Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 11:06 AM EDT

PDB ID	:	9NLH
EMDB ID	:	EMD-29405
Title	:	E.coli Initiation complex with YheS-EQ2
Authors	:	Singh, S.; Hunt, J.F.
Deposited on	:	2025-03-03
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

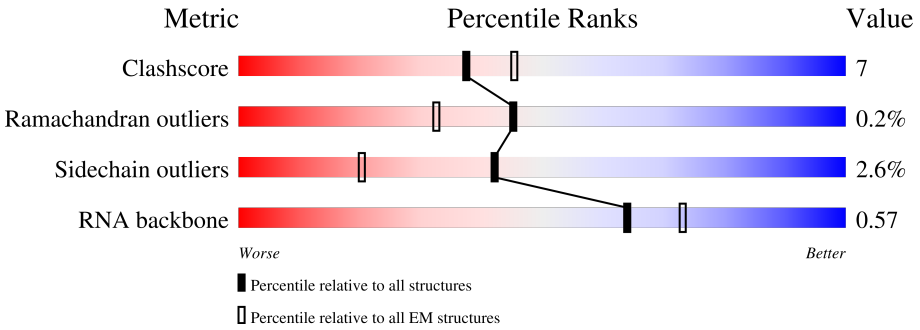
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	220	45%, 84%, 15%
2	13	142	84%, 16%
3	14	122	80%, 20%
4	15	143	84%, 15%
5	16	136	76%, 23%
6	17	120	82%, 18%
7	18	116	71%, 28%

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Mol	Chain	Length	Quality of chain
8	19	114	89% 9%
9	2	271	81% 17%
10	20	117	85% 15%
11	21	103	77% 20%
12	22	110	70% 29%
13	23	93	81% 19%
14	24	102	80% 20%
15	25	94	9% 79% 20%
16	27	75	85% 15%
17	28	77	83% 16%
18	29	63	5% 67% 32%
19	3	209	84% 15%
20	30	58	78% 22%
21	32	56	75% 23%
22	33	50	84% 14%
23	34	46	83% 15%
24	35	64	84% 16%
25	36	38	71% 29%
26	4	201	79% 21%
27	5	177	20% 65% 34%
28	6	176	16% 74% 24%
29	9	149	77% 76% 23%
30	H	526	12% 72% 27%
31	M	9	100%
32	R1	2903	67% 27% 6%

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Mol	Chain	Length	Quality of chain
33	R2	119	61% 31% 8%
34	R3	1539	61% 34% 5%
35	T	78	60% 24% 10% 5%
36	sb	218	9% 97%
37	sc	206	99%
38	sd	205	98%
39	se	157	98%
40	sf	100	24% 98%
41	sg	151	11% 98%
42	sh	129	98%
43	si	127	13% 95% 5%
44	sj	98	22% 100%
45	sk	116	8% 100%
46	sl	123	97%
47	sm	114	24% 99%
48	sn	100	8% 97%
49	so	88	94% 6%
50	sp	82	9% 100%
51	sq	80	99%
52	sr	65	12% 100%
53	ss	79	22% 99%
54	st	85	5% 100%
55	su	65	15% 91% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	H2U	T	20	X	-	-	-
35	4OC	T	32	X	-	-	-
35	5MU	T	54	X	-	-	-
35	PSU	T	55	X	-	-	-
35	4SU	T	8	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149471 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 Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	220	1353	804	270	277	2	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	13	142	1129	714	212	199	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	14	122	938	587	180	165	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	15	143	1045	649	206	189	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	16	136	1074	686	205	177	6	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	17	120	960	593	196	166	5	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	18	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	19	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	271	Total 2082	C 1288	N 423	O 364	S 7	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	20	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	21	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	23	93	Total 738	C 466	N 139	O 131	S 2	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	24	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	25	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	75	Total 575	C 356	N 116	O 102	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	28	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	29	63	Total 509	C 313	N 99	O 95	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	209	Total 1565	C 979	N 288	O 294	S 4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	30	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 25 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 30 is a protein called YheS.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	526	Total	C	N	O	S	0	0
			4173	2638	748	777	10		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	9	Total	C	N	O	P	0	0
			195	88	40	58	9		

- Molecule 32 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R1	1847	G	A	conflict	GB 2019144442

- Molecule 33 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 35 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	T	78	Total	C	N	O	P	S	0	0
			1649	740	295	536	76	2		

- Molecule 36 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	sc	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	sd	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 40 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	sf	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	sh	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 43 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	si	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	sj	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	sk	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	sl	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	sm	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	sn	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 49 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	so	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	sp	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	sq	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	sr	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ss	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	st	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

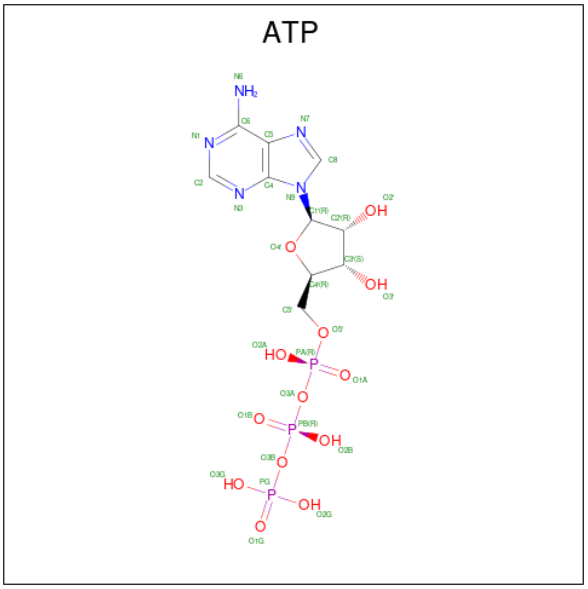
- Molecule 55 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	su	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	17	1	Total Mg 1 1	0
56	2	2	Total Mg 2 2	0
56	3	1	Total Mg 1 1	0
56	M	1	Total Mg 1 1	0
56	R1	188	Total Mg 188 188	0
56	R3	70	Total Mg 70 70	0

- Molecule 57 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
57	H	1	Total C N O P 31 10 5 13 3	0
57	H	1	Total C N O P 31 10 5 13 3	0

- Molecule 58 is SODIUM ION (three-letter code: NA) (formula: Na).

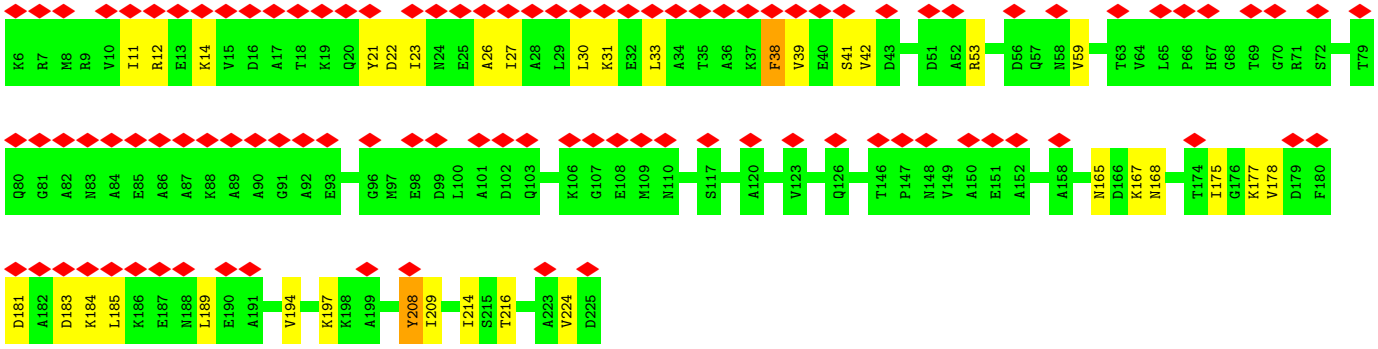
Mol	Chain	Residues	Atoms	AltConf
58	H	2	Total Na 2 2	0

3 Residue-property plots (i)

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

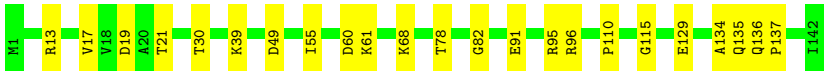
• Molecule 1: Large ribosomal subunit protein uL1

Chain 1:



• Molecule 2: Large ribosomal subunit protein uL13

Chain 13:

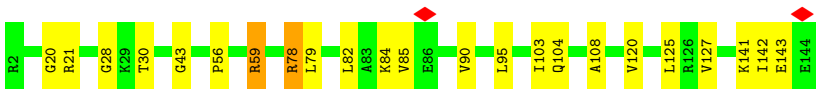


• Molecule 3: 50S ribosomal protein L14

Chain 14:

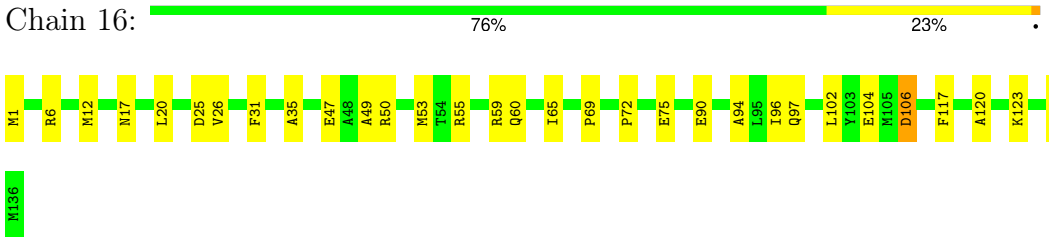
• Molecule 4: 50S ribosomal protein L15

Chain 15:



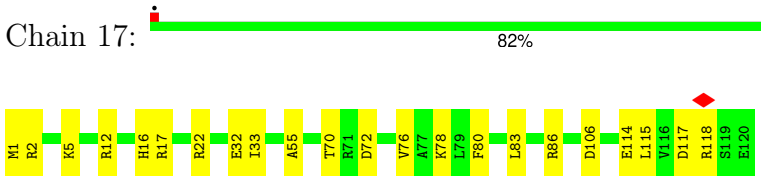
• Molecule 5: 50S ribosomal protein L16

Chain 16:



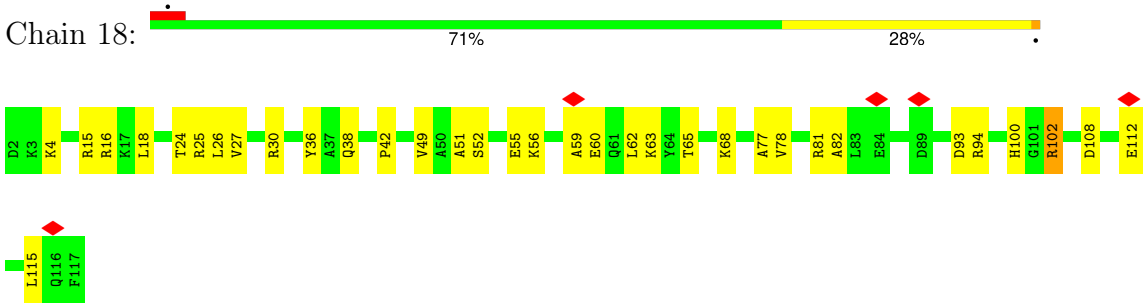
• Molecule 6: Large ribosomal subunit protein bL17

Chain 17:



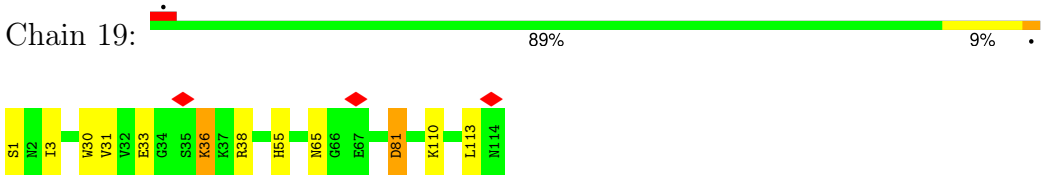
• Molecule 7: Large ribosomal subunit protein uL18

Chain 18:



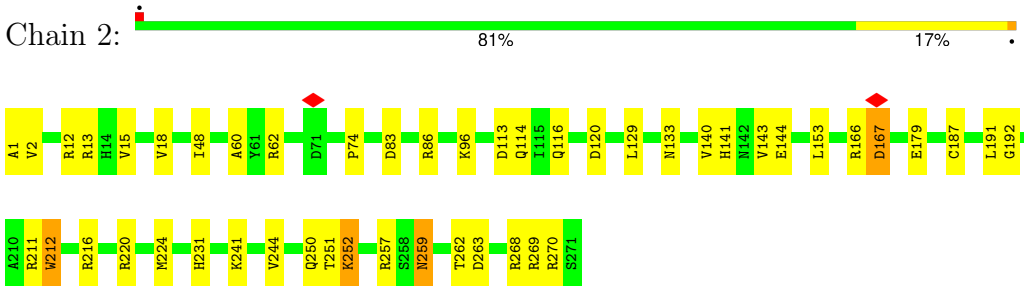
• Molecule 8: 50S ribosomal protein L19

Chain 19:



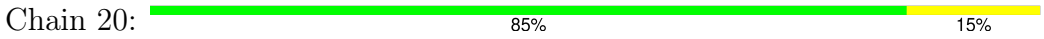
• Molecule 9: 50S ribosomal protein L2

Chain 2:

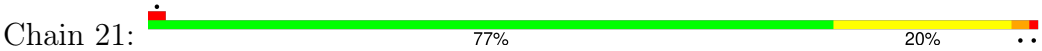


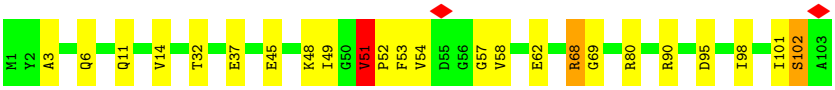
• Molecule 10: Large ribosomal subunit protein bL20

Chain 20:

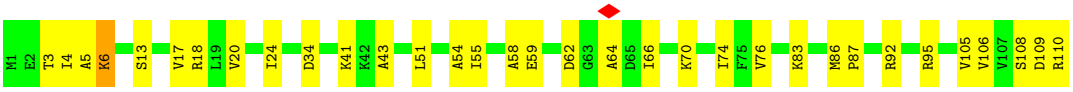


• Molecule 11: Large ribosomal subunit protein bL21

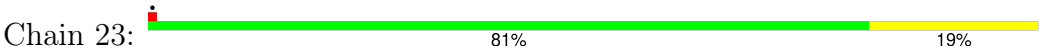


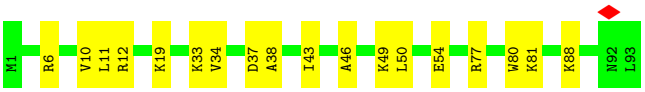


• Molecule 12: Large ribosomal subunit protein uL22

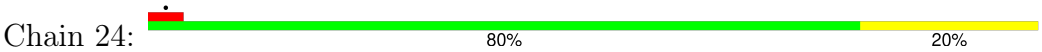


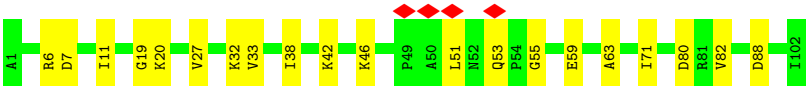
• Molecule 13: Large ribosomal subunit protein uL23



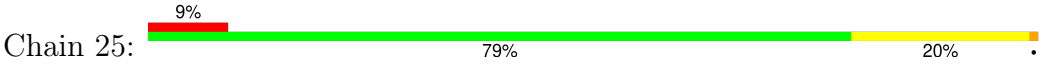


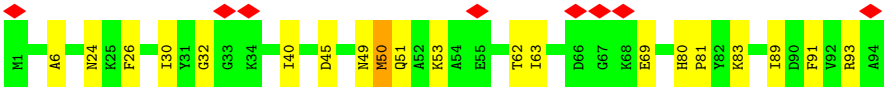
• Molecule 14: Large ribosomal subunit protein uL24



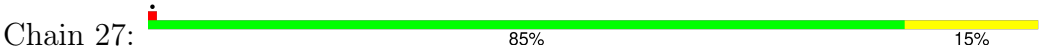


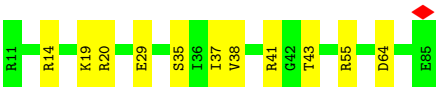
• Molecule 15: Large ribosomal subunit protein bL25





• Molecule 16: 50S ribosomal protein L27



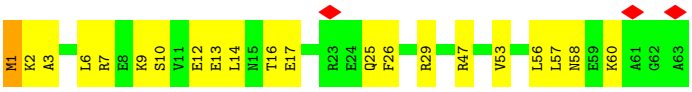


• Molecule 17: 50S ribosomal protein L28

Chain 28:

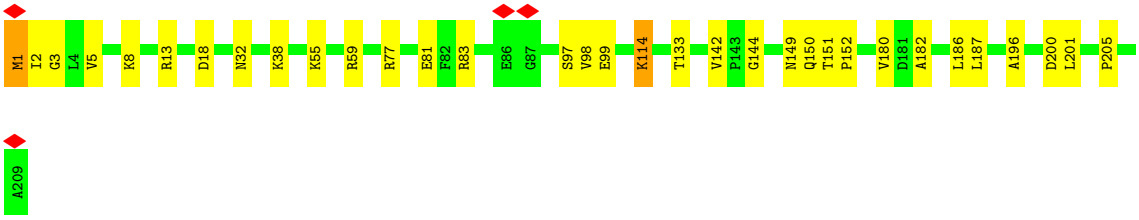
• Molecule 18: Large ribosomal subunit protein uL29

