204:ARG:HA	1.83	0.60
47:u:230:LEU:HD12	47:u:256:ILE:HG23	1.83	0.60
48:v:302:ASN:HB2	51:y:820:SER:HB2	1.83	0.60
26:R:162:LEU:HD21	26:R:191:GLU:HG3	1.82	0.60
38:h:95:SER:O	38:h:99:LYS:HG3	2.01	0.60
9:A:155:G:C5	9:A:164:A:N6	2.69	0.60
9:A:615:C:H2'	9:A:616:A:C8	2.36	0.60
9:A:1156:U:OP1	18:J:71:LYS:NZ	2.33	0.60
9:A:489:A:C6	9:A:512:A:C6	2.89	0.60
9:A:1813:A:H3'	9:A:1814:G:H8	1.65	0.60
11:C:92:ILE:HG21	28:T:17:LEU:HD11	1.82	0.60
27:S:128:THR:OG1	27:S:131:ARG:NH2	2.30	0.60
34:c:166:VAL:HG13	34:c:176:VAL:HG22	1.83	0.60
38:h:54:VAL:HG11	38:h:56:MET:HE1	1.83	0.60
51:y:68:ARG:HH12	51:y:109:ILE:HA	1.66	0.60
44:q:30:GLU:OE2	44:q:31:ASP:OD1	2.19	0.60
45:r:22:VAL:HG23	45:r:36:LEU:HA	1.83	0.60
9:A:1386:A:N6	9:A:1387:G:C2	2.69	0.60
10:B:21:LYS:NZ	26:R:156:ALA:HA	2.17	0.60
29:V:201:LYS:HD3	29:V:204:ARG:HE	1.66	0.60
1:l:319:PHE:HA	1:l:329:ILE:H	1.67	0.60
9:A:388:U:H2'	9:A:389:A:C8	2.37	0.60
9:A:940:U:H2'	9:A:941:C:H6	1.63	0.60
29:V:41:VAL:HG11	29:V:113:VAL:HG22	1.82	0.60
45:r:44:GLY:HA3	45:r:83:ILE:HG22	1.83	0.60
47:u:343:ASP:OD1	51:y:698:MET:HG2	2.02	0.60
31:Z:59:LEU:HD22	43:o:308:LEU:CD1	2.30	0.60
43:o:273:ASP:HA	43:o:280:LYS:HE2	1.84	0.60
45:r:192:ARG:CB	45:r:278:VAL:CG1	2.80	0.60
48:v:405:ILE:HG12	51:y:855:LEU:HD21	1.83	0.60
9:A:393:U:C5'	51:y:146:ARG:HH22	2.14	0.60
9:A:545:A:HO2'	9:A:546:G:C1'	2.15	0.60
9:A:634:A:H2'	9:A:635:G:C8	2.36	0.60
9:A:1139:C:H5	9:A:1149:A:H62	1.48	0.60
33:b:37:TYR:HE1	33:b:113:GLY:HA2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:468:THR:H	48:v:383:LYS:HE2	1.65	0.59
5:6:351:TYR:O	5:6:355:ASN:ND2	2.35	0.59
9:A:1315:U:C4	9:A:1316:C:N4	2.70	0.59
9:A:1402:A:N6	9:A:1441:U:O2	2.35	0.59
9:A:1518:C:H5''	9:A:1519:U:H5''	1.84	0.59
27:S:49:VAL:O	27:S:114:VAL:HG12	2.02	0.59
9:A:1759:G:H5'	9:A:1774:C:H1'	1.83	0.59
45:r:178:ASN:O	45:r:182:ARG:HB2	2.02	0.59
5:6:310:ALA:CB	47:u:401:LEU:HD13	2.32	0.59
5:6:317:ARG:NH1	47:u:398:PHE:H	2.00	0.59
9:A:996:A:H2'	9:A:997:A:C8	2.38	0.59
20:L:129:ALA:HB1	20:L:216:MET:HE1	1.84	0.59
6:7:23:A:H2	31:Z:108:LYS:NZ	1.87	0.59
9:A:1231:C:C5	9:A:1232:U:C5	2.91	0.59
44:q:63:GLY:O	44:q:64:LYS:C	2.41	0.59
5:6:313:ILE:CD1	47:u:446:ILE:HG21	2.32	0.59
9:A:1174:U:H2'	9:A:1175:G:C8	2.37	0.59
1:1:548:ARG:HB2	1:1:555:PRO:HD2	1.85	0.59
11:C:160:ILE:HB	11:C:169:ILE:HG23	1.85	0.59
13:E:140:ARG:HE	13:E:141:PRO:HD2	1.66	0.59
20:L:108:LYS:HB2	20:L:233:LEU:HD22	1.84	0.59
38:h:22:ILE:HD12	38:h:91:LEU:HD21	1.84	0.59
48:v:408:THR:HB	51:y:858:GLN:HB3	1.84	0.59
9:A:1444:U:P	30:Y:15:ARG:HH22	2.25	0.59
41:m:50:CYS:HB2	41:m:110:VAL:HG12	1.85	0.59
47:u:137:THR:HA	47:u:140:ARG:HG3	1.84	0.59
1:1:478:ILE:HD12	1:1:497:GLN:HG2	1.83	0.59
9:A:570:C:C2	9:A:571:U:C6	2.91	0.59
47:u:124:PRO:HA	47:u:127:VAL:HG22	1.84	0.59
9:A:909:G:C2	9:A:910:G:C4	2.90	0.59
9:A:1037:G:H4'	9:A:1845:A:H4'	1.85	0.59
10:B:128:VAL:CG2	10:B:140:PHE:HD2	2.01	0.59
20:L:179:THR:HG21	20:L:198:ALA:N	2.12	0.59
23:O:139:CYS:SG	23:O:140:VAL:N	2.76	0.59
31:Z:55:THR:HB	43:o:308:LEU:CD2	2.33	0.59
9:A:570:C:C4	9:A:571:U:C4	2.91	0.58
9:A:1287:A:OP2	9:A:1288:U:H5	1.85	0.58
10:B:68:ILE:HG13	10:B:143:LEU:HD11	1.85	0.58
45:r:7:ARG:HB2	45:r:9:TYR:O	2.03	0.58
45:r:142:TYR:HB2	45:r:148:GLY:HA2	1.85	0.58
27:S:56:ASN:HB2	27:S:108:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:307:ARG:HD2	47:u:309:ASN:HB2	1.85	0.58
9:A:1386:A:C6	9:A:1387:G:C5	2.92	0.58
9:A:1598:G:H2'	36:e:81:GLY:H	1.68	0.58
32:a:58:VAL:HG12	32:a:71:LEU:HA	1.85	0.58
9:A:1483:A:C4'	31:Z:160:SER:HB2	2.31	0.58
30:Y:145:TYR:O	30:Y:146:ARG:C	2.45	0.58
48:v:372:VAL:HG23	48:v:384:ILE:HD13	1.84	0.58
3:4:299:SER:O	5:6:345:GLN:NE2	2.37	0.58
10:B:86:ILE:HD13	10:B:113:LEU:HD22	1.85	0.58
47:u:91:ARG:HH21	47:u:173:LEU:HD22	1.68	0.58
9:A:77:A:H2'	9:A:78:C:C6	2.39	0.58
49:w:27:U:H2'	49:w:28:G:C8	2.39	0.58
9:A:809:A:H2'	9:A:810:A:O4'	2.03	0.58
9:A:1719:A:H2'	9:A:1720:U:H5'	1.85	0.58
24:P:64:ALA:CB	24:P:67:ASP:HB2	2.24	0.58
40:k:134:SER:HA	40:k:139:HIS:HA	1.84	0.58
18:J:81:VAL:HG11	18:J:86:LEU:HD13	1.86	0.58
25:Q:58:VAL:HG23	25:Q:59:PHE:N	2.18	0.58
47:u:51:MET:HB3	47:u:89:VAL:HG21	1.85	0.58
4:5:206:LYS:HA	4:5:269:LEU:H	1.69	0.58
9:A:1520:G:N3	9:A:1520:G:H2'	2.18	0.58
9:A:1654:G:OP1	35:d:82:ARG:HD2	2.04	0.58
28:T:104:ARG:HG3	28:T:107:ARG:NH2	2.19	0.58
44:q:42:LEU:C	44:q:44:ASN:H	2.08	0.58
34:c:152:SER:HB2	34:c:170:TRP:HD1	1.69	0.58
44:q:77:ILE:HG22	44:q:94:LYS:HB2	1.86	0.57
45:r:229:LEU:HB3	45:r:235:TYR:HB3	1.86	0.57
9:A:421:G:H5'	10:B:98:LYS:HG3	1.86	0.57
9:A:916:A:C8	17:I:73:ARG:NH2	2.72	0.57
34:c:249:CYS:SG	34:c:258:ILE:HG23	2.44	0.57
47:u:417:GLN:HB3	47:u:420:LYS:HB3	1.86	0.57
9:A:338:G:H2'	9:A:339:A:H8	1.68	0.57
9:A:909:G:C6	9:A:910:G:C6	2.92	0.57
9:A:1283:C:N4	41:m:102:LYS:HE3	2.19	0.57
9:A:1417:C:H1'	35:d:3:GLY:HA2	1.87	0.57
23:O:59:SER:OG	23:O:63:LYS:NZ	2.34	0.57
44:q:95:TYR:HD2	44:q:103:LEU:HD21	1.68	0.57
9:A:154:U:H2'	27:S:4:ASN:HD21	1.70	0.57
9:A:585:C:C2'	9:A:586:G:H5'	2.35	0.57
9:A:1287:A:OP2	9:A:1288:U:C5	2.57	0.57
9:A:1362:U:H5''	9:A:1363:C:C5	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:110:MET:HA	23:O:113:MET:HE2	1.86	0.57
26:R:120:PRO:HA	26:R:137:LEU:HD21	1.86	0.57
45:r:64:ARG:HE	45:r:67:ARG:HB2	1.70	0.57
45:r:197:VAL:CG1	45:r:211:ALA:HB3	2.34	0.57
51:y:570:LEU:HD22	51:y:612:THR:HG21	1.85	0.57
9:A:614:C:C5	9:A:626:G:C4	2.92	0.57
9:A:1208:A:N1	9:A:1209:A:C6	2.72	0.57
12:D:53:ILE:HG23	12:D:77:LEU:HD11	1.87	0.57
45:r:197:VAL:HG12	45:r:211:ALA:HB3	1.86	0.57
31:Z:89:GLU:HB3	43:o:309:ILE:HB	1.84	0.57
47:u:481:GLN:O	47:u:494:GLY:N	2.38	0.57
1:1:291:GLY:HA3	1:1:363:GLU:H	1.69	0.57
9:A:1690:U:N3	9:A:1691:U:C5	2.73	0.57
34:c:70:VAL:HG12	34:c:79:LEU:HB3	1.86	0.57
9:A:845:G:H3'	9:A:846:G:H8	1.70	0.57
50:x:307:ASN:HA	50:x:312:LEU:HD13	1.87	0.57
4:5:473:ALA:HB1	48:v:369:ARG:HH21	1.69	0.57
9:A:613:G:O2'	9:A:626:G:H4'	2.04	0.57
9:A:1424:G:O2'	9:A:1425:G:H5'	2.05	0.57
9:A:1514:G:OP1	39:i:10:HIS:CD2	2.58	0.57
9:A:1690:U:C2	9:A:1691:U:C5	2.92	0.57
24:P:85:CYS:SG	24:P:90:ILE:HB	2.44	0.57
32:a:65:ARG:HH22	39:i:22:ARG:HA	1.70	0.57
48:v:349:GLN:HB2	51:y:833:ALA:HB1	1.87	0.57
6:7:3:A:C2	25:Q:43:ASN:N	2.68	0.56
7:8:31:SER:HA	7:8:37:LYS:HA	1.87	0.56
9:A:489:A:N1	9:A:512:A:C2	2.73	0.56
9:A:851:C:H5''	9:A:852:G:H5'	1.86	0.56
9:A:1386:A:N6	9:A:1387:G:N1	2.53	0.56
22:N:124:VAL:HG21	22:N:134:LEU:HD21	1.87	0.56
42:n:32:VAL:HG23	42:n:42:ILE:HG13	1.87	0.56
9:A:27:A2M:O5'	9:A:27:A2M:H8	2.05	0.56
9:A:857:U:H2'	9:A:858:A:C8	2.41	0.56
20:L:88:ILE:HG13	20:L:93:ILE:HD12	1.87	0.56
9:A:12:U:O2'	9:A:13:C:O4'	2.19	0.56
9:A:447:A:H4'	11:C:3:ARG:HB3	1.88	0.56
9:A:1315:U:C4	9:A:1316:C:C5	2.94	0.56
9:A:1457:U:C2	9:A:1458:G:C8	2.93	0.56
9:A:1484:A:H2'	9:A:1485:U:C6	2.40	0.56
9:A:1754:G:H2'	9:A:1755:C:H4'	1.87	0.56
11:C:107:GLY:HA2	11:C:189:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:193:ASP:HB2	31:Z:196:GLY:HA3	1.87	0.56
44:q:62:ARG:O	44:q:63:GLY:C	2.48	0.56
45:r:196:GLU:HG3	45:r:233:PRO:HB3	1.86	0.56
9:A:660:C:C5	10:B:98:LYS:HE2	2.40	0.56
9:A:913:A:C6	15:G:98:ARG:HG3	2.40	0.56
9:A:1004:U:P	23:O:165:ARG:HH21	2.28	0.56
9:A:1416:C:C2	9:A:1425:G:N2	2.73	0.56
19:K:39:VAL:HG22	19:K:45:ARG:N	2.19	0.56
35:d:143:LYS:O	35:d:143:LYS:HG3	2.04	0.56
38:h:19:ARG:HG2	38:h:92:HIS:HD2	1.70	0.56
38:h:118:ASP:O	38:h:119:ALA:OXT	2.22	0.56
48:v:220:PHE:O	48:v:229:ARG:NH2	2.37	0.56
9:A:489:A:C2	9:A:512:A:N3	2.74	0.56
9:A:1397:U:O4	30:Y:12:VAL:HA	2.06	0.56
15:G:192:PHE:O	15:G:193:GLN:C	2.48	0.56
9:A:992:A:N7	25:Q:15:ARG:NH1	2.53	0.56
12:D:50:LEU:HG	12:D:54:ARG:HD2	1.87	0.56
47:u:319:SER:HB3	47:u:379:VAL:HB	1.88	0.56
49:w:21:G:H2'	49:w:22:C:C6	2.41	0.56
9:A:60:G:H22	9:A:316:G:H21	1.53	0.56
9:A:194:C:H2'	9:A:195:C:C6	2.41	0.56
27:S:21:GLU:HG2	27:S:28:TYR:HE2	1.70	0.56
34:c:164:ILE:HG22	34:c:178:ASN:HA	1.88	0.56
47:u:11:ALA:HB2	47:u:34:VAL:HG21	1.87	0.56
48:v:246:ILE:HD11	50:x:26:ARG:HH22	1.69	0.56
9:A:511:U:H2'	9:A:512:A:C8	2.41	0.56
9:A:931:C:H5''	23:O:157:GLN:OE1	2.06	0.56
9:A:1513:C:H2'	9:A:1514:G:H8	1.71	0.56
29:V:19:LEU:HD21	29:V:69:VAL:HG11	1.88	0.56
9:A:987:A:N1	23:O:120:MET:HE1	2.20	0.56
9:A:1189:A:H2'	9:A:1190:A:C8	2.41	0.56
45:r:63:ILE:O	45:r:63:ILE:CD1	2.45	0.56
45:r:220:THR:HB	45:r:223:MET:HB2	1.87	0.56
47:u:300:TYR:HD2	47:u:376:ARG:HH12	1.54	0.56
9:A:1351:G:C2	9:A:1379:A:C4	2.93	0.56
9:A:1826:G:C2'	9:A:1827:U:H5'	2.36	0.56
19:K:4:ASP:HB2	20:L:173:LYS:O	2.06	0.56
48:v:263:THR:HG21	48:v:328:CYS:HB2	1.88	0.56
9:A:1174:U:H2'	9:A:1175:G:H8	1.72	0.55
24:P:92:ALA:CB	24:P:125:LYS:HB2	2.36	0.55
46:t:442:ALA:HA	46:t:456:TRP:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:w:9:G:H2'	49:w:20:A:C5	2.41	0.55
9:A:888:U:H3	9:A:900:C:H42	1.53	0.55
9:A:1357:A:H5''	20:L:112:VAL:HG11	1.89	0.55
10:B:42:LEU:HD13	10:B:72:ILE:HD11	1.88	0.55
9:A:1249:C:H2'	9:A:1250:A:N7	2.21	0.55
10:B:82:MET:CE	10:B:85:THR:C	2.80	0.55
25:Q:58:VAL:CG2	25:Q:59:PHE:CD2	2.90	0.55
45:r:73:VAL:HA	45:r:85:LEU:HD23	1.87	0.55
45:r:156:ALA:HB3	45:r:180:ILE:HG21	1.88	0.55
49:w:26:C:H2'	49:w:27:U:C6	2.40	0.55
9:A:1859:A:C2	9:A:1860:A:C4	2.94	0.55
22:N:140:VAL:HG13	22:N:142:LEU:HG	1.87	0.55
26:R:104:ILE:HD11	26:R:189:VAL:HG22	1.89	0.55
9:A:884:C:C2	9:A:904:A:H2	2.25	0.55
9:A:1514:G:OP1	39:i:10:HIS:CE1	2.60	0.55
30:Y:89:SER:HB3	30:Y:112:LEU:HD13	1.88	0.55
33:b:17:TYR:HB3	33:b:25:LEU:HD11	1.89	0.55
49:w:67:C:H2'	49:w:68:U:C6	2.40	0.55
51:y:735:GLU:HA	51:y:738:VAL:HG12	1.88	0.55
9:A:688:U:H2'	15:G:103:LYS:HD2	1.88	0.55
9:A:1499:U:H5''	31:Z:176:LEU:HD22	1.88	0.55
9:A:1523:C:C4	37:f:141:ARG:NH1	2.74	0.55
31:Z:195:THR:HA	31:Z:201:LYS:HE2	1.88	0.55
47:u:201:LEU:O	47:u:233:ARG:NH2	2.38	0.55
48:v:349:GLN:OE1	48:v:393:MET:N	2.37	0.55
7:8:258:VAL:CB	51:y:857:LEU:HB2	2.36	0.55
9:A:919:A:H3'	17:l:16:LEU:HD23	1.89	0.55
9:A:1231:C:C4	9:A:1232:U:C5	2.94	0.55
9:A:1386:A:C5	9:A:1387:G:C8	2.94	0.55
9:A:1666:C:H2'	9:A:1667:U:O4'	2.07	0.55
13:E:58:GLU:HA	44:q:62:ARG:HH12	1.71	0.55
27:S:132:ARG:HG3	27:S:133:LEU:HG	1.88	0.55
44:q:51:CYS:SG	44:q:53:ASP:HB3	2.47	0.55
9:A:389:A:H2'	9:A:390:C:C6	2.42	0.55
20:L:180:VAL:HG13	20:L:219:ILE:HD13	1.88	0.55
35:d:142:ASN:OD1	35:d:142:ASN:O	2.24	0.55
50:x:44:ASP:OD1	50:x:47:GLY:N	2.39	0.55
9:A:1544:C:H4'	30:Y:80:GLN:NE2	2.21	0.55
29:V:139:VAL:HG11	42:n:47:LYS:HB2	1.89	0.55
9:A:1232:U:H2'	9:A:1233:G:H8	1.71	0.55
20:L:183:LYS:HG2	20:L:196:ILE:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:127:PRO:HG2	22:N:152:SER:HB3	1.88	0.54
24:P:72:TYR:CZ	24:P:76:LEU:HB2	2.42	0.54
29:V:201:LYS:HA	29:V:204:ARG:HG3	1.89	0.54
34:c:88:ARG:HG2	34:c:100:ARG:HB2	1.89	0.54
9:A:1154:U:H2'	20:L:192:LEU:HD21	1.89	0.54
9:A:1606:G:H5''	35:d:87:VAL:HG13	1.88	0.54
9:A:1865:C:O2	25:Q:92:ARG:HG2	2.07	0.54
26:R:134:GLU:HB3	26:R:138:ASN:HD21	1.73	0.54
9:A:608:C:C2'	9:A:609:U:O5'	2.54	0.54
10:B:82:MET:HE1	10:B:85:THR:HG21	1.80	0.54
32:a:92:ALA:O	32:a:96:ARG:HB2	2.08	0.54
47:u:476:ARG:NH1	51:y:794:THR:OG1	2.40	0.54
9:A:338:G:H2'	9:A:339:A:C8	2.43	0.54
9:A:522:A:H5''	12:D:145:PRO:HD2	1.89	0.54
9:A:1244:U:H2'	9:A:1245:G:H8	1.73	0.54
25:Q:58:VAL:HG22	25:Q:59:PHE:CD2	2.42	0.54
32:a:65:ARG:NH2	39:i:22:ARG:HA	2.23	0.54
47:u:483:ARG:NH2	51:y:797:SER:O	2.40	0.54
51:y:722:GLU:OE1	51:y:742:LYS:NZ	2.41	0.54
9:A:652:U:H2'	9:A:653:A:H8	1.71	0.54
9:A:1416:C:O2	9:A:1425:G:C2	2.61	0.54
51:y:781:ARG:HH11	51:y:817:THR:HG21	1.72	0.54
1:1:544:PHE:HB2	1:1:559:VAL:HB	1.89	0.54
2:3:36:GLN:HA	2:3:41:ALA:HB3	1.89	0.54
3:4:164:SER:CB	7:8:83:PRO:CB	2.86	0.54
9:A:536:A:H3'	9:A:537:C:C5'	2.37	0.54
9:A:1618:C:H2'	9:A:1619:A:C8	2.43	0.54
11:C:18:TRP:HH2	11:C:31:PRO:HD3	1.73	0.54
17:I:63:VAL:HG21	17:I:71:ILE:HG12	1.89	0.54
23:O:182:LYS:O	23:O:186:ASN:ND2	2.41	0.54
30:Y:94:ALA:O	30:Y:95:TYR:C	2.45	0.54
49:w:40:C:H2'	49:w:41:A:H8	1.72	0.54
9:A:640:A:P	14:F:115:ARG:HH22	2.30	0.54
9:A:1125:C:H5''	21:M:128:PHE:CZ	2.43	0.54
9:A:1704:C:O5'	9:A:1704:C:H6	1.90	0.54
45:r:191:ILE:O	45:r:238:THR:HA	2.08	0.54
51:y:358:VAL:HG21	51:y:378:ILE:HD11	1.90	0.54
9:A:60:G:N2	9:A:316:G:H21	2.06	0.54
9:A:1452:A:C5	9:A:1476:A:C2	2.96	0.54
34:c:175:LYS:HB3	34:c:184:LEU:HD11	1.89	0.54
38:h:118:ASP:C	38:h:119:ALA:OXT	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:302:GLY:HA2	43:o:309:ILE:HG23	1.90	0.54
45:r:24:VAL:HA	45:r:34:VAL:HG23	1.90	0.54
45:r:142:TYR:CE2	45:r:151:ASP:HB3	2.42	0.54
24:P:72:TYR:CE2	24:P:76:LEU:HB2	2.43	0.54
25:Q:75:VAL:O	25:Q:79:ILE:HG12	2.07	0.54
35:d:140:ALA:O	35:d:143:LYS:O	2.25	0.54
37:f:22:GLY:CA	37:f:56:ALA:HB3	2.34	0.54
11:C:100:ARG:HH12	11:C:122:LYS:HA	1.72	0.53
28:T:57:VAL:HB	28:T:60:PHE:CE1	2.40	0.53
46:t:167:GLN:O	46:t:169:GLN:N	2.37	0.53
22:N:77:ILE:HA	22:N:99:ILE:O	2.08	0.53
39:i:21:CYS:HB3	39:i:25:SER:N	2.23	0.53
9:A:1323:U:H2'	9:A:1324:G:C8	2.44	0.53
9:A:1349:G:C8	9:A:1350:U:H5	2.23	0.53
16:H:31:TYR:HE2	16:H:33:MET:HE3	1.73	0.53
47:u:561:SER:O	47:u:565:HIS:N	2.39	0.53
6:7:23:A:N1	31:Z:108:LYS:CD	2.70	0.53
45:r:73:VAL:HG13	45:r:83:ILE:HG13	1.90	0.53
51:y:52:ALA:HA	51:y:55:LYS:HE2	1.89	0.53
1:1:509:LEU:HD21	1:1:532:ARG:HD2	1.91	0.53
1:1:682:TRP:HA	1:1:693:LYS:HA	1.91	0.53
34:c:46:THR:H	34:c:53:GLY:HA2	1.73	0.53
44:q:46:ARG:HA	44:q:59:CYS:O	2.09	0.53
1:1:525:TYR:OH	1:1:548:ARG:NH2	2.41	0.53
9:A:1315:U:H2'	9:A:1316:C:H6	1.72	0.53
9:A:1337:C:H2'	9:A:1338:G:H8	1.72	0.53
23:O:57:ILE:HG23	23:O:59:SER:H	1.74	0.53
27:S:50:VAL:HG22	27:S:111:LEU:HB3	1.91	0.53
44:q:78:LEU:HB2	44:q:92:ILE:HB	1.90	0.53
47:u:337:ASP:N	47:u:337:ASP:OD1	2.41	0.53
49:w:58:A:H3'	49:w:59:A:C8	2.36	0.53
3:4:307:PHE:O	47:u:538:LYS:NZ	2.42	0.53
9:A:107:A:C6	9:A:108:G:C6	2.97	0.53
9:A:386:C:H2'	9:A:387:C:C6	2.43	0.53
23:O:70:SER:OG	23:O:71:LEU:N	2.42	0.53
31:Z:49:ILE:HD12	43:o:309:ILE:CD1	2.39	0.53
45:r:190:LYS:HG2	45:r:278:VAL:O	2.09	0.53
45:r:192:ARG:HG2	45:r:238:THR:HG22	1.90	0.53
45:r:214:ALA:HB3	45:r:258:ILE:HA	1.90	0.53
45:r:222:ASN:O	45:r:224:PRO:HD3	2.09	0.53
47:u:109:GLN:HA	47:u:112:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:270:GLN:HB2	47:u:306:MET:HE1	1.90	0.53
9:A:660:C:H5''	13:E:3:LYS:HD3	1.89	0.53
9:A:1093:A:H4'	18:J:3:ARG:HH22	1.74	0.53
20:L:128:VAL:HG11	20:L:155:ILE:HA	1.90	0.53
31:Z:170:THR:HG22	31:Z:187:LYS:HG2	1.90	0.53
51:y:589:MET:O	51:y:595:GLN:NE2	2.41	0.53
1:1:616:TRP:HA	1:1:623:VAL:HA	1.90	0.53
9:A:1647:A:OP1	30:Y:138:ARG:NH1	2.42	0.53
12:D:111:GLN:HE21	12:D:123:ILE:HG13	1.73	0.53
23:O:32:ASP:HA	23:O:46:LYS:HA	1.91	0.53
51:y:694:GLU:OE2	51:y:715:HIS:NE2	2.42	0.53
9:A:877:C:H2'	9:A:878:G:C8	2.44	0.53
44:q:77:ILE:HA	44:q:94:LYS:HA	1.90	0.53
47:u:544:GLN:O	47:u:548:GLU:N	2.41	0.53
48:v:304:ASP:OD1	48:v:304:ASP:N	2.42	0.53
9:A:1690:U:H2'	9:A:1691:U:H6	1.72	0.52
45:r:155:HIS:CE1	45:r:159:ASP:HB2	2.44	0.52
9:A:429:C:C2	9:A:430:C:C6	2.98	0.52
9:A:615:C:OP1	44:q:64:LYS:HG2	2.09	0.52
9:A:1116:C:H5'	47:u:63:LYS:HE2	1.91	0.52
9:A:1536:G:H2'	9:A:1537:A:C8	2.44	0.52
20:L:179:THR:HG22	20:L:180:VAL:N	2.25	0.52
27:S:49:VAL:CB	27:S:114:VAL:HG12	2.34	0.52
29:V:76:MET:HA	29:V:155:CYS:SG	2.48	0.52
48:v:262:ILE:O	48:v:335:ASN:ND2	2.41	0.52
49:w:24:U:H2'	49:w:25:G:C8	2.45	0.52
50:x:169:GLU:O	50:x:521:SER:N	2.43	0.52
9:A:862:A:C8	18:J:107:SER:HA	2.44	0.52
9:A:1452:A:HO2'	9:A:1475:G:N2	2.07	0.52
9:A:1672:U:O3'	30:Y:76:GLY:HA3	2.09	0.52
45:r:44:GLY:HA3	45:r:83:ILE:CG2	2.39	0.52
28:T:104:ARG:HG3	28:T:107:ARG:HH22	1.74	0.52
30:Y:45:ARG:O	30:Y:46:THR:C	2.49	0.52
44:q:59:CYS:HA	44:q:89:ALA:O	2.10	0.52
45:r:192:ARG:CG	45:r:278:VAL:HG11	2.38	0.52
51:y:358:VAL:HG22	51:y:374:ILE:HG13	1.90	0.52
5:6:317:ARG:HH12	47:u:398:PHE:H	1.57	0.52
6:7:3:A:H2	25:Q:43:ASN:H	1.50	0.52
9:A:44:U:H2'	9:A:45:A:H2'	1.92	0.52
9:A:358:C:O2'	9:A:359:U:H5'	2.08	0.52
9:A:909:G:C5	9:A:910:G:N7	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1667:U:H2'	9:A:1668:U:C6	2.44	0.52
40:k:135:HIS:HB2	40:k:138:ARG:O	2.09	0.52
45:r:72:VAL:HG12	45:r:90:VAL:HG22	1.92	0.52
51:y:130:MET:HA	51:y:134:ASN:HB2	1.92	0.52
51:y:831:LEU:HD21	51:y:846:ARG:HB2	1.90	0.52
5:6:322:TYR:HB3	5:6:332:VAL:HA	1.92	0.52
9:A:497:C:N3	9:A:498:C:C4	2.78	0.52
9:A:1798:C:H2'	9:A:1799:G:O4'	2.10	0.52
12:D:110:LEU:HB2	12:D:147:PHE:HB3	1.90	0.52
34:c:14:HIS:CE1	34:c:35:SER:HB2	2.44	0.52
9:A:1607:A:OP1	35:d:87:VAL:HG22	2.10	0.52
9:A:1673:U:H5''	30:Y:78:VAL:HG23	1.91	0.52
9:A:1808:U:H2'	9:A:1809:A:C8	2.45	0.52
9:A:1844:U:H2'	9:A:1845:A:C8	2.45	0.52
9:A:113:G:N2	9:A:292:A:C4	2.78	0.52
20:L:179:THR:HG23	20:L:221:ASP:O	2.09	0.52
21:M:109:LEU:HG	21:M:111:PHE:HD2	1.75	0.52
26:R:199:LEU:O	26:R:203:LYS:HB2	2.08	0.52
43:o:241:ILE:HD13	43:o:314:TRP:HA	1.92	0.52
11:C:68:ARG:HB3	11:C:76:VAL:HG11	1.91	0.52
12:D:53:ILE:HD13	12:D:81:LEU:HD21	1.91	0.52
26:R:141:ARG:HD2	26:R:146:GLN:HG2	1.92	0.52
30:Y:10:VAL:CG2	30:Y:25:CYS:HB3	2.40	0.52
46:t:85:ASN:HA	46:t:131:SER:HA	1.91	0.52
50:x:31:GLN:HG3	51:y:591:MET:O	2.10	0.52
9:A:1283:C:N4	41:m:102:LYS:HB3	2.25	0.52
9:A:1514:G:OP1	39:i:10:HIS:CG	2.63	0.52
9:A:1797:U:H2'	9:A:1798:C:C6	2.44	0.52
10:B:58:LYS:HG3	10:B:59:LYS:HG3	1.92	0.52
23:O:187:LYS:HG3	47:u:21:VAL:HG21	1.92	0.52
24:P:28:PHE:HE1	25:Q:58:VAL:HG11	1.75	0.52
34:c:292:SER:HB2	34:c:297:THR:HB	1.92	0.52
47:u:408:THR:HA	47:u:411:LEU:HB2	1.91	0.52
2:3:81:ASP:O	2:3:85:CYS:N	2.41	0.51
9:A:1351:G:N2	9:A:1379:A:C4	2.78	0.51
9:A:1438:A:H2'	9:A:1439:A:C8	2.45	0.51
51:y:333:LEU:HD13	51:y:374:ILE:HG22	1.91	0.51
9:A:27:A2M:CM'	9:A:483:C:H1'	2.38	0.51
10:B:40:ILE:HD13	10:B:62:PHE:HE1	1.75	0.51
21:M:65:PRO:HA	21:M:74:GLN:HE22	1.74	0.51
36:e:50:PHE:HE2	36:e:87:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:x:195:CYS:HA	50:x:359:ARG:HA	1.92	0.51
9:A:1276:A:O2'	32:a:51:SER:HA	2.10	0.51
9:A:1349:G:H2'	9:A:1350:U:C6	2.45	0.51
9:A:1757:G:H8	9:A:1777:G:H1	1.59	0.51
18:J:69:LEU:HD11	18:J:129:PHE:HB2	1.92	0.51
23:O:76:ASN:O	47:u:13:LYS:HE2	2.09	0.51
5:6:344:LYS:HG3	5:6:351:TYR:HE2	1.75	0.51
9:A:409:C:C2	9:A:432:G:N2	2.79	0.51
9:A:634:A:H2'	9:A:635:G:N7	2.25	0.51
9:A:694:G:H8	9:A:694:G:O5'	1.93	0.51
2:3:151:GLN:O	2:3:189:ILE:N	2.43	0.51
9:A:180:G:H2'	9:A:181:A:C8	2.46	0.51
9:A:304:C:H2'	9:A:308:G:C2	2.45	0.51
9:A:489:A:N6	9:A:512:A:N6	2.58	0.51
9:A:905:C:H2'	9:A:906:U:C6	2.46	0.51
9:A:1295:A:H3'	9:A:1296:U:H6	1.75	0.51
10:B:152:LYS:H	10:B:152:LYS:HD2	1.75	0.51
15:G:63:PHE:HA	15:G:95:ILE:O	2.10	0.51
22:N:7:VAL:HG12	22:N:191:ARG:HG2	1.92	0.51
27:S:45:TRP:CZ3	27:S:121:ILE:CD1	2.93	0.51
31:Z:45:ARG:HH11	31:Z:85:GLU:HG3	1.76	0.51
32:a:80:ARG:HD3	32:a:87:PRO:HA	1.93	0.51
49:w:56:G:H2'	49:w:57:A:N7	2.26	0.51
9:A:77:A:H5'	27:S:154:ARG:HB3	1.92	0.51
26:R:139:LYS:HB3	26:R:141:ARG:CZ	2.40	0.51
36:e:63:PRO:HG2	36:e:96:LEU:HD23	1.92	0.51
51:y:449:GLU:OE2	51:y:501:ARG:NH1	2.44	0.51
9:A:409:C:N3	9:A:432:G:C2	2.78	0.51
45:r:23:ASN:HB2	45:r:37:LEU:HD23	1.91	0.51
9:A:215:G:H2'	9:A:216:C:C6	2.46	0.51
9:A:489:A:N1	9:A:512:A:N1	2.59	0.51
9:A:797:C:C4'	9:A:798:G:OP2	2.57	0.51
9:A:1422:G:H2'	9:A:1422:G:N3	2.24	0.51
20:L:60:TRP:HE1	20:L:90:GLU:CD	2.18	0.51
23:O:175:GLU:OE1	23:O:187:LYS:NZ	2.41	0.51
34:c:173:LEU:HD13	34:c:187:ASN:HD21	1.76	0.51
38:h:97:ILE:O	38:h:100:GLN:CG	2.53	0.51
45:r:225:ILE:HG22	45:r:251:LEU:HD12	1.92	0.51
51:y:602:ASP:OD1	51:y:602:ASP:N	2.41	0.51
2:3:8:ARG:O	2:3:12:GLY:N	2.40	0.51
5:6:324:LYS:O	47:u:449:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:877:C:C2	9:A:910:G:N2	2.78	0.51
9:A:1316:C:H2'	9:A:1317:C:C6	2.46	0.51
34:c:17:TRP:HB2	34:c:36:ARG:HG3	1.93	0.51
34:c:32:LEU:HB3	34:c:69:VAL:HG21	1.92	0.51
47:u:80:GLN:HA	47:u:83:ILE:HB	1.93	0.51
47:u:564:GLU:HA	47:u:567:ARG:HB2	1.92	0.51
51:y:833:ALA:HB2	51:y:844:MET:HE3	1.92	0.51
3:4:263:ILE:O	3:4:265:LEU:N	2.44	0.51
9:A:566:U:H3'	9:A:567:C:H6	1.76	0.51
9:A:1149:A:H2'	9:A:1149:A:N3	2.24	0.51
50:x:25:PHE:O	50:x:26:ARG:NE	2.44	0.51
51:y:422:GLU:HB3	51:y:433:ASN:HD21	1.76	0.51
9:A:15:U:H2'	9:A:16:G:O4'	2.11	0.50
9:A:497:C:O2'	9:A:498:C:H5'	2.11	0.50
9:A:877:C:C2	9:A:910:G:C2	2.99	0.50
9:A:1259:A:H3'	9:A:1259:A:N3	2.27	0.50
9:A:1351:G:N1	9:A:1379:A:N6	2.56	0.50
31:Z:55:THR:HB	43:o:308:LEU:HD22	1.93	0.50
36:e:50:PHE:HD1	36:e:54:THR:HB	1.75	0.50
45:r:160:PRO:HB3	45:r:177:ILE:HG21	1.93	0.50
47:u:443:VAL:HG22	47:u:447:TYR:HB2	1.93	0.50
51:y:511:TYR:OH	51:y:611:ARG:NH1	2.44	0.50
3:4:299:SER:CB	5:6:345:GLN:HG2	2.40	0.50
5:6:204:ALA:O	5:6:208:ILE:N	2.45	0.50
9:A:287:U:H2'	9:A:288:G:C8	2.46	0.50
9:A:570:C:H2'	9:A:571:U:O4'	2.11	0.50
9:A:1258:A:N1	9:A:1663:A:H2'	2.27	0.50
9:A:1377:U:H2'	22:N:102:ARG:HH21	1.76	0.50
9:A:1661:A:C8	39:i:14:PHE:HB2	2.46	0.50
23:O:62:LEU:O	23:O:88:THR:OG1	2.24	0.50
34:c:203:ASP:HB2	34:c:205:SER:H	1.77	0.50
51:y:468:GLU:HA	51:y:471:GLU:HB2	1.93	0.50
1:1:546:ILE:O	1:1:557:ASP:N	2.36	0.50
5:6:326:ASP:OD1	5:6:326:ASP:N	2.42	0.50
9:A:614:C:C5	9:A:626:G:N3	2.79	0.50
9:A:1543:U:H2'	30:Y:77:HIS:HE1	1.77	0.50
26:R:83:TYR:HB2	26:R:202:ILE:HG12	1.93	0.50
43:o:250:THR:O	43:o:251:ARG:NH1	2.43	0.50
45:r:191:ILE:HG22	45:r:251:LEU:HD22	1.92	0.50
45:r:229:LEU:HD13	45:r:232:PRO:HA	1.93	0.50
47:u:387:VAL:HG12	47:u:410:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:558:LEU:O	47:u:562:ARG:N	2.44	0.50
51:y:330:ILE:O	51:y:334:ASN:ND2	2.44	0.50
1:1:342:TRP:HA	1:1:349:LEU:HA	1.93	0.50
9:A:441:C:H2'	9:A:442:C:C6	2.47	0.50
47:u:564:GLU:O	47:u:568:ILE:N	2.41	0.50
48:v:265:LYS:NZ	48:v:335:ASN:OD1	2.39	0.50
4:5:210:GLU:O	4:5:214:PHE:N	2.45	0.50
16:H:34:ASP:O	16:H:79:PHE:HA	2.11	0.50
33:b:108:LYS:O	33:b:111:MET:HG2	2.12	0.50
34:c:241:PHE:HE1	34:c:261:LEU:HD11	1.75	0.50
43:o:246:LEU:HD22	43:o:250:THR:HG21	1.93	0.50
1:1:481:PHE:HB2	1:1:494:THR:HB	1.92	0.50
9:A:113:G:N1	9:A:292:A:C5	2.79	0.50
9:A:539:C:H41	9:A:542:U:H5''	1.77	0.50
9:A:556:U:H3'	9:A:557:U:C5'	2.42	0.50
9:A:1859:A:H61	9:A:1860:A:N6	2.05	0.50
14:F:86:VAL:HA	14:F:89:GLN:HG2	1.94	0.50
5:6:313:ILE:HG21	47:u:399:ASN:HA	1.94	0.50
9:A:541:U:H2'	9:A:542:U:H5	1.77	0.50
9:A:1653:U:H2'	9:A:1654:G:C8	2.47	0.50
18:J:39:THR:O	18:J:43:LYS:HG2	2.11	0.50
25:Q:39:PHE:HE2	25:Q:68:TYR:HD2	1.59	0.50
9:A:1:U:O2	9:A:3:C:C5	2.64	0.50
9:A:5:U:H2'	9:A:6:G:C8	2.47	0.50
9:A:497:C:N4	9:A:498:C:N4	2.59	0.50
31:Z:109:LEU:HD21	31:Z:115:VAL:HA	1.94	0.50
32:a:90:VAL:HG21	32:a:95:ARG:HB3	1.94	0.50
35:d:114:GLU:HG2	35:d:124:THR:HG22	1.94	0.50
41:m:121:LYS:O	41:m:125:GLU:N	2.40	0.50
22:N:15:VAL:HG12	22:N:19:LEU:HD23	1.93	0.50
45:r:71:VAL:HG21	45:r:85:LEU:HD13	1.94	0.50
45:r:190:LYS:HA	45:r:239:THR:O	2.11	0.50
45:r:209:LYS:HG3	45:r:213:ARG:HB2	1.94	0.50
5:6:316:VAL:HG21	47:u:446:ILE:CD1	2.41	0.49
9:A:75:G:H4'	9:A:76:U:H5'	1.94	0.49
9:A:497:C:N4	9:A:498:C:H41	2.10	0.49
9:A:1310:U:H2'	9:A:1311:C:C6	2.47	0.49
21:M:86:PRO:HD2	22:N:200:ASP:HB3	1.95	0.49
31:Z:59:LEU:HD13	43:o:308:LEU:CG	2.39	0.49
34:c:249:CYS:HG	34:c:291:TRP:NE1	2.10	0.49
45:r:265:LYS:O	45:r:266:ARG:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:112:VAL:HA	47:u:115:ILE:HB	1.93	0.49
1:1:518:HIS:HB2	1:1:527:CYS:HB2	1.94	0.49
9:A:536:A:P	9:A:537:C:H5''	2.52	0.49
9:A:1860:A:O2'	9:A:1862:G:H8	1.95	0.49
10:B:10:TYR:HE2	10:B:12:LYS:HB3	1.78	0.49
33:b:83:MET:HB3	33:b:116:LEU:HD12	1.93	0.49
44:q:46:ARG:O	44:q:59:CYS:N	2.43	0.49
44:q:100:ALA:HA	44:q:103:LEU:HD22	1.94	0.49
10:B:40:ILE:HD13	10:B:62:PHE:CE1	2.48	0.49
35:d:39:LEU:O	35:d:96:SER:HB3	2.13	0.49
40:k:119:ARG:HD2	40:k:139:HIS:HB3	1.93	0.49
48:v:261:VAL:HG23	48:v:262:ILE:HG13	1.94	0.49
9:A:191:A:H62	9:A:208:G:H21	1.60	0.49
9:A:609:U:H2'	9:A:610:G:H8	1.76	0.49
20:L:136:HIS:HB3	20:L:162:ILE:CG2	2.43	0.49
21:M:41:ILE:HD12	21:M:47:ARG:HG2	1.95	0.49
34:c:66:VAL:HA	34:c:82:SER:HB2	1.94	0.49
41:m:93:LYS:HZ3	41:m:102:LYS:HD3	1.77	0.49
45:r:183:ARG:NH1	49:w:54:U:H4'	2.26	0.49
9:A:1348:G:N3	9:A:1348:G:H5''	2.26	0.49
9:A:1813:A:C6	9:A:1814:G:C4	3.00	0.49
27:S:50:VAL:CG2	27:S:111:LEU:HB3	2.42	0.49
31:Z:26:THR:O	31:Z:30:ALA:HB2	2.13	0.49
31:Z:190:LEU:HB2	31:Z:200:PRO:HD3	1.93	0.49
32:a:63:ALA:HB3	32:a:68:TYR:HE1	1.76	0.49
34:c:101:PHE:CE2	34:c:136:GLY:HA2	2.47	0.49
51:y:601:ALA:O	51:y:606:GLN:NE2	2.46	0.49
9:A:29:G:H4'	13:E:129:SER:HB2	1.93	0.49
9:A:608:C:H2'	9:A:609:U:O5'	2.12	0.49
9:A:1092:G:C2	9:A:1158:G:C5	2.99	0.49
9:A:1249:C:H2'	9:A:1250:A:C5	2.47	0.49
9:A:1311:C:H42	40:k:97:LYS:NZ	2.10	0.49
47:u:567:ARG:HB3	47:u:572:ARG:HA	1.95	0.49
49:w:35:U:H2'	49:w:36:A:C8	2.48	0.49
4:5:473:ALA:HB1	48:v:369:ARG:NH2	2.27	0.49
6:7:3:A:H2	25:Q:43:ASN:N	2.09	0.49
9:A:394:G:P	51:y:150:ARG:HH22	2.35	0.49
9:A:845:G:H3'	9:A:846:G:C8	2.47	0.49
9:A:1673:U:O3'	30:Y:78:VAL:HG21	2.13	0.49
21:M:18:GLU:HG3	21:M:69:ILE:HG22	1.94	0.49
21:M:106:LEU:HD21	22:N:19:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:85:ILE:HG21	33:b:111:MET:HG3	1.94	0.49
45:r:91:SER:H	45:r:94:GLU:HB2	1.78	0.49
49:w:50:U:H3	49:w:62:A:N6	2.11	0.49
5:6:316:VAL:HG11	47:u:446:ILE:CD1	2.42	0.49
9:A:496:C:H2'	9:A:497:C:C6	2.48	0.49
9:A:566:U:H3'	9:A:567:C:C6	2.47	0.49
9:A:1047:C:H42	9:A:1071:G:H1	1.59	0.49
9:A:1221:G:H2'	9:A:1222:G:C8	2.48	0.49
9:A:1342:U:H4'	9:A:1343:U:H6	1.78	0.49
18:J:18:GLU:CD	18:J:67:GLY:HA2	2.38	0.49
42:n:32:VAL:O	42:n:41:SER:HA	2.13	0.49
47:u:319:SER:HA	47:u:322:VAL:HG12	1.93	0.49
26:R:84:ASN:HD21	26:R:97:VAL:HG22	1.78	0.49
9:A:71:G:H2'	9:A:72:C:O4'	2.12	0.49
9:A:74:G:H5''	9:A:76:U:O2	2.12	0.49
9:A:825:A:H2'	9:A:826:A:C8	2.48	0.49
9:A:877:C:O2	9:A:910:G:C2	2.66	0.49
9:A:1500:G:H2'	9:A:1501:C:O4'	2.13	0.49
23:O:52:THR:HG22	23:O:58:ALA:H	1.77	0.49
24:P:65:ASP:HA	24:P:68:GLU:HG3	1.95	0.49
40:k:140:TYR:HA	40:k:146:LEU:O	2.12	0.49
47:u:23:LYS:HB3	47:u:26:PRO:HD2	1.95	0.49
9:A:1229:G:H2'	9:A:1230:C:O4'	2.13	0.48