Chain 29:



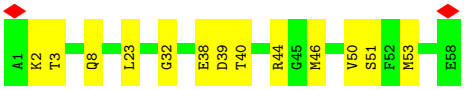
• Molecule 19: 50S ribosomal protein L3

Chain 3:



• Molecule 20: 50S ribosomal protein L30

Chain 30:



• Molecule 21: 50S ribosomal protein L32

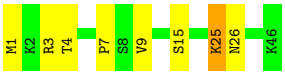
Chain 32:

• Molecule 22: Large ribosomal subunit protein bL33

Chain 33:

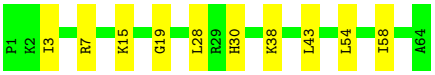
• Molecule 23: 50S ribosomal protein L34

Chain 34:



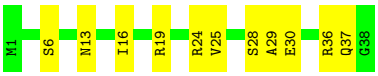
• Molecule 24: Large ribosomal subunit protein bL35

Chain 35:



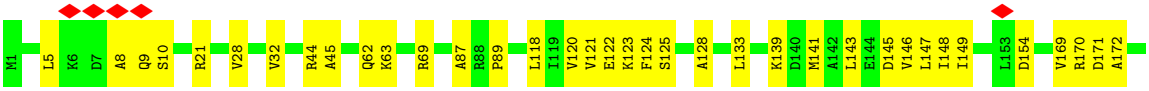
• Molecule 25: 50S ribosomal protein L36

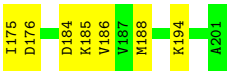
Chain 36:



• Molecule 26: Large ribosomal subunit protein uL4

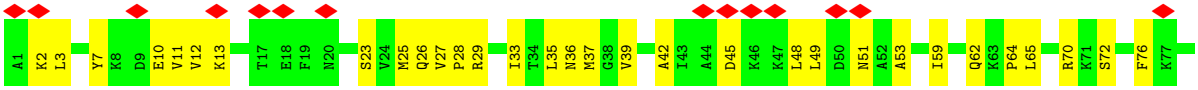
Chain 4:

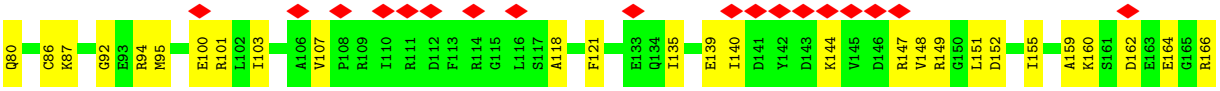


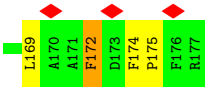


• Molecule 27: 50S ribosomal protein L5

Chain 5:

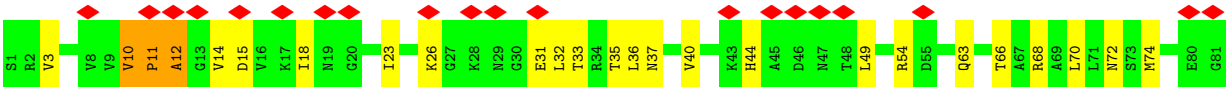


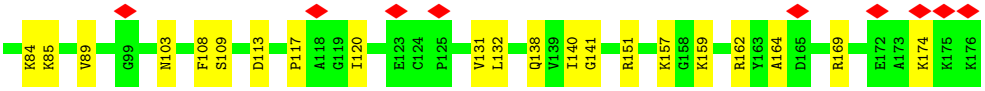




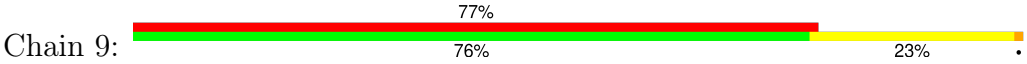
• Molecule 28: Large ribosomal subunit protein uL6

Chain 6:

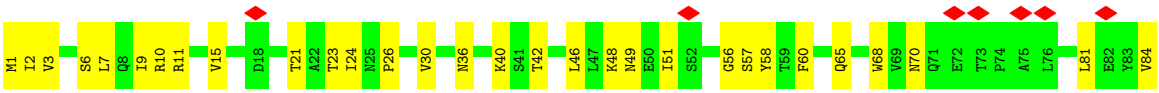


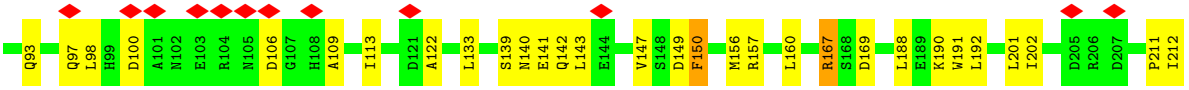


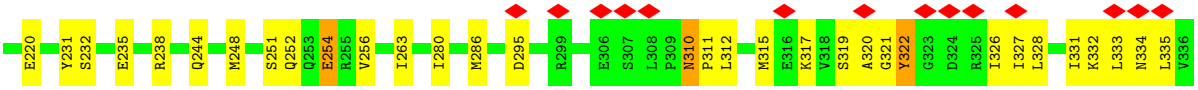
• Molecule 29: Large ribosomal subunit protein bL9

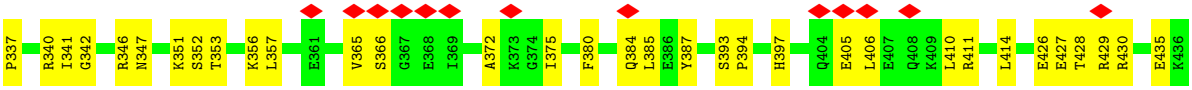


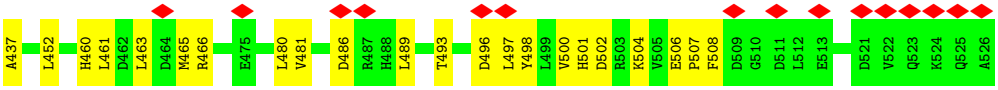
• Molecule 30: YheS







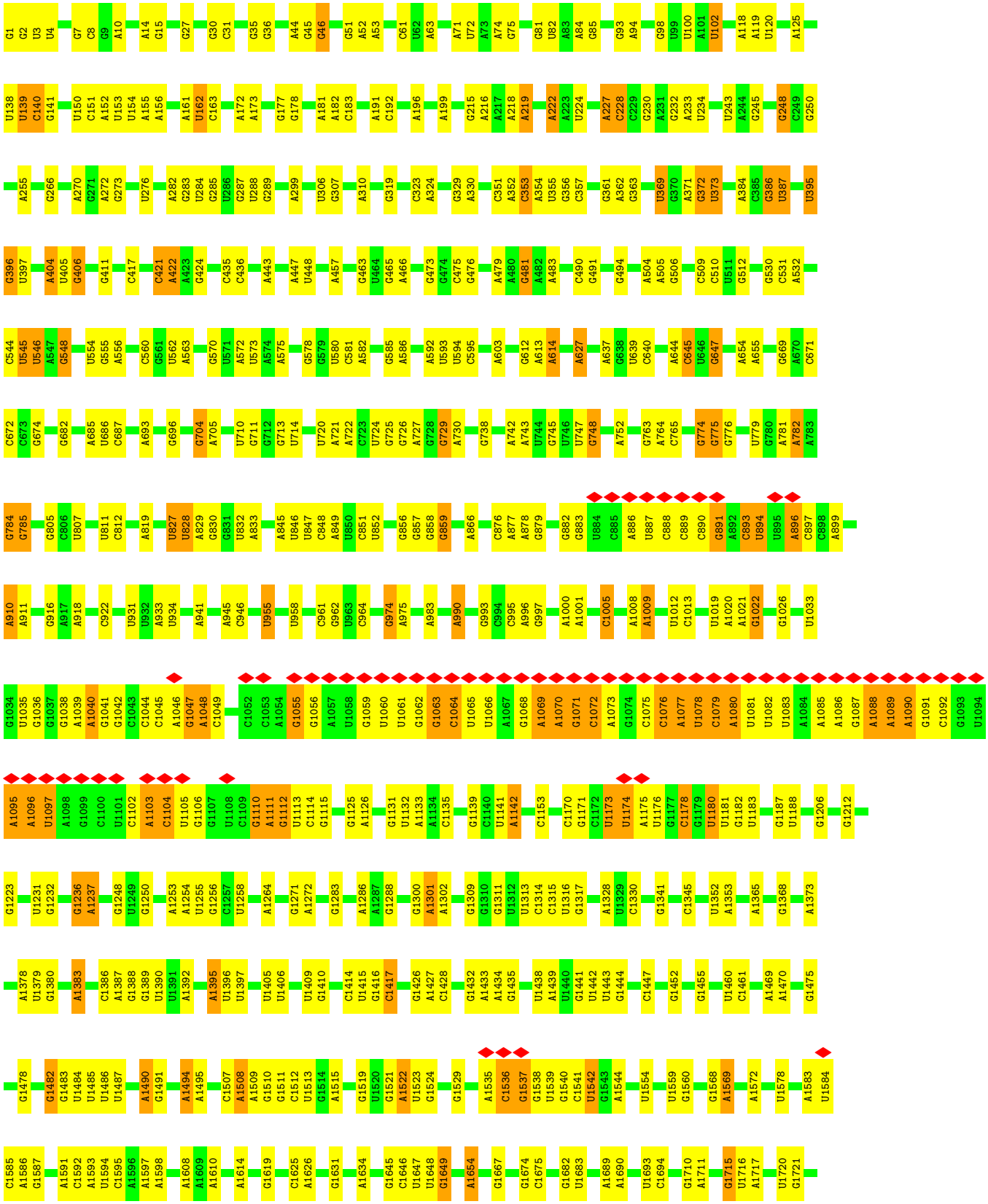


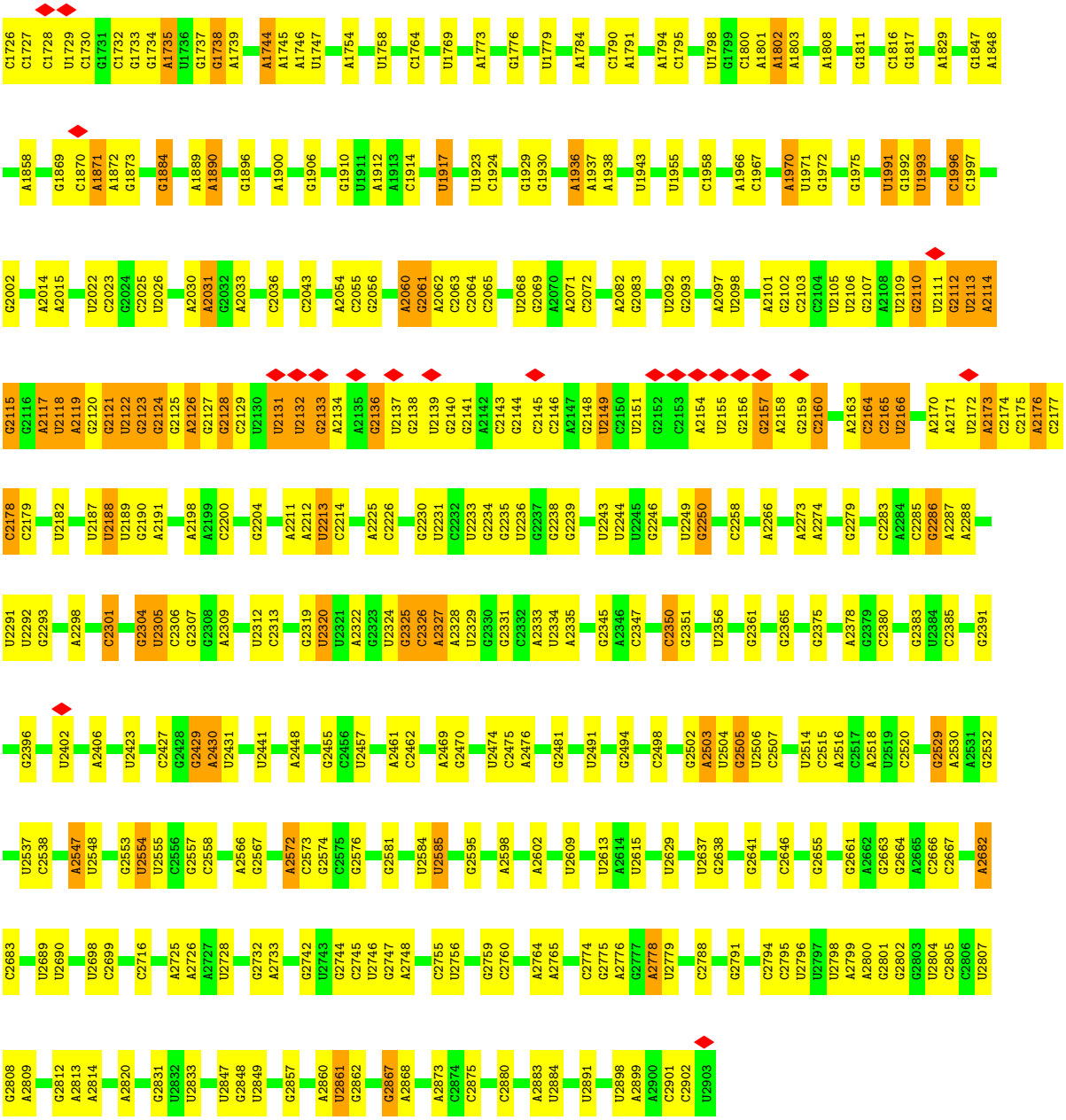


• Molecule 31: mRNA

There are no outlier residues recorded for this chain.

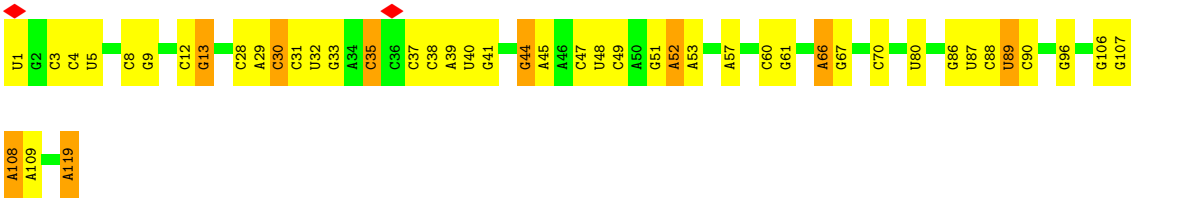
• Molecule 32: 23S ribosomal RNA





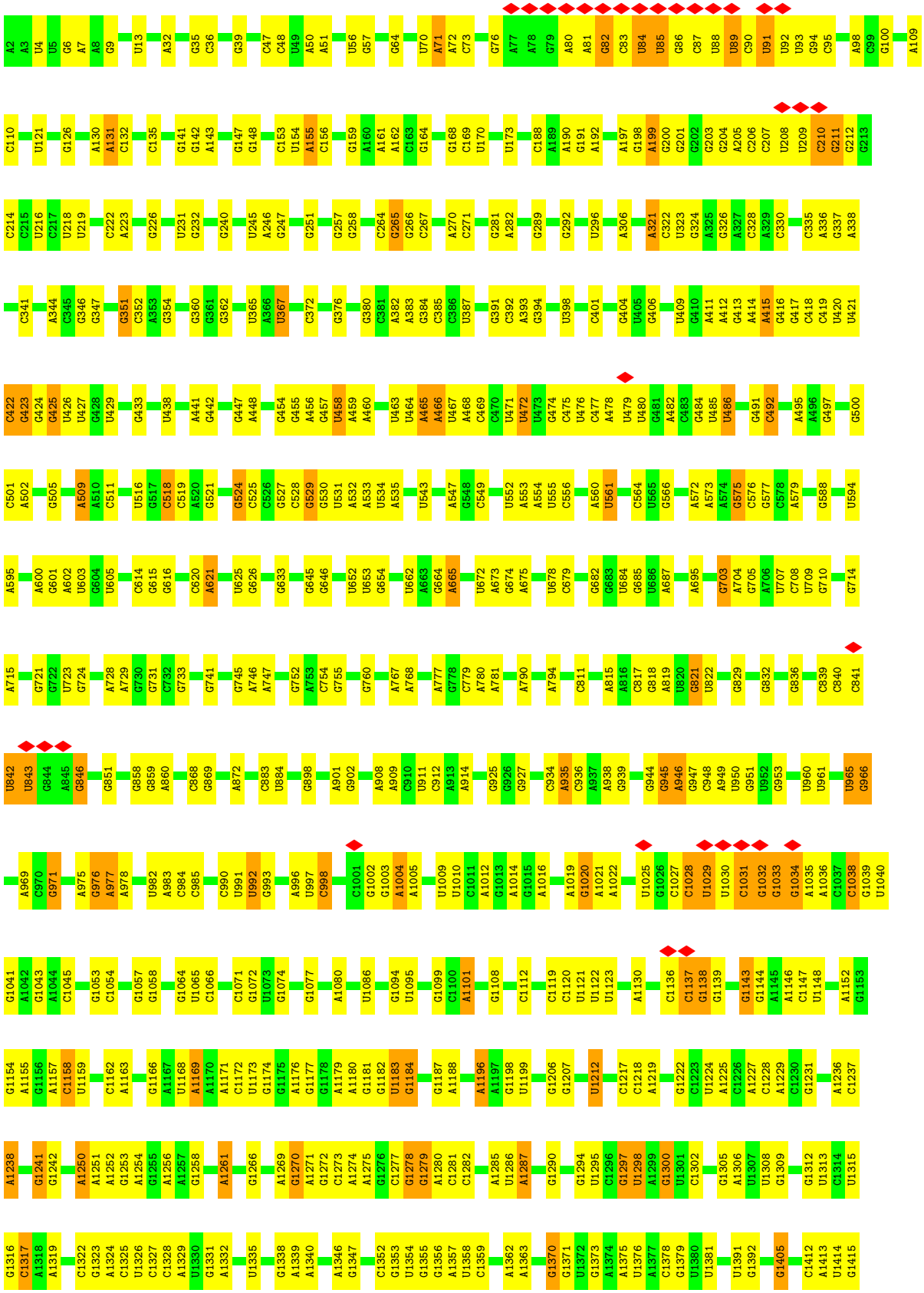
• Molecule 33: 5S ribosomal RNA

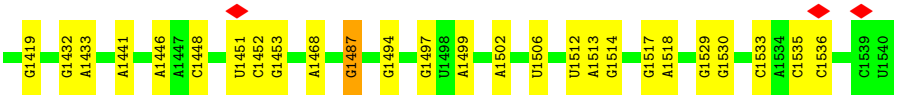
Chain R2:



• Molecule 34: 16S ribosomal RNA

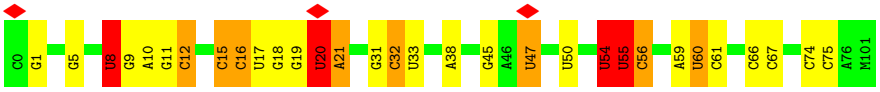
Chain R3:





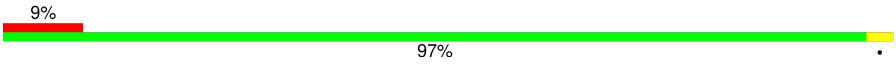
• Molecule 35: tRNA

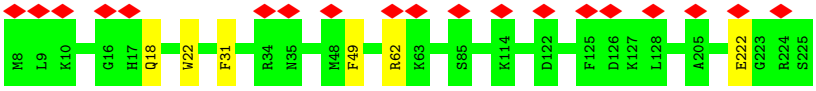
Chain T:



• Molecule 36: Small ribosomal subunit protein uS2

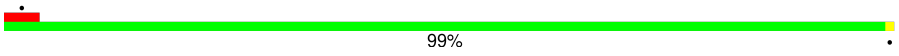
Chain sb:

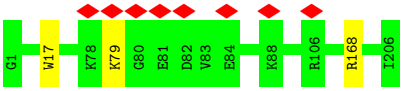




• Molecule 37: Small ribosomal subunit protein uS3

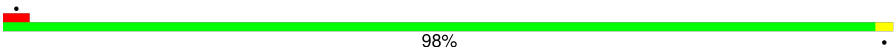
Chain sc:





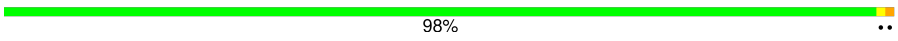
• Molecule 38: 30S ribosomal protein S4

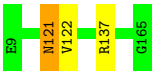
Chain sd:



• Molecule 39: Small ribosomal subunit protein uS5

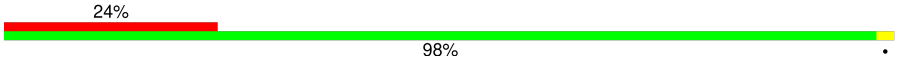
Chain se:

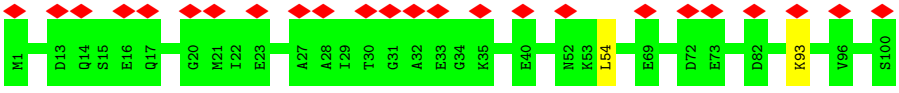




• Molecule 40: 30S ribosomal protein S6, non-modified isoform

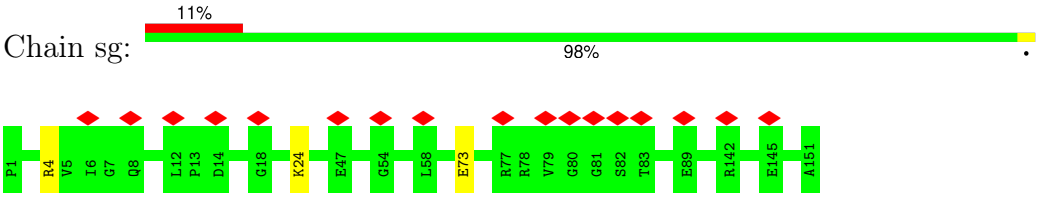
Chain sf:





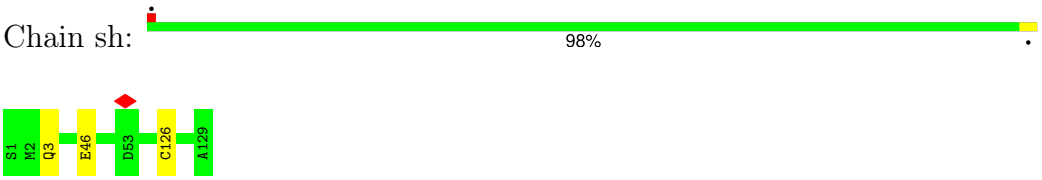
• Molecule 41: 30S ribosomal protein S7

Chain sg:



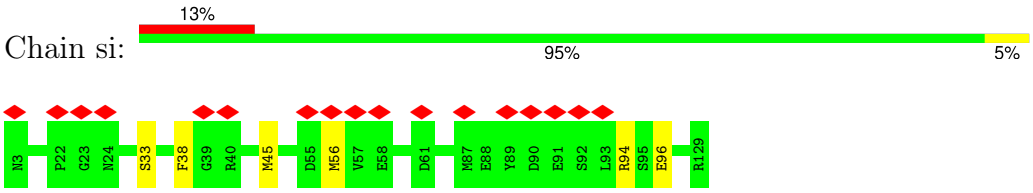
• Molecule 42: 30S ribosomal protein S8

Chain sh:



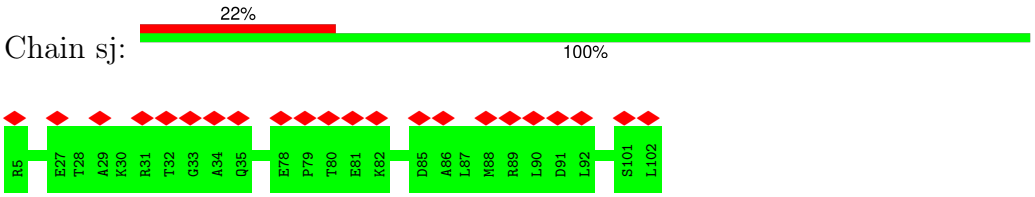
• Molecule 43: Small ribosomal subunit protein uS9

Chain si:



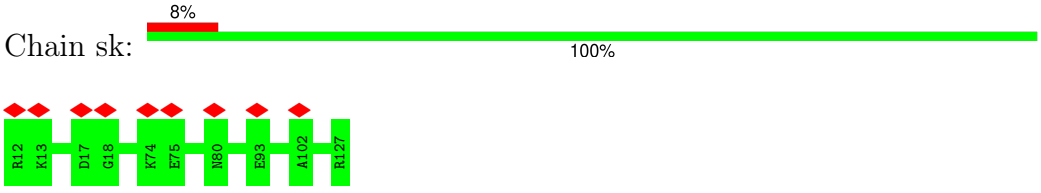
• Molecule 44: 30S ribosomal protein S10

Chain sj:



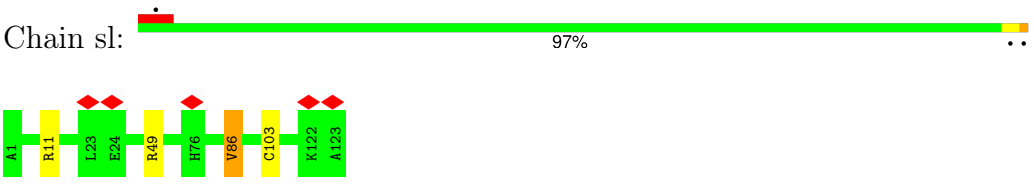
• Molecule 45: Small ribosomal subunit protein uS11

Chain sk:



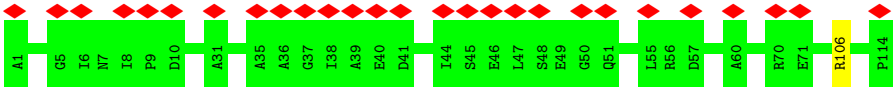
• Molecule 46: Small ribosomal subunit protein uS12

Chain sl:

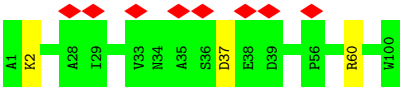


• Molecule 47: 30S ribosomal protein S13

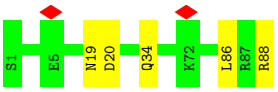
Chain sm:



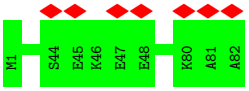
• Molecule 48: Small ribosomal subunit protein uS14



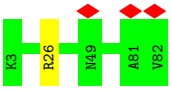
• Molecule 49: Small ribosomal subunit protein uS15



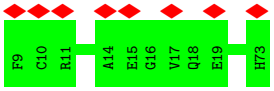
• Molecule 50: Small ribosomal subunit protein bS16



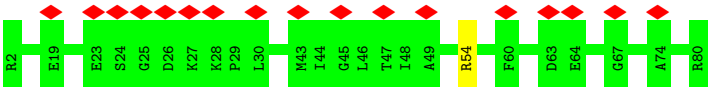
• Molecule 51: Small ribosomal subunit protein uS17



• Molecule 52: 30S ribosomal protein S18

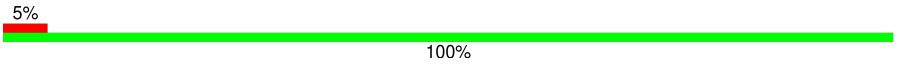


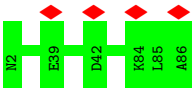
• Molecule 53: 30S ribosomal protein S19



• Molecule 54: 30S ribosomal protein S20

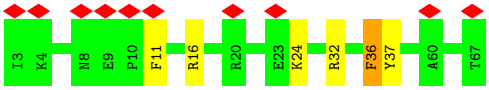
Chain st:





• Molecule 55: Small ribosomal subunit protein bS21

Chain su:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.474	Depositor
Minimum map value	-1.478	Depositor
Average map value	0.089	Depositor
Map value standard deviation	0.244	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, ATP, PSU, H2U, 4SU, 4OC, FME, NA

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	0.24	0/1361	0.49	0/1796
2	13	0.32	0/1152	0.53	0/1551
3	14	0.31	0/947	0.60	0/1268
4	15	0.32	0/1054	0.58	0/1403
5	16	0.33	0/1093	0.59	0/1460
6	17	0.31	0/973	0.59	0/1301
7	18	0.30	0/902	0.55	0/1209
8	19	0.32	0/929	0.57	1/1242 (0.1%)
9	2	0.33	0/2121	0.56	0/2852
10	20	0.37	0/960	0.54	0/1278
11	21	0.33	0/829	0.59	0/1107
12	22	0.30	0/864	0.55	0/1156
13	23	0.30	0/744	0.54	0/994
14	24	0.29	0/787	0.52	0/1051
15	25	0.30	0/766	0.50	0/1025
16	27	0.32	0/582	0.55	0/769
17	28	0.31	0/635	0.58	0/848
18	29	0.29	0/510	0.56	0/677
19	3	0.32	0/1586	0.55	0/2134
20	30	0.27	0/453	0.56	0/605
21	32	0.32	0/450	0.57	0/599
22	33	0.32	0/416	0.53	0/554
23	34	0.31	0/380	0.63	0/498
24	35	0.31	0/513	0.55	0/676
25	36	0.30	0/303	0.56	0/397
26	4	0.31	0/1571	0.52	0/2113
27	5	0.27	0/1434	0.53	0/1926
28	6	0.72	3/1343 (0.2%)	0.95	5/1816 (0.3%)
29	9	0.26	0/1122	0.57	1/1515 (0.1%)
30	H	0.28	0/4253	0.53	0/5752
31	M	0.36	0/219	0.66	0/339
32	R1	0.53	0/69797	0.79	8/108890 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	R2	0.40	0/2847	0.81	1/4440 (0.0%)
34	R3	0.42	0/36963	0.78	2/57662 (0.0%)
35	T	0.42	0/1716	0.77	0/2672
36	sb	0.26	0/1735	0.50	0/2338
37	sc	0.28	0/1651	0.53	0/2225
38	sd	0.28	0/1665	0.55	0/2227
39	se	0.30	0/1169	0.57	0/1573
40	sf	0.27	0/835	0.59	1/1128 (0.1%)
41	sg	0.28	0/1195	0.56	0/1602
42	sh	0.29	0/989	0.54	0/1326
43	si	0.27	0/1034	0.63	0/1375
44	sj	0.27	0/796	0.60	0/1077
45	sk	0.28	0/885	0.54	0/1195
46	sl	0.30	0/969	0.60	0/1300
47	sm	0.25	0/892	0.58	0/1193
48	sn	0.26	0/817	0.60	0/1088
49	so	0.28	0/722	0.55	0/964
50	sp	0.31	0/659	0.59	0/884
51	sq	0.30	0/657	0.56	0/881
52	sr	0.27	0/544	0.52	0/731
53	ss	0.25	0/652	0.52	0/877
54	st	0.28	0/671	0.50	0/888
55	su	0.27	0/550	0.65	0/728
All	All	0.45	3/161662 (0.0%)	0.73	19/241175 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	21	0	1
28	6	0	1
29	9	0	1
35	T	8	0
39	se	0	1
46	sl	0	1
All	All	8	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	11	PRO	N-CD	19.75	1.75	1.47
28	6	11	PRO	CB-CG	-11.31	0.93	1.50
28	6	11	PRO	CG-CD	-7.59	1.25	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	6	11	PRO	N-CD-CG	-19.69	73.67	103.20
28	6	11	PRO	CB-CG-CD	17.68	175.45	106.50
28	6	11	PRO	CA-CB-CG	-14.77	75.94	104.00
28	6	11	PRO	CA-N-CD	-13.91	92.03	111.50
32	R1	1313	U	C2-N1-C1'	6.36	125.34	117.70
40	sf	54	LEU	CA-CB-CG	6.15	129.45	115.30
28	6	10	VAL	C-N-CD	6.13	141.27	128.40
34	R3	754	C	C2-N1-C1'	6.04	125.45	118.80
32	R1	1314	C	C2-N1-C1'	5.53	124.89	118.80
32	R1	2902	C	N3-C2-O2	-5.50	118.05	121.90
29	9	90	LEU	CA-CB-CG	5.48	127.91	115.30
34	R3	509	A	N7-C8-N9	5.42	116.51	113.80
32	R1	1917	U	N3-C2-O2	-5.41	118.41	122.20
32	R1	955	U	C2-N1-C1'	5.31	124.07	117.70
8	19	113	LEU	CA-CB-CG	5.13	127.10	115.30
32	R1	955	U	N3-C2-O2	-5.13	118.61	122.20
33	R2	35	C	N1-C2-O2	5.10	121.96	118.90
32	R1	2301	C	C2-N1-C1'	5.09	124.40	118.80
32	R1	2503	A	OP1-P-O3'	5.01	116.22	105.20

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	8	4SU	C2',C3'
35	T	20	H2U	C2',C3'
35	T	32	4OC	C1',C2'
35	T	54	5MU	C4'
35	T	55	PSU	C4'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	21	51	VAL	Peptide
28	6	12	ALA	Peptide
29	9	8	LYS	Peptide
39	se	121	ASN	Peptide

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Mol	Chain	Res	Type	Group
46	sl	86	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	23	0
2	13	1129	0	1162	17	0
3	14	938	0	1012	16	0
4	15	1045	0	1117	15	0
5	16	1074	0	1157	18	0
6	17	960	0	1000	13	0
7	18	892	0	923	26	0
8	19	917	0	965	9	0
9	2	2082	0	2157	33	0
10	20	947	0	1022	16	0
11	21	816	0	839	18	0
12	22	857	0	922	22	0
13	23	738	0	807	13	0
14	24	779	0	834	10	0
15	25	753	0	780	11	0
16	27	575	0	592	8	0
17	28	625	0	655	8	0
18	29	509	0	543	15	0
19	3	1565	0	1616	22	0
20	30	449	0	491	8	0
21	32	444	0	461	11	0
22	33	409	0	440	5	0
23	34	377	0	418	7	0
24	35	504	0	574	7	0
25	36	302	0	343	7	0
26	4	1552	0	1619	28	0
27	5	1410	0	1447	41	0
28	6	1323	0	1374	30	0
29	9	1111	0	1148	26	0
30	H	4173	0	4184	108	0
31	M	195	0	99	0	0
32	R1	62318	0	31345	515	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	R2	2546	0	1292	39	0
34	R3	33012	0	16617	298	0
35	T	1649	0	853	16	0
36	sb	1704	0	1732	0	0
37	sc	1624	0	1699	0	0
38	sd	1643	0	1710	0	0
39	se	1156	0	1199	0	0
40	sf	817	0	808	0	0
41	sg	1181	0	1240	0	0
42	sh	979	0	1034	0	0
43	si	1022	0	1070	0	0
44	sj	786	0	828	0	0
45	sk	869	0	878	0	0
46	sl	955	0	1019	0	0
47	sm	883	0	944	0	0
48	sn	805	0	847	0	0
49	so	714	0	737	0	0
50	sp	649	0	666	0	0
51	sq	648	0	691	0	0
52	sr	535	0	552	0	0
53	ss	637	0	665	0	0
54	st	665	0	714	0	0
55	su	544	0	579	0	0
56	17	1	0	0	0	0
56	2	2	0	0	0	0
56	3	1	0	0	0	0
56	M	1	0	0	0	0
56	R1	188	0	0	0	0
56	R3	70	0	0	0	0
57	H	62	0	24	4	0
58	H	2	0	0	0	0
All	All	149471	0	101603	1337	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 7.