11:C:68:ARG:HE	11:C:76:VAL:HG11	1.77	0.48
11:C:122:LYS:HE2	11:C:124:CYS:SG	2.53	0.48
20:L:179:THR:HG22	20:L:180:VAL:H	1.78	0.48
41:m:45:ARG:HG2	41:m:72:HIS:CD2	2.48	0.48
44:q:29:LYS:HG2	44:q:30:GLU:N	2.28	0.48
47:u:562:ARG:HD3	47:u:562:ARG:HA	1.60	0.48
2:3:9:ALA:O	2:3:13:LYS:N	2.44	0.48
9:A:1377:U:H2'	22:N:102:ARG:NH2	2.28	0.48
9:A:1850:MA6:H93	9:A:1850:MA6:N7	2.27	0.48
11:C:44:LEU:HD13	11:C:72:ILE:HD11	1.95	0.48
11:C:100:ARG:HH21	11:C:118:GLU:HG2	1.78	0.48
47:u:476:ARG:HB2	51:y:795:TYR:HE1	1.78	0.48
5:6:323:CYS:HB3	47:u:448:GLN:CB	2.37	0.48
9:A:5:U:H2'	9:A:6:G:H8	1.78	0.48
9:A:1575:G:H2'	9:A:1576:G:C8	2.47	0.48
22:N:65:ILE:HG23	22:N:74:VAL:HG21	1.95	0.48
26:R:96:LEU:O	26:R:179:PRO:HG2	2.13	0.48
34:c:87:LEU:HB2	34:c:101:PHE:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:437:PHE:HA	1:1:451:THR:H	1.78	0.48
9:A:520:A:C4	9:A:521:A:C8	3.02	0.48
9:A:640:A:H2'	9:A:641:A:C8	2.49	0.48
9:A:963:A:H2'	9:A:964:A:C8	2.49	0.48
9:A:1277:C:O5'	9:A:1277:C:H6	1.95	0.48
9:A:1407:U:H2'	9:A:1408:U:C6	2.49	0.48
15:G:43:LEU:HB3	15:G:72:PHE:CE2	2.48	0.48
29:V:91:ARG:HD3	36:e:103:HIS:CE1	2.48	0.48
45:r:86:SER:HB2	45:r:88:ARG:HG2	1.95	0.48
47:u:520:ARG:HA	47:u:523:LEU:HD12	1.95	0.48
9:A:91:A:H61	27:S:89:THR:HG23	1.78	0.48
9:A:1598:G:H3'	36:e:80:ARG:HG2	1.96	0.48
13:E:61:GLN:O	13:E:62:PRO:C	2.55	0.48
15:G:146:VAL:HG22	15:G:152:ARG:HG2	1.95	0.48
46:t:441:ILE:O	46:t:457:GLY:N	2.47	0.48
50:x:360:TYR:HE1	50:x:374:ARG:HG3	1.78	0.48
5:6:326:ASP:N	47:u:449:SER:OG	2.46	0.48
9:A:883:U:O2	9:A:904:A:N6	2.47	0.48
9:A:1379:A:H2'	9:A:1380:C:C6	2.49	0.48
9:A:1757:G:H8	9:A:1777:G:H22	1.61	0.48
9:A:1826:G:H2'	9:A:1827:U:H5'	1.94	0.48
23:O:101:HIS:ND1	23:O:101:HIS:O	2.46	0.48
30:Y:86:GLN:HE22	30:Y:122:ALA:HB2	1.77	0.48
43:o:243:VAL:HB	43:o:283:ALA:HB3	1.94	0.48
47:u:179:GLN:NE2	47:u:231:GLU:OE1	2.46	0.48
48:v:208:LEU:HD21	48:v:246:ILE:HB	1.95	0.48
3:4:288:GLN:CB	5:6:348:GLN:NE2	2.75	0.48
7:8:258:VAL:HA	51:y:857:LEU:HD22	1.96	0.48
9:A:113:G:C2	9:A:292:A:C2	3.02	0.48
9:A:113:G:N3	9:A:292:A:C2	2.82	0.48
9:A:1556:A:N3	9:A:1556:A:H2'	2.27	0.48
9:A:1699:A:H5'	9:A:1702:G:H4'	1.95	0.48
9:A:1758:G:H4'	9:A:1774:C:C6	2.49	0.48
11:C:102:ILE:HD12	11:C:239:PRO:HD3	1.94	0.48
18:J:77:PRO:HG2	18:J:79:PHE:CE2	2.49	0.48
20:L:104:ASP:HB3	20:L:130:ILE:HG23	1.95	0.48
20:L:182:CYS:SG	20:L:183:LYS:N	2.87	0.48
50:x:301:ASP:HB3	50:x:309:PRO:HD3	1.94	0.48
51:y:339:ALA:HA	51:y:342:LYS:HD2	1.94	0.48
51:y:515:ASP:H	51:y:579:HIS:CE1	2.32	0.48
9:A:1064:C:OP1	24:P:149:ARG:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1587:G:C6	35:d:67:ARG:HG2	2.48	0.48
22:N:183:LEU:HB3	22:N:189:ILE:HG12	1.95	0.48
31:Z:138:VAL:HG22	31:Z:184:ILE:HD13	1.96	0.48
34:c:51:ASN:HB3	34:c:53:GLY:H	1.79	0.48
34:c:178:ASN:HB3	34:c:181:ASN:OD1	2.14	0.48
35:d:75:MET:HA	35:d:78:ILE:HG13	1.95	0.48
44:q:63:GLY:O	44:q:66:ARG:N	2.44	0.48
45:r:227:ILE:HD12	45:r:235:TYR:CD2	2.39	0.48
49:w:44:G:H5'	49:w:45:G:C6	2.49	0.48
50:x:28:MET:HE1	51:y:591:MET:HE1	1.96	0.48
9:A:1386:A:C5	9:A:1387:G:C4	3.01	0.48
10:B:35:ARG:HH11	10:B:35:ARG:HB2	1.79	0.48
26:R:143:LYS:HB2	26:R:143:LYS:HE2	1.54	0.48
28:T:55:ILE:HD13	28:T:75:ILE:HG23	1.95	0.48
50:x:225:HIS:O	50:x:374:ARG:NH2	2.45	0.48
51:y:643:LYS:HG3	51:y:650:LEU:HB2	1.96	0.48
2:3:170:LEU:O	2:3:174:MET:N	2.39	0.48
5:6:325:ILE:HD13	5:6:329:GLN:HB3	1.95	0.48
9:A:543:C:H5''	9:A:544:G:C8	2.48	0.48
9:A:1101:U:H2'	9:A:1102:G:C8	2.48	0.48
9:A:1209:A:N1	9:A:1691:U:C4	2.81	0.48
9:A:1322:G:H2'	9:A:1323:U:O4'	2.13	0.48
38:h:68:THR:OG1	38:h:70:CYS:O	2.28	0.48
41:m:46:GLN:OE1	41:m:112:LYS:NZ	2.38	0.48
1:1:380:ASP:N	1:1:389:VAL:O	2.42	0.47
9:A:291:G:H2'	9:A:292:A:C8	2.48	0.47
9:A:1242:U:O2'	9:A:1518:C:H5'	2.14	0.47
9:A:1621:U:O2'	9:A:1622:U:H2'	2.14	0.47
16:H:8:LEU:HD13	18:J:53:ILE:HD11	1.95	0.47
29:V:16:ASP:N	50:x:384:ALA:HB1	2.29	0.47
38:h:118:ASP:O	38:h:119:ALA:C	2.57	0.47
50:x:322:ASN:OD1	50:x:323:PHE:N	2.47	0.47
50:x:447:LEU:HB2	50:x:473:PRO:HG3	1.96	0.47
9:A:751:G:H3'	9:A:752:G:H5''	1.96	0.47
9:A:1266:C:H2'	9:A:1267:C:C6	2.49	0.47
9:A:1285:G:OP1	41:m:105:GLY:O	2.32	0.47
10:B:21:LYS:HZ1	26:R:156:ALA:HA	1.78	0.47
25:Q:43:ASN:HA	25:Q:66:LYS:HA	1.96	0.47
26:R:146:GLN:HA	26:R:149:TYR:HD2	1.79	0.47
40:k:138:ARG:HD2	40:k:149:CYS:HA	1.96	0.47
41:m:26:LEU:HD22	41:m:90:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:103:LEU:HB3	44:q:109:LEU:HB2	1.95	0.47
45:r:239:THR:HG21	45:r:247:GLY:HA3	1.96	0.47
47:u:52:LEU:HD12	47:u:89:VAL:HG23	1.96	0.47
48:v:208:LEU:HG	48:v:242:TYR:HD1	1.78	0.47
50:x:432:LEU:HD12	50:x:476:PHE:HZ	1.78	0.47
1:l:378:LEU:N	1:l:391:PHE:O	2.45	0.47
9:A:429:C:H2'	9:A:430:C:H6	1.78	0.47
9:A:1851:MA6:H93	9:A:1851:MA6:N7	2.28	0.47
34:c:143:GLN:HE21	34:c:143:GLN:HB2	1.56	0.47
39:i:13:LYS:HB2	39:i:13:LYS:HE2	1.51	0.47
44:q:40:LYS:HG3	44:q:48:GLU:OE2	2.14	0.47
45:r:196:GLU:HB3	45:r:270:ASN:HB3	1.95	0.47
50:x:31:GLN:HE22	50:x:67:SER:N	2.10	0.47
1:l:549:MET:HA	1:l:554:VAL:HG13	1.96	0.47
9:A:982:G:H2'	9:A:983:A:C8	2.49	0.47
9:A:1257:G:H4'	9:A:1258:A:C5'	2.44	0.47
9:A:1402:A:N6	9:A:1441:U:C2	2.83	0.47
9:A:1405:A:H2'	9:A:1406:G:O4'	2.14	0.47
9:A:1754:G:C2'	9:A:1755:C:OP1	2.63	0.47
9:A:1760:G:H21	9:A:1772:C:H3'	1.80	0.47
9:A:1788:A:H2'	9:A:1789:G:O4'	2.14	0.47
9:A:16:G:H2'	9:A:17:C:C6	2.49	0.47
9:A:484:A2M:HM'3	9:A:484:A2M:H1'	1.47	0.47
9:A:644:OMG:HM23	9:A:644:OMG:H1'	1.55	0.47
9:A:1457:U:C2	9:A:1458:G:N7	2.81	0.47
30:Y:24:HIS:CD2	30:Y:26:LYS:HD2	2.50	0.47
37:f:86:ARG:HH11	37:f:106:LYS:HD2	1.79	0.47
44:q:104:LYS:HG2	44:q:109:LEU:O	2.14	0.47
9:A:429:C:O2	9:A:430:C:C6	2.67	0.47
9:A:440:G:O2'	9:A:1737:G:H1'	2.14	0.47
9:A:666:U:O5'	9:A:666:U:H6	1.96	0.47
9:A:1719:A:C2'	9:A:1720:U:H5'	2.43	0.47
27:S:159:ARG:NE	27:S:173:ALA:HB2	2.30	0.47
31:Z:53:THR:HG22	31:Z:91:VAL:HG11	1.96	0.47
48:v:209:GLN:HG2	48:v:209:GLN:H	1.37	0.47
9:A:652:U:H2'	9:A:653:A:C8	2.48	0.47
9:A:912:C:H3'	9:A:913:A:H5''	1.97	0.47
9:A:940:U:H3	9:A:1002:U:H3	1.63	0.47
9:A:958:G:H2'	9:A:959:G:C8	2.49	0.47
9:A:1101:U:H2'	9:A:1102:G:H8	1.79	0.47
9:A:1311:C:H42	40:k:97:LYS:HZ1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1550:G:H3'	9:A:1579:A:H61	1.80	0.47
9:A:1575:G:H2'	9:A:1576:G:H8	1.79	0.47
9:A:1742:C:C2	9:A:1793:A:C2	3.02	0.47
11:C:254:LYS:HB2	11:C:254:LYS:HE3	1.67	0.47
15:G:27:LEU:O	15:G:31:GLU:N	2.43	0.47
20:L:131:GLY:HA3	20:L:216:MET:HB3	1.95	0.47
22:N:76:VAL:HG12	22:N:123:VAL:HB	1.96	0.47
29:V:19:LEU:HD22	29:V:109:LEU:HD21	1.97	0.47
30:Y:81:ILE:HG13	30:Y:82:TYR:N	2.28	0.47
31:Z:193:ASP:CG	31:Z:196:GLY:HA3	2.40	0.47
44:q:38:VAL:HG22	44:q:77:ILE:HD13	1.95	0.47
45:r:104:LYS:HD2	45:r:104:LYS:HA	1.54	0.47
47:u:561:SER:HA	47:u:564:GLU:HB2	1.97	0.47
51:y:339:ALA:O	51:y:345:THR:HG21	2.14	0.47
9:A:656:G:C2	9:A:1154:U:C4	3.03	0.47
11:C:35:PRO:HB2	11:C:36:HIS:CD2	2.49	0.47
13:E:49:GLY:HA2	13:E:75:ILE:HG13	1.97	0.47
20:L:191:VAL:HG11	20:L:236:PHE:CD1	2.49	0.47
22:N:206:ASP:O	22:N:207:PRO:C	2.56	0.47
25:Q:53:ILE:HD13	25:Q:53:ILE:HA	1.73	0.47
27:S:72:ARG:HA	27:S:98:ARG:HA	1.96	0.47
44:q:33:GLN:HB3	44:q:92:ILE:HG13	1.97	0.47
50:x:70:ALA:CB	51:y:597:ASN:HB3	2.45	0.47
50:x:397:ASN:N	50:x:397:ASN:OD1	2.48	0.47
9:A:305:U:H2'	9:A:308:G:H5''	1.96	0.47
9:A:520:A:C6	9:A:521:A:N7	2.83	0.47
17:I:76:LYS:HA	17:I:81:ALA:HB2	1.96	0.47
20:L:204:ILE:HG23	20:L:222:CYS:HB3	1.95	0.47
25:Q:7:ASN:HB2	25:Q:10:ARG:O	2.14	0.47
47:u:140:ARG:HA	51:y:465:HIS:O	2.15	0.47
9:A:107:A:N6	9:A:108:G:O6	2.48	0.47
9:A:695:C:C2'	9:A:696:G:C8	2.80	0.47
9:A:1486:A:O2'	20:L:118:ALA:CB	2.63	0.47
23:O:117:TRP:HB3	23:O:153:THR:HA	1.97	0.47
27:S:135:PRO:HB3	27:S:140:ARG:HB3	1.97	0.47
35:d:72:VAL:O	35:d:76:THR:HG23	2.15	0.47
37:f:125:HIS:CD2	37:f:131:VAL:HG11	2.50	0.47
41:m:69:CYS:SG	41:m:76:LEU:HD21	2.54	0.47
5:6:43:ALA:HB1	5:6:47:GLU:H	1.80	0.46
9:A:532:C:H2'	9:A:533:A:C8	2.50	0.46
25:Q:28:ARG:O	25:Q:29:CYS:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:16:LYS:O	30:Y:17:LYS:C	2.56	0.46
30:Y:105:LYS:HB3	30:Y:105:LYS:HE3	1.56	0.46
34:c:152:SER:HB2	34:c:170:TRP:CD1	2.49	0.46
45:r:209:LYS:HB3	45:r:213:ARG:HH21	1.79	0.46
9:A:77:A:C1'	27:S:176:ILE:HD13	2.39	0.46
9:A:454:U:H2'	9:A:455:A:C8	2.49	0.46
9:A:631:U:H5'	9:A:631:U:H6	1.80	0.46
9:A:1132:C:H2'	9:A:1133:A:O4'	2.15	0.46
15:G:61:ILE:HA	15:G:93:VAL:HG23	1.97	0.46
22:N:177:MET:O	22:N:181:GLU:HG2	2.15	0.46
34:c:116:ASP:O	34:c:117:ASN:HB2	2.15	0.46
34:c:256:ILE:HB	34:c:270:LEU:HB2	1.97	0.46
51:y:763:GLY:HA2	51:y:767:ASP:HB2	1.98	0.46
9:A:339:A:H2'	9:A:340:C:H5	1.79	0.46
9:A:562:U:H2'	9:A:563:G:C8	2.50	0.46
9:A:818:A:H2'	9:A:819:G:C8	2.51	0.46
10:B:19:ASN:OD1	26:R:192:GLY:HA3	2.16	0.46
30:Y:10:VAL:HG23	30:Y:25:CYS:HB3	1.97	0.46
31:Z:45:ARG:NH1	31:Z:85:GLU:HG3	2.30	0.46
33:b:96:VAL:HG11	33:b:116:LEU:HB3	1.96	0.46
45:r:247:GLY:HA2	45:r:250:VAL:HG22	1.96	0.46
47:u:143:ARG:HD3	51:y:465:HIS:HB2	1.96	0.46
50:x:31:GLN:HB3	51:y:593:HIS:CE1	2.50	0.46
1:l:612:ASN:H	1:l:627:GLY:HA2	1.80	0.46
9:A:186:C:H2'	9:A:187:G:H8	1.75	0.46
9:A:879:C:H2'	9:A:880:G:H5''	1.97	0.46
9:A:1199:A:H2'	9:A:1200:A:C8	2.50	0.46
10:B:82:MET:HE2	10:B:85:THR:C	2.38	0.46
34:c:216:ALA:O	34:c:229:THR:HA	2.16	0.46
43:o:270:LEU:HD11	43:o:279:SER:HB2	1.97	0.46
9:A:936:G:O2'	17:I:105:ASN:HB3	2.16	0.46
9:A:1578:U:H5''	9:A:1579:A:O4'	2.15	0.46
11:C:123:LEU:HD12	11:C:236:ILE:HG23	1.95	0.46
13:E:51:VAL:HG13	13:E:70:VAL:HB	1.96	0.46
13:E:124:LYS:HG2	13:E:129:SER:HA	1.96	0.46
15:G:172:THR:O	15:G:176:VAL:HG23	2.15	0.46
20:L:176:LYS:HD3	20:L:176:LYS:HA	1.62	0.46
22:N:68:ILE:CG2	22:N:73:ASP:HB2	2.46	0.46
27:S:162:LEU:O	27:S:169:PRO:HA	2.16	0.46
38:h:21:ARG:HH21	38:h:88:LEU:HD23	1.80	0.46
38:h:70:CYS:HB2	38:h:71:GLY:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:38:MET:HB2	39:i:38:MET:HE3	1.72	0.46
45:r:138:PHE:CE1	45:r:166:LEU:HD11	2.51	0.46
48:v:243:LEU:HB3	48:v:249:MET:SD	2.55	0.46
9:A:409:C:C2	9:A:432:G:C2	3.04	0.46
9:A:497:C:C2	9:A:498:C:C6	3.04	0.46
9:A:1074:C:H2'	9:A:1075:C:H6	1.81	0.46
9:A:1225:U:O2'	9:A:1226:G:H5'	2.15	0.46
9:A:1862:G:H4'	9:A:1863:A:OP1	2.16	0.46
10:B:137:THR:HG21	26:R:13:LYS:HB3	1.98	0.46
16:H:55:LEU:O	16:H:56:CYS:HB2	2.15	0.46
23:O:180:ASP:OD1	23:O:180:ASP:N	2.49	0.46
24:P:107:THR:HG23	25:Q:69:VAL:HG11	1.97	0.46
31:Z:16:ILE:HG23	32:a:64:TRP:HH2	1.81	0.46
37:f:87:GLN:O	37:f:88:LYS:C	2.59	0.46
45:r:36:LEU:HD11	45:r:83:ILE:HG21	1.97	0.46
45:r:71:VAL:HB	45:r:85:LEU:HB3	1.97	0.46
47:u:567:ARG:HA	47:u:573:GLN:HG3	1.97	0.46
47:u:567:ARG:HE	47:u:572:ARG:HG3	1.80	0.46
49:w:67:C:H2'	49:w:68:U:H6	1.79	0.46
50:x:72:PHE:HA	51:y:600:HIS:O	2.16	0.46
51:y:792:LEU:HD21	51:y:807:LEU:HD21	1.98	0.46
38:h:55:ARG:HE	38:h:87:ARG:HH11	1.64	0.46
41:m:24:THR:HA	41:m:27:ILE:HG12	1.97	0.46
47:u:549:GLN:HA	47:u:552:LEU:HB3	1.98	0.46
1:1:512:VAL:HG13	1:1:530:VAL:HG13	1.98	0.46
9:A:317:C:H5	27:S:183:ARG:HH11	1.63	0.46
9:A:541:U:H2'	9:A:542:U:C5	2.51	0.46
9:A:1386:A:N6	9:A:1387:G:C5	2.84	0.46
23:O:75:GLN:NE2	47:u:17:GLU:OE2	2.49	0.46
24:P:44:VAL:HG13	24:P:53:ILE:HB	1.96	0.46
24:P:142:ARG:HG3	24:P:143:LYS:N	2.31	0.46
26:R:190:LEU:HB3	26:R:195:LEU:HD13	1.97	0.46
33:b:60:LEU:HD21	33:b:94:VAL:HG13	1.97	0.46
34:c:137:VAL:O	34:c:137:VAL:CG2	2.63	0.46
9:A:527:C:H2'	9:A:528:A:C8	2.50	0.46
9:A:1021:U:OP1	17:I:132:LYS:NZ	2.47	0.46
17:I:129:TYR:HB3	17:I:135:LEU:HG	1.98	0.46
21:M:35:CYS:HA	21:M:38:ILE:HG12	1.98	0.46
22:N:78:SER:HA	22:N:125:THR:HG22	1.98	0.46
22:N:183:LEU:HA	22:N:183:LEU:HD23	1.67	0.46
25:Q:7:ASN:HD22	25:Q:9:GLY:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:58:VAL:HG23	25:Q:59:PHE:CG	2.50	0.46
27:S:45:TRP:CE3	27:S:121:ILE:HD11	2.51	0.46
29:V:142:SER:HB3	42:n:47:LYS:O	2.16	0.46
34:c:109:LEU:HA	34:c:109:LEU:HD23	1.65	0.46
37:f:31:THR:HG23	37:f:37:GLY:HA2	1.98	0.46
40:k:139:HIS:O	40:k:147:THR:HA	2.16	0.46
9:A:287:U:H2'	9:A:288:G:H8	1.81	0.46
9:A:379:C:H3'	26:R:181:GLN:HE22	1.81	0.46
9:A:489:A:N6	9:A:512:A:C6	2.84	0.46
9:A:494:C:N4	9:A:509:OMG:HN22	2.14	0.46
9:A:1017:U:H1'	17:I:52:VAL:HG22	1.98	0.46
15:G:81:ARG:HA	15:G:84:GLU:HG3	1.97	0.46
23:O:166:LYS:HE3	23:O:166:LYS:HB3	1.74	0.46
31:Z:55:THR:HB	43:o:308:LEU:HD21	1.97	0.46
37:f:25:LYS:HE2	37:f:25:LYS:HB2	1.68	0.46
51:y:785:GLU:HG2	51:y:813:LEU:HD11	1.96	0.46
9:A:539:C:N4	9:A:542:U:H5''	2.31	0.45
9:A:614:C:N4	9:A:626:G:C2	2.84	0.45
9:A:683:OMG:HM23	9:A:683:OMG:H1'	1.56	0.45
9:A:824:C:H2'	9:A:825:A:C8	2.51	0.45
9:A:862:A:N7	18:J:107:SER:HA	2.31	0.45
9:A:1529:C:O3'	35:d:89:PRO:HG3	2.17	0.45
9:A:1813:A:H3'	9:A:1814:G:C8	2.49	0.45
9:A:1844:U:H2'	9:A:1845:A:H8	1.80	0.45
25:Q:26:CYS:O	25:Q:27:ALA:HB3	2.16	0.45
30:Y:96:TYR:CD2	30:Y:108:ILE:HD13	2.51	0.45
41:m:31:LEU:HD12	41:m:31:LEU:HA	1.70	0.45
47:u:411:LEU:HD23	47:u:432:GLN:HG2	1.98	0.45
49:w:30:G:H2'	49:w:31:C:C6	2.51	0.45
2:3:154:ASP:O	2:3:158:LEU:N	2.45	0.45
9:A:155:G:C6	9:A:164:A:C6	3.04	0.45
9:A:156:G:H1	9:A:162:C:H42	1.63	0.45
9:A:982:G:H2'	9:A:983:A:H8	1.82	0.45
9:A:1333:U:H4'	31:Z:147:ALA:HB2	1.98	0.45
9:A:1513:C:H2'	9:A:1514:G:C8	2.52	0.45
24:P:75:MET:HE3	24:P:75:MET:HB2	1.70	0.45
27:S:35:GLU:HA	27:S:51:ARG:HA	1.98	0.45
29:V:203:ASN:O	29:V:204:ARG:C	2.57	0.45
32:a:80:ARG:HG3	32:a:85:LEU:HB2	1.97	0.45
34:c:147:HIS:HE1	34:c:167:SER:HB2	1.81	0.45
44:q:109:LEU:HD13	44:q:112:HIS:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:r:31:GLY:HA3	45:r:45:MET:HE2	1.98	0.45
47:u:389:ASP:N	47:u:389:ASP:OD1	2.47	0.45
47:u:446:ILE:HG23	47:u:447:TYR:HD1	1.81	0.45
3:4:329:SER:O	48:v:401:TYR:OH	2.34	0.45
9:A:388:U:H2'	9:A:389:A:H8	1.79	0.45
19:K:43:THR:O	19:K:44:GLY:C	2.58	0.45
20:L:133:TYR:O	20:L:134:ASN:C	2.59	0.45
20:L:173:LYS:H	20:L:173:LYS:HG2	1.58	0.45
21:M:106:LEU:HD23	21:M:106:LEU:HA	1.68	0.45
22:N:147:LEU:HB3	22:N:163:CYS:SG	2.55	0.45
27:S:137:ARG:O	27:S:141:ILE:HG13	2.16	0.45
37:f:144:ARG:O	37:f:145:THR:C	2.59	0.45
45:r:112:LEU:HD21	45:r:135:ALA:HB2	1.99	0.45
45:r:231:ALA:CB	49:w:73:C:N3	2.78	0.45
47:u:266:PRO:HA	47:u:267:PRO:HD3	1.82	0.45
47:u:329:ILE:O	47:u:434:ASN:ND2	2.41	0.45
47:u:399:ASN:HB3	47:u:402:LYS:HZ3	1.81	0.45
47:u:411:LEU:HA	47:u:414:VAL:HB	1.97	0.45
15:G:37:LYS:HD3	15:G:41:ARG:HH21	1.81	0.45
17:I:39:LYS:HA	17:I:42:LYS:HE2	1.98	0.45
45:r:142:TYR:HB2	45:r:148:GLY:CA	2.46	0.45
51:y:78:LYS:HA	51:y:81:GLU:HG2	1.99	0.45
3:4:288:GLN:CA	5:6:348:GLN:HE21	2.29	0.45
9:A:223:C:N3	9:A:299:A:C2	2.84	0.45
9:A:303:C:H2'	9:A:304:C:O4'	2.16	0.45
9:A:434:G:H2'	9:A:435:A:C8	2.52	0.45
9:A:880:G:H5'	9:A:880:G:N3	2.31	0.45
9:A:1043:G:H2'	9:A:1044:G:O4'	2.16	0.45
10:B:36:TYR:CD1	10:B:36:TYR:C	2.94	0.45
28:T:10:ARG:HG3	28:T:24:VAL:HB	1.99	0.45
31:Z:49:ILE:CD1	43:o:309:ILE:HD11	2.43	0.45
37:f:98:VAL:HG11	37:f:106:LYS:HG3	1.98	0.45
47:u:171:GLU:HA	47:u:174:TYR:HB3	1.97	0.45
48:v:385:ASP:OD2	48:v:390:HIS:N	2.49	0.45
15:G:36:LEU:HD21	15:G:82:GLU:HG3	1.98	0.45
24:P:99:ALA:HB2	24:P:108:PRO:HA	1.98	0.45
31:Z:162:ASP:N	31:Z:163:PRO:HD2	2.32	0.45
35:d:39:LEU:HD21	35:d:52:TRP:CZ3	2.52	0.45
38:h:19:ARG:HG2	38:h:92:HIS:CD2	2.52	0.45
45:r:64:ARG:HG2	45:r:67:ARG:HE	1.81	0.45
3:4:301:ASP:O	3:4:305:GLY:N	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:330:G:C2	9:A:331:C:C2	3.04	0.45
9:A:1349:G:N7	9:A:1350:U:O4	2.50	0.45
9:A:1865:C:H1'	25:Q:7:ASN:HD21	1.82	0.45
11:C:52:LEU:HA	11:C:52:LEU:HD23	1.68	0.45
11:C:128:LYS:HG2	11:C:140:VAL:HB	1.99	0.45
20:L:255:LEU:HD12	20:L:255:LEU:HA	1.79	0.45
27:S:16:ILE:HD12	27:S:16:ILE:HA	1.73	0.45
32:a:59:LYS:HG3	32:a:72:THR:HG22	1.98	0.45
45:r:219:SER:HA	45:r:225:ILE:HD11	1.99	0.45
49:w:9:G:C6	49:w:20:A:H1'	2.52	0.45
8:9:5:TRP:HB3	9:A:1852:C:H5	1.81	0.45
9:A:27:A2M:HM'3	9:A:27:A2M:H1'	1.72	0.45
9:A:92:A:H4'	9:A:93:U:OP2	2.16	0.45
9:A:176:U:H2'	9:A:177:G:C8	2.51	0.45
9:A:998:A:N7	9:A:999:G:H1'	2.32	0.45
9:A:1284:A:H5''	9:A:1286:G:O4'	2.17	0.45
9:A:1511:U:H2'	9:A:1512:C:C6	2.52	0.45
9:A:1791:A:H4'	27:S:75:LEU:HD11	1.98	0.45
11:C:152:PRO:HG2	27:S:216:ARG:HG3	1.98	0.45
15:G:30:LEU:HD11	15:G:82:GLU:HB3	1.98	0.45
15:G:73:GLN:HA	15:G:76:GLN:HB2	1.99	0.45
20:L:183:LYS:HG3	20:L:197:PRO:HD2	1.99	0.45
22:N:60:LEU:HA	22:N:63:ARG:HD2	1.98	0.45
27:S:221:LYS:HE3	27:S:221:LYS:HB3	1.66	0.45
31:Z:156:LEU:H	31:Z:156:LEU:HD12	1.82	0.45
45:r:168:LEU:HD13	45:r:172:GLU:HB3	1.98	0.45
45:r:209:LYS:HA	45:r:209:LYS:HD2	1.80	0.45
49:w:35:U:H2'	49:w:36:A:H8	1.82	0.45
3:4:164:SER:HA	7:8:85:PRO:O	2.16	0.45
9:A:883:U:O2	9:A:904:A:C6	2.70	0.45
9:A:1134:G:H2'	9:A:1135:C:C6	2.52	0.45
9:A:1275:G:C4	9:A:1506:A:C6	3.05	0.45
9:A:1647:A:N1	9:A:1675:A:H5''	2.32	0.45
15:G:73:GLN:HB3	15:G:135:PHE:CE1	2.52	0.45
17:I:114:ARG:HD3	17:I:114:ARG:HA	1.80	0.45
22:N:51:LEU:O	22:N:54:THR:HG22	2.15	0.45
31:Z:193:ASP:OD1	31:Z:196:GLY:HA3	2.17	0.45
33:b:60:LEU:HD23	33:b:60:LEU:HA	1.81	0.45
44:q:64:LYS:HB3	44:q:65:LEU:H	1.32	0.45
47:u:91:ARG:HE	47:u:91:ARG:HB2	1.56	0.45
50:x:35:LYS:H	50:x:35:LYS:HG3	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:80:GLU:HA	5:6:118:PRO:CB	2.47	0.45
9:A:625:G:H1	13:E:65:ALA:HB2	1.82	0.45
9:A:1859:A:C5	9:A:1860:A:N7	2.84	0.45
11:C:60:GLU:HB3	28:T:18:LEU:HD11	1.99	0.45
18:J:42:MET:HE2	18:J:42:MET:HB3	1.80	0.45
18:J:95:PRO:HB2	20:L:182:CYS:SG	2.57	0.45
22:N:68:ILE:HG21	22:N:73:ASP:HB2	1.99	0.45
23:O:52:THR:O	23:O:52:THR:OG1	2.35	0.45
26:R:150:ASP:HA	26:R:153:LYS:HD2	1.99	0.45
47:u:548:GLU:O	47:u:552:LEU:N	2.37	0.45
47:u:551:GLN:O	47:u:555:THR:N	2.43	0.45
48:v:339:PHE:HA	48:v:342:GLU:HB3	1.98	0.45
5:6:286:ALA:HA	5:6:332:VAL:HG21	1.99	0.44
9:A:588:G:H4'	9:A:589:G:H5'	1.98	0.44
9:A:1092:G:C2	9:A:1158:G:C6	3.04	0.44
9:A:1234:C:H4'	9:A:1246:A:N1	2.33	0.44
9:A:1440:C:H2'	9:A:1441:U:C6	2.52	0.44
10:B:104:LYS:HD3	13:E:8:ARG:HH11	1.82	0.44
24:P:72:TYR:O	24:P:73:ALA:C	2.57	0.44
24:P:141:ARG:NH1	25:Q:22:ARG:HH12	2.15	0.44
28:T:18:LEU:HD23	28:T:18:LEU:HA	1.84	0.44
31:Z:66:ILE:HG21	43:o:307:HIS:CB	2.48	0.44
35:d:80:GLY:HA3	35:d:92:PHE:CE1	2.49	0.44
41:m:14:VAL:HG21	41:m:126:GLU:HG3	1.99	0.44
48:v:367:ALA:O	48:v:371:ILE:HG12	2.17	0.44
49:w:50:U:H3	49:w:62:A:H61	1.66	0.44
9:A:497:C:C4	9:A:498:C:N4	2.85	0.44
9:A:1416:C:H2'	9:A:1417:C:C6	2.52	0.44
12:D:173:VAL:O	12:D:177:ASN:HB2	2.17	0.44
16:H:26:GLN:H	16:H:26:GLN:HG2	1.32	0.44
24:P:103:ASN:OD1	24:P:103:ASN:N	2.50	0.44
47:u:500:ALA:HB1	47:u:502:ARG:HB2	1.99	0.44
9:A:1277:C:H2'	9:A:1278:A:H8	1.81	0.44
9:A:1349:G:C4	9:A:1350:U:C6	3.05	0.44
9:A:1418:C:O2'	9:A:1419:C:H2'	2.18	0.44
12:D:125:HIS:O	12:D:128:VAL:HG22	2.18	0.44
17:I:46:THR:O	17:I:47:PRO:C	2.58	0.44
28:T:12:PHE:CZ	28:T:21:LYS:HB3	2.53	0.44
31:Z:158:ILE:HD11	31:Z:167:TYR:HB2	2.00	0.44
31:Z:223:ILE:HG13	31:Z:224:SER:N	2.33	0.44
37:f:15:VAL:HG13	37:f:68:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:r:242:LEU:HD12	45:r:243:GLU:HG2	1.99	0.44
47:u:386:GLU:HG2	47:u:413:TRP:CG	2.52	0.44
48:v:229:ARG:HD3	48:v:229:ARG:HA	1.68	0.44
48:v:267:VAL:HG13	48:v:270:ARG:HG3	1.98	0.44
9:A:878:G:H1	9:A:908:A:H61	1.65	0.44
9:A:1208:A:N6	9:A:1209:A:H62	2.15	0.44
9:A:1288:U:O4	40:k:97:LYS:NZ	2.49	0.44
9:A:1813:A:C5	9:A:1814:G:C5	3.05	0.44
10:B:10:TYR:CE2	10:B:12:LYS:HB3	2.52	0.44
16:H:8:LEU:O	16:H:10:PRO:HD3	2.17	0.44
26:R:65:PHE:HB2	26:R:109:TYR:OH	2.16	0.44
29:V:68:ILE:HD12	29:V:68:ILE:HA	1.65	0.44
29:V:103:LEU:HA	29:V:103:LEU:HD23	1.82	0.44
30:Y:44:PRO:HG3	30:Y:77:HIS:HB3	1.99	0.44
45:r:197:VAL:HB	45:r:208:VAL:HG12	1.99	0.44
50:x:73:HIS:CG	51:y:602:ASP:HB3	2.53	0.44
5:6:344:LYS:HA	5:6:347:TRP:HB2	1.98	0.44
9:A:517:OMC:HM23	9:A:517:OMC:H1'	1.74	0.44
9:A:571:U:O2	9:A:571:U:H2'	2.18	0.44
9:A:911:C:H2'	9:A:912:C:C6	2.53	0.44
11:C:11:ARG:HA	11:C:28:ALA:HB2	1.99	0.44
11:C:126:VAL:HG22	11:C:139:LEU:HD13	2.00	0.44
15:G:166:VAL:HG22	15:G:173:PHE:HZ	1.83	0.44
26:R:158:ILE:HD12	26:R:158:ILE:HA	1.72	0.44
34:c:272:GLN:O	34:c:273:GLU:C	2.61	0.44
37:f:20:ILE:HD13	37:f:30:ILE:HA	2.00	0.44
40:k:120:GLU:HG2	40:k:129:GLY:HA2	1.97	0.44
47:u:483:ARG:N	47:u:492:SER:O	2.43	0.44
47:u:562:ARG:O	47:u:566:GLN:NE2	2.51	0.44
47:u:567:ARG:O	47:u:572:ARG:N	2.50	0.44
48:v:93:LYS:O	48:v:97:ASP:N	2.50	0.44
48:v:205:LEU:H	48:v:205:LEU:HG	1.36	0.44
51:y:596:ASP:OD1	51:y:596:ASP:N	2.49	0.44
9:A:115:U:H2'	9:A:116:OMU:C6	2.48	0.44
9:A:909:G:N1	9:A:910:G:C5	2.85	0.44
9:A:1587:G:C6	35:d:67:ARG:CG	3.01	0.44
9:A:1757:G:H1'	9:A:1776:G:H22	1.83	0.44
19:K:15:ARG:HA	20:L:259:THR:HG21	2.00	0.44
20:L:98:LEU:HD11	20:L:136:HIS:CG	2.53	0.44
41:m:75:ASN:HB2	41:m:127:TYR:CG	2.52	0.44
48:v:231:ASN:HA	48:v:235:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:322:ASP:HB3	48:v:325:LEU:HD12	2.00	0.44
49:w:3:C:H2'	49:w:4:A:C8	2.53	0.44
51:y:146:ARG:O	51:y:150:ARG:NE	2.51	0.44
9:A:47:G:C6	9:A:48:C:C4	3.06	0.44
9:A:178:C:H2'	9:A:179:C:C6	2.53	0.44
9:A:1335:G:H2'	9:A:1336:C:O4'	2.18	0.44
9:A:1560:U:H2'	9:A:1561:A:C8	2.53	0.44
9:A:1810:U:H2'	9:A:1811:C:C6	2.53	0.44
9:A:1840:U:C4	9:A:1841:C:C5	3.06	0.44
9:A:1842:C:H2'	9:A:1843:G:C8	2.53	0.44
28:T:100:LYS:HE2	28:T:100:LYS:HB2	1.86	0.44
31:Z:16:ILE:HD13	39:i:22:ARG:HH11	1.82	0.44
34:c:130:LYS:HE2	34:c:130:LYS:HB3	1.84	0.44
38:h:101:ILE:HD12	38:h:101:ILE:HA	1.74	0.44
40:k:120:GLU:HG2	40:k:129:GLY:CA	2.48	0.44
47:u:685:GLN:O	47:u:689:LYS:N	2.50	0.44
9:A:28:U:H2'	9:A:29:G:H8	1.83	0.44
11:C:79:ASP:HB3	11:C:82:TYR:HB2	2.00	0.44
22:N:125:THR:O	22:N:147:LEU:HB2	2.18	0.44
24:P:138:ASP:HB2	24:P:139:SER:H	1.60	0.44
27:S:70:HIS:O	27:S:98:ARG:NH2	2.50	0.44
33:b:103:ASN:HD22	33:b:103:ASN:HA	1.59	0.44
34:c:143:GLN:HA	34:c:146:SER:HB2	2.00	0.44
35:d:75:MET:HE2	35:d:75:MET:HB2	1.88	0.44
41:m:83:LYS:HB2	41:m:83:LYS:HE2	1.81	0.44
44:q:78:LEU:CB	44:q:92:ILE:HB	2.47	0.44
47:u:330:PRO:O	47:u:333:PRO:HD3	2.17	0.44
49:w:44:G:H5'	49:w:45:G:N1	2.33	0.44
51:y:386:ASN:OD1	51:y:386:ASN:N	2.50	0.44
3:4:277:ALA:O	3:4:281:ASP:N	2.44	0.44
5:6:289:ASN:HA	5:6:332:VAL:HG22	2.00	0.44
9:A:111:A:O2'	9:A:112:U:H5'	2.18	0.44
9:A:223:C:C4	9:A:299:A:N1	2.85	0.44
9:A:543:C:H5''	9:A:544:G:C5	2.53	0.44
9:A:1074:C:H2'	9:A:1075:C:C6	2.53	0.44
9:A:1273:C:N4	9:A:1506:A:H1'	2.33	0.44
14:F:82:ARG:H	14:F:82:ARG:HG2	1.61	0.44
17:I:130:LYS:HD2	17:I:137:PRO:O	2.17	0.44
22:N:67:ALA:O	22:N:68:ILE:C	2.61	0.44
41:m:49:LEU:HB3	41:m:111:VAL:HB	1.99	0.44
47:u:87:GLU:HG2	47:u:170:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:y:439:ARG:HH22	51:y:441:ARG:HH21	1.65	0.44
9:A:1181:A:H2'	9:A:1182:A:H8	1.79	0.43
9:A:1859:A:C6	9:A:1860:A:C5	3.05	0.43
14:F:105:ARG:CZ	14:F:105:ARG:HB3	2.46	0.43
15:G:57:ARG:HD2	15:G:57:ARG:HA	1.72	0.43
19:K:28:ASP:C	19:K:30:ALA:N	2.73	0.43
32:a:15:LEU:HD23	32:a:79:LEU:HD11	2.00	0.43
41:m:44:LYS:HB3	41:m:46:GLN:HG2	1.99	0.43
41:m:91:LEU:H	41:m:91:LEU:HG	1.63	0.43
47:u:280:SER:OG	47:u:321:ARG:NH1	2.51	0.43
47:u:515:PRO:O	47:u:520:ARG:NH2	2.50	0.43
48:v:331:ASP:OD1	48:v:331:ASP:N	2.50	0.43
48:v:353:ILE:HG12	48:v:371:ILE:HG13	2.00	0.43
50:x:394:LYS:HD2	50:x:447:LEU:HD11	2.00	0.43
9:A:124:U:C4	9:A:125:C:C4	3.06	0.43
9:A:300:U:H2'	9:A:301:A:C8	2.53	0.43
9:A:656:G:N1	9:A:1154:U:C4	2.86	0.43
9:A:862:A:C5	18:J:107:SER:HA	2.53	0.43
9:A:1294:G:H3'	9:A:1295:A:H8	1.84	0.43
9:A:1351:G:O6	9:A:1379:A:N6	2.49	0.43
27:S:181:THR:H	27:S:184:VAL:HG12	1.83	0.43
31:Z:72:VAL:HG12	32:a:20:VAL:HB	2.00	0.43
37:f:6:PRO:HG2	37:f:58:GLU:HG2	1.99	0.43
47:u:407:VAL:HG22	47:u:411:LEU:HD13	2.00	0.43
47:u:555:THR:HA	47:u:558:LEU:HB2	2.00	0.43
51:y:815:LEU:HA	51:y:818:VAL:HG12	2.01	0.43
5:6:252:TYR:O	5:6:257:GLN:N	2.50	0.43
9:A:454:U:H2'	9:A:455:A:H8	1.83	0.43
9:A:1192:U:H2'	9:A:1193:U:C6	2.53	0.43
9:A:1824:A:N1	44:q:44:ASN:HA	2.33	0.43
11:C:233:LYS:HD3	11:C:233:LYS:HA	1.78	0.43
15:G:37:LYS:O	15:G:38:ALA:C	2.60	0.43
18:J:34:ILE:O	18:J:38:LEU:HG	2.18	0.43
20:L:120:GLN:HE21	20:L:120:GLN:HB3	1.55	0.43
24:P:100:THR:HB	24:P:105:THR:HG22	1.99	0.43
31:Z:140:GLY:HA3	31:Z:182:LEU:HD22	2.01	0.43
33:b:79:HIS:HD2	33:b:97:TYR:HB2	1.83	0.43
41:m:33:ARG:HD2	41:m:91:LEU:HD23	2.01	0.43
43:o:242:ARG:N	43:o:313:GLU:O	2.48	0.43
50:x:34:SER:OG	50:x:57:ASN:OD1	2.37	0.43
51:y:508:LEU:HD23	51:y:508:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1308:U:H1'	40:k:140:TYR:OH	2.19	0.43
9:A:1380:C:H2'	9:A:1381:G:C8	2.54	0.43
22:N:76:VAL:HG23	22:N:87:VAL:HG13	2.00	0.43
22:N:179:ALA:HA	22:N:182:VAL:HG12	2.00	0.43
26:R:195:LEU:O	26:R:199:LEU:HB2	2.18	0.43
33:b:110:GLU:C	37:f:117:ILE:HD11	2.44	0.43
34:c:270:LEU:HA	34:c:270:LEU:HD23	1.53	0.43
35:d:143:LYS:O	35:d:143:LYS:CG	2.66	0.43
36:e:60:LYS:HA	36:e:60:LYS:HD3	1.74	0.43
9:A:55:U:OP2	9:A:506:G:H4'	2.19	0.43
9:A:146:G:H2'	9:A:147:A:O4'	2.18	0.43
9:A:367:U:H4'	9:A:371:A:C8	2.54	0.43
9:A:496:C:H2'	9:A:497:C:H6	1.83	0.43
9:A:1852:C:H2'	9:A:1853:C:C6	2.53	0.43
24:P:31:CYS:HA	24:P:44:VAL:HA	2.01	0.43
31:Z:59:LEU:HD21	43:o:306:ASP:O	2.19	0.43
33:b:119:PHE:HE1	37:f:117:ILE:HG23	1.83	0.43
34:c:147:HIS:CE1	34:c:167:SER:HB2	2.53	0.43
34:c:207:CYS:HB2	34:c:221:LEU:HG	2.00	0.43
48:v:307:GLY:HA2	48:v:311:LYS:HB2	2.01	0.43
51:y:145:ILE:HD13	51:y:145:ILE:HA	1.83	0.43
1:1:544:PHE:CZ	1:1:565:ILE:HG12	2.54	0.43
3:4:124:VAL:HA	3:4:129:VAL:HA	1.99	0.43
9:A:941:C:H2'	9:A:942:G:C8	2.52	0.43
9:A:1209:A:C2	9:A:1691:U:N3	2.86	0.43
9:A:1560:U:H2'	9:A:1561:A:H8	1.83	0.43
9:A:1866:A:H5'	25:Q:95:ARG:HD2	2.00	0.43
13:E:16:HIS:CE1	13:E:20:GLN:HG3	2.53	0.43
21:M:58:MET:HE3	21:M:58:MET:HB3	1.80	0.43
22:N:82:THR:O	22:N:204:TYR:HB2	2.19	0.43
23:O:28:LYS:HD3	23:O:48:LEU:HD13	2.00	0.43
27:S:10:THR:C	27:S:128:THR:HB	2.38	0.43
32:a:47:LYS:HD3	32:a:47:LYS:HA	1.75	0.43
34:c:10:THR:HG22	34:c:308:ARG:HG2	2.00	0.43
35:d:39:LEU:HA	35:d:39:LEU:HD23	1.31	0.43
43:o:245:ASN:HB3	43:o:310:LEU:HA	2.00	0.43
51:y:580:SER:OG	51:y:623:GLN:OE1	2.37	0.43