All (1337) 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)
32:R1:1040:A:H61	32:R1:1115:G:H1	1.03	0.95
34:R3:509:A:H8	34:R3:543:U:HO2'	1.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1064:C:N3	32:R1:1073:A:N1	2.19	0.91
34:R3:1009:U:H3	34:R3:1020:G:H1	1.19	0.90
32:R1:883:G:N1	32:R1:893:C:N3	2.24	0.84
4:15:78:ARG:NH2	32:R1:627:A:OP1	2.12	0.83
27:5:35:LEU:HD11	27:5:151:LEU:HD13	1.62	0.82
30:H:312:LEU:HD12	30:H:335:LEU:HB2	1.60	0.82
34:R3:664:G:H22	34:R3:741:G:H1	1.26	0.81
32:R1:1040:A:N6	32:R1:1115:G:H1	1.77	0.81
32:R1:2124:G:N2	32:R1:2175:C:O2	2.12	0.81
32:R1:1064:C:O2	32:R1:1073:A:N6	2.13	0.81
28:6:117:PRO:HD2	28:6:120:ILE:HD13	1.63	0.80
12:22:5:ALA:HB2	12:22:54:ALA:HB2	1.66	0.78
32:R1:883:G:N2	32:R1:893:C:O2	2.11	0.78
32:R1:2304:G:H22	32:R1:2312:U:H3	1.28	0.78
34:R3:71:A:N6	34:R3:100:G:N3	2.32	0.77
1:1:181:ASP:H	1:1:184:LYS:HD2	1.49	0.77
35:T:59:A:O2’	35:T:60:U:O5’	2.03	0.77
34:R3:998:C:O2	34:R3:1043:G:N2	2.17	0.77
18:29:6:LEU:HD22	18:29:7:ARG:HH21	1.49	0.77
28:6:11:PRO:HD2	28:6:14:VAL:HG22	1.64	0.77
29:9:132:PHE:HB2	29:9:140:ALA:HB3	1.67	0.76
7:18:63:LYS:NZ	33:R2:51:G:OP1	2.19	0.75
30:H:212:ILE:HG13	30:H:212:ILE:O	1.87	0.75
18:29:6:LEU:HD22	18:29:7:ARG:NH2	2.01	0.74
7:18:60:GLU:N	7:18:60:GLU:OE2	2.20	0.74
32:R1:1063:G:H3’	32:R1:1064:C:H4’	1.70	0.74
32:R1:481:G:O2’	32:R1:506:G:N2	2.20	0.74
32:R1:1529:G:H1	32:R1:1542:U:H3	1.35	0.73
28:6:103:ASN:ND2	28:6:113:ASP:OD1	2.20	0.73
28:6:174:LYS:HG3	32:R1:2529:G:H4’	1.70	0.73
34:R3:998:C:N3	34:R3:1043:G:N1	2.36	0.73
1:1:31:LYS:NZ	1:1:178:VAL:O	2.22	0.73
11:21:45:GLU:OE2	11:21:45:GLU:N	2.22	0.73
11:21:80:ARG:NH2	32:R1:572:A:OP2	2.22	0.73
34:R3:1137:C:O2’	34:R3:1138:G:N2	2.23	0.72
32:R1:1521:G:H3’	32:R1:1522:A:H5”	1.71	0.72
32:R1:2115:G:H21	32:R1:2119:A:H62	1.38	0.72
34:R3:76:G:H1	34:R3:93:U:H3	1.37	0.72
9:2:216:ARG:NH2	32:R1:781:A:OP1	2.23	0.71
32:R1:475:C:O2	32:R1:479:A:N6	2.22	0.71
1:1:59:VAL:H	1:1:165:ASN:HD21	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:883:G:O6	32:R1:893:C:N4	2.24	0.71
28:6:32:LEU:HB3	28:6:74:MET:HE2	1.73	0.70
32:R1:284:U:O2	32:R1:356:G:N2	2.24	0.70
32:R1:2682:A:H61	32:R1:2728:U:H1'	1.56	0.70
29:9:62:LEU:O	29:9:66:ASN:ND2	2.23	0.70
19:3:59:ARG:NH2	32:R1:2831:G:OP2	2.23	0.70
34:R3:84:U:O2'	34:R3:85:U:O2	2.09	0.70
29:9:27:ARG:NH1	32:R1:2092:U:OP2	2.25	0.70
32:R1:284:U:H3	32:R1:356:G:H1	1.37	0.70
12:22:6:LYS:HB3	32:R1:494:G:H4'	1.74	0.70
32:R1:890:C:H2'	32:R1:891:G:H4'	1.73	0.69
34:R3:842:U:H5"	34:R3:843:U:H4'	1.72	0.69
30:H:322:TYR:OH	30:H:356:LYS:NZ	2.24	0.69
32:R1:2126:A:H62	32:R1:2163:A:H4'	1.57	0.69
34:R3:1238:A:OP1	34:R3:1335:U:O2'	2.09	0.69
19:3:180:VAL:HG22	19:3:187:LEU:HD12	1.74	0.69
32:R1:962:G:H21	32:R1:2250:G:H1	1.38	0.69
34:R3:505:G:H5'	34:R3:534:U:H2'	1.75	0.69
5:16:75:GLU:HB2	5:16:90:GLU:HG3	1.75	0.69
32:R1:1900:A:H1'	32:R1:1970:A:H2'	1.75	0.69
32:R1:2794:C:O2	32:R1:2802:G:N2	2.14	0.69
9:2:270:ARG:NH2	32:R1:1798:U:OP2	2.26	0.68
34:R3:687:A:N6	34:R3:703:G:O2'	2.25	0.68
32:R1:745:G:O2'	32:R1:748:G:O2'	2.11	0.68
29:9:133:GLN:NE2	29:9:135:HIS:O	2.26	0.68
30:H:192:LEU:HB3	30:H:212:ILE:HD12	1.75	0.68
34:R3:509:A:H8	34:R3:543:U:O2'	1.74	0.68
11:21:37:GLU:N	11:21:37:GLU:OE1	2.27	0.68
32:R1:1597:A:H5"	32:R1:1598:A:H5'	1.76	0.68
30:H:11:ARG:NH1	30:H:42:THR:OG1	2.26	0.68
30:H:6:SER:H	30:H:21:THR:HG22	1.59	0.68
12:22:34:ASP:OD2	21:32:36:LYS:NZ	2.27	0.68
35:T:47:U:O2'	35:T:50:U:OP1	2.11	0.68
7:18:24:THR:HG22	7:18:42:PRO:HD3	1.75	0.67
32:R1:2126:A:O2'	32:R1:2173:A:N1	2.25	0.67
32:R1:2794:C:N3	32:R1:2802:G:N1	2.29	0.67
27:5:45:ASP:HB3	27:5:48:LEU:HB3	1.76	0.67
30:H:254:GLU:OE1	30:H:254:GLU:N	2.25	0.67
32:R1:848:C:H2'	32:R1:849:A:H8	1.60	0.67
34:R3:971:G:OP2	34:R3:1231:G:N2	2.26	0.67
34:R3:1356:G:H2'	34:R3:1357:A:C8	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:17:22:ARG:HG3	6:17:70:THR:HA	1.76	0.67
30:H:394:PRO:HD3	30:H:427:GLU:HB2	1.75	0.67
32:R1:140:C:OP2	32:R1:141:G:N2	2.26	0.67
9:2:13:ARG:NH2	32:R1:1693:U:O2'	2.27	0.67
9:2:141:HIS:ND1	9:2:192:GLY:O	2.26	0.67
32:R1:1055:G:O6	32:R1:1104:C:N4	2.27	0.67
32:R1:1090:A:H2'	32:R1:1091:G:H8	1.59	0.67
32:R1:306:U:H3	32:R1:310:A:H62	1.42	0.66
5:16:20:LEU:HD13	15:25:81:PRO:HG2	1.76	0.66
8:19:3:ILE:HD11	19:3:186:LEU:HD21	1.78	0.66
34:R3:1054:C:O2	34:R3:1196:A:N6	2.28	0.66
26:4:5:LEU:HD12	26:4:10:SER:HB2	1.76	0.66
19:3:2:ILE:HG13	19:3:3:GLY:N	2.09	0.66
10:20:87:VAL:HG13	11:21:49:ILE:HG21	1.77	0.66
24:35:7:ARG:NH1	32:R1:243:U:OP2	2.29	0.66
27:5:135:ILE:HG22	27:5:140:ILE:HG21	1.76	0.66
32:R1:1536:C:O2'	32:R1:1537:G:N2	2.29	0.66
13:23:46:ALA:O	13:23:50:LEU:HB2	1.96	0.66
6:17:106:ASP:OD2	32:R1:1649:G:O2'	2.13	0.65
32:R1:1779:U:OP2	32:R1:1784:A:N6	2.30	0.65
3:14:2:ILE:CD1	3:14:6:THR:HG21	2.26	0.65
29:9:51:ARG:HG2	29:9:55:GLU:HB2	1.79	0.65
32:R1:2124:G:H2'	32:R1:2125:G:O4'	1.96	0.65
3:14:70:ARG:NH2	32:R1:2683:C:O2	2.29	0.65
1:1:168:ASN:ND2	32:R1:2178:C:O2'	2.30	0.65
25:36:13:ASN:HD22	25:36:29:ALA:HB2	1.62	0.65
30:H:1:MET:H1	30:H:26:PRO:HD3	1.62	0.65
32:R1:1044:C:O2'	32:R1:1111:A:N6	2.30	0.65
30:H:372:ALA:HB3	30:H:375:ILE:HG13	1.80	0.64
32:R1:882:G:H21	32:R1:896:A:H62	1.45	0.64
32:R1:1478:G:H1	32:R1:1513:U:H3	1.45	0.64
34:R3:1277:C:H2'	34:R3:1279:G:H21	1.60	0.64
3:14:2:ILE:HD13	3:14:6:THR:HG21	1.79	0.64
16:27:43:THR:H	32:R1:2331:G:H4'	1.60	0.64
32:R1:1432:G:H2'	32:R1:1433:A:C8	2.31	0.64
30:H:405:GLU:HG3	30:H:406:LEU:H	1.62	0.64
29:9:80:ILE:HD12	29:9:146:VAL:HG22	1.78	0.64
32:R1:1509:A:H2'	32:R1:1510:G:H8	1.61	0.64
32:R1:1073:A:H4'	32:R1:2474:U:H4'	1.79	0.64
32:R1:1:G:H2'	32:R1:2:G:H8	1.62	0.64
34:R3:222:C:H2'	34:R3:223:A:H8	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:15:85:VAL:HG11	4:15:90:VAL:HG22	1.80	0.64
32:R1:918:A:N3	33:R2:80:U:O2'	2.30	0.64
24:35:38:LYS:NZ	32:R1:2365:G:O6	2.32	0.64
32:R1:1936:A:H2	32:R1:1943:U:H3	1.45	0.63
2:13:13:ARG:NH2	2:13:49:ASP:O	2.30	0.63
32:R1:270:A:N1	32:R1:369:U:O2'	2.31	0.63
32:R1:1482:G:H2'	32:R1:1483:G:H8	1.62	0.63
20:30:39:ASP:OD2	20:30:44:ARG:NH1	2.31	0.63
30:H:220:GLU:OE2	30:H:238:ARG:NH1	2.31	0.63
34:R3:714:G:H2'	34:R3:715:A:C8	2.33	0.63
12:22:5:ALA:O	32:R1:494:G:O2'	2.17	0.63
19:3:38:LYS:NZ	19:3:81:GLU:OE1	2.32	0.63
32:R1:1087:G:H8	32:R1:1088:A:H4'	1.64	0.63
13:23:11:LEU:O	18:29:29:ARG:NH2	2.29	0.62
32:R1:2134:A:N7	32:R1:2157:G:O2'	2.25	0.62
33:R2:30:C:H1'	33:R2:57:A:H61	1.63	0.62
34:R3:203:G:H1'	34:R3:465:A:H61	1.62	0.62
34:R3:1222:G:OP2	34:R3:1322:C:N4	2.31	0.62
34:R3:1218:C:H2'	34:R3:1219:A:C8	2.34	0.62
28:6:12:ALA:O	28:6:14:VAL:N	2.31	0.62
30:H:341:ILE:HG22	30:H:496:ASP:HB2	1.81	0.62
32:R1:1721:G:O2'	32:R1:1739:A:N6	2.32	0.62
32:R1:2137:U:H2'	32:R1:2138:G:H8	1.64	0.62
14:24:27:VAL:HG13	14:24:33:VAL:HG12	1.82	0.62
13:23:38:ALA:HB1	13:23:43:ILE:HD11	1.80	0.62
17:28:11:PRO:HB3	17:28:29:LEU:HD23	1.81	0.62
26:4:145:ASP:HB3	26:4:184:ASP:HB2	1.81	0.62
30:H:98:LEU:HB2	30:H:113:ILE:HG21	1.81	0.62
34:R3:380:G:N2	34:R3:383:A:OP2	2.31	0.62
32:R1:141:G:N2	32:R1:141:G:OP2	2.32	0.62
32:R1:704:G:H2'	32:R1:726:G:H22	1.63	0.62
7:18:25:ARG:NH2	33:R2:8:C:O3'	2.33	0.62
32:R1:1645:G:H5"	32:R1:1646:C:H5'	1.81	0.62
17:28:5:GLN:NE2	17:28:75:GLU:OE2	2.27	0.62
4:15:20:GLY:HA2	4:15:28:GLY:HA2	1.82	0.61
34:R3:1218:C:H2'	34:R3:1219:A:H8	1.64	0.61
12:22:59:GLU:OE2	12:22:66:ILE:HD13	1.99	0.61
28:6:89:VAL:HG11	28:6:162:ARG:HH21	1.64	0.61
30:H:139:SER:OG	30:H:141:GLU:OE1	2.16	0.61
34:R3:1266:G:N2	34:R3:1269:A:OP2	2.19	0.61
26:4:123:LYS:NZ	26:4:125:SER:OG	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:42:ALA:HA	27:5:45:ASP:HB2	1.83	0.61
30:H:36:ASN:ND2	30:H:460:HIS:O	2.32	0.61
30:H:40:LYS:HB3	30:H:202:ILE:HD13	1.82	0.61
6:17:17:ARG:NH2	32:R1:2002:G:OP1	2.34	0.61
7:18:100:HIS:NE2	33:R2:37:C:O2	2.26	0.61
9:2:143:VAL:HB	9:2:153:LEU:HB2	1.81	0.61
34:R3:1154:G:H2'	34:R3:1155:A:H8	1.64	0.61
1:1:41:SER:HA	1:1:177:LYS:HA	1.82	0.61
9:2:60:ALA:O	9:2:62:ARG:NH1	2.34	0.61
11:21:14:VAL:HG21	11:21:98:ILE:HG13	1.83	0.61
27:5:147:ARG:HD2	27:5:148:VAL:H	1.66	0.61
32:R1:704:G:H1'	32:R1:727:A:H61	1.65	0.61
26:4:45:ALA:HA	26:4:87:ALA:O	2.01	0.61
34:R3:674:G:H2'	34:R3:675:A:H8	1.66	0.61
9:2:1:ALA:N	9:2:198:GLU:OE1	2.34	0.61
32:R1:1019:U:H3	32:R1:1142:A:H62	1.48	0.60
34:R3:200:G:H2'	34:R3:201:G:H8	1.66	0.60
8:19:55:HIS:HA	19:3:13:ARG:HH21	1.65	0.60
32:R1:45:G:H5"	32:R1:46:G:H5'	1.82	0.60
32:R1:1071:G:H1'	32:R1:1089:A:H2'	1.83	0.60
32:R1:1417:C:HO2'	32:R1:1587:G:HO2'	1.48	0.60
13:23:54:GLU:OE1	13:23:88:LYS:NZ	2.33	0.60
16:27:14:ARG:NH1	32:R1:2279:G:N7	2.45	0.60
23:34:25:LYS:NZ	23:34:26:ASN:OD1	2.34	0.60
33:R2:31:C:H1'	33:R2:53:A:H61	1.67	0.60
34:R3:1004:A:H2'	34:R3:1005:A:C8	2.36	0.60
34:R3:1241:G:H2'	34:R3:1242:G:H8	1.67	0.60
2:13:68:LYS:NZ	32:R1:1022:G:O6	2.28	0.60
18:29:10:SER:O	18:29:14:LEU:HD12	2.00	0.60
28:6:138:GLN:OE1	32:R1:2759:G:N2	2.31	0.60
30:H:319:SER:HB3	30:H:366:SER:HB3	1.83	0.60
30:H:341:ILE:HG13	30:H:481:VAL:HG13	1.83	0.60
10:20:91:ARG:NH2	32:R1:1153:C:OP1	2.30	0.60
11:21:68:ARG:NH1	32:R1:1223:G:OP1	2.34	0.60
3:14:109:SER:O	3:14:111:LYS:N	2.35	0.60
17:28:9:LYS:NZ	32:R1:397:U:OP2	2.32	0.60
27:5:118:ALA:O	27:5:166:ARG:NE	2.32	0.60
28:6:37:ASN:ND2	28:6:63:GLN:OE1	2.34	0.60
32:R1:2788:C:O2'	32:R1:2809:A:N3	2.34	0.60
2:13:91:GLU:HG3	2:13:95:ARG:HH21	1.67	0.59
33:R2:66:A:OP2	33:R2:108:A:N6	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:31:GLU:OE2	28:6:33:THR:OG1	2.19	0.59
32:R1:1073:A:N6	32:R1:1075:C:O2	2.36	0.59
35:T:54:5MU:OP2	35:T:54:5MU:H4'	2.01	0.59
30:H:327:ILE:HG22	30:H:328:LEU:HG	1.84	0.59
32:R1:2505:G:HO2'	32:R1:2576:G:H1	1.50	0.59
34:R3:1077:G:N2	34:R3:1080:A:OP2	2.25	0.59
25:36:19:ARG:NE	32:R1:2756:U:OP2	2.33	0.59
32:R1:1912:A:HO2'	34:R3:1494:G:HO2'	1.51	0.59
33:R2:5:U:OP1	33:R2:61:G:O2'	2.20	0.59
35:T:20:H2U:O2'	35:T:21:A:O5'	2.12	0.59
30:H:461:LEU:O	30:H:466:ARG:NH1	2.36	0.59
32:R1:1079:C:H2'	32:R1:1080:A:C8	2.38	0.59
34:R3:458:U:O2	34:R3:474:G:N2	2.35	0.59
19:3:1:MET:HG2	19:3:205:PRO:HG2	1.83	0.59
28:6:35:THR:HG22	28:6:36:LEU:H	1.68	0.59
7:18:30:ARG:NH2	33:R2:48:U:OP1	2.26	0.59
32:R1:177:G:H3'	32:R1:178:G:H8	1.68	0.59
7:18:36:TYR:OH	33:R2:28:C:OP1	2.21	0.58
27:5:59:ILE:O	27:5:101:ARG:NH2	2.36	0.58
32:R1:2326:C:O2'	32:R1:2327:A:OP1	2.20	0.58
32:R1:2848:G:O2'	32:R1:2868:A:N6	2.37	0.58
18:29:58:ASN:ND2	32:R1:72:U:O4	2.36	0.58
32:R1:2131:U:H5'	32:R1:2132:U:H5"	1.85	0.58
32:R1:2804:U:H2'	32:R1:2805:C:C6	2.38	0.58
29:9:80:ILE:HD13	29:9:94:ILE:HD12	1.86	0.58
32:R1:859:G:O2'	32:R1:916:G:O6	2.16	0.58
34:R3:415:A:H61	34:R3:427:U:H3	1.49	0.58
7:18:68:LYS:NZ	33:R2:49:C:O3'	2.35	0.58
34:R3:1002:G:H2'	34:R3:1003:G:C8	2.39	0.58
9:2:144:GLU:HB2	9:2:187:CYS:HB3	1.86	0.58
32:R1:476:G:N1	32:R1:479:A:OP2	2.36	0.58
1:1:214:ILE:HG22	1:1:224:VAL:HB	1.85	0.58
9:2:167:ASP:OD1	9:2:167:ASP:N	2.36	0.58
34:R3:126:G:OP1	34:R3:605:U:O2'	2.16	0.58
34:R3:422:C:O2'	34:R3:423:G:N2	2.37	0.58
30:H:251:SER:O	30:H:254:GLU:OE2	2.21	0.58
32:R1:1056:G:N7	32:R1:1102:C:N4	2.52	0.58
15:25:32:GLY:HA3	15:25:93:ARG:HB2	1.84	0.57
32:R1:2857:G:N2	32:R1:2860:A:OP2	2.35	0.57
34:R3:938:A:N3	34:R3:1376:U:O2'	2.32	0.57
6:17:86:ARG:NE	6:17:117:ASP:OD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:856:G:H2'	32:R1:857:G:C8	2.39	0.57
32:R1:1667:G:O2'	32:R1:1991:U:O4	2.13	0.57
34:R3:842:U:H4'	34:R3:846:G:C5	2.39	0.57
18:29:47:ARG:NH2	32:R1:61:C:OP2	2.37	0.57
27:5:12:VAL:HG12	27:5:27:VAL:HG11	1.87	0.57
28:6:18:ILE:HG13	28:6:23:ILE:HD13	1.87	0.57
34:R3:552:U:H2'	34:R3:553:A:H8	1.68	0.57
19:3:77:ARG:NH1	19:3:200:ASP:OD1	2.37	0.57
30:H:351:LYS:HG2	30:H:500:VAL:HG21	1.86	0.57
32:R1:1103:A:H5"	32:R1:1104:C:C5	2.40	0.57
32:R1:1447:C:O2'	32:R1:1544:A:N3	2.37	0.57
27:5:3:LEU:HB3	27:5:172:PHE:HE1	1.70	0.57
12:22:87:PRO:HB3	32:R1:1614:A:C6	2.40	0.57
26:4:44:ARG:NH2	32:R1:1248:G:OP1	2.37	0.57
34:R3:1306:A:N6	34:R3:1331:G:O2'	2.38	0.57
9:2:129:LEU:HD12	9:2:133:ASN:HB2	1.87	0.57
30:H:244:GLN:O	30:H:248:MET:HG3	2.04	0.57
32:R1:1414:C:H2'	32:R1:1415:U:C6	2.40	0.57
32:R1:2812:G:H2'	32:R1:2813:A:C8	2.39	0.57
9:2:120:ASP:HB3	29:9:91:PHE:HE2	1.69	0.57
28:6:108:PHE:O	32:R1:2666:C:N4	2.36	0.57
32:R1:1316:U:H2'	32:R1:1317:G:H8	1.70	0.57
32:R1:1754:A:N1	32:R1:2716:C:O2'	2.35	0.57
34:R3:996:A:H2'	34:R3:997:U:C6	2.40	0.57
35:T:8:4SU:O2	35:T:8:4SU:O2'	2.20	0.57
35:T:59:A:O2'	35:T:60:U:O4'	2.23	0.57
27:5:10:GLU:OE1	27:5:10:GLU:N	2.37	0.56
3:14:105:ARG:NH1	8:19:33:GLU:OE2	2.38	0.56
26:4:118:LEU:HA	26:4:186:VAL:O	2.05	0.56
30:H:3:VAL:HG22	30:H:23:THR:HG22	1.88	0.56
32:R1:554:U:H2'	32:R1:555:G:O4'	2.05	0.56
32:R1:555:G:HO2'	32:R1:556:A:H8	1.52	0.56
34:R3:222:C:H2'	34:R3:223:A:C8	2.41	0.56
34:R3:674:G:H2'	34:R3:675:A:C8	2.40	0.56
28:6:40:VAL:O	28:6:54:ARG:NH2	2.37	0.56
30:H:24:ILE:HG12	30:H:30:VAL:HG21	1.87	0.56
18:29:13:GLU:HB3	18:29:57:LEU:HD11	1.88	0.56
5:16:106:ASP:OD2	5:16:106:ASP:C	2.44	0.56
32:R1:1387:A:H5'	32:R1:1469:A:H1'	1.87	0.56
29:9:9:VAL:HB	29:9:12:LEU:O	2.05	0.56
29:9:135:HIS:H	29:9:138:VAL:HB	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1469:A:H2'	32:R1:1470:A:C8	2.40	0.56
32:R1:1509:A:H2'	32:R1:1510:G:C8	2.39	0.56
29:9:69:ALA:O	29:9:73:ASN:ND2	2.39	0.56
34:R3:602:A:H2'	34:R3:603:U:H6	1.71	0.56
32:R1:1056:G:N3	32:R1:1086:A:H1'	2.20	0.55
32:R1:2637:U:H2'	32:R1:2638:G:O4'	2.05	0.55
16:27:29:GLU:OE2	32:R1:922:C:O2'	2.21	0.55
34:R3:1352:C:H2'	34:R3:1353:G:C8	2.42	0.55
1:1:12:ARG:NH2	32:R1:2176:A:OP1	2.29	0.55
27:5:72:SER:OG	27:5:80:GLN:N	2.39	0.55
30:H:2:ILE:HG12	30:H:24:ILE:HB	1.88	0.55
32:R1:1063:G:N2	32:R1:1070:A:OP1	2.39	0.55
32:R1:1288:G:OP2	32:R1:1288:G:N2	2.31	0.55
34:R3:1305:G:O2'	34:R3:1306:A:O4'	2.24	0.55
11:21:51:VAL:HG23	11:21:52:PRO:CD	2.37	0.55
9:2:257:ARG:NH1	9:2:263:ASP:OD1	2.37	0.55
30:H:256:VAL:HG22	30:H:286:MET:HE3	1.88	0.55
32:R1:1055:G:H2'	32:R1:1056:G:C8	2.42	0.55
32:R1:1077:A:N6	32:R1:1089:A:OP2	2.39	0.55
6:17:33:ILE:HG13	6:17:114:GLU:HB3	1.87	0.55
12:22:59:GLU:HA	12:22:64:ALA:HA	1.89	0.55
12:22:74:ILE:HD12	12:22:105:VAL:HG22	1.89	0.55
14:24:71:ILE:HD12	14:24:82:VAL:HG21	1.89	0.55
18:29:13:GLU:HA	18:29:16:THR:HG22	1.87	0.55
30:H:192:LEU:HD12	30:H:212:ILE:CD1	2.36	0.55
32:R1:1386:C:H2'	32:R1:1387:A:H8	1.72	0.55
34:R3:1412:C:H2'	34:R3:1413:A:C8	2.41	0.55
12:22:109:ASP:O	12:22:110:ARG:NE	2.36	0.55
15:25:6:ALA:HB1	15:25:40:ILE:HG23	1.89	0.55
32:R1:1173:U:H2'	32:R1:1174:U:O4'	2.06	0.55
32:R1:2595:G:N2	32:R1:2598:A:OP2	2.28	0.55
34:R3:1294:G:H2'	34:R3:1295:U:C6	2.42	0.55
14:24:51:LEU:O	14:24:53:GLN:NE2	2.40	0.55
27:5:62:GLN:HE21	27:5:94:ARG:NH1	2.05	0.55
32:R1:354:A:H2'	32:R1:355:U:O4'	2.07	0.55
32:R1:851:C:H2'	32:R1:852:U:C6	2.42	0.55
32:R1:2122:U:O4	32:R1:2176:A:N6	2.40	0.55
32:R1:2128:G:H2'	32:R1:2129:C:C6	2.42	0.55
32:R1:2391:G:O2'	32:R1:2429:G:N2	2.40	0.54
28:6:15:ASP:HB3	28:6:26:LYS:HE2	1.89	0.54
32:R1:1096:A:OP2	32:R1:1096:A:H8	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R2:51:G:H2'	33:R2:52:A:O4'	2.06	0.54
2:13:17:VAL:HG23	2:13:137:PRO:HB2	1.88	0.54
14:24:42:LYS:HD2	14:24:59:GLU:HG2	1.88	0.54
26:4:143:LEU:HD13	26:4:146:VAL:HG11	1.89	0.54
32:R1:955:U:H5	32:R1:962:G:H1	1.56	0.54
32:R1:2061:G:N2	32:R1:2062:A:O2'	2.40	0.54
32:R1:2324:U:H3'	32:R1:2325:G:H5'	1.90	0.54
3:14:58:LEU:HD11	3:14:86:LEU:HD12	1.90	0.54
32:R1:84:A:N1	32:R1:98:G:O2'	2.34	0.54
34:R3:673:A:H2'	34:R3:674:G:C8	2.42	0.54
15:25:24:ASN:ND2	15:25:45:ASP:OD2	2.40	0.54
26:4:5:LEU:HD23	26:4:120:VAL:HG12	1.90	0.54
32:R1:2328:A:H2'	32:R1:2329:U:C6	2.42	0.54
9:2:259:ASN:OD1	9:2:262:THR:OG1	2.19	0.54
26:4:176:ASP:OD1	26:4:176:ASP:N	2.39	0.54
32:R1:878:A:N6	32:R1:899:A:O2'	2.41	0.54
32:R1:1912:A:O2'	34:R3:1494:G:O2'	2.23	0.54
7:18:62:LEU:HD22	7:18:65:THR:HG23	1.88	0.54
32:R1:1045:C:N4	32:R1:1111:A:OP2	2.41	0.54
34:R3:337:G:H2'	34:R3:338:A:C8	2.43	0.54
34:R3:652:U:O4	34:R3:752:G:O2'	2.21	0.54
29:9:9:VAL:HG11	29:9:12:LEU:HB3	1.90	0.54
32:R1:1432:G:H2'	32:R1:1433:A:H8	1.73	0.54
32:R1:2125:G:N3	32:R1:2173:A:N6	2.55	0.54
32:R1:2554:U:H2'	32:R1:2555:U:C6	2.43	0.54
34:R3:409:U:H3	34:R3:433:G:H1	1.55	0.54
16:27:37:ILE:HG22	16:27:38:VAL:HG23	1.90	0.54
27:5:33:ILE:HD12	27:5:155:ILE:HG12	1.89	0.54
30:H:321:GLY:HA2	30:H:326:ILE:HA	1.90	0.54
32:R1:1095:A:H2'	32:R1:1096:A:C8	2.43	0.54
32:R1:1746:A:H2'	32:R1:1747:U:C6	2.43	0.54
32:R1:2457:U:H5	32:R1:2494:G:H1	1.55	0.54
34:R3:811:C:O2'	34:R3:901:A:N1	2.41	0.54
2:13:30:THR:HG21	32:R1:1005:C:O2'	2.07	0.53
6:17:1:MET:N	32:R1:1654:A:OP2	2.35	0.53
10:20:49:ARG:NH1	32:R1:993:G:OP1	2.35	0.53
10:20:87:VAL:HA	11:21:49:ILE:HD13	1.89	0.53
21:32:53:VAL:HG23	21:32:54:ILE:H	1.73	0.53
32:R1:1019:U:OP1	32:R1:1035:U:O2'	2.19	0.53
32:R1:1847:G:O2'	32:R1:1848:A:H8	1.92	0.53
32:R1:2106:U:H2'	32:R1:2107:G:C8	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:672:U:H2'	34:R3:673:A:H8	1.73	0.53
34:R3:1071:C:H2'	34:R3:1072:G:H8	1.73	0.53
23:34:4:THR:HG22	32:R1:687:C:H1'	1.90	0.53
32:R1:827:U:O2'	32:R1:2068:U:N3	2.41	0.53
32:R1:2812:G:H2'	32:R1:2813:A:H8	1.74	0.53
27:5:28:PRO:HB3	27:5:159:ALA:HB2	1.91	0.53
32:R1:140:C:H2'	32:R1:141:G:H5'	1.90	0.53
32:R1:645:C:H2'	32:R1:647:G:N7	2.23	0.53
35:T:20:H2U:HO2'	35:T:21:A:P	2.31	0.53
1:1:30:LEU:HA	1:1:33:LEU:HG	1.90	0.53
32:R1:2112:G:O2'	32:R1:2115:G:N2	2.42	0.53
34:R3:56:U:H2'	34:R3:57:G:H8	1.73	0.53
34:R3:296:U:O2'	34:R3:556:C:O2	2.25	0.53
15:25:30:ILE:HD11	15:25:63:ILE:HD12	1.90	0.53
32:R1:1236:G:O2'	32:R1:1237:A:O5'	2.27	0.53
32:R1:1591:A:H2'	32:R1:1592:C:C6	2.44	0.53
34:R3:203:G:N2	34:R3:204:G:O6	2.39	0.53
34:R3:620:C:O2'	34:R3:621:A:O5'	2.27	0.53
34:R3:944:G:N1	34:R3:1338:G:OP2	2.34	0.53
34:R3:1287:A:H2	34:R3:1353:G:H1'	1.74	0.53
30:H:84:VAL:HG21	30:H:133:LEU:HD11	1.91	0.53
32:R1:1720:U:H2'	32:R1:1721:G:O4'	2.09	0.53
32:R1:2025:C:H2'	32:R1:2026:U:C6	2.44	0.53
32:R1:2115:G:H21	32:R1:2119:A:N6	2.05	0.53
34:R3:588:G:N2	34:R3:653:U:O4	2.33	0.53
32:R1:1869:G:N2	32:R1:1872:A:OP2	2.26	0.53
34:R3:998:C:N4	34:R3:1043:G:O6	2.42	0.53
32:R1:372:G:H1'	32:R1:373:U:H5	1.74	0.53
32:R1:1056:G:H1'	32:R1:1086:A:H8	1.73	0.53
34:R3:662:U:O2'	34:R3:836:G:OP1	2.26	0.53
3:14:105:ARG:HD2	3:14:108:ARG:HH21	1.74	0.53
15:25:80:HIS:ND1	15:25:83:LYS:HB2	2.24	0.53
26:4:143:LEU:HB3	26:4:146:VAL:HG11	1.91	0.53
33:R2:1:U:H3	33:R2:119:A:H2	1.57	0.53
34:R3:1355:G:H2'	34:R3:1356:G:H8	1.74	0.53
19:3:149:ASN:OD1	19:3:150:GLN:N	2.31	0.52
26:4:154:ASP:OD1	26:4:154:ASP:N	2.42	0.52
29:9:50:ARG:HH12	29:9:54:LEU:HD13	1.74	0.52
34:R3:1306:A:H1'	34:R3:1332:A:N1	2.25	0.52
24:35:15:LYS:NZ	24:35:19:GLY:O	2.42	0.52
32:R1:2031:A:N3	32:R1:2455:G:O2'	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:56:U:H2'	34:R3:57:G:C8	2.44	0.52