5:6:260:LYS:O	5:6:262:PHE:N	2.51	0.43
5:6:313:ILE:HG13	47:u:400:PRO:HD2	2.01	0.43
9:A:85:A:H2'	9:A:86:C:C6	2.54	0.43
9:A:116:OMU:HM23	9:A:116:OMU:H1'	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:155:G:C5	9:A:164:A:C6	3.07	0.43
9:A:367:U:N3	51:y:144:LYS:HE3	2.29	0.43
9:A:1064:C:O3'	24:P:149:ARG:NH2	2.51	0.43
9:A:1445:U:H1'	9:A:1580:A:N6	2.34	0.43
9:A:1643:U:H2'	9:A:1644:C:C6	2.54	0.43
16:H:41:TYR:CE1	50:x:73:HIS:HE1	2.37	0.43
21:M:61:ILE:HD11	21:M:69:ILE:HD12	1.99	0.43
22:N:59:LEU:HD23	22:N:59:LEU:HA	1.73	0.43
24:P:123:GLY:O	24:P:124:MET:C	2.60	0.43
35:d:98:SER:O	35:d:99:VAL:C	2.61	0.43
38:h:24:LEU:HD21	38:h:39:LEU:HD22	2.00	0.43
38:h:34:LYS:HG3	38:h:35:VAL:N	2.33	0.43
45:r:43:GLU:N	45:r:82:TYR:OH	2.52	0.43
45:r:189:VAL:O	45:r:240:THR:HA	2.19	0.43
1:l:528:VAL:HB	1:l:545:GLU:HB2	1.99	0.43
9:A:289:G:H2'	9:A:290:U:C6	2.54	0.43
9:A:1208:A:C2	9:A:1209:A:C4	3.07	0.43
9:A:1448:A:H2'	9:A:1449:G:O4'	2.18	0.43
9:A:1819:A:O2'	9:A:1820:G:H5'	2.18	0.43
20:L:212:LYS:HD2	20:L:212:LYS:HA	1.75	0.43
21:M:18:GLU:HG2	21:M:70:SER:H	1.84	0.43
29:V:88:MET:O	29:V:91:ARG:HG3	2.19	0.43
31:Z:115:VAL:HB	31:Z:150:MET:HE1	2.00	0.43
31:Z:177:LEU:HD23	31:Z:177:LEU:HA	1.84	0.43
35:d:75:MET:HG3	35:d:79:TYR:CE2	2.54	0.43
50:x:70:ALA:HB2	51:y:597:ASN:HB3	2.01	0.43
9:A:501:C:O2	9:A:501:C:H2'	2.19	0.43
9:A:909:G:N1	9:A:910:G:C4	2.87	0.43
9:A:1053:C:H2'	9:A:1054:G:H8	1.84	0.43
9:A:1338:G:H2'	9:A:1339:U:O4'	2.19	0.43
9:A:1544:C:H4'	30:Y:80:GLN:HE22	1.83	0.43
12:D:144:ILE:HG22	12:D:146:SER:H	1.84	0.43
15:G:49:LYS:O	15:G:60:ILE:HA	2.19	0.43
23:O:28:LYS:HA	23:O:50:THR:HA	2.00	0.43
27:S:18:VAL:HG11	27:S:24:LEU:HG	2.01	0.43
50:x:381:MET:HB2	50:x:391:ILE:HD13	2.00	0.43
51:y:459:MET:HB3	51:y:672:PRO:HB3	2.01	0.43
2:3:210:VAL:O	2:3:214:MET:N	2.51	0.43
5:6:207:CYS:O	5:6:211:ALA:N	2.52	0.43
9:A:511:U:H2'	9:A:512:A:H8	1.80	0.43
9:A:895:G:H2'	9:A:896:U:O3'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:972:A:OP2	9:A:973:C:H5	2.02	0.43
21:M:32:LYS:HB3	21:M:32:LYS:HE2	1.75	0.43
27:S:131:ARG:N	27:S:131:ARG:HD2	2.33	0.43
29:V:30:ILE:HG23	29:V:117:ILE:HD11	2.00	0.43
33:b:28:MET:HB3	33:b:28:MET:HE2	1.69	0.43
34:c:5:MET:H	34:c:5:MET:HG3	1.49	0.43
36:e:69:THR:O	36:e:73:VAL:HG12	2.19	0.43
44:q:51:CYS:HB2	44:q:55:VAL:O	2.19	0.43
44:q:64:LYS:HD3	44:q:64:LYS:HA	1.75	0.43
45:r:77:ASP:HB3	45:r:80:LYS:O	2.18	0.43
47:u:257:HIS:CD2	47:u:358:LEU:HA	2.54	0.43
49:w:29:G:H3'	49:w:30:G:H8	1.84	0.43
3:4:261:ARG:HA	7:8:204:VAL:O	2.19	0.42
9:A:1125:C:OP1	23:O:150:ILE:HG13	2.18	0.42
9:A:1239:U:H5''	33:b:124:LYS:HD2	1.99	0.42
9:A:1690:U:C2	9:A:1691:U:C6	3.07	0.42
17:I:40:LEU:HD23	17:I:40:LEU:HA	1.84	0.42
22:N:41:ARG:HB2	22:N:47:TYR:CE1	2.54	0.42
27:S:49:VAL:CG1	27:S:114:VAL:HG12	2.26	0.42
27:S:229:ALA:O	27:S:230:LYS:C	2.61	0.42
29:V:109:LEU:O	29:V:113:VAL:HG23	2.19	0.42
31:Z:193:ASP:CB	31:Z:196:GLY:HA3	2.49	0.42
35:d:39:LEU:HG	35:d:47:PRO:HG3	1.99	0.42
40:k:116:ARG:HD3	40:k:116:ARG:HA	1.49	0.42
45:r:234:ARG:HE	45:r:234:ARG:HB2	1.48	0.42
48:v:393:MET:N	48:v:393:MET:SD	2.92	0.42
49:w:71:U:H2'	49:w:72:A:O4'	2.19	0.42
51:y:421:GLY:N	51:y:440:VAL:HG13	2.34	0.42
5:6:131:ALA:HB3	5:6:135:GLY:HA3	2.02	0.42
9:A:113:G:N2	9:A:292:A:N3	2.67	0.42
9:A:364:A:H2'	9:A:365:C:C6	2.54	0.42
9:A:1267:C:H2'	9:A:1268:C:C6	2.53	0.42
9:A:1752:C:H6	9:A:1779:G:H1	1.67	0.42
19:K:62:MET:HE3	19:K:62:MET:HB2	1.91	0.42
20:L:213:LEU:HA	20:L:216:MET:HE2	2.01	0.42
21:M:109:LEU:HG	21:M:111:PHE:CD2	2.54	0.42
45:r:22:VAL:O	45:r:68:ASN:HA	2.20	0.42
45:r:142:TYR:O	45:r:143:LYS:HB2	2.19	0.42
47:u:416:GLU:O	47:u:425:GLN:NE2	2.52	0.42
49:w:27:U:H2'	49:w:28:G:H8	1.84	0.42
51:y:439:ARG:HH12	51:y:441:ARG:HE	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:316:VAL:HG23	5:6:321:VAL:HA	2.01	0.42
8:9:13:LEU:HA	8:9:13:LEU:HD12	1.75	0.42
9:A:387:C:H2'	9:A:388:U:C6	2.54	0.42
9:A:421:G:OP1	10:B:98:LYS:HA	2.20	0.42
9:A:898:U:H4'	9:A:898:U:OP1	2.20	0.42
9:A:1189:A:H2'	9:A:1190:A:H8	1.83	0.42
9:A:1728:U:H2'	9:A:1729:U:C1'	2.48	0.42
9:A:1729:U:O2	9:A:1806:A:C2	2.72	0.42
15:G:66:VAL:O	15:G:67:PRO:C	2.58	0.42
21:M:66:VAL:HG13	21:M:69:ILE:HG13	2.01	0.42
22:N:34:MET:HE3	22:N:34:MET:HB3	1.73	0.42
23:O:82:ARG:HH11	23:O:191:ASP:HB3	1.84	0.42
34:c:202:PRO:HG2	34:c:243:PRO:HA	2.01	0.42
45:r:105:SER:HA	45:r:108:VAL:HB	2.01	0.42
47:u:205:LEU:HD11	47:u:259:LEU:HD21	2.00	0.42
47:u:341:LEU:HD11	47:u:347:ILE:HG13	2.01	0.42
47:u:352:GLN:HG2	47:u:364:PRO:HB3	2.01	0.42
49:w:41:A:H2'	49:w:42:G:H8	1.84	0.42
3:4:93:ARG:O	3:4:130:GLU:HA	2.19	0.42
9:A:77:A:C2	27:S:175:LYS:HG3	2.55	0.42
9:A:1284:A:OP2	41:m:104:VAL:HG13	2.19	0.42
9:A:1295:A:H3'	9:A:1296:U:C6	2.55	0.42
9:A:1310:U:C5'	40:k:130:VAL:HG13	2.47	0.42
18:J:46:TYR:CE1	20:L:256:TRP:HZ2	2.37	0.42
22:N:107:THR:HG22	22:N:115:ALA:O	2.18	0.42
23:O:62:LEU:HD13	23:O:91:VAL:HG11	2.01	0.42
24:P:43:HIS:ND1	24:P:55:ARG:HB3	2.34	0.42
44:q:82:ARG:HB3	44:q:85:GLN:O	2.20	0.42
47:u:233:ARG:HA	47:u:236:GLN:HB3	2.01	0.42
47:u:320:THR:HG21	47:u:384:VAL:HG23	2.00	0.42
47:u:552:LEU:HA	47:u:555:THR:HB	2.01	0.42
7:8:41:ILE:HA	7:8:78:ILE:H	1.84	0.42
9:A:548:C:H2'	9:A:549:C:C6	2.54	0.42
9:A:558:G:H1'	9:A:559:G:C8	2.54	0.42
9:A:655:A:N3	9:A:655:A:H5'	2.35	0.42
9:A:1097:G:H4'	22:N:32:PHE:CD1	2.55	0.42
9:A:1386:A:C5	9:A:1387:G:N7	2.88	0.42
9:A:1827:U:H2'	9:A:1828:C:C6	2.54	0.42
22:N:3:GLY:HA3	22:N:5:LEU:HD22	2.00	0.42
25:Q:58:VAL:CG2	25:Q:59:PHE:CG	3.02	0.42
25:Q:58:VAL:HG23	25:Q:59:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:95:LYS:HA	27:S:95:LYS:HD2	1.81	0.42
34:c:137:VAL:O	34:c:137:VAL:HG23	2.16	0.42
45:r:223:MET:SD	45:r:246:GLU:HB3	2.59	0.42
45:r:223:MET:CB	45:r:250:VAL:HG21	2.37	0.42
50:x:315:GLU:O	50:x:319:ILE:HG12	2.19	0.42
50:x:365:LEU:HD22	50:x:369:ILE:HG21	2.02	0.42
51:y:673:PHE:HA	51:y:676:HIS:ND1	2.34	0.42
1:l:390:THR:O	1:l:405:ILE:N	2.40	0.42
9:A:14:C:H2'	9:A:15:U:C6	2.54	0.42
9:A:35:C:H2'	9:A:36:U:C6	2.55	0.42
9:A:107:A:H2'	9:A:108:G:C8	2.55	0.42
9:A:410:G:C5	9:A:431:G:N1	2.88	0.42
9:A:606:G:H4'	9:A:607:U:OP1	2.20	0.42
9:A:750:C:H41	9:A:793:G:H1'	1.85	0.42
9:A:1096:G:H2'	9:A:1097:G:O4'	2.19	0.42
9:A:1585:U:C4	35:d:67:ARG:NE	2.87	0.42
9:A:1703:OMC:H1'	9:A:1703:OMC:HM23	1.85	0.42
9:A:1719:A:N7	9:A:1720:U:C5	2.87	0.42
9:A:1819:A:H2'	9:A:1820:G:O4'	2.20	0.42
9:A:1833:C:OP1	9:A:1840:U:H4'	2.20	0.42
22:N:104:THR:O	22:N:105:PRO:C	2.60	0.42
23:O:146:ARG:HE	23:O:146:ARG:HB3	1.58	0.42
27:S:162:LEU:HD23	27:S:162:LEU:HA	1.59	0.42
31:Z:151:LYS:HB2	31:Z:151:LYS:HE3	1.68	0.42
33:b:111:MET:HE2	33:b:111:MET:HB3	1.89	0.42
36:e:78:LYS:H	36:e:78:LYS:HG2	1.53	0.42
42:n:13:ARG:HH11	50:x:419:ALA:HB1	1.83	0.42
45:r:243:GLU:HG2	45:r:243:GLU:H	1.53	0.42
47:u:109:GLN:HE21	47:u:109:GLN:HB2	1.69	0.42
48:v:208:LEU:O	48:v:212:THR:N	2.50	0.42
51:y:120:LEU:HD23	51:y:120:LEU:HA	1.91	0.42
9:A:944:A:H5''	24:P:134:PRO:CB	2.49	0.42
9:A:1305:C:H2'	9:A:1306:U:C6	2.54	0.42
9:A:1542:C:O3'	9:A:1543:U:O4'	2.38	0.42
15:G:166:VAL:HG22	15:G:173:PHE:CZ	2.54	0.42
18:J:111:MET:HE2	18:J:111:MET:HB3	1.86	0.42
20:L:65:LYS:HD3	20:L:65:LYS:HA	1.87	0.42
20:L:126:ALA:HB1	20:L:151:ILE:HD13	2.01	0.42
27:S:5:ILE:O	27:S:13:GLN:HA	2.20	0.42
28:T:14:THR:HG23	28:T:21:LYS:HG2	2.01	0.42
34:c:90:TRP:HA	34:c:97:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:64:THR:HG22	38:h:77:TRP:HE3	1.84	0.42
44:q:40:LYS:HE3	44:q:48:GLU:OE2	2.19	0.42
45:r:59:ILE:H	45:r:59:ILE:HG13	1.39	0.42
7:8:49:ILE:O	7:8:53:TYR:N	2.53	0.42
9:A:13:C:H1'	9:A:1356:G:N2	2.35	0.42
9:A:77:A:H2	27:S:175:LYS:HG3	1.84	0.42
9:A:106:C:H5''	9:A:431:G:O2'	2.19	0.42
9:A:113:G:C2	9:A:292:A:N3	2.87	0.42
9:A:200:G:H5'	9:A:200:G:N3	2.34	0.42
9:A:376:A:H2'	9:A:377:G:O4'	2.19	0.42
9:A:483:C:OP1	13:E:76:LYS:HE2	2.20	0.42
9:A:866:U:H2'	9:A:867:G:C8	2.54	0.42
9:A:1372:U:H2'	9:A:1373:C:O4'	2.20	0.42
9:A:1386:A:N7	9:A:1387:G:C5	2.88	0.42
9:A:1410:C:H2'	9:A:1411:G:C8	2.54	0.42
17:I:132:LYS:HD3	17:I:132:LYS:HA	1.80	0.42
26:R:87:ASN:HB3	26:R:90:LEU:HG	2.01	0.42
28:T:23:MET:HE1	28:T:75:ILE:HG13	2.01	0.42
32:a:96:ARG:HD3	32:a:96:ARG:HA	1.61	0.42
37:f:121:ARG:HG3	37:f:131:VAL:HB	2.02	0.42
41:m:42:LEU:HD13	41:m:110:VAL:HG11	2.02	0.42
41:m:89:VAL:HG23	41:m:91:LEU:HG	2.02	0.42
45:r:190:LYS:HG2	45:r:278:VAL:C	2.44	0.42
47:u:11:ALA:HB1	47:u:31:LEU:HD23	2.02	0.42
48:v:249:MET:HB2	48:v:281:ILE:HG12	2.02	0.42
48:v:284:GLU:OE1	51:y:586:ARG:NH1	2.52	0.42
2:3:173:TRP:O	2:3:177:TYR:N	2.52	0.42
3:4:307:PHE:C	47:u:538:LYS:HZ1	2.28	0.42
9:A:155:G:C2	9:A:164:A:C6	3.08	0.42
9:A:216:C:C2'	9:A:217:A:H5'	2.50	0.42
9:A:380:G:H1'	26:R:5:ARG:CZ	2.50	0.42
9:A:393:U:C5'	51:y:146:ARG:NH2	2.75	0.42
9:A:1220:A:H2'	9:A:1221:G:O4'	2.19	0.42
9:A:1231:C:C5	9:A:1232:U:C4	3.05	0.42
9:A:1391:C:H2'	9:A:1392:U:O4'	2.19	0.42
9:A:1425:G:H5''	30:Y:31:LEU:HD21	2.02	0.42
9:A:1603:G:H4'	37:f:38:ARG:NE	2.35	0.42
21:M:33:ARG:HD3	21:M:33:ARG:HA	1.95	0.42
21:M:34:VAL:HG12	21:M:38:ILE:HD13	2.01	0.42
25:Q:40:VAL:HG23	25:Q:69:VAL:HB	2.01	0.42
26:R:121:LEU:O	26:R:122:GLY:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:3:GLU:O	34:c:4:GLN:C	2.63	0.42
44:q:47:LEU:HB2	44:q:59:CYS:HB2	2.02	0.42
45:r:194:ASP:CB	45:r:272:GLN:HB3	2.48	0.42
45:r:201:GLY:HA2	45:r:266:ARG:HB3	2.02	0.42
47:u:483:ARG:O	47:u:492:SER:N	2.45	0.42
49:w:52:G:H2'	49:w:53:A:C8	2.54	0.42
51:y:70:ALA:HA	51:y:73:ILE:HG22	2.02	0.42
1:1:562:LYS:HA	1:1:562:LYS:HD2	1.87	0.42
5:6:185:MET:O	5:6:189:LEU:N	2.50	0.42
9:A:520:A:C6	9:A:521:A:C5	3.08	0.42
9:A:847:A:H3'	9:A:848:U:H6	1.84	0.42
9:A:1053:C:H2'	9:A:1054:G:C8	2.55	0.42
9:A:1317:C:H2'	9:A:1318:G:C8	2.55	0.42
9:A:1813:A:N6	9:A:1814:G:C2	2.88	0.42
22:N:97:THR:HA	22:N:98:PRO:HD3	1.90	0.42
26:R:74:ARG:HB2	26:R:109:TYR:CE1	2.54	0.42
26:R:146:GLN:H	26:R:146:GLN:HG3	1.48	0.42
27:S:32:MET:HE2	27:S:32:MET:HB3	1.83	0.42
30:Y:93:VAL:HG13	30:Y:105:LYS:HD2	2.02	0.42
31:Z:48:ILE:O	31:Z:87:TYR:HB2	2.19	0.42
36:e:48:VAL:HG22	36:e:49:LEU:HG	2.02	0.42
47:u:14[B]:ARG:NH2	47:u:17:GLU:OE1	2.53	0.42
48:v:233:ILE:HD11	48:v:273:VAL:HB	2.01	0.42
48:v:261:VAL:HG21	48:v:274:LEU:HG	2.02	0.42
50:x:304:ASN:OD1	50:x:311:ASN:ND2	2.53	0.42
51:y:439:ARG:HH12	51:y:441:ARG:HH21	1.68	0.42
5:6:184:VAL:O	5:6:188:LEU:N	2.46	0.41
5:6:312:VAL:HG12	5:6:330:ARG:HH11	1.85	0.41
5:6:324:LYS:O	47:u:448:GLN:N	2.53	0.41
9:A:70:G:H1'	9:A:80:G:N2	2.35	0.41
9:A:520:A:C5	9:A:521:A:N7	2.88	0.41
9:A:1049:A:OP1	9:A:1854:U:O2'	2.38	0.41
9:A:1259:A:OP2	9:A:1259:A:C2	2.73	0.41
9:A:1712:A:C6	9:A:1713:C:C4	3.08	0.41
11:C:153:LEU:O	11:C:155:LYS:HG2	2.20	0.41
12:D:163:SER:O	12:D:164:PRO:C	2.62	0.41
16:H:20:LYS:HE2	16:H:20:LYS:HB2	1.47	0.41
20:L:84:PHE:HB2	20:L:86:LEU:HG	2.02	0.41
20:L:130:ILE:HD11	20:L:158:ALA:C	2.45	0.41
20:L:182:CYS:O	20:L:183:LYS:C	2.61	0.41
21:M:71:ILE:H	21:M:71:ILE:HG12	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:118:GLU:H	27:S:118:GLU:HG2	1.60	0.41
32:a:65:ARG:CD	39:i:25:SER:HB3	2.50	0.41
34:c:219:TRP:CZ3	34:c:226:HIS:HB2	2.55	0.41
44:q:37:GLN:HE21	44:q:37:GLN:HB3	1.62	0.41
45:r:200:TYR:O	45:r:266:ARG:HB3	2.20	0.41
51:y:502:ILE:HD12	51:y:502:ILE:HA	1.88	0.41
9:A:164:A:H2'	9:A:165:G:N3	2.35	0.41
9:A:538:U:H2'	9:A:539:C:O4'	2.19	0.41
9:A:824:C:C6	12:D:144:ILE:HG13	2.55	0.41
9:A:932:G:H4'	9:A:993:G:O2'	2.20	0.41
9:A:1093:A:H4'	18:J:3:ARG:NH2	2.35	0.41
9:A:1120:U:H1'	9:A:1121:G:C8	2.55	0.41
9:A:1163:C:H2'	9:A:1164:G:H8	1.85	0.41
9:A:1311:C:N4	40:k:97:LYS:HZ1	2.17	0.41
9:A:1386:A:C8	9:A:1387:G:C8	3.08	0.41
16:H:56:CYS:SG	16:H:57:VAL:N	2.93	0.41
19:K:45:ARG:HE	19:K:45:ARG:HB3	1.41	0.41
21:M:92:ASP:O	21:M:93:GLN:C	2.62	0.41
42:n:59:LEU:HD12	42:n:59:LEU:HA	1.76	0.41
45:r:36:LEU:HD21	45:r:83:ILE:HD13	2.01	0.41
47:u:542:ILE:HG23	47:u:543:LEU:HD12	2.02	0.41
49:w:41:A:H2'	49:w:42:G:C8	2.56	0.41
9:A:61:A:C2	9:A:336:A:O4'	2.73	0.41
9:A:432:G:H2'	9:A:433:A:C8	2.55	0.41
9:A:570:C:N4	9:A:571:U:C4	2.88	0.41
9:A:674:C:H2'	9:A:675:U:C6	2.55	0.41
9:A:738:C:H2'	9:A:739:C:C6	2.54	0.41
9:A:818:A:H2'	9:A:819:G:H8	1.84	0.41
9:A:1720:U:C4	9:A:1814:G:N2	2.87	0.41
9:A:1805:G:C6	9:A:1806:A:C6	3.08	0.41
9:A:1811:C:H2'	9:A:1812:U:O4'	2.20	0.41
9:A:1815:A:H2'	9:A:1816:G:O4'	2.20	0.41
11:C:29:PRO:HG2	11:C:46:ILE:HD11	2.02	0.41
15:G:58:LYS:HE2	15:G:58:LYS:HB2	1.83	0.41
24:P:56:VAL:HG11	24:P:61:LYS:HG2	2.03	0.41
26:R:141:ARG:O	26:R:142:SER:C	2.63	0.41
27:S:45:TRP:CZ3	27:S:121:ILE:HD13	2.55	0.41
27:S:124:LEU:HD23	27:S:124:LEU:HA	1.79	0.41
28:T:60:PHE:HA	28:T:70:THR:O	2.20	0.41
32:a:95:ARG:C	32:a:97:SER:N	2.77	0.41
33:b:58:LYS:HB3	33:b:58:LYS:HE3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:246:TYR:HD2	34:c:262:GLU:HB2	1.85	0.41
45:r:190:LYS:HB2	45:r:238:THR:HB	2.01	0.41
47:u:286:SER:HA	51:y:728:GLY:HA2	2.01	0.41
48:v:223:PHE:HB3	48:v:224:ASN:H	1.75	0.41
49:w:31:C:H3'	49:w:32:C:C6	2.56	0.41
50:x:448:LYS:HE3	50:x:448:LYS:HB3	1.72	0.41
51:y:499:VAL:HA	51:y:502:ILE:HG22	2.02	0.41
4:5:522:TYR:O	48:v:402:GLN:NE2	2.53	0.41
9:A:119:PSU:H2'	9:A:120:U:C6	2.56	0.41
9:A:1049:A:OP1	9:A:1855:G:H5'	2.20	0.41
9:A:1105:G:O3'	16:H:69:GLY:HA3	2.20	0.41
9:A:1199:A:C6	9:A:1200:A:C5	3.08	0.41
11:C:115:THR:HB	11:C:118:GLU:H	1.86	0.41
17:I:55:ARG:HE	17:I:55:ARG:HB3	1.71	0.41
22:N:62:ALA:O	22:N:66:VAL:HG23	2.20	0.41
22:N:117:ARG:HD3	22:N:117:ARG:HA	1.56	0.41
24:P:121:ARG:HA	24:P:121:ARG:NE	2.36	0.41
25:Q:21:ILE:O	25:Q:21:ILE:HG13	2.19	0.41
26:R:38:ILE:HG12	26:R:96:LEU:HD21	2.03	0.41
29:V:193:LYS:HE3	29:V:193:LYS:HB3	1.67	0.41
30:Y:42:ILE:HD13	30:Y:42:ILE:HA	1.89	0.41
39:i:21:CYS:HB3	39:i:25:SER:H	1.85	0.41
43:o:243:VAL:HG22	43:o:312:VAL:HG12	2.03	0.41
47:u:549:GLN:O	47:u:553:ALA:N	2.49	0.41
1:1:489:ILE:HA	1:1:490:PRO:HD2	1.90	0.41
3:4:163:VAL:O	7:8:83:PRO:C	2.64	0.41
3:4:265:LEU:O	3:4:269:LEU:N	2.50	0.41
3:4:267:SER:HA	7:8:341:LEU:CB	2.50	0.41
9:A:473:A:H5'	9:A:473:A:H8	1.86	0.41
9:A:928:G:H2'	9:A:929:G:C8	2.55	0.41
9:A:1529:C:O2'	35:d:89:PRO:HD3	2.21	0.41
26:R:25:ARG:O	26:R:28:GLU:HG2	2.20	0.41
31:Z:133:GLY:HA2	31:Z:155:GLY:HA3	2.03	0.41
31:Z:162:ASP:O	31:Z:163:PRO:C	2.61	0.41
40:k:94:LYS:HD2	40:k:94:LYS:HA	1.95	0.41
45:r:176:LEU:HG	45:r:180:ILE:HD11	2.02	0.41
48:v:273:VAL:O	48:v:277:LEU:N	2.40	0.41
4:5:227:VAL:O	4:5:231:LEU:N	2.46	0.41
8:9:7:LYS:HG2	8:9:11:ARG:HD2	2.03	0.41
9:A:95:G:H5''	12:D:2:PRO:HG2	2.02	0.41
9:A:1164:G:O2'	9:A:1165:G:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1532:C:O2	9:A:1636:G:H5'	2.20	0.41
9:A:1650:A:H61	9:A:1674:G:H1'	1.85	0.41
9:A:1754:G:O2'	9:A:1755:C:P	2.75	0.41
10:B:126:VAL:HB	10:B:142:VAL:HG13	2.02	0.41
12:D:115:PHE:HA	12:D:120:ALA:HB3	2.02	0.41
16:H:21:LYS:HD2	17:I:15:ALA:HB2	2.03	0.41
21:M:57:LEU:O	21:M:58:MET:C	2.64	0.41
24:P:34:PHE:HE1	24:P:100:THR:HA	1.85	0.41
30:Y:113:ILE:HG12	30:Y:120:LEU:HD12	2.02	0.41
32:a:53:LYS:HB3	32:a:53:LYS:HE3	1.48	0.41
34:c:54:ILE:HD12	34:c:54:ILE:HA	1.94	0.41
34:c:90:TRP:CZ3	34:c:97:THR:HG22	2.55	0.41
45:r:123:LYS:HB2	45:r:126:GLN:HG2	2.03	0.41
45:r:234:ARG:HH22	49:w:1:A:H1'	1.86	0.41
47:u:57:LEU:HD23	47:u:57:LEU:HA	1.93	0.41
47:u:113:LEU:HD12	47:u:113:LEU:HA	1.92	0.41
47:u:481:GLN:HG2	47:u:499:TYR:CD1	2.56	0.41
51:y:594:LEU:HD22	51:y:598:ILE:HD13	2.03	0.41
3:4:287:LEU:CB	47:u:543:LEU:HD11	2.50	0.41
9:A:409:C:H5''	9:A:426:A:H5'	2.02	0.41
9:A:1092:G:C6	9:A:1158:G:C6	3.08	0.41
9:A:1755:C:H2'	9:A:1777:G:C2	2.55	0.41
9:A:1805:G:C4	9:A:1806:A:C8	3.09	0.41
10:B:152:LYS:HE3	10:B:152:LYS:HB3	1.70	0.41
17:I:33:VAL:HG21	17:I:66:VAL:HG21	2.03	0.41
21:M:23:ARG:HB3	34:c:170:TRP:HZ3	1.86	0.41
26:R:48:VAL:HG11	26:R:54:LYS:HD2	2.02	0.41
26:R:178:ARG:H	26:R:178:ARG:HG3	1.37	0.41
35:d:33:TRP:HZ2	35:d:102:ARG:HG3	1.86	0.41
35:d:42:HIS:HA	35:d:83:GLN:HG3	2.02	0.41
44:q:68:LYS:HB2	44:q:69:VAL:H	1.74	0.41
45:r:64:ARG:HG3	45:r:67:ARG:HB2	2.02	0.41
47:u:342:LEU:HA	47:u:346:GLY:HA2	2.02	0.41
50:x:68:GLN:HE21	50:x:68:GLN:HB3	1.58	0.41
50:x:412:LYS:HD3	50:x:416:GLN:HB3	2.02	0.41
51:y:760:LYS:HB2	51:y:760:LYS:HE2	1.89	0.41
8:9:14:LYS:HE3	8:9:14:LYS:HB2	1.59	0.41
9:A:75:G:N3	9:A:76:U:N3	2.65	0.41
9:A:1529:C:H2'	9:A:1530:U:C6	2.55	0.41
9:A:1742:C:C2	9:A:1793:A:N1	2.88	0.41
23:O:78:GLU:O	23:O:79:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:125:LYS:CB	25:Q:58:VAL:HG12	2.48	0.41
28:T:110:ARG:HG3	28:T:126:GLY:HA3	2.03	0.41
30:Y:61:GLU:CD	30:Y:61:GLU:H	2.28	0.41
34:c:143:GLN:O	34:c:144:ASP:C	2.63	0.41
34:c:290:ALA:O	34:c:298:LEU:HD12	2.19	0.41
49:w:53:A:H2'	49:w:54:U:O4'	2.21	0.41
50:x:71:TYR:CZ	51:y:563:ARG:HD2	2.56	0.41
1:1:658:GLU:O	1:1:667:VAL:N	2.51	0.41
5:6:324:LYS:HB2	47:u:447:TYR:CG	2.56	0.41
9:A:116:OMU:HN3	9:A:347:G:H1	1.69	0.41
9:A:390:C:H2'	9:A:391:C:O4'	2.21	0.41
9:A:522:A:OP1	12:D:146:SER:HB3	2.21	0.41
9:A:614:C:C5	9:A:626:G:C2	3.09	0.41
9:A:868:G:C5	15:G:115:LYS:HB3	2.55	0.41
9:A:1045:U:H2'	9:A:1046:U:O4'	2.21	0.41
9:A:1058:A:H2'	9:A:1059:G:C8	2.55	0.41
9:A:1073:U:H2'	9:A:1074:C:C6	2.56	0.41
10:B:82:MET:HE3	10:B:82:MET:HB2	1.68	0.41
13:E:133:LEU:HA	13:E:133:LEU:HD23	1.89	0.41
15:G:51:ILE:O	15:G:58:LYS:HA	2.20	0.41
18:J:75:ILE:HD13	18:J:75:ILE:HA	1.82	0.41
22:N:39:TYR:HB2	22:N:50:ASN:HD22	1.86	0.41
22:N:137:ALA:O	22:N:138:SER:C	2.64	0.41
24:P:25:GLU:H	24:P:25:GLU:HG3	1.66	0.41
26:R:22:HIS:HD2	26:R:25:ARG:HG3	1.85	0.41
27:S:1:MET:HG3	27:S:106:LEU:O	2.21	0.41
29:V:192:LYS:HA	29:V:192:LYS:HD3	1.81	0.41
31:Z:38:GLU:HB3	31:Z:49:ILE:HB	2.03	0.41
38:h:30:LYS:HD3	38:h:30:LYS:HA	1.94	0.41
44:q:35:TYR:HB2	44:q:52:PHE:CD1	2.56	0.41
47:u:531:ALA:HA	47:u:534:LEU:HB3	2.03	0.41
47:u:535:GLU:HA	47:u:538:LYS:HD2	2.02	0.41
47:u:558:LEU:HA	47:u:561:SER:HB2	2.02	0.41
48:v:261:VAL:HG11	48:v:274:LEU:HD21	2.02	0.41
50:x:80:PHE:CD2	50:x:82:LEU:HG	2.56	0.41
51:y:347:ARG:H	51:y:347:ARG:HG2	1.66	0.41
51:y:369:GLY:HA3	51:y:425:LEU:HD11	2.02	0.41
51:y:458:ILE:HG22	51:y:459:MET:HE2	2.03	0.41
51:y:855:LEU:HD23	51:y:855:LEU:HA	1.84	0.41
4:5:466:LEU:O	48:v:384:ILE:HB	2.20	0.41
5:6:186:VAL:O	5:6:190:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:210:U:H2'	9:A:211:G:O4'	2.21	0.41
9:A:339:A:H2'	9:A:340:C:C5	2.55	0.41
9:A:1336:C:H2'	9:A:1337:C:O4'	2.21	0.41
11:C:19:MET:SD	11:C:108:ARG:HD2	2.60	0.41
11:C:108:ARG:O	11:C:109:PHE:C	2.63	0.41
13:E:86:PRO:HD2	13:E:130:LEU:HD23	2.02	0.41
18:J:86:LEU:HD21	18:J:113:HIS:HB2	2.03	0.41
22:N:36:GLN:H	22:N:36:GLN:HG3	1.68	0.41
26:R:65:PHE:HA	26:R:187:GLY:O	2.21	0.41
29:V:171:GLU:HG3	36:e:106:GLN:HE22	1.86	0.41
31:Z:64:ARG:NH2	32:a:76:ILE:HD11	2.36	0.41
34:c:146:SER:O	34:c:147:HIS:C	2.62	0.41
45:r:80:LYS:HA	45:r:80:LYS:HD3	1.81	0.41
47:u:254:GLU:HG3	47:u:358:LEU:HD21	2.03	0.41
47:u:304:ARG:NH1	47:u:315:MET:SD	2.94	0.41
51:y:552:CYS:HB3	51:y:556:TYR:CZ	2.55	0.41
3:4:106:TYR:O	47:u:569:LEU:HD23	2.20	0.40
5:6:313:ILE:HA	5:6:316:VAL:HG12	2.01	0.40
7:8:219:GLU:CB	47:u:558:LEU:HD21	2.51	0.40
8:9:2:ARG:HB3	8:9:5:TRP:CD1	2.56	0.40
9:A:379:C:O5'	26:R:181:GLN:NE2	2.54	0.40
9:A:392:A:O2'	10:B:83:GLN:NE2	2.54	0.40
9:A:433:A:H2'	9:A:434:G:C8	2.56	0.40
9:A:804:U:H4'	18:J:122:GLY:O	2.22	0.40
9:A:874:G:H2'	9:A:875:A:C8	2.57	0.40
9:A:1208:A:C6	9:A:1209:A:N6	2.90	0.40
9:A:1470:C:H2'	9:A:1471:C:H6	1.85	0.40
30:Y:90:LYS:HE2	30:Y:90:LYS:HB3	1.88	0.40
31:Z:225:GLU:HG3	34:c:187:ASN:HB3	2.03	0.40
35:d:51:ASN:HB3	35:d:54:TYR:HD2	1.86	0.40
37:f:82:TRP:CD1	37:f:82:TRP:H	2.39	0.40
42:n:21:THR:HG22	42:n:27:CYS:O	2.21	0.40
51:y:801:SER:HA	51:y:842:VAL:HA	2.03	0.40
9:A:375:U:H2'	9:A:376:A:C8	2.56	0.40
9:A:1031:A2M:H1'	9:A:1031:A2M:HM'3	1.55	0.40
9:A:1237:C:O5'	9:A:1237:C:H6	2.03	0.40
9:A:1414:A:C5	9:A:1415:C:C4	3.09	0.40
9:A:1626:C:H2'	9:A:1627:C:C6	2.56	0.40
9:A:1831:A:O2'	9:A:1852:C:H5'	2.22	0.40
22:N:30:LEU:HD11	22:N:35:GLU:HA	2.03	0.40
23:O:42:ARG:HA	23:O:42:ARG:HD2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:58:VAL:HG22	25:Q:59:PHE:N	2.35	0.40
26:R:153:LYS:HA	26:R:156:ALA:HB3	2.03	0.40
28:T:55:ILE:H	28:T:55:ILE:HG12	1.49	0.40
30:Y:12:VAL:HG11	30:Y:90:LYS:HB3	2.03	0.40
30:Y:96:TYR:HA	30:Y:100:VAL:HG23	2.02	0.40
35:d:33:TRP:CZ2	35:d:102:ARG:HG3	2.56	0.40
37:f:13:LEU:HD11	37:f:56:ALA:HB1	2.03	0.40
40:k:121:CYS:HA	40:k:122:PRO:HD3	1.96	0.40
45:r:142:TYR:HE2	45:r:151:ASP:HB3	1.83	0.40
47:u:490:THR:OG1	47:u:491:LEU:N	2.54	0.40
1:1:530:VAL:HB	1:1:543:ASN:HB2	2.03	0.40
5:6:180:ALA:O	5:6:184:VAL:N	2.52	0.40
9:A:67:C:H42	27:S:167:LYS:HB2	1.86	0.40
9:A:1190:A:H2'	9:A:1191:C:O4'	2.22	0.40
9:A:1452:A:H5''	21:M:48:ASN:OD1	2.22	0.40
13:E:68:LYS:HB3	13:E:91:LEU:HD22	2.03	0.40
26:R:148:LYS:HE2	26:R:148:LYS:HB3	1.82	0.40
28:T:23:MET:HE3	28:T:23:MET:HB3	1.87	0.40
29:V:76:MET:HE2	29:V:76:MET:HB2	1.75	0.40
29:V:109:LEU:O	29:V:110:GLN:C	2.63	0.40
36:e:57:LYS:HE3	36:e:77:LEU:HD22	2.03	0.40
45:r:174:GLU:HA	45:r:177:ILE:HG12	2.03	0.40
47:u:35:MET:HE2	47:u:51:MET:HE3	2.03	0.40
47:u:80:GLN:HG2	47:u:169:ARG:HE	1.87	0.40
47:u:290:LEU:HA	47:u:329:ILE:HD13	2.04	0.40
47:u:323:LEU:HD12	47:u:323:LEU:HA	1.91	0.40
9:A:41:G:H1	9:A:481:C:H42	1.68	0.40
9:A:509:OMG:H1'	9:A:509:OMG:HM23	1.80	0.40
9:A:1092:G:N1	9:A:1158:G:C6	2.89	0.40
9:A:1157:G:H5'	9:A:1157:G:N3	2.36	0.40
9:A:1527:C:C4	9:A:1528:G:C8	3.09	0.40
9:A:1740:C:H2'	9:A:1741:U:C6	2.56	0.40
10:B:42:LEU:HD23	10:B:42:LEU:HA	1.97	0.40
10:B:111:VAL:HG12	10:B:140:PHE:CB	2.51	0.40
13:E:135:LYS:HD3	13:E:137:LYS:HE2	2.03	0.40
15:G:29:GLU:O	15:G:32:MET:HB3	2.22	0.40
15:G:37:LYS:HD3	15:G:41:ARG:NH2	2.36	0.40
16:H:75:GLU:H	16:H:75:GLU:CD	2.30	0.40
20:L:64:THR:HG23	20:L:67:GLY:H	1.86	0.40
20:L:192:LEU:O	20:L:226:ALA:HA	2.22	0.40
22:N:69:GLU:H	22:N:69:GLU:HG2	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:72:TYR:CD2	24:P:72:TYR:C	2.97	0.40
27:S:203:LYS:HE3	27:S:203:LYS:HB2	1.79	0.40
29:V:201:LYS:HE2	29:V:201:LYS:HB2	1.83	0.40
31:Z:59:LEU:HD11	43:o:308:LEU:HG	1.98	0.40
34:c:19:THR:O	34:c:288:SER:HB3	2.22	0.40
35:d:64:LEU:HA	35:d:64:LEU:HD23	1.70	0.40
35:d:75:MET:HE3	35:d:104:LEU:HD21	2.04	0.40
37:f:116:LYS:HE3	37:f:116:LYS:HB3	1.86	0.40
40:k:138:ARG:H	40:k:138:ARG:HG2	1.51	0.40
47:u:279:VAL:HA	47:u:282:VAL:HG12	2.02	0.40
47:u:385:PRO:O	47:u:388:LYS:NZ	2.53	0.40
48:v:51:VAL:O	48:v:55:MET:N	2.51	0.40
51:y:769:PHE:CD2	51:y:775:VAL:HG11	2.56	0.40
9:A:517:OMC:H2'	9:A:518:G:O4'	2.21	0.40
9:A:563:G:N3	9:A:564:A:C8	2.90	0.40
9:A:990:A:N6	9:A:992:A:C2	2.90	0.40
9:A:1031:A2M:H2'	9:A:1032:C:C6	2.56	0.40
9:A:1114:U:H2'	9:A:1119:A:N6	2.37	0.40
9:A:1157:G:N3	9:A:1157:G:H2'	2.37	0.40
9:A:1203:G:C6	9:A:1204:A:C6	3.09	0.40
9:A:1529:C:H5'	9:A:1666:C:OP1	2.22	0.40
9:A:1595:U:H2'	9:A:1596:U:C6	2.56	0.40
9:A:1805:G:C2	9:A:1806:A:C4	3.09	0.40
9:A:1805:G:N1	9:A:1806:A:C5	2.90	0.40
11:C:125:LYS:HA	11:C:159:THR:HA	2.03	0.40
19:K:30:ALA:HA	22:N:138:SER:O	2.22	0.40
22:N:13:GLU:HG3	22:N:17:LYS:HE2	2.04	0.40
27:S:63:MET:HA	27:S:98:ARG:O	2.22	0.40
34:c:147:HIS:HB3	34:c:171:ASP:CG	2.47	0.40
35:d:11:GLN:O	35:d:15:VAL:HG23	2.21	0.40
44:q:42:LEU:HD23	44:q:42:LEU:HA	1.62	0.40
45:r:20:VAL:HG13	45:r:71:VAL:HG23	2.04	0.40
47:u:448:GLN:O	47:u:493:PHE:N	2.50	0.40
51:y:825:MET:HE2	51:y:825:MET:HB2	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	443/813 (54%)	414 (94%)	26 (6%)	3 (1%)	18	50
2	3	209/218 (96%)	205 (98%)	3 (1%)	1 (0%)	24	56
3	4	251/357 (70%)	229 (91%)	19 (8%)	3 (1%)	10	40
4	5	307/564 (54%)	301 (98%)	6 (2%)	0	100	100
5	6	348/374 (93%)	318 (91%)	30 (9%)	0	100	100
7	8	313/352 (89%)	276 (88%)	35 (11%)	2 (1%)	21	52
8	9	22/25 (88%)	22 (100%)	0	0	100	100
10	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
11	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
12	D	175/194 (90%)	174 (99%)	1 (1%)	0	100	100
13	E	138/143 (96%)	134 (97%)	3 (2%)	1 (1%)	18	50
14	F	43/59 (73%)	43 (100%)	0	0	100	100
15	G	171/194 (88%)	163 (95%)	7 (4%)	1 (1%)	21	52
16	H	79/84 (94%)	76 (96%)	2 (2%)	1 (1%)	9	38
17	I	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
18	J	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	48
19	K	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
20	L	218/293 (74%)	215 (99%)	2 (1%)	1 (0%)	24	56
21	M	123/135 (91%)	121 (98%)	2 (2%)	0	100	100
22	N	205/295 (70%)	201 (98%)	3 (2%)	1 (0%)	24	56
23	O	209/264 (79%)	193 (92%)	16 (8%)	0	100	100
24	P	131/151 (87%)	123 (94%)	7 (5%)	1 (1%)	16	48
25	Q	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
26	R	194/208 (93%)	194 (100%)	0	0	100	100
27	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	T	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
29	V	180/204 (88%)	175 (97%)	5 (3%)	0	100	100
30	Y	139/146 (95%)	136 (98%)	3 (2%)	0	100	100
31	Z	225/243 (93%)	223 (99%)	2 (1%)	0	100	100
32	a	97/165 (59%)	97 (100%)	0	0	100	100
33	b	108/145 (74%)	107 (99%)	1 (1%)	0	100	100
34	c	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
35	d	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
36	e	64/125 (51%)	64 (100%)	0	0	100	100
37	f	140/152 (92%)	134 (96%)	6 (4%)	0	100	100
38	h	101/119 (85%)	97 (96%)	4 (4%)	0	100	100
39	i	48/56 (86%)	47 (98%)	0	1 (2%)	5	31
40	k	49/156 (31%)	44 (90%)	4 (8%)	1 (2%)	6	32
41	m	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
42	n	61/69 (88%)	59 (97%)	1 (2%)	1 (2%)	7	35
43	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
44	q	99/144 (69%)	83 (84%)	12 (12%)	4 (4%)	2	21
45	r	273/315 (87%)	255 (93%)	17 (6%)	1 (0%)	30	60
46	t	346/472 (73%)	337 (97%)	5 (1%)	4 (1%)	10	40
47	u	705/1382 (51%)	672 (95%)	32 (4%)	1 (0%)	48	78
48	v	380/445 (85%)	350 (92%)	30 (8%)	0	100	100
50	x	415/548 (76%)	386 (93%)	29 (7%)	0	100	100
51	y	636/913 (70%)	610 (96%)	25 (4%)	1 (0%)	43	72
All	All	9485/12718 (75%)	9077 (96%)	378 (4%)	30 (0%)	37	65

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	282	PRO
1	1	427	PRO
3	4	264	GLY
16	H	56	CYS
24	P	136	PRO
44	q	94	LYS

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Mol	Chain	Res	Type
45	r	54	ARG
46	t	167	GLN
46	t	168	PRO
46	t	248	ARG
7	8	154	PRO
42	n	39	SER
44	q	63	GLY
44	q	69	VAL
1	1	499	PRO
20	L	171	GLY
22	N	98	PRO
46	t	247	PRO
51	y	849	PRO
3	4	263	ILE
39	i	11	PRO
44	q	64	LYS
2	3	206	ASP
3	4	320	PRO
13	E	116	PRO
7	8	310	PRO
47	u	539	PRO
18	J	29	PRO
15	G	190	PRO
40	k	102	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	97/701 (14%)	95 (98%)	2 (2%)	47	64
5	6	49/335 (15%)	48 (98%)	1 (2%)	48	64
8	9	23/24 (96%)	23 (100%)	0	100	100
10	B	129/142 (91%)	117 (91%)	12 (9%)	8	32
11	C	220/225 (98%)	195 (89%)	25 (11%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	158/168 (94%)	149 (94%)	9 (6%)	18	45
13	E	112/115 (97%)	101 (90%)	11 (10%)	7	30
14	F	38/48 (79%)	35 (92%)	3 (8%)	11	37
15	G	159/174 (91%)	135 (85%)	24 (15%)	3	16
16	H	73/76 (96%)	61 (84%)	12 (16%)	2	14
17	I	130/131 (99%)	121 (93%)	9 (7%)	14	41
18	J	112/113 (99%)	108 (96%)	4 (4%)	31	54
19	K	65/67 (97%)	57 (88%)	8 (12%)	4	22
20	L	186/225 (83%)	157 (84%)	29 (16%)	2	15
21	M	114/122 (93%)	98 (86%)	16 (14%)	3	18
22	N	173/243 (71%)	159 (92%)	14 (8%)	11	36
23	O	192/231 (83%)	190 (99%)	2 (1%)	68	74
24	P	104/119 (87%)	84 (81%)	20 (19%)	1	9
25	Q	86/98 (88%)	74 (86%)	12 (14%)	3	18
26	R	172/180 (96%)	154 (90%)	18 (10%)	6	28
27	S	200/218 (92%)	174 (87%)	26 (13%)	4	20
28	T	107/115 (93%)	96 (90%)	11 (10%)	7	29
29	V	156/170 (92%)	144 (92%)	12 (8%)	12	38
30	Y	117/121 (97%)	107 (92%)	10 (8%)	10	35
31	Z	190/202 (94%)	153 (80%)	37 (20%)	1	9
32	a	90/136 (66%)	83 (92%)	7 (8%)	11	37
33	b	100/130 (77%)	89 (89%)	11 (11%)	6	26
34	c	272/275 (99%)	229 (84%)	43 (16%)	2	15
35	d	112/115 (97%)	99 (88%)	13 (12%)	5	24
36	e	58/103 (56%)	50 (86%)	8 (14%)	3	19
37	f	123/132 (93%)	108 (88%)	15 (12%)	5	22
38	h	94/107 (88%)	82 (87%)	12 (13%)	4	21
39	i	44/49 (90%)	41 (93%)	3 (7%)	14	42
40	k	47/140 (34%)	34 (72%)	13 (28%)	0	3
41	m	104/108 (96%)	95 (91%)	9 (9%)	9	34
42	n	56/62 (90%)	46 (82%)	10 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	o	64/277 (23%)	59 (92%)	5 (8%)	11	37
44	q	77/123 (63%)	61 (79%)	16 (21%)	1	8
45	r	247/280 (88%)	199 (81%)	48 (19%)	1	9
47	u	528/1259 (42%)	518 (98%)	10 (2%)	50	65
48	v	206/406 (51%)	198 (96%)	8 (4%)	28	53
50	x	206/494 (42%)	197 (96%)	9 (4%)	25	50
51	y	563/811 (69%)	554 (98%)	9 (2%)	55	68
All	All	6153/9370 (66%)	5577 (91%)	576 (9%)	10	32