11:21:57:GLY:HA2	11:21:102:SER:HB3	1.92	0.52
34:R3:1297:G:H4'	34:R3:1298:U:O5'	2.09	0.52
4:15:82:LEU:HD22	4:15:90:VAL:HG21	1.90	0.52
30:H:147:VAL:HA	30:H:150:PHE:HD2	1.74	0.52
12:22:4:ILE:HG12	12:22:106:VAL:HG22	1.91	0.52
14:24:32:LYS:HB3	14:24:63:ALA:HB1	1.91	0.52
30:H:393:SER:O	30:H:397:HIS:HB2	2.10	0.52
30:H:501:HIS:ND1	30:H:502:ASP:OD1	2.43	0.52
32:R1:139:U:HO2'	32:R1:140:C:H6	1.57	0.52
34:R3:602:A:H2'	34:R3:603:U:C6	2.45	0.52
34:R3:1020:G:H2'	34:R3:1021:A:C8	2.45	0.52
1:1:175:ILE:HD12	1:1:189:LEU:HG	1.91	0.52
11:21:6:GLN:HB3	11:21:11:GLN:HG2	1.90	0.52
32:R1:918:A:O2'	33:R2:96:G:N2	2.43	0.52
32:R1:1090:A:H2'	32:R1:1091:G:C8	2.42	0.52
32:R1:2127:G:H2'	32:R1:2128:G:C8	2.45	0.52
32:R1:2375:G:N2	32:R1:2378:A:OP2	2.33	0.52
3:14:66:LYS:HD2	3:14:81:GLY:H	1.75	0.52
5:16:53:MET:HG2	5:16:120:ALA:HB2	1.90	0.52
13:23:33:LYS:HG3	13:23:80:TRP:CE3	2.45	0.52
32:R1:2292:U:H2'	32:R1:2293:G:H8	1.75	0.52
35:T:11:G:H2'	35:T:12:C:O4'	2.10	0.52
10:20:4:LYS:NZ	32:R1:447:A:OP1	2.40	0.52
32:R1:1591:A:H2'	32:R1:1592:C:H6	1.75	0.52
32:R1:1779:U:H5	32:R1:1784:A:N7	2.07	0.52
32:R1:1802:A:H2'	32:R1:1803:A:C8	2.44	0.52
32:R1:2469:A:N6	32:R1:2481:G:O2'	2.43	0.52
34:R3:1010:U:H3	34:R3:1019:A:H2	1.58	0.52
34:R3:1251:A:H2'	34:R3:1252:A:C8	2.45	0.52
1:1:53:ARG:HH21	30:H:167:ARG:HH21	1.56	0.52
7:18:27:VAL:HA	7:18:93:ASP:HB3	1.92	0.52
9:2:179:GLU:OE2	9:2:269:ARG:NH1	2.43	0.51
16:27:64:ASP:N	16:27:64:ASP:OD1	2.42	0.51
30:H:489:LEU:O	30:H:493:THR:OG1	2.25	0.51
32:R1:227:A:HO2'	32:R1:228:C:P	2.33	0.51
32:R1:2258:C:O2'	32:R1:2427:C:OP2	2.25	0.51
26:4:45:ALA:HB2	26:4:89:PRO:HD3	1.90	0.51
30:H:252:GLN:O	30:H:256:VAL:HG23	2.10	0.51
32:R1:645:C:H2'	32:R1:647:G:C8	2.45	0.51
32:R1:2134:A:C5	32:R1:2158:A:H5'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:423:G:H22	34:R3:424:G:H21	1.56	0.51
12:22:83:LYS:HG2	12:22:95:ARG:HD3	1.92	0.51
34:R3:745:G:H2'	34:R3:746:A:H8	1.76	0.51
34:R3:1157:A:N7	34:R3:1180:A:N6	2.59	0.51
18:29:3:ALA:O	18:29:7:ARG:HG2	2.10	0.51
32:R1:2121:G:N1	32:R1:2178:C:O2	2.43	0.51
21:32:4:GLN:HE22	32:R1:2054:A:H2'	1.75	0.51
27:5:65:LEU:HD13	33:R2:41:G:H2'	1.92	0.51
32:R1:1426:G:O2'	32:R1:1572:A:N6	2.43	0.51
32:R1:2106:U:H2'	32:R1:2107:G:H8	1.75	0.51
32:R1:2190:G:H2'	32:R1:2191:A:C8	2.46	0.51
32:R1:2532:G:N2	32:R1:2663:G:O2'	2.43	0.51
34:R3:426:U:H2'	34:R3:427:U:C6	2.46	0.51
34:R3:1034:G:H2'	34:R3:1035:A:O4'	2.11	0.51
2:13:134:ALA:O	32:R1:2898:U:O2'	2.23	0.51
4:15:103:ILE:HG23	4:15:104:GLN:HG2	1.92	0.51
27:5:7:TYR:HA	27:5:11:VAL:HB	1.93	0.51
30:H:191:TRP:CD1	30:H:192:LEU:HD23	2.46	0.51
30:H:192:LEU:HD12	30:H:212:ILE:HD11	1.92	0.51
32:R1:1592:C:H2'	32:R1:1593:A:H8	1.75	0.51
32:R1:2319:G:HO2'	32:R1:2320:U:H6	1.59	0.51
33:R2:32:U:C2	33:R2:33:G:C8	2.98	0.51
32:R1:1:G:H2'	32:R1:2:G:C8	2.44	0.51
32:R1:1682:G:H2'	32:R1:1683:U:C6	2.45	0.51
11:21:52:PRO:HB2	11:21:53:PHE:CD2	2.45	0.51
30:H:157:ARG:HH12	30:H:347:ASN:HD22	1.58	0.51
3:14:68:GLY:HA3	3:14:78:ARG:HA	1.93	0.51
10:20:47:ARG:NH1	32:R1:560:C:O2'	2.44	0.51
32:R1:2101:A:H2'	32:R1:2102:G:H8	1.76	0.51
32:R1:2327:A:H2'	32:R1:2328:A:C8	2.46	0.51
24:35:3:ILE:HD11	32:R1:592:A:C2	2.45	0.51
32:R1:1064:C:H42	32:R1:1073:A:H2	1.59	0.51
32:R1:1538:G:H2'	32:R1:1539:U:C6	2.46	0.51
32:R1:2291:U:H2'	32:R1:2292:U:C6	2.45	0.51
30:H:65:GLN:N	30:H:169:ASP:OD2	2.32	0.50
30:H:320:ALA:HB2	30:H:357:LEU:HD22	1.93	0.50
32:R1:1405:U:H2'	32:R1:1406:U:C6	2.46	0.50
34:R3:417:G:H2'	34:R3:418:C:C6	2.47	0.50
27:5:51:ASN:OD1	27:5:149:ARG:NH2	2.44	0.50
33:R2:86:G:C6	33:R2:88:C:H1'	2.46	0.50
5:16:50:ARG:HD3	5:16:65:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1:MET:HG3	19:3:2:ILE:N	2.26	0.50
30:H:139:SER:OG	30:H:140:ASN:N	2.44	0.50
30:H:428:THR:HG22	30:H:429:ARG:H	1.76	0.50
32:R1:644:A:H2'	32:R1:645:C:O4'	2.11	0.50
34:R3:191:G:H2'	34:R3:192:A:H8	1.77	0.50
7:18:51:ALA:HB3	7:18:78:VAL:HB	1.93	0.50
29:9:18:GLN:HE21	29:9:44:ILE:HD11	1.76	0.50
32:R1:139:U:O2'	32:R1:140:C:H5'	2.12	0.50
32:R1:351:C:H2'	32:R1:352:A:H8	1.76	0.50
32:R1:2136:G:H1	32:R1:2156:G:H1'	1.76	0.50
21:32:15:ARG:NH2	32:R1:1264:A:OP1	2.36	0.50
32:R1:2861:U:H2'	32:R1:2862:G:H8	1.77	0.50
2:13:39:LYS:NZ	32:R1:1009:A:OP2	2.44	0.50
13:23:34:VAL:HG23	13:23:81:LYS:HB3	1.93	0.50
30:H:46:LEU:HB2	30:H:51:ILE:HD11	1.94	0.50
32:R1:2213:U:H5"	32:R1:2214:C:OP2	2.12	0.50
32:R1:2557:G:H2'	32:R1:2558:C:C6	2.46	0.50
34:R3:159:G:N2	34:R3:162:A:OP2	2.43	0.50
34:R3:321:A:H2'	34:R3:322:C:C6	2.47	0.50
29:9:116:ARG:HB2	29:9:131:SER:HB2	1.94	0.50
34:R3:859:G:H2'	34:R3:860:A:C8	2.47	0.50
34:R3:1016:A:HO2'	34:R3:1217:C:HO2'	1.56	0.50
3:14:69:VAL:HG11	3:14:104:THR:HG21	1.94	0.50
4:15:56:PRO:HG2	4:15:59:ARG:HB2	1.94	0.50
30:H:7:LEU:HD12	30:H:56:GLY:HA3	1.94	0.50
30:H:322:TYR:HE2	30:H:353:THR:HG22	1.76	0.50
32:R1:287:G:H2'	32:R1:288:U:C6	2.46	0.50
32:R1:1727:C:H2'	32:R1:1728:C:O4'	2.11	0.50
34:R3:422:C:HO2'	34:R3:423:G:N2	2.09	0.50
34:R3:728:A:H2'	34:R3:729:A:C8	2.47	0.50
27:5:39:VAL:HG21	27:5:49:LEU:HD13	1.94	0.50
30:H:149:ASP:OD1	30:H:150:PHE:N	2.37	0.50
32:R1:3:U:H2'	32:R1:4:U:C6	2.47	0.50
32:R1:639:U:H2'	32:R1:640:C:C6	2.47	0.50
32:R1:2115:G:O2'	32:R1:2166:U:O2	2.24	0.50
32:R1:2324:U:H3'	32:R1:2325:G:C5'	2.41	0.50
34:R3:984:C:H2'	34:R3:985:C:H6	1.76	0.50
34:R3:1028:C:H2'	34:R3:1029:U:H4'	1.94	0.50
21:32:25:THR:OG1	21:32:26:SER:N	2.43	0.49
26:4:5:LEU:HD22	26:4:122:GLU:HG2	1.93	0.49
32:R1:421:C:HO2'	32:R1:422:A:P	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2140:G:H2'	32:R1:2141:G:H8	1.75	0.49
32:R1:2243:U:H2'	32:R1:2244:U:C6	2.47	0.49
32:R1:2698:U:H2'	32:R1:2699:C:C6	2.46	0.49
34:R3:50:A:O2'	34:R3:360:G:N2	2.45	0.49
34:R3:746:A:H2'	34:R3:747:A:C8	2.47	0.49
34:R3:1028:C:O2'	34:R3:1030:U:O4	2.25	0.49
34:R3:367:U:H3	34:R3:393:A:H62	1.59	0.49
34:R3:1305:G:O2'	34:R3:1306:A:H8	1.94	0.49
17:28:71:ARG:NH1	17:28:77:TYR:OH	2.32	0.49
19:3:133:THR:HG21	32:R1:1993:U:H4'	1.95	0.49
32:R1:351:C:H2'	32:R1:352:A:C8	2.47	0.49
32:R1:882:G:N2	32:R1:894:U:O2	2.39	0.49
32:R1:1858:A:N6	32:R1:1884:G:O2'	2.43	0.49
32:R1:2847:U:H2'	32:R1:2848:G:O4'	2.12	0.49
34:R3:790:A:OP1	35:T:38:A:O2'	2.27	0.49
34:R3:1074:G:O2'	34:R3:1101:A:N1	2.33	0.49
34:R3:1183:U:O2'	34:R3:1184:G:OP1	2.28	0.49
3:14:1:MET:HG3	3:14:67:LYS:HD2	1.93	0.49
4:15:108:ALA:HB3	4:15:125:LEU:HD22	1.93	0.49
5:16:69:PRO:HA	5:16:94:ALA:HB2	1.94	0.49
29:9:99:ILE:HG12	29:9:130:VAL:HG21	1.93	0.49
30:H:435:GLU:OE2	57:H:602:ATP:O3'	2.20	0.49
32:R1:2804:U:H2'	32:R1:2805:C:H6	1.75	0.49
32:R1:2898:U:H2'	32:R1:2899:A:H8	1.77	0.49
34:R3:821:G:H2'	34:R3:822:U:C6	2.48	0.49
32:R1:848:C:H2'	32:R1:849:A:C8	2.43	0.49
32:R1:1511:G:H2'	32:R1:1512:C:C6	2.47	0.49
32:R1:1744:A:H3'	32:R1:1745:A:H8	1.78	0.49
32:R1:2138:G:O6	32:R1:2154:A:N6	2.45	0.49
32:R1:2898:U:H2'	32:R1:2899:A:C8	2.48	0.49
34:R3:555:U:H2'	34:R3:556:C:C6	2.48	0.49
34:R3:1432:G:O2'	34:R3:1468:A:N6	2.46	0.49
7:18:56:LYS:HA	7:18:59:ALA:HB3	1.94	0.49
32:R1:1096:A:H5"	32:R1:1097:U:OP2	2.13	0.49
32:R1:2638:G:H1'	32:R1:2778:A:H61	1.77	0.49
34:R3:1253:G:H2'	34:R3:1254:A:C8	2.47	0.49
30:H:426:GLU:OE1	30:H:427:GLU:N	2.43	0.49
34:R3:419:C:O2	34:R3:425:G:N2	2.46	0.49
4:15:127:VAL:HG11	4:15:142:ILE:HG21	1.94	0.49
9:2:15:VAL:HG22	9:2:205:GLY:HA3	1.95	0.49
9:2:231:HIS:HA	9:2:241:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:H:263:ILE:HD13	30:H:280:ILE:HG13	1.94	0.49
32:R1:889:C:H2'	32:R1:890:C:O4'	2.12	0.49
32:R1:1114:C:H2'	32:R1:1115:G:C8	2.48	0.49
32:R1:1594:U:H2'	32:R1:1595:C:C6	2.47	0.49
32:R1:2801:G:H2'	32:R1:2802:G:H8	1.78	0.49
2:13:129:GLU:OE1	2:13:129:GLU:N	2.46	0.49
9:2:224:MET:HG2	32:R1:782:A:C2	2.48	0.49
30:H:406:LEU:HG	30:H:410:LEU:HD13	1.93	0.49
32:R1:182:A:H2'	32:R1:183:C:H6	1.78	0.49
32:R1:1386:C:H2'	32:R1:1387:A:C8	2.47	0.49
32:R1:1912:A:H62	32:R1:1917:U:H5	1.60	0.49
34:R3:524:G:H2'	34:R3:525:C:C6	2.48	0.49
9:2:211:ARG:HD2	9:2:211:ARG:HA	1.59	0.48
14:24:11:ILE:HD11	14:24:19:GLY:HA2	1.95	0.48
15:25:62:THR:HG23	15:25:69:GLU:HG2	1.94	0.48
15:25:80:HIS:CE1	15:25:83:LYS:HD2	2.48	0.48
22:33:5:ARG:NH1	32:R1:2285:C:OP2	2.40	0.48
23:34:1:MET:N	32:R1:1619:G:O2'	2.46	0.48
30:H:353:THR:HG23	57:H:601:ATP:O2A	2.13	0.48
3:14:63:VAL:HG12	3:14:107:LEU:HD11	1.95	0.48
9:2:251:THR:OG1	9:2:252:LYS:N	2.46	0.48
15:25:26:PHE:HE2	15:25:89:ILE:HG13	1.77	0.48
30:H:498:TYR:CD1	30:H:507:PRO:HA	2.48	0.48
32:R1:1441:G:H2'	32:R1:1442:U:C6	2.48	0.48
34:R3:1328:C:H2'	34:R3:1329:A:C8	2.48	0.48
34:R3:1355:G:H2'	34:R3:1356:G:C8	2.48	0.48
22:33:33:LEU:HD11	32:R1:2286:G:C5	2.49	0.48
30:H:191:TRP:HD1	30:H:192:LEU:HD23	1.78	0.48
32:R1:307:G:N2	32:R1:310:A:OP2	2.41	0.48
33:R2:28:C:H2'	33:R2:29:A:C8	2.49	0.48
34:R3:198:G:H2'	34:R3:199:A:C8	2.48	0.48
1:1:21:TYR:HB2	1:1:26:ALA:HB2	1.95	0.48
32:R1:1871:A:H8	32:R1:1872:A:C8	2.32	0.48
34:R3:131:A:H2'	34:R3:132:C:C6	2.47	0.48
34:R3:147:G:H2'	34:R3:148:G:C8	2.49	0.48
34:R3:191:G:H2'	34:R3:192:A:C8	2.48	0.48
13:23:49:LYS:HG3	13:23:50:LEU:HD12	1.95	0.48
34:R3:1166:G:N2	34:R3:1169:A:OP2	2.39	0.48
34:R3:1253:G:H2'	34:R3:1254:A:H8	1.78	0.48
26:4:149:ILE:HD12	26:4:188:MET:HG2	1.94	0.48
34:R3:384:G:H2'	34:R3:385:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:220:ARG:HE	9:2:220:ARG:HB2	1.38	0.48
12:22:24:ILE:O	12:22:24:ILE:HG13	2.13	0.48
32:R1:155:A:H2'	32:R1:156:A:C8	2.48	0.48