All (576) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	554	VAL
1	1	566	ILE
5	6	326	ASP
10	B	15	THR
10	B	35	ARG
10	B	40	ILE
10	B	46	THR
10	B	69	ARG
10	B	79	LYS
10	B	86	ILE
10	B	103	GLU
10	B	114	SER
10	B	118	ARG
10	B	128	VAL
10	B	152	LYS
11	C	12	VAL
11	C	26	VAL
11	C	33	THR
11	C	40	GLU
11	C	41	CYS
11	C	45	ILE
11	C	57	THR
11	C	91	SER
11	C	102	ILE
11	C	105	THR
11	C	111	VAL
11	C	134	LYS
11	C	141	THR

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Mol	Chain	Res	Type
11	C	143	ASP
11	C	166	THR
11	C	169	ILE
11	C	173	ILE
11	C	176	ASP
11	C	183	VAL
11	C	198	ARG
11	C	220	THR
11	C	227	VAL
11	C	232	ASN
11	C	236	ILE
11	C	248	ILE
12	D	14	VAL
12	D	32	ILE
12	D	65	GLU
12	D	95	ASP
12	D	102	ILE
12	D	128	VAL
12	D	138	ARG
12	D	149	VAL
12	D	155	LYS
13	E	4	CYS
13	E	55	VAL
13	E	66	ILE
13	E	82	THR
13	E	94	ILE
13	E	102	VAL
13	E	105	PHE
13	E	115	ILE
13	E	125	VAL
13	E	130	LEU
13	E	139	GLU
14	F	82	ARG
14	F	93	VAL
14	F	103	THR
15	G	23	ILE
15	G	25	GLN
15	G	29	GLU
15	G	30	LEU
15	G	46	THR
15	G	51	ILE
15	G	53	VAL

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Mol	Chain	Res	Type
15	G	62	ILE
15	G	72	PHE
15	G	92	VAL
15	G	113	LYS
15	G	121	THR
15	G	123	THR
15	G	139	ILE
15	G	144	ILE
15	G	147	LYS
15	G	148	LEU
15	G	154	ILE
15	G	156	VAL
15	G	166	VAL
15	G	171	GLU
15	G	180	LEU
15	G	183	LYS
15	G	185	VAL
16	H	8	LEU
16	H	13	GLU
16	H	23	ARG
16	H	25	VAL
16	H	26	GLN
16	H	35	VAL
16	H	36	LYS
16	H	40	CYS
16	H	43	ILE
16	H	53	VAL
16	H	59	CYS
16	H	61	THR
17	I	16	LEU
17	I	22	VAL
17	I	35	GLU
17	I	63	VAL
17	I	87	ASP
17	I	106	ARG
17	I	121	ARG
17	I	140	LYS
17	I	150	VAL
18	J	25	VAL
18	J	55	ASP
18	J	72	CYS
18	J	74	VAL

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Mol	Chain	Res	Type
19	K	32	ILE
19	K	39	VAL
19	K	42	VAL
19	K	50	PHE
19	K	52	THR
19	K	64	GLU
19	K	79	VAL
19	K	81	LYS
20	L	83	LEU
20	L	88	ILE
20	L	104	ASP
20	L	109	ILE
20	L	116	THR
20	L	120	GLN
20	L	122	THR
20	L	123	ARG
20	L	128	VAL
20	L	130	ILE
20	L	147	VAL
20	L	173	LYS
20	L	180	VAL
20	L	184	VAL
20	L	209	VAL
20	L	213	LEU
20	L	227	ARG
20	L	230	THR
20	L	236	PHE
20	L	240	THR
20	L	252	THR
20	L	253	PRO
20	L	254	ASP
20	L	255	LEU
20	L	259	THR
20	L	260	VAL
20	L	262	THR
20	L	270	THR
20	L	276	THR
21	M	8	THR
21	M	9	VAL
21	M	47	ARG
21	M	61	ILE
21	M	66	VAL

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Mol	Chain	Res	Type
21	M	69	ILE
21	M	71	ILE
21	M	72	LYS
21	M	73	LEU
21	M	77	GLU
21	M	88	VAL
21	M	95	ILE
21	M	102	THR
21	M	108	LEU
21	M	110	ASP
21	M	127	ASN
22	N	5	LEU
22	N	7	VAL
22	N	11	LYS
22	N	30	LEU
22	N	33	GLN
22	N	35	GLU
22	N	87	VAL
22	N	97	THR
22	N	107	THR
22	N	111	GLN
22	N	124	VAL
22	N	131	HIS
22	N	177	MET
22	N	198	MET
23	O	78	GLU
23	O	210	VAL
24	P	23	GLU
24	P	26	ASN
24	P	30	VAL
24	P	40	THR
24	P	42	VAL
24	P	44	VAL
24	P	50	LYS
24	P	52	THR
24	P	55	ARG
24	P	57	THR
24	P	61	LYS
24	P	62	VAL
24	P	81	VAL
24	P	88	LEU
24	P	100	THR

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Mol	Chain	Res	Type
24	P	107	THR
24	P	113	GLN
24	P	116	LEU
24	P	133	THR
24	P	142	ARG
25	Q	7	ASN
25	Q	12	LYS
25	Q	19	GLN
25	Q	40	VAL
25	Q	46	GLU
25	Q	58	VAL
25	Q	63	VAL
25	Q	64	LEU
25	Q	67	LEU
25	Q	75	VAL
25	Q	84	VAL
25	Q	87	ARG
26	R	29	LEU
26	R	46	VAL
26	R	53	LYS
26	R	72	CYS
26	R	96	LEU
26	R	110	ARG
26	R	119	LEU
26	R	133	GLU
26	R	135	GLU
26	R	136	ILE
26	R	137	LEU
26	R	138	ASN
26	R	143	LYS
26	R	146	GLN
26	R	158	ILE
26	R	162	LEU
26	R	163	GLU
26	R	182	CYS
27	S	2	LYS
27	S	5	ILE
27	S	6	SER
27	S	13	GLN
27	S	16	ILE
27	S	19	ASP
27	S	22	ARG

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Mol	Chain	Res	Type
27	S	30	LYS
27	S	36	VAL
27	S	69	THR
27	S	89	THR
27	S	93	LYS
27	S	97	VAL
27	S	100	CYS
27	S	118	GLU
27	S	120	ASP
27	S	121	ILE
27	S	125	THR
27	S	128	THR
27	S	144	LEU
27	S	153	VAL
27	S	171	THR
27	S	176	ILE
27	S	179	LEU
27	S	184	VAL
27	S	201	LYS
28	T	6	THR
28	T	8	ARG
28	T	44	LEU
28	T	47	MET
28	T	50	THR
28	T	55	ILE
28	T	69	THR
28	T	97	TYR
28	T	102	THR
28	T	104	ARG
28	T	124	ASN
29	V	26	ASP
29	V	28	VAL
29	V	29	GLN
29	V	41	VAL
29	V	68	ILE
29	V	69	VAL
29	V	81	ARG
29	V	83	ASN
29	V	92	ILE
29	V	126	THR
29	V	139	VAL
29	V	187	SER

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Mol	Chain	Res	Type
30	Y	7	LEU
30	Y	20	THR
30	Y	22	VAL
30	Y	35	ASN
30	Y	81	ILE
30	Y	89	SER
30	Y	100	VAL
30	Y	101	ASP
30	Y	105	LYS
30	Y	116	ASP
31	Z	3	VAL
31	Z	4	GLN
31	Z	26	THR
31	Z	31	GLU
31	Z	38	GLU
31	Z	42	THR
31	Z	47	GLU
31	Z	51	LEU
31	Z	59	LEU
31	Z	62	LYS
31	Z	66	ILE
31	Z	84	VAL
31	Z	85	GLU
31	Z	86	LEU
31	Z	89	GLU
31	Z	93	THR
31	Z	94	ARG
31	Z	115	VAL
31	Z	120	TYR
31	Z	122	VAL
31	Z	141	LYS
31	Z	142	LEU
31	Z	143	ARG
31	Z	153	VAL
31	Z	154	ASP
31	Z	158	ILE
31	Z	169	ASP
31	Z	179	GLN
31	Z	181	VAL
31	Z	193	ASP
31	Z	195	THR
31	Z	205	PRO

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Mol	Chain	Res	Type
31	Z	214	LYS
31	Z	217	ILE
31	Z	223	ILE
31	Z	225	GLU
31	Z	227	LYS
32	a	37	ASP
32	a	40	VAL
32	a	66	HIS
32	a	90	VAL
32	a	95	ARG
32	a	96	ARG
32	a	98	ARG
33	b	25	LEU
33	b	75	VAL
33	b	84	ILE
33	b	85	ILE
33	b	88	GLU
33	b	94	VAL
33	b	96	VAL
33	b	101	THR
33	b	103	ASN
33	b	108	LYS
33	b	112	ILE
34	c	6	THR
34	c	12	LYS
34	c	14	HIS
34	c	26	GLN
34	c	39	THR
34	c	48	ASP
34	c	54	ILE
34	c	64	HIS
34	c	65	PHE
34	c	89	LEU
34	c	93	THR
34	c	97	THR
34	c	99	ARG
34	c	100	ARG
34	c	102	VAL
34	c	107	ASP
34	c	116	ASP
34	c	132	TRP
34	c	137	VAL

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Mol	Chain	Res	Type
34	c	143	GLN
34	c	144	ASP
34	c	159	ASN
34	c	165	ILE
34	c	168	CYS
34	c	170	TRP
34	c	186	THR
34	c	189	ILE
34	c	191	HIS
34	c	197	THR
34	c	198	VAL
34	c	203	ASP
34	c	207	CYS
34	c	223	GLU
34	c	227	LEU
34	c	229	THR
34	c	230	LEU
34	c	239	LEU
34	c	265	ILE
34	c	266	ILE
34	c	267	VAL
34	c	274	VAL
34	c	287	THR
34	c	314	ILE
35	d	12	GLN
35	d	38	LYS
35	d	39	LEU
35	d	66	LEU
35	d	84	ARG
35	d	87	VAL
35	d	88	MET
35	d	96	SER
35	d	97	LYS
35	d	110	LEU
35	d	114	GLU
35	d	138	VAL
35	d	142	ASN
36	e	54	THR
36	e	58	LEU
36	e	73	VAL
36	e	78	LYS
36	e	79	ILE

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Mol	Chain	Res	Type
36	e	90	GLU
36	e	107	VAL
36	e	110	THR
37	f	5	ILE
37	f	7	GLU
37	f	12	ILE
37	f	16	LEU
37	f	59	LEU
37	f	60	THR
37	f	62	ASP
37	f	70	ILE
37	f	83	PHE
37	f	88	LYS
37	f	98	VAL
37	f	117	ILE
37	f	136	THR
37	f	141	ARG
37	f	145	THR
38	h	18	HIS
38	h	39	LEU
38	h	50	VAL
38	h	58	THR
38	h	68	THR
38	h	70	CYS
38	h	78	ASP
38	h	91	LEU
38	h	101	ILE
38	h	112	VAL
38	h	113	GLU
38	h	116	ILE
39	i	10	HIS
39	i	13	LYS
39	i	53	ILE
40	k	98	VAL
40	k	99	LYS
40	k	100	LEU
40	k	102	VAL
40	k	103	LEU
40	k	106	TYR
40	k	114	ILE
40	k	116	ARG
40	k	117	LEU

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Mol	Chain	Res	Type
40	k	135	HIS
40	k	136	PHE
40	k	137	ASP
40	k	138	ARG
41	m	15	ASN
41	m	62	VAL
41	m	66	GLU
41	m	74	ILE
41	m	91	LEU
41	m	93	LYS
41	m	94	ILE
41	m	124	ILE
41	m	132	LYS
42	n	6	VAL
42	n	9	ILE
42	n	17	VAL
42	n	28	THR
42	n	32	VAL
42	n	39	SER
42	n	46	VAL
42	n	56	LEU
42	n	58	LEU
42	n	62	GLU
43	o	240	THR
43	o	245	ASN
43	o	286	SER
43	o	297	ILE
43	o	313	GLU
44	q	27	VAL
44	q	33	GLN
44	q	37	GLN
44	q	38	VAL
44	q	41	MET
44	q	46	ARG
44	q	64	LYS
44	q	65	LEU
44	q	68	LYS
44	q	79	VAL
44	q	81	LEU
44	q	85	GLN
44	q	103	LEU
44	q	106	TYR

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Mol	Chain	Res	Type
44	q	109	LEU
44	q	115	ILE
45	r	7	ARG
45	r	11	HIS
45	r	19	VAL
45	r	20	VAL
45	r	24	VAL
45	r	27	ILE
45	r	34	VAL
45	r	36	LEU
45	r	37	LEU
45	r	42	ILE
45	r	47	LEU
45	r	49	SER
45	r	57	ARG
45	r	59	ILE
45	r	72	VAL
45	r	74	ILE
45	r	80	LYS
45	r	83	ILE
45	r	88	ARG
45	r	94	GLU
45	r	111	ILE
45	r	112	LEU
45	r	120	GLU
45	r	124	ASP
45	r	150	TYR
45	r	151	ASP
45	r	162	ILE
45	r	163	LEU
45	r	178	ASN
45	r	184	LEU
45	r	189	VAL
45	r	195	ILE
45	r	196	GLU
45	r	197	VAL
45	r	199	CYS
45	r	202	TYR
45	r	208	VAL
45	r	221	GLU
45	r	225	ILE
45	r	229	LEU

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Mol	Chain	Res	Type
45	r	234	ARG
45	r	242	LEU
45	r	243	GLU
45	r	246	GLU
45	r	250	VAL
45	r	251	LEU
45	r	253	GLN
45	r	262	ILE
47	u	109	GLN
47	u	331	ILE
47	u	337	ASP
47	u	340	ARG
47	u	448	GLN
47	u	459	VAL
47	u	562	ARG
47	u	563	LYS
47	u	568	ILE
47	u	572	ARG
48	v	203	SER
48	v	205	LEU
48	v	226	PRO
48	v	237	LEU
48	v	243	LEU
48	v	246	ILE
48	v	377	ASN
48	v	392	VAL
50	x	68	GLN
50	x	77	GLU
50	x	80	PHE
50	x	81	GLN
50	x	368	ASP
50	x	385	ASN
50	x	466	LEU
50	x	471	PHE
50	x	475	GLU
51	y	67	ILE
51	y	77	THR
51	y	102	VAL
51	y	116	TYR
51	y	140	THR
51	y	340	ARG
51	y	597	ASN

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Mol	Chain	Res	Type
51	y	779	LEU
51	y	841	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
8	9	22	GLN
10	B	65	ASN
10	B	83	GLN
11	C	36	HIS
11	C	179	ASN
11	C	188	ASN
12	D	124	HIS
12	D	154	GLN
13	E	61	GLN
15	G	162	GLN
16	H	26	GLN
17	I	58	HIS
18	J	64	ASN
18	J	70	ASN
19	K	2	GLN
20	L	120	GLN
20	L	235	ASN
21	M	48	ASN
21	M	74	GLN
21	M	118	GLN
22	N	33	GLN
22	N	132	GLN
22	N	193	HIS
24	P	113	GLN
25	Q	72	HIS
26	R	84	ASN
26	R	138	ASN
26	R	168	GLN
27	S	4	ASN
27	S	81	HIS
27	S	177	GLN
28	T	15	ASN
28	T	89	HIS
28	T	112	ASN
28	T	124	ASN
29	V	51	HIS

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Mol	Chain	Res	Type
29	V	79	HIS
29	V	83	ASN
29	V	165	ASN
29	V	186	ASN
30	Y	86	GLN
30	Y	97	GLN
31	Z	4	GLN
31	Z	145	GLN
31	Z	179	GLN
33	b	79	HIS
33	b	103	ASN
34	c	26	GLN
34	c	143	GLN
34	c	159	ASN
34	c	162	ASN
34	c	188	HIS
35	d	51	ASN
36	e	45	ASN
37	f	10	GLN
37	f	73	ASN
37	f	135	HIS
38	h	18	HIS
38	h	28	ASN
38	h	81	GLN
38	h	92	HIS
39	i	26	ASN
40	k	151	ASN
43	o	245	ASN
43	o	307	HIS
43	o	311	ASN
44	q	85	GLN
44	q	112	HIS
45	r	60	ASN
45	r	155	HIS
45	r	270	ASN
47	u	79	GLN
47	u	200	ASN
47	u	212	HIS
47	u	219	ASN
47	u	221	ASN
47	u	270	GLN
47	u	274	ASN

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Mol	Chain	Res	Type
47	u	288	ASN
47	u	392	ASN
47	u	417	GLN
47	u	448	GLN
47	u	512	GLN
47	u	566	GLN
48	v	209	GLN
48	v	283	GLN
48	v	373	ASN
48	v	402	GLN
50	x	68	GLN
50	x	73	HIS
50	x	296	ASN
50	x	326	GLN
50	x	416	GLN
50	x	456	HIS
50	x	479	GLN
51	y	118	ASN
51	y	433	ASN
51	y	460	GLN
51	y	467	GLN
51	y	520	GLN
51	y	597	ASN
51	y	670	GLN
51	y	701	HIS
51	y	717	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	w	74/75 (98%)	42 (56%)	0
6	7	21/255 (8%)	11 (52%)	3 (14%)
9	A	1710/1869 (91%)	510 (29%)	69 (4%)
All	All	1805/2199 (82%)	563 (31%)	72 (3%)

All (563) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	7	4	G
6	7	5	A
6	7	8	A

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Mol	Chain	Res	Type
6	7	11	A
6	7	15	U
6	7	16	A
6	7	17	C
6	7	18	G
6	7	20	U
6	7	22	C
6	7	23	A
9	A	2	A
9	A	3	C
9	A	4	C
9	A	10	G
9	A	11	A
9	A	17	C
9	A	23	G
9	A	33	G
9	A	34	U
9	A	41	G
9	A	43	U
9	A	44	U
9	A	45	A
9	A	46	A
9	A	56	G
9	A	58	C
9	A	59	U
9	A	62	G
9	A	64	A
9	A	65	C
9	A	67	C
9	A	68	A
9	A	72	C
9	A	73	C
9	A	74	G
9	A	76	U
9	A	78	C
9	A	99	A
9	A	100	U
9	A	103	A
9	A	110	U
9	A	115	U
9	A	126	G
9	A	129	C

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Mol	Chain	Res	Type
9	A	130	G
9	A	140	U
9	A	142	C
9	A	143	U
9	A	149	A
9	A	155	G
9	A	156	G
9	A	158	A
9	A	160	U
9	A	163	U
9	A	165	G
9	A	168	C
9	A	171	A
9	A	173	A
9	A	175	A
9	A	182	C
9	A	184	G
9	A	190	G
9	A	197	U
9	A	198	U
9	A	199	C
9	A	200	G
9	A	202	G
9	A	203	G
9	A	204	G
9	A	206	G
9	A	207	G
9	A	208	G
9	A	209	A
9	A	220	U
9	A	291	G
9	A	292	A
9	A	295	C
9	A	302	A
9	A	305	U
9	A	306	C
9	A	307	G
9	A	308	G
9	A	309	G
9	A	314	U
9	A	318	A
9	A	319	C

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Mol	Chain	Res	Type
9	A	320	G
9	A	321	C
9	A	323	C
9	A	324	C
9	A	325	C
9	A	326	C
9	A	327	G
9	A	328	U
9	A	329	G
9	A	332	G
9	A	340	C
9	A	347	G
9	A	362	C
9	A	364	A
9	A	368	U
9	A	369	C
9	A	370	G
9	A	371	A
9	A	372	U
9	A	381	C
9	A	385	G
9	A	386	C
9	A	392	A
9	A	393	U
9	A	394	G
9	A	399	C
9	A	407	G
9	A	409	C
9	A	417	C
9	A	419	G
9	A	421	G
9	A	438	G
9	A	447	A
9	A	448	A
9	A	450	C
9	A	452	G
9	A	465	A
9	A	467	G
9	A	470	G
9	A	471	G
9	A	472	C
9	A	473	A

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Mol	Chain	Res	Type
9	A	474	G
9	A	476	A
9	A	482	G
9	A	487	U
9	A	492	C
9	A	496	C
9	A	502	C
9	A	508	A
9	A	509	OMG
9	A	512	A
9	A	525	A
9	A	533	A
9	A	534	G
9	A	536	A
9	A	537	C
9	A	538	U
9	A	539	C
9	A	540	U
9	A	541	U
9	A	542	U
9	A	543	C
9	A	544	G
9	A	545	A
9	A	546	G
9	A	547	G
9	A	550	C
9	A	554	A
9	A	556	U
9	A	557	U
9	A	558	G
9	A	559	G
9	A	563	G
9	A	564	A
9	A	565	G
9	A	566	U
9	A	568	C
9	A	576	A
9	A	583	A
9	A	589	G
9	A	590	A
9	A	591	U
9	A	593	C

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Mol	Chain	Res	Type
9	A	594	A
9	A	599	A
9	A	600	G
9	A	601	G
9	A	603	C
9	A	604	A
9	A	606	G
9	A	607	U
9	A	608	C
9	A	609	U
9	A	615	C
9	A	617	G
9	A	624	C
9	A	626	G
9	A	627	U
9	A	628	A
9	A	630	U
9	A	631	U
9	A	632	C
9	A	633	C
9	A	634	A
9	A	635	G
9	A	638	C
9	A	639	C
9	A	643	A
9	A	655	A
9	A	660	C
9	A	668	A2M
9	A	669	A
9	A	670	A
9	A	671	A
9	A	672	A
9	A	673	G
9	A	684	G
9	A	687	C
9	A	688	U
9	A	689	U
9	A	691	G
9	A	692	G
9	A	693	A
9	A	734	C
9	A	735	C

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Mol	Chain	Res	Type
9	A	738	C
9	A	748	C
9	A	749	U
9	A	751	G
9	A	752	G
9	A	753	C
9	A	791	C
9	A	797	C
9	A	798	G
9	A	799	U
9	A	800	U
9	A	801	U
9	A	811	A
9	A	821	G
9	A	822	PSU
9	A	823	PSU
9	A	827	A
9	A	830	A
9	A	836	G
9	A	838	G
9	A	839	C
9	A	840	C
9	A	841	G
9	A	842	C
9	A	847	A
9	A	861	A
9	A	862	A
9	A	869	A
9	A	870	A
9	A	872	A
9	A	873	G
9	A	880	G
9	A	886	A
9	A	887	U
9	A	888	U
9	A	889	U
9	A	890	U
9	A	891	G
9	A	892	U
9	A	894	G
9	A	895	G
9	A	896	U

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Mol	Chain	Res	Type
9	A	897	U
9	A	898	U
9	A	899	U
9	A	900	C
9	A	903	A
9	A	909	G
9	A	912	C
9	A	913	A
9	A	914	U
9	A	917	U
9	A	919	A
9	A	920	A
9	A	922	A
9	A	930	C
9	A	933	G
9	A	949	G
9	A	950	C
9	A	960	U
9	A	963	A
9	A	965	U
9	A	969	U
9	A	970	G
9	A	971	G
9	A	972	A
9	A	985	G
9	A	986	G
9	A	988	C
9	A	989	C
9	A	990	A
9	A	992	A
9	A	997	A
9	A	999	G
9	A	1002	U
9	A	1008	A
9	A	1016	U
9	A	1017	U
9	A	1023	A
9	A	1034	A
9	A	1061	U
9	A	1062	A
9	A	1081	PSU
9	A	1083	A

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Mol	Chain	Res	Type
9	A	1085	C
9	A	1089	G
9	A	1109	C
9	A	1112	U
9	A	1113	A
9	A	1114	U
9	A	1115	U
9	A	1116	C
9	A	1117	C
9	A	1120	U
9	A	1133	A
9	A	1138	C
9	A	1139	C
9	A	1150	A
9	A	1153	C
9	A	1154	U
9	A	1155	U
9	A	1165	G
9	A	1166	G
9	A	1170	A
9	A	1183	A
9	A	1195	A
9	A	1207	G
9	A	1208	A
9	A	1209	A
9	A	1215	C
9	A	1216	C
9	A	1217	A
9	A	1220	A
9	A	1224	G
9	A	1226	G
9	A	1240	A
9	A	1242	U
9	A	1243	PSU
9	A	1250	A
9	A	1251	A
9	A	1253	A
9	A	1256	G
9	A	1257	G
9	A	1259	A
9	A	1264	C
9	A	1273	C

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Mol	Chain	Res	Type
9	A	1274	G
9	A	1275	G
9	A	1284	A
9	A	1286	G
9	A	1287	A
9	A	1288	U
9	A	1290	G
9	A	1294	G
9	A	1295	A
9	A	1301	A
9	A	1302	G
9	A	1303	C
9	A	1308	U
9	A	1313	A
9	A	1322	G
9	A	1326	U
9	A	1332	A
9	A	1342	U
9	A	1348	G
9	A	1355	C
9	A	1357	A
9	A	1371	U
9	A	1372	U
9	A	1378	A
9	A	1397	U
9	A	1402	A
9	A	1416	C
9	A	1417	C
9	A	1418	C
9	A	1419	C
9	A	1420	G
9	A	1421	A
9	A	1422	G
9	A	1423	C
9	A	1424	G
9	A	1433	C
9	A	1435	C
9	A	1436	C
9	A	1437	C
9	A	1438	A
9	A	1442	U
9	A	1446	A

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Mol	Chain	Res	Type
9	A	1454	A
9	A	1455	A
9	A	1463	U
9	A	1464	C
9	A	1466	G
9	A	1474	A
9	A	1484	A
9	A	1487	A
9	A	1488	C
9	A	1489	A
9	A	1490	G
9	A	1497	G
9	A	1498	A
9	A	1507	G
9	A	1509	U
9	A	1510	G
9	A	1512	C
9	A	1513	C
9	A	1518	C
9	A	1519	U
9	A	1520	G
9	A	1521	C
9	A	1522	A
9	A	1523	C
9	A	1524	G
9	A	1531	A
9	A	1532	C
9	A	1533	A
9	A	1534	C
9	A	1535	U
9	A	1536	G
9	A	1538	C
9	A	1539	U
9	A	1541	G
9	A	1542	C
9	A	1543	U
9	A	1552	G
9	A	1553	C
9	A	1555	U
9	A	1556	A
9	A	1557	C
9	A	1566	G

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Mol	Chain	Res	Type
9	A	1570	G
9	A	1578	U
9	A	1580	A
9	A	1584	G
9	A	1585	U
9	A	1587	G
9	A	1588	A
9	A	1593	C
9	A	1594	A
9	A	1598	G
9	A	1599	U
9	A	1601	A
9	A	1602	U
9	A	1603	G
9	A	1606	G
9	A	1618	C
9	A	1619	A
9	A	1621	U
9	A	1623	A
9	A	1624	U
9	A	1629	C
9	A	1637	A
9	A	1639	G
9	A	1643	U
9	A	1646	C
9	A	1654	G
9	A	1663	A
9	A	1665	G
9	A	1671	G
9	A	1687	C
9	A	1691	U
9	A	1692	U
9	A	1693	G
9	A	1695	A
9	A	1696	C
9	A	1697	A
9	A	1698	C
9	A	1699	A
9	A	1700	C
9	A	1701	C
9	A	1702	G
9	A	1715	A

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Mol	Chain	Res	Type
9	A	1719	A
9	A	1721	U
9	A	1722	G
9	A	1733	U
9	A	1744	G
9	A	1745	A
9	A	1747	C
9	A	1750	C
9	A	1752	C
9	A	1753	C
9	A	1755	C
9	A	1756	C
9	A	1757	G
9	A	1758	G
9	A	1759	G
9	A	1760	G
9	A	1772	C
9	A	1773	C
9	A	1774	C
9	A	1775	U
9	A	1776	G
9	A	1777	G
9	A	1778	C
9	A	1779	G
9	A	1780	G
9	A	1781	A
9	A	1782	G
9	A	1783	C
9	A	1785	C
9	A	1800	A
9	A	1801	A
9	A	1805	G
9	A	1807	C
9	A	1808	U
9	A	1813	A
9	A	1819	A
9	A	1820	G
9	A	1822	A
9	A	1823	A
9	A	1824	A
9	A	1825	A
9	A	1826	G

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Mol	Chain	Res	Type
9	A	1827	U
9	A	1831	A
9	A	1832	A
9	A	1835	A
9	A	1838	U
9	A	1849	G
9	A	1851	MA6
9	A	1861	G
9	A	1862	G
9	A	1863	A
9	A	1865	C
9	A	1867	U
9	A	1868	U
9	A	1869	A
49	w	4	A
49	w	5	G
49	w	7	G
49	w	8	U
49	w	9	G
49	w	10	G
49	w	11	C
49	w	14	A
49	w	15	G
49	w	16	C
49	w	17	G
49	w	18	G
49	w	19	A
49	w	20	A
49	w	21	G
49	w	26	C
49	w	27	U
49	w	29	G
49	w	30	G
49	w	34	A
49	w	35	U
49	w	41	A
49	w	43	A
49	w	44	G
49	w	45	G
49	w	46	U
49	w	47	C
49	w	48	G

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Mol	Chain	Res	Type
49	w	51	G
49	w	52	G
49	w	55	C
49	w	56	G
49	w	57	A
49	w	58	A
49	w	59	A
49	w	60	C
49	w	62	A
49	w	64	C
49	w	71	U
49	w	73	C
49	w	74	C
49	w	75	A

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	7	3	A
6	7	4	G
6	7	17	C
9	A	1	U
9	A	43	U
9	A	72	C
9	A	203	G
9	A	291	G
9	A	306	C
9	A	307	G
9	A	368	U
9	A	369	C
9	A	371	A
9	A	392	A
9	A	557	U
9	A	563	G
9	A	589	G
9	A	593	C
9	A	606	G
9	A	614	C
9	A	630	U
9	A	670	A
9	A	797	C
9	A	838	G

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Mol	Chain	Res	Type
9	A	839	C
9	A	840	C
9	A	861	A
9	A	868	G
9	A	912	C
9	A	985	G
9	A	1016	U
9	A	1020	A
9	A	1081	PSU
9	A	1112	U
9	A	1114	U
9	A	1119	A
9	A	1138	C
9	A	1165	G
9	A	1302	G
9	A	1341	C
9	A	1355	C
9	A	1371	U
9	A	1434	C
9	A	1488	C
9	A	1497	G
9	A	1509	U
9	A	1519	U
9	A	1520	G
9	A	1521	C
9	A	1522	A
9	A	1533	A
9	A	1542	C
9	A	1556	A
9	A	1580	A
9	A	1581	C
9	A	1587	G
9	A	1598	G
9	A	1600	G
9	A	1604	G
9	A	1637	A
9	A	1695	A
9	A	1700	C
9	A	1701	C
9	A	1744	G
9	A	1756	C
9	A	1757	G

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Mol	Chain	Res	Type
9	A	1775	U
9	A	1777	G
9	A	1778	C
9	A	1781	A
9	A	1825	A
9	A	1831	A

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

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	5MU	A	814	9	19,22,23	1.55	5 (26%)	27,32,35	2.38	9 (33%)
9	OMU	A	116	9	19,22,23	1.36	3 (15%)	25,31,34	1.94	5 (20%)
9	UR3	A	1830	9	19,22,23	1.04	2 (10%)	26,32,35	2.27	8 (30%)
9	OMC	A	517	9	19,22,23	0.95	1 (5%)	25,31,34	1.18	2 (8%)
9	OMG	A	644	9	23,26,27	1.36	4 (17%)	32,38,41	2.15	9 (28%)
9	PSU	A	823	9	18,21,22	1.60	5 (27%)	21,30,33	2.18	4 (19%)
9	A2M	A	159	9	22,25,26	1.50	4 (18%)	30,36,39	2.20	9 (30%)
9	PSU	A	1081	9	18,21,22	1.73	5 (27%)	21,30,33	2.49	6 (28%)
9	A2M	A	1031	9	22,25,26	1.55	6 (27%)	30,36,39	2.34	9 (30%)
9	PSU	A	822	9	18,21,22	1.55	4 (22%)	21,30,33	2.39	5 (23%)
9	MA6	A	1850	9	23,26,27	1.53	4 (17%)	33,38,41	2.53	13 (39%)
9	5MC	A	1374	9	19,22,23	1.70	3 (15%)	26,32,35	1.51	6 (23%)
9	OMG	A	683	9	23,26,27	1.33	4 (17%)	32,38,41	2.21	6 (18%)
9	A2M	A	484	9	22,25,26	1.53	4 (18%)	30,36,39	2.32	8 (26%)
9	A2M	A	1678	9	22,25,26	1.54	6 (27%)	30,36,39	2.13	10 (33%)
9	MA6	A	1851	9	23,26,27	1.57	5 (21%)	33,38,41	2.38	14 (42%)
9	PSU	A	1243	9	18,21,22	1.54	5 (27%)	21,30,33	2.20	4 (19%)
9	OMC	A	1703	9	19,22,23	1.04	2 (10%)	25,31,34	1.20	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PSU	A	612	9	18,21,22	1.51	5 (27%)	21,30,33	2.18	4 (19%)
9	PSU	A	119	9	18,21,22	1.47	4 (22%)	21,30,33	2.32	5 (23%)
9	A2M	A	27	9	22,25,26	1.55	6 (27%)	30,36,39	2.31	10 (33%)
9	A2M	A	166	9	22,25,26	1.53	5 (22%)	30,36,39	2.25	9 (30%)
9	OMU	A	121	9	19,22,23	1.46	4 (21%)	25,31,34	1.96	6 (24%)
9	OMC	A	174	9	19,22,23	0.91	0	25,31,34	1.17	2 (8%)
9	OMG	A	509	9	23,26,27	1.38	4 (17%)	32,38,41	2.15	6 (18%)
9	A2M	A	668	9	22,25,26	1.53	6 (27%)	30,36,39	2.06	11 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	5MU	A	814	9	-	0/7/25/26	0/2/2/2
9	OMU	A	116	9	-	1/9/27/28	0/2/2/2
9	UR3	A	1830	9	-	2/7/25/26	0/2/2/2
9	OMC	A	517	9	-	1/9/27/28	0/2/2/2
9	OMG	A	644	9	-	2/9/27/28	0/3/3/3
9	PSU	A	823	9	-	1/7/25/26	0/2/2/2
9	A2M	A	159	9	-	1/9/27/28	0/3/3/3
9	PSU	A	1081	9	-	2/7/25/26	0/2/2/2
9	A2M	A	1031	9	-	1/9/27/28	0/3/3/3
9	PSU	A	822	9	-	0/7/25/26	0/2/2/2
9	MA6	A	1850	9	-	1/11/29/30	0/3/3/3
9	5MC	A	1374	9	-	0/7/25/26	0/2/2/2
9	OMG	A	683	9	-	1/9/27/28	0/3/3/3
9	A2M	A	484	9	-	1/9/27/28	0/3/3/3
9	A2M	A	1678	9	-	0/9/27/28	0/3/3/3
9	MA6	A	1851	9	-	4/11/29/30	0/3/3/3
9	PSU	A	1243	9	-	0/7/25/26	0/2/2/2
9	OMC	A	1703	9	-	2/9/27/28	0/2/2/2
9	PSU	A	612	9	-	1/7/25/26	0/2/2/2
9	PSU	A	119	9	-	1/7/25/26	0/2/2/2
9	A2M	A	27	9	-	1/9/27/28	0/3/3/3
9	A2M	A	166	9	-	0/9/27/28	0/3/3/3
9	OMU	A	121	9	-	0/9/27/28	0/2/2/2
9	OMC	A	174	9	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	OMG	A	509	9	-	2/9/27/28	0/3/3/3
9	A2M	A	668	9	-	3/9/27/28	0/3/3/3