32:R1:807:U:O2'	32:R1:2060:A:N1	2.45	0.48
32:R1:1079:C:N4	32:R1:1088:A:O4'	2.47	0.48
32:R1:1315:C:O2'	32:R1:1392:A:N3	2.42	0.48
32:R1:1486:U:H2'	32:R1:1487:U:C6	2.49	0.48
32:R1:2581:G:OP2	32:R1:2581:G:N2	2.46	0.48
8:19:33:GLU:OE1	8:19:36:LYS:NZ	2.46	0.48
27:5:162:ASP:OD1	27:5:162:ASP:N	2.46	0.48
32:R1:693:A:O2'	32:R1:1353:A:N3	2.46	0.48
32:R1:2123:G:N2	32:R1:2124:G:O6	2.46	0.48
34:R3:1086:U:H3	34:R3:1099:G:H22	1.62	0.48
32:R1:1095:A:O2'	32:R1:1096:A:O5'	2.21	0.48
32:R1:151:C:H2'	32:R1:152:A:H8	1.79	0.48
32:R1:1726:C:H2'	32:R1:1727:C:C6	2.49	0.48
34:R3:335:C:O2'	34:R3:1433:A:N3	2.42	0.48
34:R3:1513:A:H2'	34:R3:1514:G:C8	2.49	0.48
26:4:147:LEU:HD11	26:4:170:ARG:HE	1.78	0.47
27:5:36:ASN:OD1	27:5:152:ASP:HB3	2.14	0.47
32:R1:713:G:H2'	32:R1:714:U:C6	2.49	0.47
32:R1:742:A:H2'	32:R1:743:A:C8	2.49	0.47
32:R1:1889:A:H2'	32:R1:1890:A:C8	2.49	0.47
34:R3:939:G:H21	34:R3:1375:A:H2	1.60	0.47
12:22:3:THR:HG21	12:22:58:ALA:HB2	1.96	0.47
17:28:60:LYS:NZ	32:R1:372:G:OP2	2.42	0.47
25:36:28:SER:O	28:6:169:ARG:NH2	2.47	0.47
32:R1:774:G:O2'	32:R1:775:G:O5'	2.32	0.47
32:R1:1072:C:N4	32:R1:1092:C:OP2	2.47	0.47
34:R3:447:G:N1	34:R3:486:U:OP1	2.42	0.47
34:R3:1004:A:O2'	34:R3:1005:A:O4'	2.30	0.47
34:R3:1162:C:H2'	34:R3:1163:A:C8	2.49	0.47
30:H:7:LEU:HG	30:H:9:ILE:HG13	1.97	0.47
32:R1:910:A:H2'	32:R1:911:A:C8	2.49	0.47
32:R1:1538:G:H2'	32:R1:1539:U:H6	1.77	0.47
34:R3:82:G:N2	34:R3:87:C:O2	2.47	0.47
34:R3:1171:A:H2'	34:R3:1172:C:C6	2.49	0.47
5:16:17:ASN:OD1	5:16:97:GLN:NE2	2.46	0.47
28:6:109:SER:HB3	32:R1:2667:C:N3	2.29	0.47
30:H:2:ILE:HG22	30:H:60:PHE:HB2	1.97	0.47
30:H:385:LEU:HD21	30:H:437:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2291:U:OP1	32:R1:2380:C:O2'	2.31	0.47
34:R3:944:G:O2'	34:R3:1339:A:N6	2.47	0.47
1:1:208:TYR:CE1	1:1:209:ILE:HG12	2.49	0.47
5:16:35:ALA:HB2	5:16:102:LEU:HD11	1.95	0.47
27:5:45:ASP:OD2	27:5:48:LEU:HD13	2.14	0.47
30:H:315:MET:HG2	30:H:331:ILE:HG12	1.95	0.47
32:R1:1170:C:H2'	32:R1:1171:G:C8	2.49	0.47
32:R1:1187:G:N2	32:R1:1188:U:O4	2.47	0.47
32:R1:2554:U:H2'	32:R1:2555:U:H6	1.79	0.47
32:R1:2725:A:O2'	32:R1:2726:A:O5'	2.33	0.47
32:R1:2747:G:O6	32:R1:2755:C:H5"	2.13	0.47
34:R3:839:C:H2'	34:R3:840:C:O4'	2.14	0.47
34:R3:1358:U:OP2	34:R3:1359:C:N4	2.41	0.47
2:13:82:GLY:HA2	32:R1:1131:G:OP1	2.15	0.47
12:22:109:ASP:N	12:22:109:ASP:OD1	2.45	0.47
28:6:85:LYS:HG2	28:6:131:VAL:HG22	1.97	0.47
32:R1:1395:A:O2'	32:R1:1396:U:H5"	2.15	0.47
32:R1:1443:U:H2'	32:R1:1444:G:H8	1.80	0.47
5:16:55:ARG:HD2	32:R1:2469:A:H4'	1.95	0.47
12:22:41:LYS:HD2	21:32:21:LEU:HD11	1.96	0.47
22:33:10:LEU:HD12	22:33:48:TYR:HB3	1.97	0.47
23:34:3:ARG:HD3	23:34:3:ARG:HA	1.69	0.47
30:H:81:LEU:HD21	30:H:143:LEU:HD22	1.97	0.47
30:H:93:GLN:O	30:H:97:GLN:HG3	2.14	0.47
30:H:192:LEU:CD1	30:H:212:ILE:CD1	2.92	0.47
30:H:461:LEU:HD13	30:H:465:MET:HB3	1.97	0.47
32:R1:958:U:H2'	33:R2:89:U:H1'	1.96	0.47
32:R1:1631:G:N2	32:R1:1634:A:OP2	2.36	0.47
32:R1:1769:U:O2'	32:R1:1958:C:OP1	2.32	0.47
34:R3:218:U:H2'	34:R3:219:U:O4'	2.15	0.47
34:R3:684:U:H2'	34:R3:685:G:O4'	2.15	0.47
34:R3:745:G:H2'	34:R3:746:A:C8	2.49	0.47
34:R3:1324:A:H2'	34:R3:1325:C:C6	2.50	0.47
34:R3:1414:U:H2'	34:R3:1415:G:H8	1.79	0.47
9:2:209:ALA:HA	9:2:212:TRP:CE2	2.50	0.47
32:R1:578:G:OP1	32:R1:1255:U:O2'	2.30	0.47
32:R1:593:U:H2'	32:R1:594:U:C6	2.49	0.47
32:R1:1511:G:H2'	32:R1:1512:C:H6	1.79	0.47
34:R3:841:C:O2'	34:R3:843:U:O4'	2.30	0.47
34:R3:1033:G:H2'	34:R3:1034:G:C8	2.49	0.47
25:36:24:ARG:NH2	32:R1:2742:G:OP1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:10:VAL:HG12	28:6:11:PRO:CD	2.45	0.47
32:R1:1071:G:H8	32:R1:1071:G:OP1	1.97	0.47
32:R1:2305:U:H2'	32:R1:2306:C:C6	2.50	0.47
34:R3:600:A:H2'	34:R3:601:G:H8	1.79	0.47
32:R1:161:A:H3'	32:R1:162:U:H5"	1.97	0.47
33:R2:28:C:H2'	33:R2:29:A:H8	1.80	0.47
4:15:43:GLY:N	32:R1:671:C:OP1	2.41	0.46
32:R1:784:G:H5'	32:R1:785:G:OP1	2.15	0.46
32:R1:2071:A:H2'	32:R1:2072:C:C6	2.51	0.46
34:R3:991:U:N3	34:R3:1212:U:O2'	2.48	0.46
35:T:54:5MU:H2'	35:T:55:PSU:O4'	2.15	0.46
30:H:317:LYS:O	30:H:366:SER:OG	2.20	0.46
32:R1:1141:U:H4'	32:R1:1142:A:O4'	2.16	0.46
32:R1:1537:G:C5	32:R1:1538:G:H1'	2.49	0.46
33:R2:44:G:O2'	33:R2:47:C:N4	2.48	0.46
1:1:11:ILE:HA	1:1:14:LYS:HB3	1.97	0.46
6:17:72:ASP:O	6:17:76:VAL:HG23	2.16	0.46
23:34:9:VAL:HG12	32:R1:125:A:H2	1.80	0.46
33:R2:39:A:H2	33:R2:44:G:C4	2.33	0.46
34:R3:362:G:N1	34:R3:365:U:OP2	2.48	0.46
1:1:194:VAL:HA	1:1:197:LYS:HG2	1.98	0.46
30:H:211:PRO:HG2	30:H:212:ILE:HG23	1.97	0.46
32:R1:155:A:H2'	32:R1:156:A:H8	1.80	0.46
32:R1:1236:G:HO2'	32:R1:1237:A:P	2.38	0.46
32:R1:1486:U:H2'	32:R1:1487:U:H6	1.80	0.46
34:R3:270:A:H2'	34:R3:271:C:C6	2.51	0.46
34:R3:1171:A:H2'	34:R3:1172:C:H6	1.81	0.46
34:R3:1236:A:H2'	34:R3:1237:C:C6	2.51	0.46
9:2:2:VAL:HG12	9:2:18:VAL:HG22	1.97	0.46
9:2:12:ARG:HG3	32:R1:729:G:OP1	2.15	0.46
10:20:5:ARG:NH2	32:R1:585:G:N7	2.62	0.46
20:30:51:SER:O	20:30:51:SER:OG	2.27	0.46
32:R1:612:G:C2	32:R1:614:A:H1'	2.51	0.46
34:R3:1326:U:H2'	34:R3:1327:C:H6	1.81	0.46
1:1:30:LEU:HD12	1:1:216:THR:HG23	1.97	0.46
9:2:48:ILE:HG22	32:R1:779:U:OP1	2.15	0.46
10:20:16:ILE:HD13	10:20:35:PHE:HD1	1.81	0.46
30:H:49:ASN:OD1	30:H:58:TYR:OH	2.27	0.46
32:R1:1433:A:H2'	32:R1:1434:A:O4'	2.16	0.46
32:R1:1592:C:H2'	32:R1:1593:A:C8	2.51	0.46
33:R2:31:C:H2'	33:R2:32:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:898:G:N2	34:R3:901:A:OP2	2.38	0.46
34:R3:991:U:H5"	34:R3:992:U:OP1	2.16	0.46
34:R3:1021:A:H2'	34:R3:1022:A:C8	2.51	0.46
34:R3:1352:C:H2'	34:R3:1353:G:H8	1.78	0.46
1:1:38:PHE:HD1	1:1:39:VAL:H	1.61	0.46
1:1:175:ILE:CD1	1:1:189:LEU:HG	2.45	0.46
7:18:102:ARG:HG2	33:R2:49:C:OP1	2.15	0.46
26:4:69:ARG:O	32:R1:674:G:H4'	2.16	0.46
30:H:295:ASP:N	30:H:295:ASP:OD1	2.49	0.46
32:R1:851:C:H2'	32:R1:852:U:H6	1.79	0.46
34:R3:198:G:H2'	34:R3:199:A:H8	1.81	0.46
34:R3:998:C:C2	34:R3:1043:G:N2	2.80	0.46
34:R3:1120:C:H2'	34:R3:1121:U:H6	1.80	0.46
6:17:2:ARG:HA	6:17:5:LYS:HD2	1.97	0.46
9:2:62:ARG:NH2	32:R1:1568:G:OP2	2.45	0.46
11:21:49:ILE:HA	11:21:54:VAL:HG23	1.98	0.46
32:R1:1710:G:H2'	32:R1:1711:A:C8	2.51	0.46
34:R3:471:U:H2'	34:R3:472:U:C6	2.51	0.46
34:R3:976:G:OP2	34:R3:1358:U:O2'	2.34	0.46
34:R3:1241:G:H2'	34:R3:1242:G:C8	2.50	0.46
9:2:140:VAL:HG23	9:2:191:LEU:HA	1.98	0.46
32:R1:2:G:H2'	32:R1:3:U:C6	2.51	0.46
32:R1:2:G:H2'	32:R1:3:U:H6	1.81	0.46
32:R1:1405:U:H2'	32:R1:1406:U:H6	1.81	0.46
33:R2:48:U:H2'	33:R2:49:C:C6	2.51	0.46
29:9:129:GLU:HG3	29:9:143:ILE:HD13	1.98	0.46
30:H:142:GLN:HB3	30:H:150:PHE:CZ	2.51	0.46
30:H:352:SER:N	57:H:601:ATP:O1B	2.46	0.46
32:R1:1485:U:H2'	32:R1:1486:U:C6	2.50	0.46
32:R1:1734:G:H2'	32:R1:1735:A:H8	1.81	0.46
32:R1:2801:G:H2'	32:R1:2802:G:C8	2.51	0.46
34:R3:1405:G:H21	34:R3:1518:A:H8	1.62	0.46
5:16:49:ALA:O	5:16:53:MET:HG3	2.15	0.45
26:4:146:VAL:HA	26:4:185:LYS:O	2.15	0.45
27:5:28:PRO:HG3	27:5:164:GLU:HB3	1.97	0.45
30:H:333:LEU:HD12	30:H:334:ASN:N	2.31	0.45
32:R1:964:C:O2'	32:R1:2273:A:N3	2.39	0.45
32:R1:1485:U:H2'	32:R1:1486:U:H6	1.80	0.45
32:R1:1585:C:H2'	32:R1:1586:A:O4'	2.16	0.45
32:R1:2163:A:H5"	32:R1:2164:C:OP2	2.16	0.45
34:R3:1040:U:H2'	34:R3:1041:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:27:41:ARG:HD3	16:27:41:ARG:HA	1.65	0.45
30:H:319:SER:O	30:H:365:VAL:HG22	2.16	0.45
32:R1:404:A:H1'	32:R1:406:G:C4	2.51	0.45
32:R1:828:U:H2'	32:R1:829:A:C8	2.50	0.45
33:R2:30:C:H2'	33:R2:31:C:H5'	1.98	0.45
34:R3:672:U:H2'	34:R3:673:A:C8	2.52	0.45
34:R3:948:C:H2'	34:R3:949:A:H8	1.82	0.45
34:R3:1033:G:O6	34:R3:1035:A:N6	2.50	0.45
34:R3:1038:C:H2'	34:R3:1039:G:H8	1.80	0.45
34:R3:1316:G:N2	34:R3:1319:A:OP2	2.49	0.45
34:R3:1405:G:O2'	34:R3:1518:A:O2'	2.34	0.45
2:13:78:THR:HB	32:R1:2641:G:H5"	1.98	0.45
12:22:70:LYS:N	12:22:108:SER:O	2.48	0.45
19:3:83:ARG:HH11	32:R1:2637:U:H5"	1.82	0.45
26:4:28:VAL:O	26:4:32:VAL:HG13	2.16	0.45
30:H:342:GLY:O	30:H:497:LEU:HA	2.15	0.45
32:R1:30:G:H2'	32:R1:31:C:C6	2.51	0.45
32:R1:465:G:H2'	32:R1:466:A:C8	2.51	0.45
34:R3:376:G:H1	34:R3:387:U:H3	1.64	0.45
34:R3:707:U:H2'	34:R3:708:C:C6	2.51	0.45
34:R3:977:A:N6	34:R3:1224:U:O4'	2.50	0.45
34:R3:1016:A:O2'	34:R3:1217:C:O2'	2.30	0.45
34:R3:1027:C:N3	34:R3:1033:G:N1	2.61	0.45
34:R3:1162:C:H2'	34:R3:1163:A:H8	1.81	0.45
5:16:47:GLU:OE2	5:16:47:GLU:C	2.54	0.45
6:17:32:GLU:OE2	6:17:78:LYS:NZ	2.34	0.45
7:18:16:ARG:NH1	32:R1:2334:U:O4	2.50	0.45
10:20:111:LYS:HZ1	11:21:48:LYS:HB3	1.80	0.45
12:22:92:ARG:HE	12:22:92:ARG:HB2	1.58	0.45
15:25:49:ASN:OD1	15:25:50:MET:N	2.49	0.45
32:R1:974:G:H1'	32:R1:975:A:C8	2.52	0.45
32:R1:2101:A:H2'	32:R1:2102:G:C8	2.51	0.45
34:R3:422:C:O2'	34:R3:423:G:H5"	2.16	0.45
34:R3:474:G:N3	34:R3:474:G:H2'	2.32	0.45
34:R3:1513:A:H2'	34:R3:1514:G:H8	1.81	0.45
2:13:60:ASP:C	2:13:60:ASP:OD2	2.54	0.45
22:33:12:SER:HB2	22:33:48:TYR:CZ	2.52	0.45
26:4:149:ILE:HD13	26:4:175:ILE:HG21	1.98	0.45
34:R3:945:G:C2	34:R3:946:A:C8	3.05	0.45
34:R3:1157:A:H4'	34:R3:1158:C:O5'	2.16	0.45
34:R3:1261:A:N6	34:R3:1274:A:O2'	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:1353:G:C2	34:R3:1370:G:C2	3.05	0.45
1:1:59:VAL:HB	1:1:165:ASN:OD1	2.17	0.45
10:20:49:ARG:HD2	32:R1:993:G:OP1	2.16	0.45
30:H:201:LEU:HD23	30:H:202:ILE:N	2.32	0.45
30:H:231:TYR:O	30:H:235:GLU:HG2	2.17	0.45
32:R1:150:U:H2'	32:R1:151:C:C6	2.52	0.45
32:R1:177:G:H3'	32:R1:178:G:C8	2.51	0.45