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1374	5MC	C5-C4	5.90	1.48	1.44
9	A	159	A2M	C5-C4	4.54	1.47	1.39
9	A	166	A2M	C5-C4	4.46	1.47	1.39
9	A	484	A2M	C5-C4	4.22	1.46	1.39
9	A	1031	A2M	C5-C4	4.19	1.46	1.39
9	A	1851	MA6	C5-C4	4.17	1.46	1.39
9	A	27	A2M	C5-C4	4.01	1.46	1.39
9	A	1850	MA6	C5-C4	3.95	1.46	1.39
9	A	1678	A2M	C5-C4	3.91	1.46	1.39
9	A	1081	PSU	C4-N3	-3.64	1.32	1.38
9	A	668	A2M	C5-C4	3.61	1.45	1.39
9	A	121	OMU	C4-N3	-3.46	1.32	1.38
9	A	823	PSU	C4-N3	-3.42	1.32	1.38
9	A	814	5MU	C4-N3	-3.42	1.32	1.38
9	A	509	OMG	C6-N1	-3.19	1.32	1.38
9	A	668	A2M	C4-N9	-3.11	1.31	1.37
9	A	484	A2M	C5-N7	-3.11	1.33	1.39
9	A	822	PSU	C4-N3	-3.09	1.33	1.38
9	A	1243	PSU	C4-N3	-3.08	1.33	1.38
9	A	1850	MA6	C4-N9	-3.05	1.31	1.37
9	A	1081	PSU	C2-N3	-3.05	1.32	1.37
9	A	612	PSU	C4-N3	-3.02	1.33	1.38
9	A	116	OMU	C4-N3	-3.02	1.33	1.38
9	A	121	OMU	C2-N3	-3.00	1.32	1.38
9	A	822	PSU	C6-C5	2.98	1.38	1.35
9	A	1851	MA6	C4-N9	-2.97	1.31	1.37
9	A	644	OMG	C6-N1	-2.97	1.33	1.38
9	A	1031	A2M	C5-N7	-2.97	1.33	1.39
9	A	509	OMG	C5-N7	-2.95	1.33	1.39
9	A	509	OMG	C5-C4	2.93	1.46	1.38
9	A	119	PSU	C4-N3	-2.91	1.33	1.38
9	A	27	A2M	C5-N7	-2.90	1.33	1.39
9	A	1374	5MC	C6-N1	-2.87	1.33	1.38
9	A	823	PSU	C6-C5	2.83	1.38	1.35
9	A	644	OMG	C5-N7	-2.83	1.33	1.39
9	A	1081	PSU	C2-N1	-2.82	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	683	OMG	C6-N1	-2.82	1.33	1.38
9	A	1678	A2M	C5-N7	-2.79	1.34	1.39
9	A	644	OMG	C5-C4	2.78	1.46	1.38
9	A	814	5MU	C2-N3	-2.74	1.33	1.38
9	A	159	A2M	C5-N7	-2.71	1.34	1.39
9	A	1850	MA6	C5-N7	-2.70	1.34	1.39
9	A	1678	A2M	C4-N9	-2.69	1.32	1.37
9	A	683	OMG	C5-N7	-2.68	1.33	1.39
9	A	1243	PSU	C6-C5	2.68	1.38	1.35
9	A	683	OMG	C5-C4	2.67	1.46	1.38
9	A	814	5MU	C6-N1	-2.67	1.33	1.38
9	A	668	A2M	C5-N7	-2.67	1.34	1.39
9	A	116	OMU	C2-N3	-2.65	1.33	1.38
9	A	27	A2M	C4-N9	-2.64	1.32	1.37
9	A	1081	PSU	C6-C5	2.61	1.38	1.35
9	A	166	A2M	C5-C6	2.60	1.48	1.41
9	A	1031	A2M	C4-N9	-2.57	1.32	1.37
9	A	119	PSU	C6-C5	2.56	1.38	1.35
9	A	1851	MA6	C5-N7	-2.55	1.34	1.39
9	A	823	PSU	C2-N3	-2.54	1.33	1.37
9	A	484	A2M	C4-N9	-2.54	1.32	1.37
9	A	166	A2M	C5-N7	-2.53	1.34	1.39
9	A	159	A2M	C5-C6	2.50	1.47	1.41
9	A	121	OMU	C5-C4	-2.49	1.38	1.43
9	A	822	PSU	C2-N3	-2.48	1.33	1.37
9	A	612	PSU	C2-N1	-2.47	1.33	1.36
9	A	116	OMU	C5-C4	-2.46	1.38	1.43
9	A	1243	PSU	C2-N1	-2.46	1.33	1.36
9	A	683	OMG	C4-N9	-2.44	1.31	1.38
9	A	1374	5MC	C6-C5	2.43	1.38	1.34
9	A	1851	MA6	C5-C6	2.42	1.47	1.41
9	A	119	PSU	C2-N3	-2.36	1.33	1.37
9	A	822	PSU	C2-N1	-2.35	1.33	1.36
9	A	612	PSU	C2-N3	-2.35	1.33	1.37
9	A	1678	A2M	C5-C6	2.33	1.47	1.41
9	A	1850	MA6	C5-C6	2.32	1.47	1.41
9	A	119	PSU	C2-N1	-2.32	1.33	1.36
9	A	1031	A2M	C5-C6	2.31	1.47	1.41
9	A	814	5MU	C6-C5	2.31	1.38	1.34
9	A	612	PSU	C6-C5	2.27	1.37	1.35
9	A	159	A2M	C4-N9	-2.27	1.33	1.37
9	A	27	A2M	C5-C6	2.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1243	PSU	C2'-C1'	-2.24	1.50	1.53
9	A	1243	PSU	C2-N3	-2.23	1.33	1.37
9	A	644	OMG	C4-N9	-2.21	1.32	1.38
9	A	1031	A2M	C8-N9	-2.20	1.33	1.37
9	A	166	A2M	C8-N7	2.20	1.35	1.31
9	A	166	A2M	C4-N9	-2.20	1.33	1.37
9	A	484	A2M	C5-C6	2.19	1.47	1.41
9	A	1830	UR3	C5-C4	-2.17	1.38	1.43
9	A	27	A2M	C8-N7	2.16	1.35	1.31
9	A	668	A2M	C5-C6	2.16	1.47	1.41
9	A	823	PSU	C2-N1	-2.16	1.33	1.36
9	A	27	A2M	C8-N9	-2.15	1.33	1.37
9	A	612	PSU	C2'-C1'	-2.15	1.50	1.53
9	A	823	PSU	C2'-C1'	-2.13	1.50	1.53
9	A	668	A2M	C8-N9	-2.12	1.33	1.37
9	A	1703	OMC	C5-C4	-2.09	1.38	1.42
9	A	121	OMU	C6-N1	-2.09	1.33	1.38
9	A	1081	PSU	C2'-C1'	-2.08	1.50	1.53
9	A	668	A2M	C8-N7	2.08	1.35	1.31
9	A	1703	OMC	C6-N1	-2.07	1.33	1.38
9	A	1678	A2M	C8-N7	2.06	1.35	1.31
9	A	1851	MA6	C8-N7	2.06	1.35	1.31
9	A	1830	UR3	C6-N1	-2.05	1.33	1.38
9	A	1031	A2M	C8-N7	2.05	1.35	1.31
9	A	1678	A2M	C8-N9	-2.05	1.34	1.37
9	A	509	OMG	C4-N9	-2.03	1.32	1.38
9	A	814	5MU	C2-N1	2.02	1.41	1.38
9	A	517	OMC	C5-C4	-2.02	1.38	1.42

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	822	PSU	N1-C2-N3	7.03	122.58	115.17
9	A	1830	UR3	C4-N3-C2	-7.00	118.95	124.58
9	A	1081	PSU	N1-C2-N3	6.92	122.47	115.17
9	A	119	PSU	N1-C2-N3	6.54	122.07	115.17
9	A	484	A2M	C2'-C1'-N9	-6.54	102.99	113.75
9	A	823	PSU	N1-C2-N3	6.51	122.03	115.17
9	A	1243	PSU	N1-C2-N3	6.44	121.96	115.17
9	A	612	PSU	N1-C2-N3	6.39	121.91	115.17
9	A	509	OMG	C5-C4-N3	-6.37	118.25	128.39
9	A	27	A2M	C2'-C1'-N9	-6.33	103.33	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1031	A2M	C2'-C1'-N9	-6.25	103.46	113.75
9	A	644	OMG	C5-C4-N3	-6.07	118.72	128.39
9	A	484	A2M	C5-C4-N3	-6.05	118.38	126.72
9	A	683	OMG	C5-C4-N3	-6.02	118.80	128.39
9	A	1031	A2M	C5-C4-N3	-5.97	118.50	126.72
9	A	166	A2M	C5-C4-N3	-5.93	118.56	126.72
9	A	1081	PSU	C3'-C2'-C1'	5.81	108.54	101.69
9	A	159	A2M	C5-C4-N3	-5.78	118.75	126.72
9	A	1678	A2M	C5-C4-N3	-5.67	118.91	126.72
9	A	27	A2M	C5-C4-N3	-5.66	118.92	126.72
9	A	1850	MA6	C9-N6-C6	-5.46	106.64	120.52
9	A	814	5MU	N3-C2-N1	5.46	121.99	114.89
9	A	159	A2M	C2'-C1'-N9	-5.41	104.85	113.75
9	A	1850	MA6	C5-C4-N3	-5.27	119.46	126.72
9	A	814	5MU	C4-N3-C2	-5.12	120.62	127.34
9	A	683	OMG	C2-N3-C4	5.10	121.09	112.30
9	A	1851	MA6	C5-C4-N3	-5.05	119.76	126.72
9	A	668	A2M	C5-C4-N3	-4.96	119.89	126.72
9	A	644	OMG	C2-N3-C4	4.90	120.74	112.30
9	A	166	A2M	C2'-C1'-N9	-4.81	105.84	113.75
9	A	121	OMU	C4-N3-C2	-4.79	120.66	126.61
9	A	116	OMU	C4-N3-C2	-4.77	120.69	126.61
9	A	683	OMG	C2'-C1'-N9	-4.76	105.21	114.24
9	A	484	A2M	N3-C4-N9	4.75	135.24	127.17
9	A	509	OMG	C2'-C1'-N9	-4.73	105.26	114.24
9	A	509	OMG	C2-N3-C4	4.64	120.30	112.30
9	A	166	A2M	N3-C4-N9	4.62	135.03	127.17
9	A	119	PSU	C4-N3-C2	-4.61	120.02	126.37
9	A	509	OMG	N9-C4-N3	4.58	135.10	125.95
9	A	822	PSU	C4-N3-C2	-4.52	120.15	126.37
9	A	159	A2M	N3-C4-N9	4.52	134.85	127.17
9	A	644	OMG	N9-C4-N3	4.50	134.95	125.95
9	A	1031	A2M	N3-C4-N9	4.49	134.80	127.17
9	A	1850	MA6	N3-C4-N9	4.45	134.73	127.17
9	A	121	OMU	N3-C2-N1	4.42	120.64	114.89
9	A	1851	MA6	C9-N6-C6	-4.40	109.32	120.52
9	A	814	5MU	C5-C4-N3	4.37	119.12	115.32
9	A	1678	A2M	N3-C4-N9	4.30	134.48	127.17
9	A	814	5MU	O4-C4-C5	-4.23	120.08	124.92
9	A	119	PSU	O2-C2-N1	-4.19	118.46	122.79
9	A	1851	MA6	C10-N6-C6	-4.19	109.85	120.52
9	A	1850	MA6	C2'-C1'-N9	-4.19	102.90	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	116	OMU	N3-C2-N1	4.18	120.34	114.89
9	A	27	A2M	N3-C4-N9	4.15	134.22	127.17
9	A	1243	PSU	O2-C2-N1	-4.15	118.51	122.79
9	A	683	OMG	N9-C4-N3	4.13	134.22	125.95
9	A	1850	MA6	C10-N6-C6	-4.11	110.05	120.52
9	A	612	PSU	C4-N3-C2	-4.08	120.75	126.37
9	A	1374	5MC	C5-C6-N1	-4.06	118.90	123.31
9	A	116	OMU	C5-C4-N3	4.06	120.49	114.80
9	A	1243	PSU	C4-N3-C2	-4.02	120.84	126.37
9	A	1851	MA6	N3-C4-N9	3.97	133.92	127.17
9	A	612	PSU	O2-C2-N1	-3.97	118.70	122.79
9	A	644	OMG	C2'-C1'-N9	-3.96	106.73	114.24
9	A	1081	PSU	C4-N3-C2	-3.93	120.95	126.37
9	A	1243	PSU	C3'-C2'-C1'	3.91	106.31	101.69
9	A	166	A2M	C2-N3-C4	3.91	121.38	111.83
9	A	1830	UR3	C1'-N1-C2	3.89	123.41	117.04
9	A	1703	OMC	C2'-C1'-N1	-3.89	106.86	114.24
9	A	119	PSU	C3'-C2'-C1'	3.89	106.28	101.69
9	A	121	OMU	C5-C4-N3	3.87	120.22	114.80
9	A	1851	MA6	C2-N1-C6	3.87	121.27	111.83
9	A	823	PSU	C4-N3-C2	-3.86	121.06	126.37
9	A	1850	MA6	C2-N1-C6	3.84	121.22	111.83
9	A	27	A2M	C4-C5-N7	-3.83	106.21	110.58
9	A	1678	A2M	C2-N3-C4	3.72	120.92	111.83
9	A	822	PSU	O2-C2-N1	-3.72	118.95	122.79
9	A	822	PSU	C3'-C2'-C1'	3.68	106.04	101.69
9	A	1850	MA6	C2-N3-C4	3.68	120.82	111.83
9	A	1031	A2M	C4-C5-N7	-3.68	106.38	110.58
9	A	668	A2M	N3-C4-N9	3.67	133.41	127.17
9	A	612	PSU	C3'-C2'-C1'	3.67	106.02	101.69
9	A	1031	A2M	C2-N3-C4	3.64	120.72	111.83
9	A	668	A2M	C4-C5-N7	-3.62	106.44	110.58
9	A	159	A2M	C2-N3-C4	3.60	120.62	111.83
9	A	1830	UR3	O3'-C3'-C2'	-3.58	100.35	111.82
9	A	27	A2M	C2-N3-C4	3.56	120.53	111.83
9	A	1850	MA6	N1-C2-N3	-3.51	123.27	128.58
9	A	166	A2M	C4-C5-N7	-3.46	106.62	110.58
9	A	121	OMU	C2'-C1'-N1	-3.46	107.67	114.24
9	A	1851	MA6	C2-N3-C4	3.45	120.27	111.83
9	A	1678	A2M	C4-C5-N7	-3.44	106.65	110.58
9	A	484	A2M	C2-N3-C4	3.43	120.20	111.83
9	A	683	OMG	C6-C5-N7	3.43	136.53	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	174	OMC	C2'-C1'-N1	-3.40	107.78	114.24
9	A	668	A2M	C2-N3-C4	3.39	120.12	111.83
9	A	823	PSU	O2-C2-N1	-3.37	119.31	122.79
9	A	1830	UR3	C5-C4-N3	3.35	119.45	115.04
9	A	814	5MU	C5-C6-N1	-3.34	119.68	123.31
9	A	116	OMU	C2'-C1'-N1	-3.33	107.92	114.24
9	A	166	A2M	N3-C2-N1	-3.31	123.58	128.58
9	A	159	A2M	C4-C5-N7	-3.29	106.82	110.58
9	A	668	A2M	C4-N9-C8	3.29	109.19	105.74
9	A	1678	A2M	N3-C2-N1	-3.26	123.64	128.58
9	A	484	A2M	C4-C5-N7	-3.24	106.88	110.58
9	A	517	OMC	C2'-C1'-N1	-3.22	108.13	114.24
9	A	668	A2M	N3-C2-N1	-3.20	123.74	128.58
9	A	1850	MA6	C4-N9-C8	3.20	109.09	105.74
9	A	1081	PSU	O2-C2-N1	-3.17	119.52	122.79
9	A	116	OMU	O4-C4-C5	-3.13	119.76	125.16
9	A	644	OMG	C6-C5-N7	3.09	135.92	130.29
9	A	1851	MA6	C4-C5-N7	-3.08	107.06	110.58
9	A	1830	UR3	O4'-C1'-N1	3.06	115.30	108.36
9	A	823	PSU	C3'-C2'-C1'	3.06	105.30	101.69
9	A	1851	MA6	N1-C6-N6	3.05	120.57	116.86
9	A	27	A2M	N3-C2-N1	-3.04	123.98	128.58
9	A	1851	MA6	N1-C2-N3	-3.03	123.99	128.58
9	A	1031	A2M	N3-C2-N1	-3.02	124.00	128.58
9	A	1851	MA6	C2'-C1'-N9	-2.97	105.92	113.30
9	A	1851	MA6	C4-N9-C8	2.94	108.83	105.74
9	A	1850	MA6	N1-C6-N6	2.92	120.41	116.86
9	A	1850	MA6	C5-C6-N6	-2.88	120.78	125.33
9	A	159	A2M	N3-C2-N1	-2.87	124.23	128.58
9	A	121	OMU	O4-C4-C5	-2.87	120.22	125.16
9	A	509	OMG	C6-C5-N7	2.84	135.46	130.29
9	A	683	OMG	C4-C5-N7	-2.83	106.19	110.67
9	A	1374	5MC	C5-C4-N3	-2.79	118.89	121.75
9	A	1850	MA6	C4-C5-N7	-2.74	107.45	110.58
9	A	1678	A2M	C4-N9-C8	2.73	108.60	105.74
9	A	1830	UR3	O2-C2-N3	-2.70	117.60	121.33
9	A	814	5MU	O2'-C2'-C3'	-2.70	103.17	111.82
9	A	27	A2M	C4-N9-C8	2.68	108.56	105.74
9	A	1851	MA6	C5-C6-N6	-2.67	121.11	125.33
9	A	814	5MU	O2-C2-N3	-2.66	116.58	121.49
9	A	27	A2M	C5-N7-C8	2.65	107.61	103.45
9	A	166	A2M	C4-N9-C8	2.62	108.49	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	509	OMG	C4-C5-N7	-2.59	106.57	110.67
9	A	668	A2M	N9-C8-N7	-2.56	110.31	113.94
9	A	1830	UR3	C6-N1-C2	-2.52	119.74	121.80
9	A	1031	A2M	C5-N7-C8	2.49	107.37	103.45
9	A	668	A2M	C5-N7-C8	2.48	107.36	103.45
9	A	644	OMG	C4-C5-N7	-2.48	106.74	110.67
9	A	668	A2M	C6-C5-N7	2.48	136.87	132.09
9	A	1031	A2M	C4-N9-C8	2.47	108.33	105.74
9	A	484	A2M	N3-C2-N1	-2.46	124.86	128.58
9	A	166	A2M	C5-N7-C8	2.45	107.31	103.45
9	A	822	PSU	C5-C6-N1	-2.44	118.76	122.14
9	A	517	OMC	O2-C2-N3	-2.40	118.54	122.33
9	A	1374	5MC	C2'-C1'-N1	-2.38	106.62	113.25
9	A	121	OMU	O2-C2-N1	-2.37	119.72	122.80
9	A	1678	A2M	C5-N7-C8	2.36	107.17	103.45
9	A	1374	5MC	O2-C2-N3	-2.36	118.61	122.33
9	A	119	PSU	C5-C6-N1	-2.36	118.86	122.14
9	A	1081	PSU	C5-C6-N1	-2.36	118.87	122.14
9	A	644	OMG	O2'-C2'-C1'	-2.33	104.56	108.99
9	A	166	A2M	C6-C5-N7	2.33	136.57	132.09
9	A	484	A2M	C4-N9-C8	2.31	108.16	105.74
9	A	159	A2M	C5-N7-C8	2.29	107.06	103.45
9	A	27	A2M	C6-C5-N7	2.29	136.50	132.09
9	A	484	A2M	C5-N7-C8	2.28	107.03	103.45
9	A	814	5MU	C3'-C2'-C1'	2.28	105.77	101.46
9	A	1678	A2M	O2'-C2'-C1'	-2.26	104.70	108.99
9	A	159	A2M	C4-N9-C8	2.25	108.11	105.74
9	A	27	A2M	N9-C8-N7	-2.24	110.76	113.94
9	A	174	OMC	O2-C2-N3	-2.22	118.82	122.33
9	A	668	A2M	C2'-C1'-N9	-2.21	110.12	113.75
9	A	1678	A2M	C6-C5-N7	2.19	136.32	132.09
9	A	1830	UR3	C3U-N3-C4	2.19	120.90	117.87
9	A	814	5MU	C2'-C3'-C4'	-2.18	98.40	102.61
9	A	1081	PSU	O2-C2-N3	-2.17	118.01	121.86
9	A	1850	MA6	C3'-C2'-C1'	2.16	105.54	101.46
9	A	644	OMG	O6-C6-C5	-2.15	120.86	126.53
9	A	644	OMG	CM2-O2'-C2'	-2.15	108.97	114.47
9	A	1374	5MC	C3'-C2'-C1'	2.13	105.50	101.46
9	A	668	A2M	C2-N1-C6	2.09	122.16	118.73
9	A	1678	A2M	N9-C8-N7	-2.09	110.97	113.94
9	A	159	A2M	C6-C5-N7	2.07	136.07	132.09
9	A	1374	5MC	N1-C2-N3	2.03	122.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1031	A2M	C6-C5-N7	2.02	135.98	132.09
9	A	1851	MA6	C10-N6-C9	-2.02	109.70	116.18
9	A	1851	MA6	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	27	A2M	C1'-C2'-O2'-CM'
9	A	116	OMU	C1'-C2'-O2'-CM2
9	A	159	A2M	C1'-C2'-O2'-CM'
9	A	484	A2M	C1'-C2'-O2'-CM'
9	A	517	OMC	C1'-C2'-O2'-CM2
9	A	644	OMG	C1'-C2'-O2'-CM2
9	A	668	A2M	O4'-C4'-C5'-O5'
9	A	1031	A2M	C1'-C2'-O2'-CM'
9	A	1703	OMC	C1'-C2'-O2'-CM2
9	A	1830	UR3	O4'-C1'-N1-C6
9	A	1830	UR3	O4'-C1'-N1-C2
9	A	1851	MA6	O4'-C4'-C5'-O5'
9	A	683	OMG	C1'-C2'-O2'-CM2
9	A	668	A2M	C3'-C4'-C5'-O5'
9	A	1851	MA6	C3'-C4'-C5'-O5'
9	A	509	OMG	O4'-C4'-C5'-O5'
9	A	1851	MA6	C5-C6-N6-C9
9	A	509	OMG	C3'-C4'-C5'-O5'
9	A	1850	MA6	C5-C6-N6-C9
9	A	1851	MA6	C4'-C5'-O5'-P
9	A	612	PSU	O4'-C4'-C5'-O5'
9	A	119	PSU	O4'-C4'-C5'-O5'
9	A	1703	OMC	O4'-C4'-C5'-O5'
9	A	1081	PSU	C4'-C5'-O5'-P
9	A	1081	PSU	O4'-C4'-C5'-O5'
9	A	823	PSU	O4'-C1'-C5-C6
9	A	644	OMG	C4'-C5'-O5'-P
9	A	668	A2M	C2'-C1'-N9-C8

There are no ring outliers.

12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	116	OMU	3	0
9	A	517	OMC	2	0
9	A	644	OMG	1	0
9	A	1031	A2M	2	0
9	A	1850	MA6	2	0
9	A	683	OMG	1	0
9	A	484	A2M	1	0
9	A	1851	MA6	1	0
9	A	1703	OMC	1	0
9	A	119	PSU	1	0
9	A	27	A2M	4	0
9	A	509	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

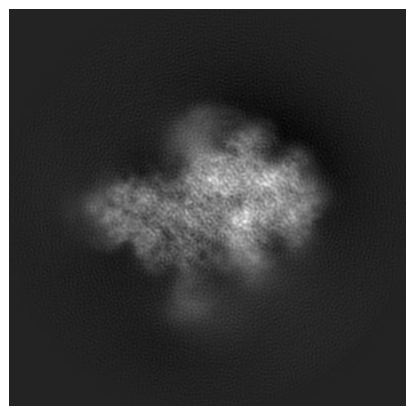
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14114. These allow visual inspection of the internal detail of the map and identification of artifacts.

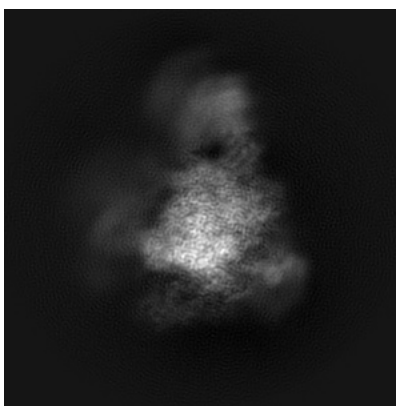
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

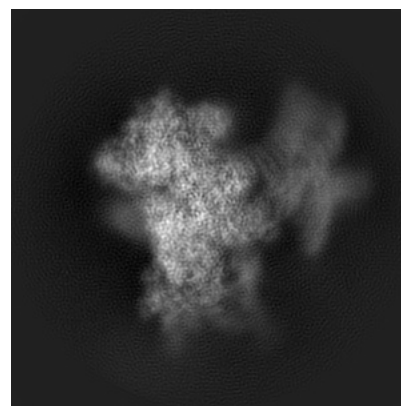
6.1.1 Primary map



X

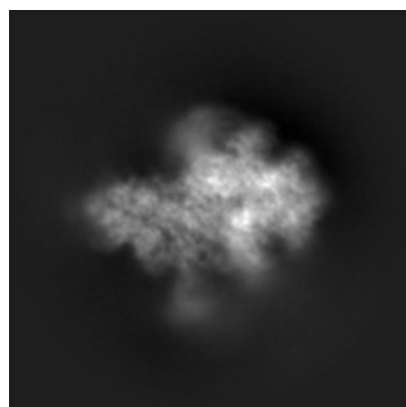


Y

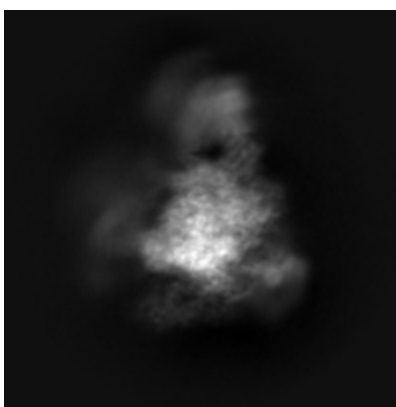


Z

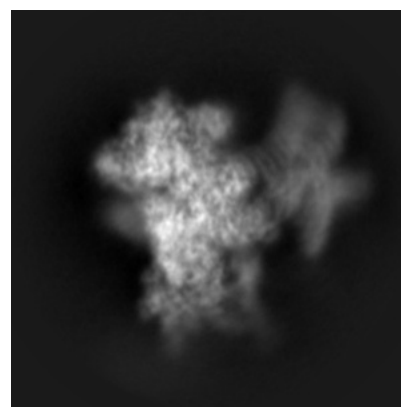
6.1.2 Raw map



X



Y

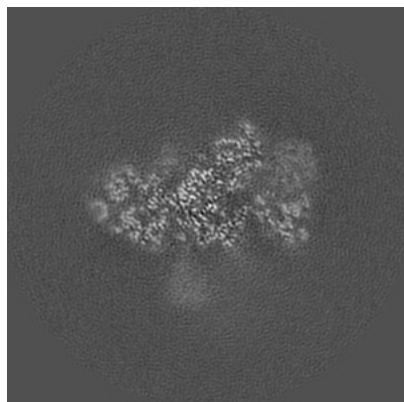


Z

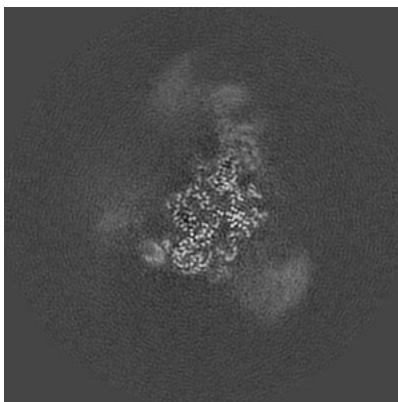
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

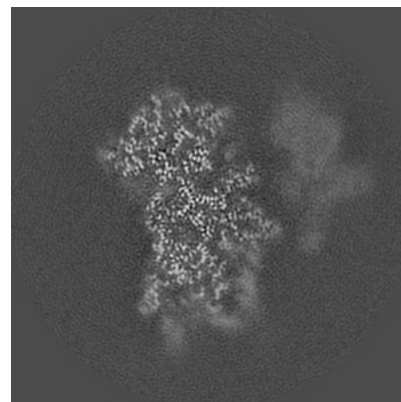
6.2.1 Primary map



X Index: 180

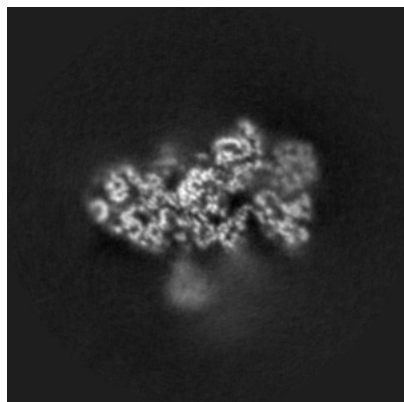


Y Index: 180

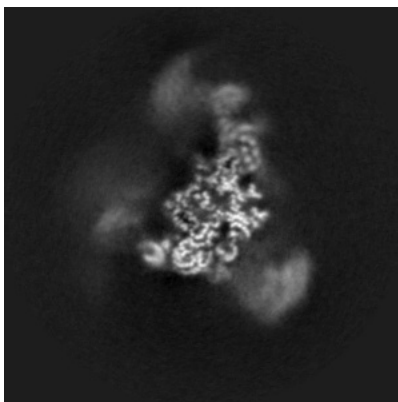


Z Index: 180

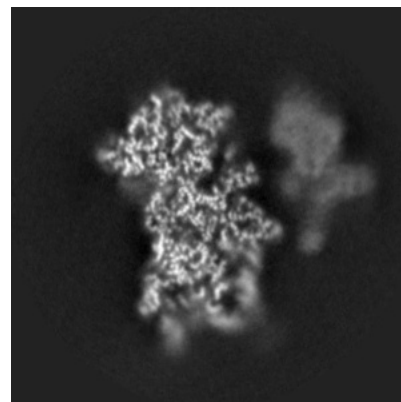
6.2.2 Raw map



X Index: 180



Y Index: 180

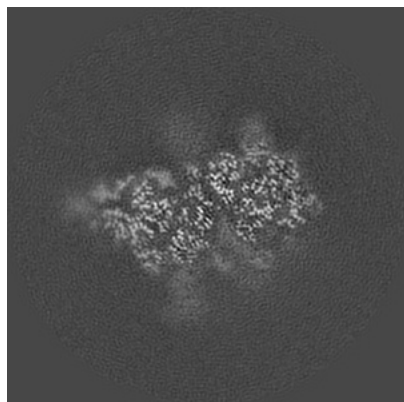


Z Index: 180

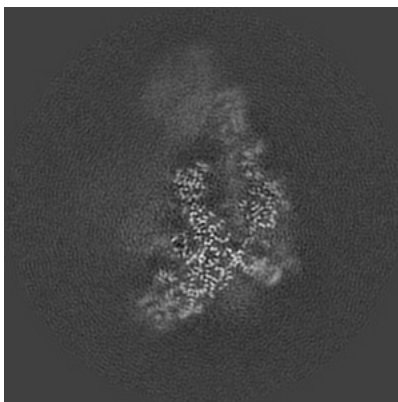
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

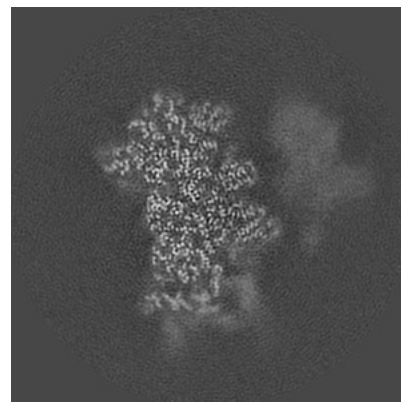
6.3.1 Primary map



X Index: 149

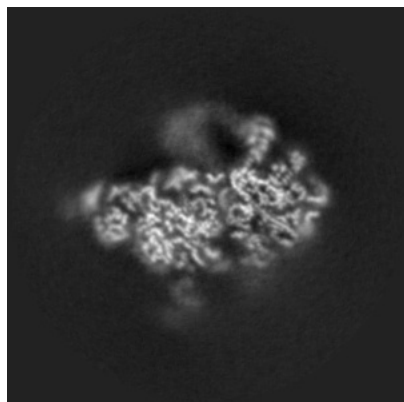


Y Index: 213

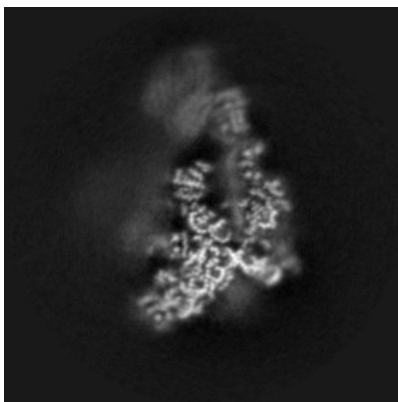


Z Index: 176

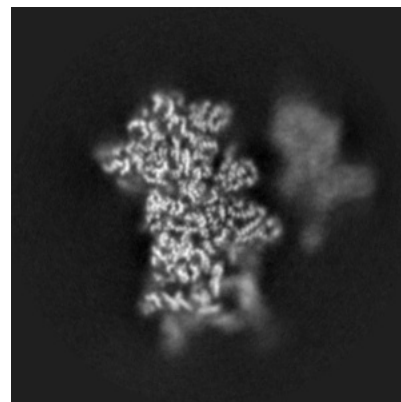
6.3.2 Raw map



X Index: 139



Y Index: 213

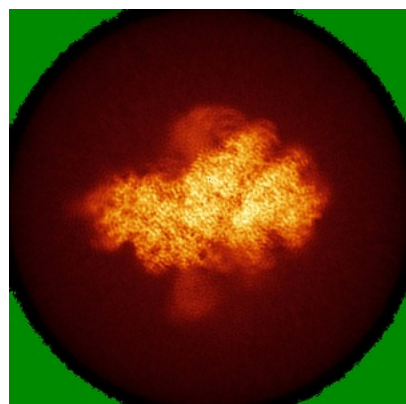


Z Index: 176

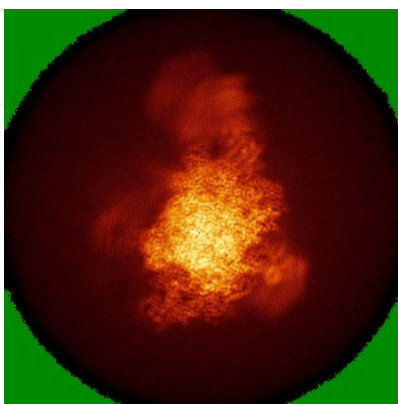
The images above show the largest variance slices of the map in three orthogonal directions.

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

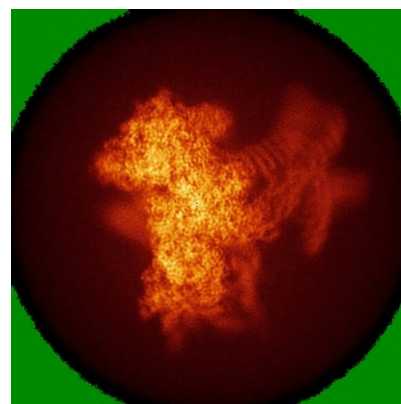
6.4.1 Primary map



X

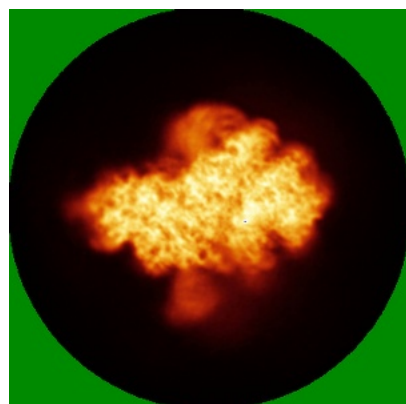


Y

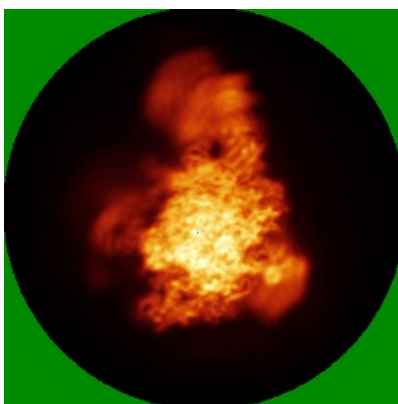


Z

6.4.2 Raw 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](#)

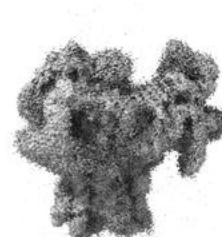
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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

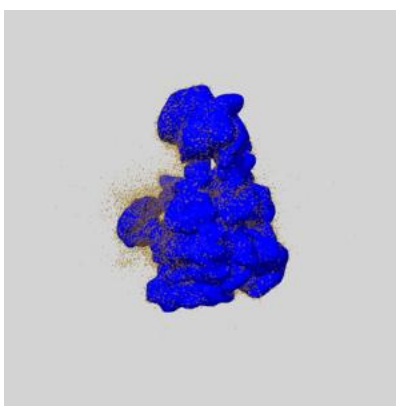
A mask typically either:

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

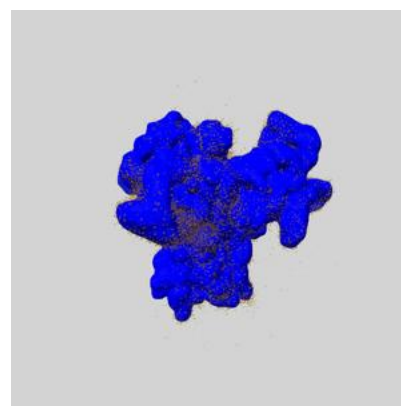
6.6.1 emd_14114_msk_1.map [i](#)



X



Y

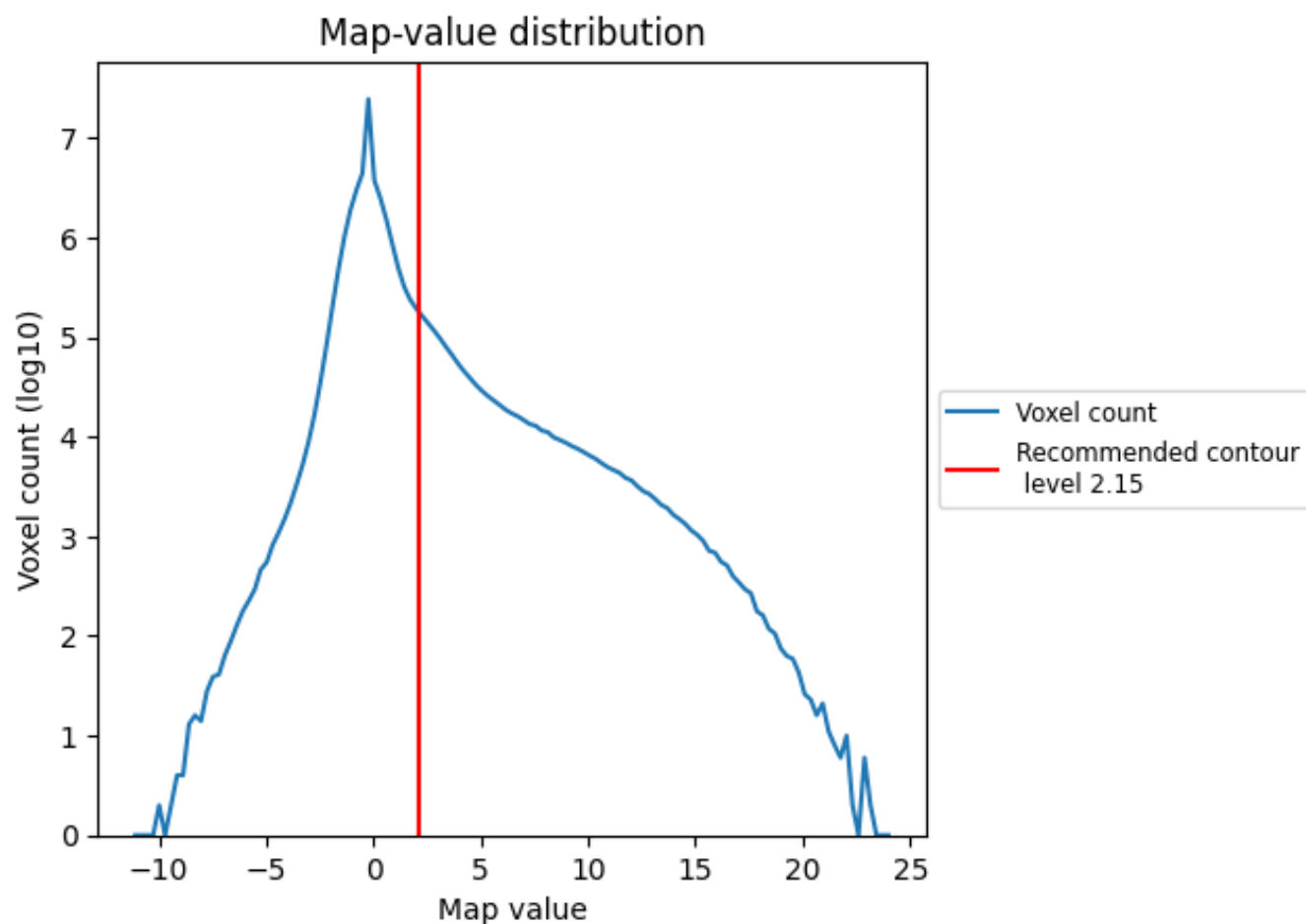


Z

7 Map analysis [i](#)

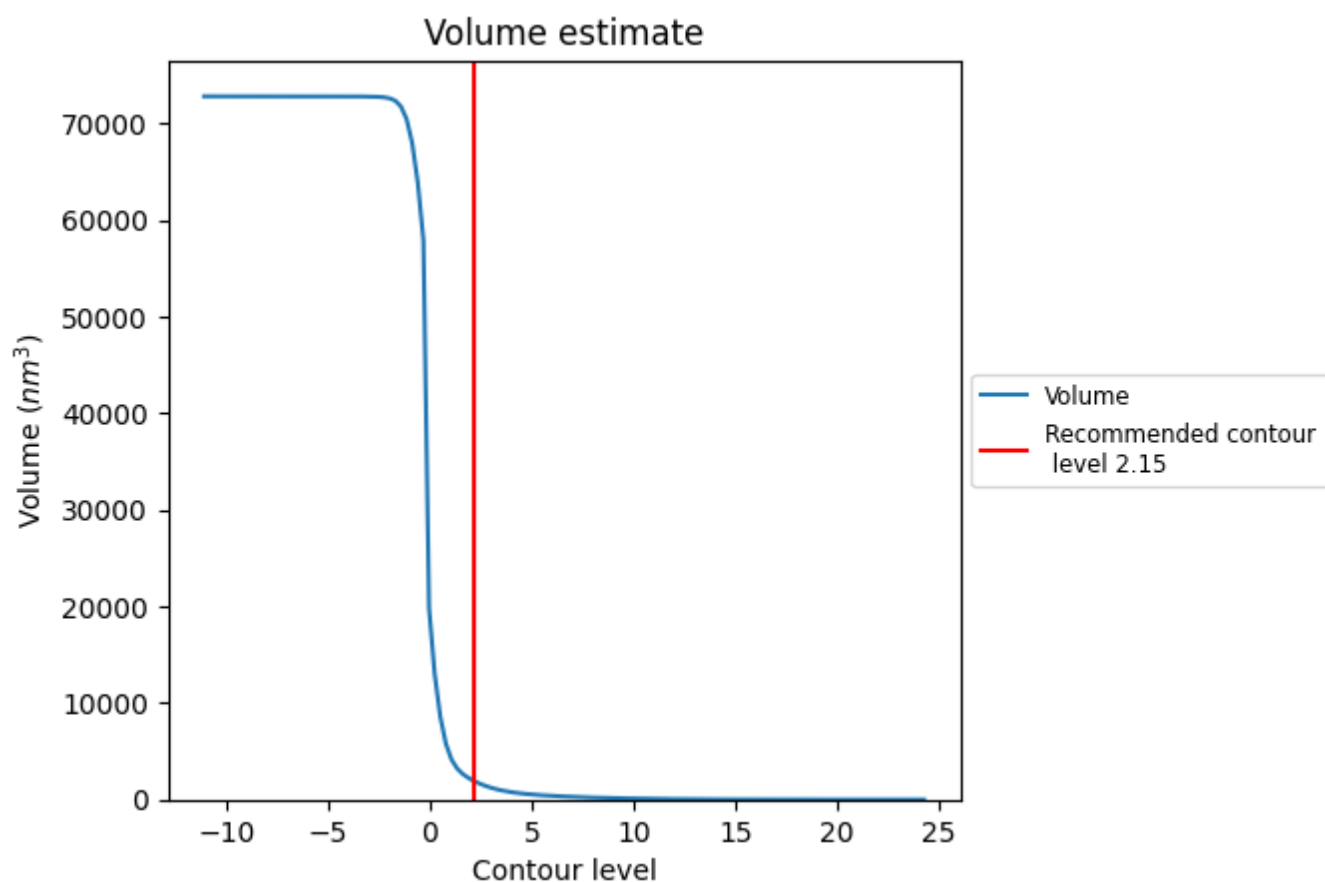
This section contains the results of statistical analysis of the map.

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.

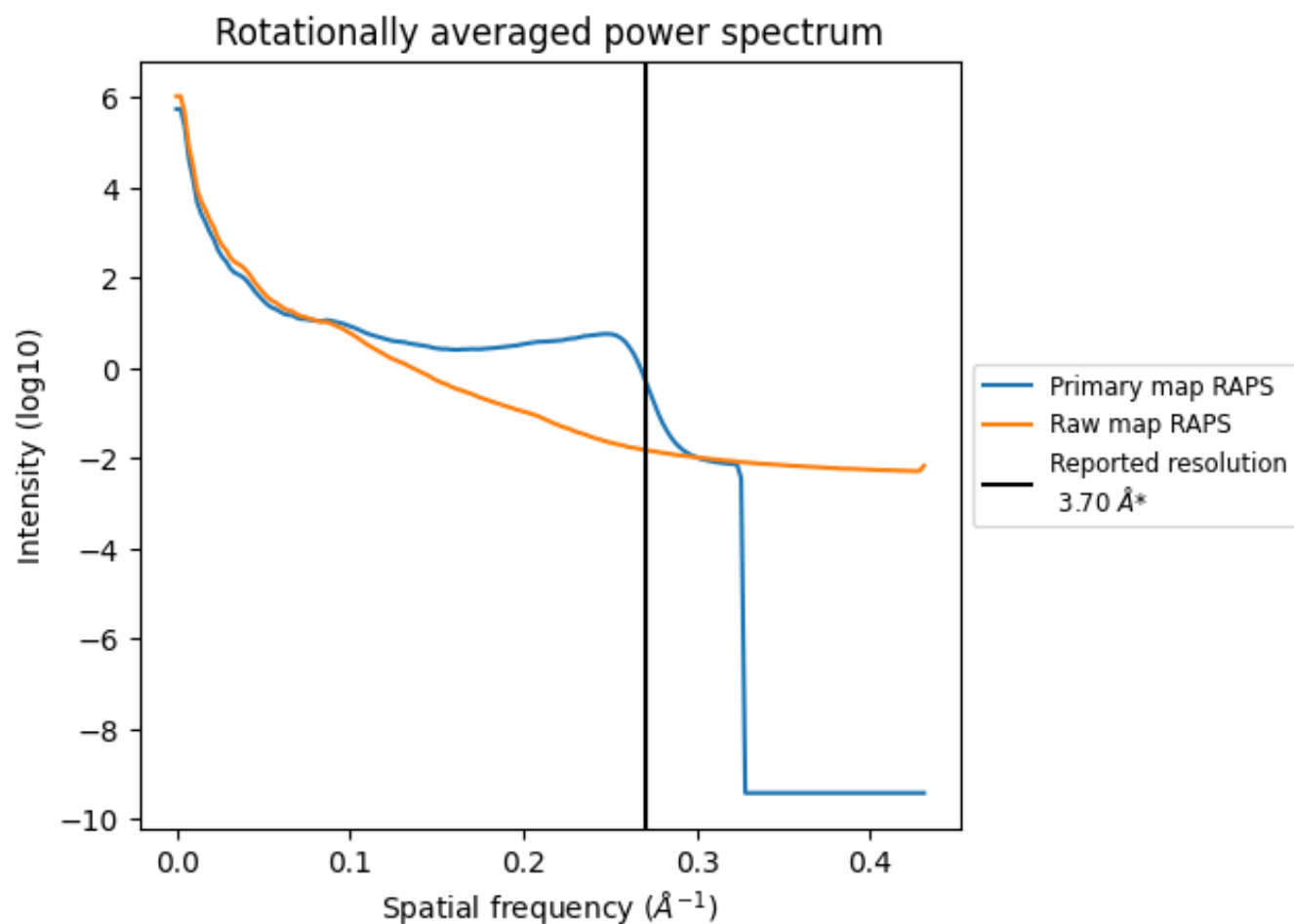
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1935 nm³; this corresponds to an approximate mass of 1748 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 ⓘ

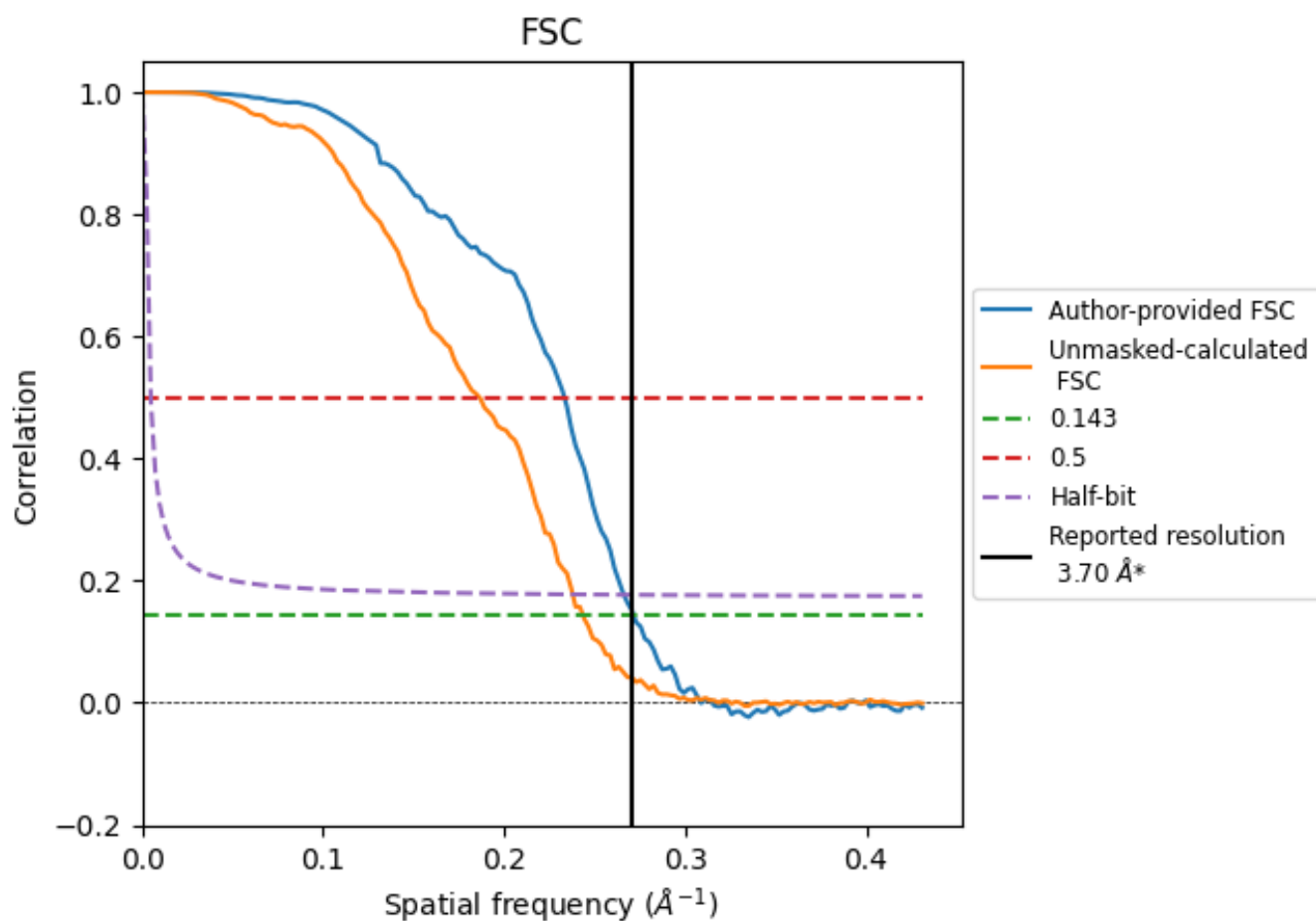


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

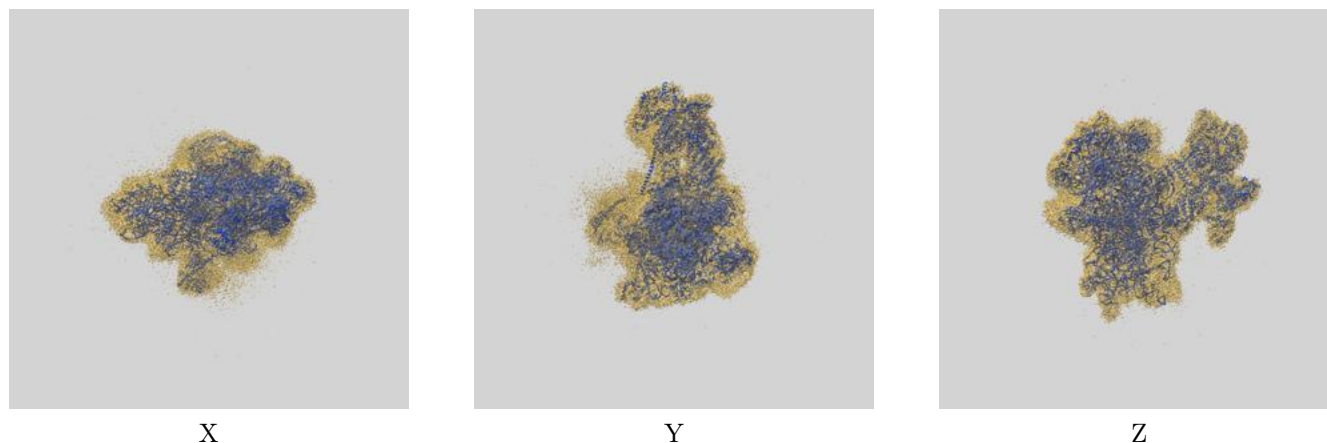
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.29	3.76
Unmasked-calculated*	4.11	5.36	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

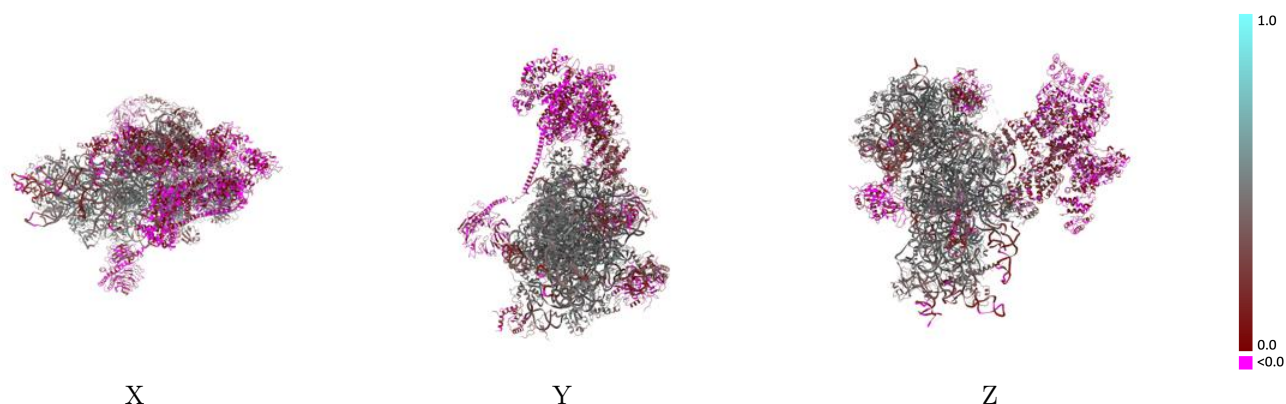
This section contains information regarding the fit between EMDB map EMD-14114 and PDB model 7QP7. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



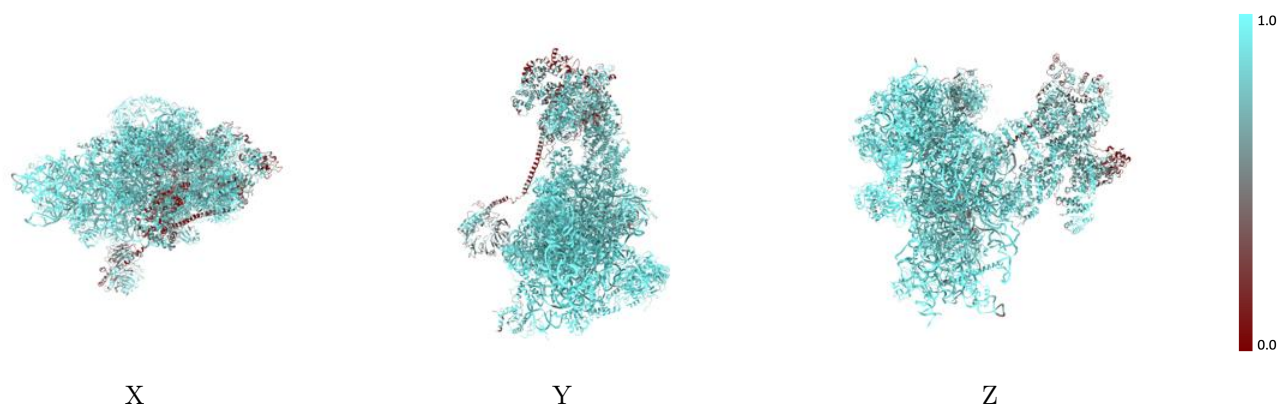
The images above show the 3D surface view of the map at the recommended contour level 2.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



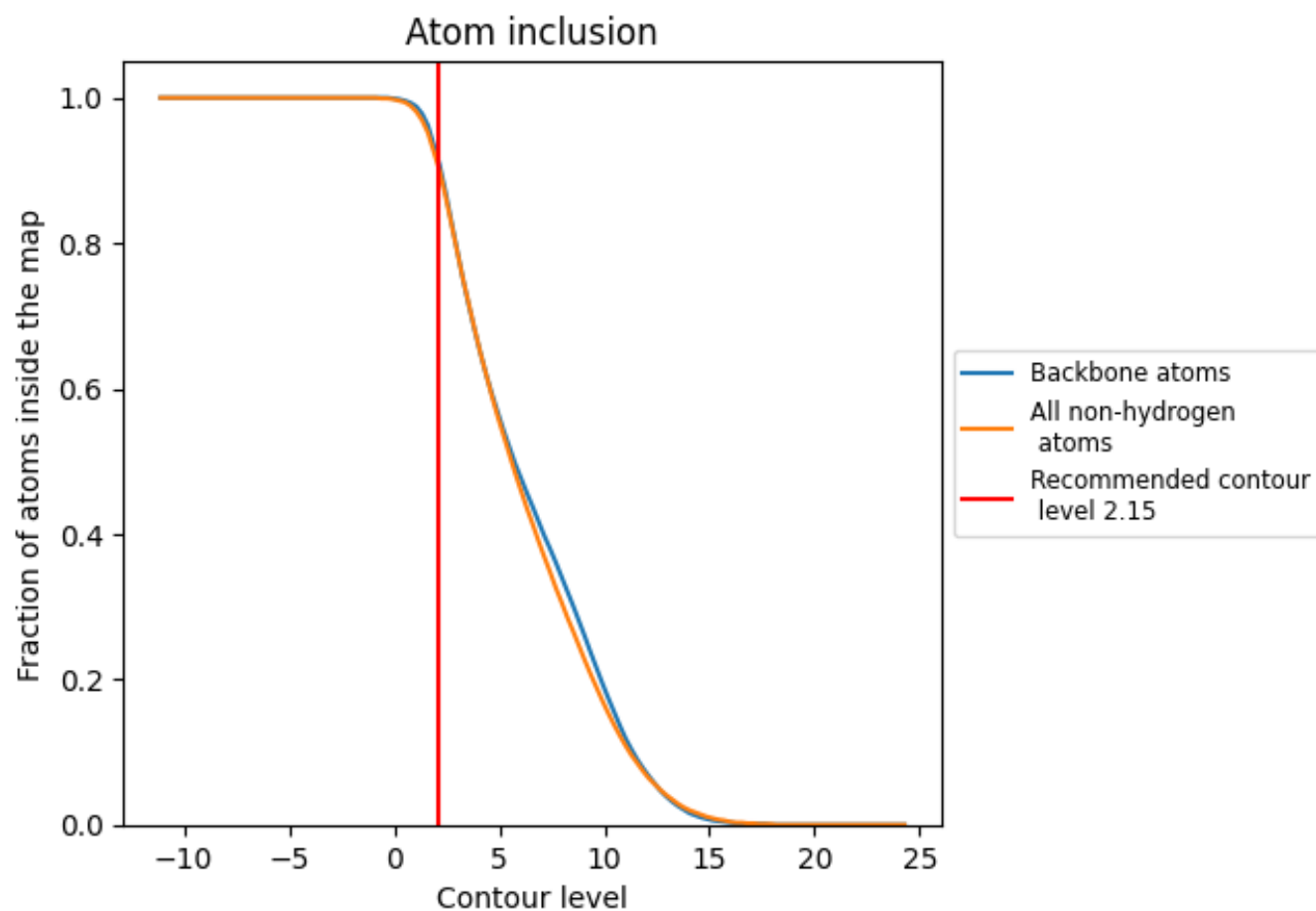
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (2.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.3370
1	 0.5900	 0.0480
3	 0.4050	 0.0230
4	 0.7400	 0.0390
5	 0.6400	 0.0290
6	 0.6270	 0.0200
7	 0.8870	 0.2360
8	 0.6980	 0.0350
9	 0.9710	 0.4920
A	 0.9850	 0.4050
B	 0.9680	 0.4940
C	 0.9720	 0.4950
D	 0.9680	 0.4890
E	 0.9700	 0.5100
F	 0.9730	 0.4820
G	 0.9300	 0.4390
H	 0.9440	 0.4800
I	 0.9800	 0.4910
J	 0.9610	 0.5170
K	 0.9720	 0.5040
L	 0.9490	 0.5010
M	 0.9250	 0.4600
N	 0.9540	 0.4940
O	 0.9210	 0.3930
P	 0.9660	 0.4860
Q	 0.9590	 0.5090
R	 0.9640	 0.4350
S	 0.9660	 0.4150
T	 0.9850	 0.4700
V	 0.9650	 0.4930
Y	 0.9650	 0.4950
Z	 0.9400	 0.4750
a	 0.9580	 0.4660
b	 0.9610	 0.4650
c	 0.9590	 0.4390



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Chain	Atom inclusion	Q-score
d	 0.9780	 0.4840
e	 0.9590	 0.4570
f	 0.9580	 0.4520
h	 0.9670	 0.4650
i	 0.9530	 0.4940
k	 0.9430	 0.3350
m	 0.8100	 0.1540
n	 0.9370	 0.4830
o	 0.8600	 0.2190
q	 0.8380	 0.3450
r	 0.9560	 0.3330
t	 0.9320	 0.0370
u	 0.7040	 0.1200
v	 0.7640	 0.0480
w	 0.9740	 0.2120
x	 0.7010	 0.1440
y	 0.7970	 0.1610