32:R1:306:U:H2'	32:R1:307:G:O4'	2.16	0.45
33:R2:44:G:H1'	33:R2:47:C:H42	1.80	0.45
34:R3:911:U:H2'	34:R3:912:C:C6	2.51	0.45
34:R3:1250:A:N3	34:R3:1370:G:O2'	2.45	0.45
34:R3:1356:G:H2'	34:R3:1357:A:H8	1.76	0.45
3:14:92:GLU:OE1	3:14:111:LYS:HB2	2.16	0.45
7:18:93:ASP:OD1	7:18:94:ARG:N	2.49	0.45
16:27:19:LYS:HD3	16:27:19:LYS:HA	1.77	0.45
32:R1:1055:G:N1	32:R1:1105:U:O2	2.46	0.45
32:R1:2064:C:H2'	32:R1:2065:C:C6	2.52	0.45
32:R1:2159:G:C6	32:R1:2160:C:N3	2.85	0.45
34:R3:246:A:C2	34:R3:282:A:C5	3.05	0.45
34:R3:982:U:H4'	34:R3:983:A:O4'	2.16	0.45
34:R3:1014:A:C2	34:R3:1219:A:H1'	2.52	0.45
34:R3:1305:G:HO2'	34:R3:1306:A:H8	1.64	0.45
1:1:38:PHE:CE2	32:R1:2127:G:H5'	2.52	0.45
4:15:82:LEU:HD13	4:15:120:VAL:HG11	1.99	0.45
11:21:69:GLY:O	11:21:90:ARG:NH1	2.49	0.45
26:4:148:ILE:HB	26:4:169:VAL:HG22	1.98	0.45
28:6:140:ILE:HG13	28:6:141:GLY:N	2.31	0.45
32:R1:962:G:N2	32:R1:2250:G:H1	2.12	0.45
7:18:36:TYR:HD2	7:18:52:SER:HB2	1.82	0.45
7:18:49:VAL:HG21	7:18:82:ALA:HA	1.99	0.45
19:3:114:LYS:HD2	19:3:196:ALA:HB2	1.97	0.45
30:H:346:ARG:O	30:H:351:LYS:NZ	2.46	0.45
30:H:506:GLU:HG3	30:H:508:PHE:H	1.81	0.45
32:R1:2140:G:H2'	32:R1:2141:G:C8	2.51	0.45
34:R3:990:C:H2'	34:R3:991:U:O4'	2.17	0.45
35:T:60:U:H5"	35:T:61:C:C5	2.52	0.45
13:23:12:ARG:HB2	13:23:33:LYS:O	2.17	0.45
17:28:30:PRO:HG2	17:28:32:LEU:HG	1.98	0.45
18:29:2:LYS:HD2	32:R1:102:U:N1	2.32	0.45
19:3:5:VAL:H	19:3:32:ASN:HD21	1.65	0.45
25:36:16:ILE:HD13	25:36:25:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:H:322:TYR:CE2	30:H:353:THR:HG22	2.52	0.45
32:R1:832:U:H2'	32:R1:833:A:H8	1.81	0.45
32:R1:1047:G:H22	32:R1:1110:G:H2'	1.82	0.45
32:R1:1373:A:H5'	32:R1:2212:A:H1'	1.99	0.45
32:R1:1494:A:H2'	32:R1:1495:A:C8	2.52	0.45
32:R1:2173:A:H8	32:R1:2174:C:C6	2.33	0.45
32:R1:2725:A:O2'	32:R1:2726:A:C8	2.67	0.45
34:R3:560:A:H4'	34:R3:561:U:H5'	1.98	0.45
34:R3:868:C:H2'	34:R3:869:G:O4'	2.16	0.45
10:20:105:PHE:O	10:20:109:VAL:HG23	2.17	0.44
30:H:160:LEU:HD21	30:H:188:LEU:HD13	1.98	0.44
32:R1:1341:G:OP1	32:R1:1397:U:N3	2.47	0.44
34:R3:142:G:H2'	34:R3:143:A:C8	2.52	0.44
34:R3:620:C:O2'	34:R3:621:A:H8	2.00	0.44
34:R3:1157:A:H5'	34:R3:1158:C:C6	2.53	0.44
35:T:60:U:H5"	35:T:61:C:H5	1.81	0.44
7:18:18:LEU:HD23	7:18:18:LEU:HA	1.81	0.44
10:20:91:ARG:HD3	32:R1:997:G:OP1	2.17	0.44
12:22:13:SER:O	12:22:17:VAL:HG23	2.18	0.44
17:28:36:ARG:NH1	32:R1:2200:C:OP2	2.51	0.44
19:3:99:GLU:HG2	19:3:182:ALA:HB2	1.99	0.44
29:9:50:ARG:NH1	29:9:51:ARG:HG3	2.32	0.44
30:H:149:ASP:CG	30:H:150:PHE:H	2.18	0.44
30:H:333:LEU:HB3	30:H:498:TYR:OH	2.17	0.44
32:R1:355:U:H2'	32:R1:356:G:C8	2.51	0.44
32:R1:372:G:O2'	32:R1:373:U:P	2.75	0.44
32:R1:975:A:H1'	32:R1:990:A:N1	2.33	0.44
32:R1:2143:C:H2'	32:R1:2144:G:O4'	2.17	0.44
32:R1:2514:U:H2'	32:R1:2515:C:C6	2.52	0.44
26:4:194:LYS:H	26:4:194:LYS:HG2	1.56	0.44
32:R1:1181:U:H2'	32:R1:1182:G:C8	2.51	0.44
32:R1:1716:U:H2'	32:R1:1717:A:H8	1.82	0.44
32:R1:2187:U:H2'	32:R1:2188:U:C6	2.52	0.44
32:R1:2553:G:H2'	32:R1:2554:U:O4'	2.17	0.44
33:R2:106:G:H2'	33:R2:107:G:O4'	2.18	0.44
34:R3:257:G:H2'	34:R3:258:G:H8	1.82	0.44
34:R3:416:G:H2'	34:R3:417:G:C8	2.53	0.44
2:13:135:GLN:NE2	32:R1:7:G:O4'	2.50	0.44
30:H:1:MET:H1	30:H:26:PRO:CD	2.30	0.44
30:H:310:ASN:HB3	30:H:311:PRO:HD3	1.99	0.44
30:H:320:ALA:N	30:H:328:LEU:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:285:G:O6	32:R1:356:G:C6	2.70	0.44
32:R1:1283:G:N2	32:R1:1286:A:OP2	2.46	0.44
32:R1:1538:G:H8	32:R1:1538:G:OP2	2.00	0.44
32:R1:1794:A:H2'	32:R1:1795:C:C6	2.52	0.44
34:R3:704:A:C4	34:R3:705:G:C8	3.05	0.44
34:R3:1057:G:H2'	34:R3:1058:G:O4'	2.18	0.44
4:15:30:THR:O	4:15:30:THR:OG1	2.35	0.44
5:16:96:ILE:HG21	5:16:126:ILE:HD12	1.99	0.44
29:9:50:ARG:NH1	29:9:54:LEU:HD13	2.32	0.44
30:H:405:GLU:OE1	30:H:405:GLU:HA	2.18	0.44
32:R1:248:G:H5'	32:R1:250:G:N7	2.33	0.44
32:R1:2745:C:H2'	32:R1:2746:U:C6	2.51	0.44
34:R3:454:G:H1	34:R3:477:C:H42	1.64	0.44
34:R3:859:G:H2'	34:R3:860:A:H8	1.81	0.44
34:R3:976:G:N7	34:R3:1362:A:N6	2.66	0.44
19:3:142:VAL:HG12	19:3:144:GLY:H	1.82	0.44
26:4:171:ASP:OD1	26:4:172:ALA:N	2.51	0.44
27:5:103:ILE:HD13	27:5:107:VAL:HG21	2.00	0.44
30:H:321:GLY:HA2	30:H:327:ILE:H	1.83	0.44
32:R1:2154:A:H2'	32:R1:2155:U:O4'	2.17	0.44
34:R3:1143:G:H2'	34:R3:1144:G:C8	2.52	0.44
34:R3:1147:C:H2'	34:R3:1148:U:C6	2.53	0.44
4:15:79:LEU:HD12	4:15:79:LEU:HA	1.80	0.44
7:18:15:ARG:NH2	33:R2:8:C:OP1	2.28	0.44
13:23:19:LYS:HD3	13:23:19:LYS:HA	1.76	0.44
15:25:30:ILE:HG12	15:25:91:PHE:HB2	2.00	0.44
30:H:384:GLN:O	30:H:387:TYR:HB3	2.18	0.44
32:R1:1103:A:H2'	32:R1:1103:A:N3	2.32	0.44
32:R1:1790:C:H2'	32:R1:1791:A:C8	2.53	0.44
32:R1:2102:G:H2'	32:R1:2103:C:H6	1.83	0.44
34:R3:553:A:H2'	34:R3:554:A:H8	1.81	0.44
34:R3:965:U:H5"	34:R3:966:G:OP1	2.18	0.44
10:20:23:TYR:HB2	10:20:28:SER:HB3	2.00	0.44
13:23:33:LYS:HG3	13:23:80:TRP:HE3	1.82	0.44
28:6:66:THR:O	28:6:70:LEU:HG	2.18	0.44
32:R1:93:G:H2'	32:R1:94:A:C8	2.53	0.44
32:R1:154:U:H2'	32:R1:155:A:H8	1.82	0.44
32:R1:1047:G:O2'	32:R1:1048:A:O4'	2.34	0.44
32:R1:1087:G:C2	32:R1:1089:A:H1'	2.53	0.44
34:R3:518:C:O2'	34:R3:530:G:N2	2.51	0.44
34:R3:1347:G:N2	34:R3:1373:G:H2'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1040:A:N1	32:R1:1115:G:N2	2.53	0.44
32:R1:1715:G:O2'	32:R1:1716:U:H6	2.01	0.44
32:R1:2515:C:H2'	32:R1:2516:A:H8	1.82	0.44
34:R3:1154:G:H2'	34:R3:1155:A:C8	2.50	0.44
34:R3:1319:A:C8	34:R3:1323:G:C6	3.05	0.44
9:2:83:ASP:OD2	9:2:86:ARG:NH1	2.51	0.43
19:3:149:ASN:HB3	32:R1:2572:A:OP2	2.17	0.43
30:H:385:LEU:HD12	30:H:385:LEU:HA	1.84	0.43
32:R1:282:A:H2'	32:R1:283:G:C8	2.53	0.43
32:R1:1389:G:H2'	32:R1:1390:U:O4'	2.18	0.43
32:R1:2230:G:H2'	32:R1:2231:U:C6	2.53	0.43
33:R2:60:C:H2'	33:R2:61:G:H8	1.82	0.43
34:R3:210:C:H4'	34:R3:211:G:C2	2.53	0.43
34:R3:908:A:H2'	34:R3:909:A:H8	1.82	0.43
34:R3:1040:U:H2'	34:R3:1041:G:C8	2.53	0.43
34:R3:1121:U:C2	34:R3:1122:U:C5	3.06	0.43
34:R3:1316:G:H2'	34:R3:1317:C:H5"	2.00	0.43
34:R3:1326:U:C2	34:R3:1327:C:C5	3.05	0.43
35:T:74:C:H2'	35:T:75:C:C6	2.53	0.43
19:3:180:VAL:HG22	19:3:187:LEU:CD1	2.46	0.43
20:30:40:THR:O	20:30:44:ARG:HG2	2.18	0.43
24:35:54:LEU:O	24:35:58:ILE:HG13	2.18	0.43
32:R1:1038:G:H2'	32:R1:1039:A:C8	2.53	0.43
32:R1:1041:G:C2	32:R1:1042:G:N7	2.86	0.43
32:R1:1482:G:C4	32:R1:1508:A:H2	2.35	0.43
32:R1:2014:A:H2'	32:R1:2015:A:C8	2.52	0.43
32:R1:2082:A:C2	32:R1:2083:G:H1'	2.53	0.43
34:R3:323:U:H2'	34:R3:324:G:O4'	2.18	0.43
34:R3:1020:G:H2'	34:R3:1021:A:H8	1.82	0.43
34:R3:1144:G:N2	34:R3:1146:A:H62	2.15	0.43
34:R3:1391:U:H2'	34:R3:1392:G:C8	2.54	0.43
1:1:167:LYS:NZ	32:R1:2179:C:O2'	2.51	0.43
3:14:38:ILE:HD11	3:14:112:PHE:HZ	1.83	0.43
3:14:105:ARG:NH2	8:19:31:VAL:HG21	2.33	0.43
27:5:169:LEU:HD23	27:5:169:LEU:HA	1.73	0.43
32:R1:1078:U:H1'	32:R1:1088:A:H2	1.82	0.43
32:R1:2113:U:H5'	32:R1:2114:A:C2	2.54	0.43
32:R1:2164:C:O2'	32:R1:2165:C:OP1	2.34	0.43
34:R3:1228:C:H2'	34:R3:1229:A:H8	1.82	0.43
7:18:108:ASP:O	7:18:112:GLU:HG2	2.19	0.43
16:27:20:ARG:HD3	32:R1:2356:U:O3'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:174:LYS:HD3	32:R1:2530:A:H5'	2.00	0.43
32:R1:435:C:H2'	32:R1:436:C:H5'	2.01	0.43
32:R1:2249:U:H3'	32:R1:2250:G:H5"	2.01	0.43
33:R2:13:G:N7	33:R2:70:C:H4'	2.34	0.43
34:R3:423:G:H22	34:R3:424:G:N2	2.16	0.43
34:R3:620:C:HO2'	34:R3:621:A:H8	1.61	0.43
34:R3:1327:C:C2	34:R3:1328:C:C5	3.07	0.43
2:13:60:ASP:OD2	2:13:61:LYS:HG2	2.18	0.43
9:2:74:PRO:O	9:2:96:LYS:HG2	2.17	0.43
11:21:3:ALA:HB2	11:21:101:ILE:HD11	1.99	0.43
26:4:62:GLN:HG3	26:4:63:LYS:HG2	2.00	0.43
32:R1:2233:U:H2'	32:R1:2234:G:C8	2.54	0.43
34:R3:109:A:C6	34:R3:326:G:C6	3.07	0.43
34:R3:264:C:H2'	34:R3:265:G:O4'	2.18	0.43
34:R3:620:C:O2'	34:R3:621:A:O4'	2.37	0.43
4:15:95:LEU:HD11	4:15:125:LEU:HD11	2.00	0.43
8:19:38:ARG:NH1	34:R3:346:G:OP1	2.50	0.43
28:6:84:LYS:HD2	28:6:84:LYS:HA	1.84	0.43
30:H:10:ARG:HA	30:H:15:VAL:HA	2.01	0.43
30:H:461:LEU:HD23	30:H:461:LEU:HA	1.87	0.43
32:R1:3:U:H2'	32:R1:4:U:H6	1.82	0.43
32:R1:288:U:H2'	32:R1:289:G:C8	2.54	0.43
32:R1:1009:A:N3	32:R1:1153:C:O2'	2.49	0.43
32:R1:2117:A:N6	32:R1:2119:A:N1	2.66	0.43
33:R2:30:C:O2'	33:R2:57:A:N1	2.50	0.43
34:R3:1122:U:H2'	34:R3:1123:U:C6	2.53	0.43
34:R3:1306:A:H1'	34:R3:1332:A:C2	2.54	0.43
7:18:56:LYS:HD2	7:18:59:ALA:HB3	2.01	0.43
22:33:35:LEU:HD11	32:R1:2286:G:N2	2.34	0.43
24:35:3:ILE:HD11	32:R1:592:A:H2	1.84	0.43
27:5:103:ILE:HD12	27:5:175:PRO:CD	2.49	0.43
32:R1:1923:U:H2'	32:R1:1924:C:C6	2.54	0.43
32:R1:2105:U:H2'	32:R1:2106:U:C6	2.53	0.43
34:R3:477:C:N4	34:R3:478:A:N1	2.66	0.43
34:R3:1119:C:H2'	34:R3:1120:C:H6	1.83	0.43
29:9:75:LEU:HD23	29:9:75:LEU:H	1.83	0.43
30:H:81:LEU:CD2	30:H:143:LEU:HB3	2.48	0.43
32:R1:546:U:H4'	32:R1:548:G:H1	1.84	0.43
32:R1:1710:G:H2'	32:R1:1711:A:H8	1.84	0.43
33:R2:3:C:H2'	33:R2:4:C:C6	2.53	0.43
34:R3:89:U:H2'	34:R3:90:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:401:C:O2'	34:R3:621:A:N3	2.35	0.43
34:R3:1370:G:C2	34:R3:1371:G:C8	3.06	0.43
1:1:42:VAL:HB	1:1:214:ILE:HD11	2.00	0.43
5:16:31:PHE:HB3	5:16:130:PHE:CE1	2.54	0.43
19:3:133:THR:CG2	32:R1:1993:U:H4'	2.48	0.43
23:34:26:ASN:CG	32:R1:682:G:H5'	2.39	0.43
32:R1:81:G:H2'	32:R1:82:U:O4'	2.18	0.43
32:R1:150:U:H2'	32:R1:151:C:H6	1.83	0.43
32:R1:1171:G:N2	32:R1:1178:C:N3	2.67	0.43
32:R1:1182:G:H2'	32:R1:1183:U:O4'	2.19	0.43
32:R1:2105:U:H2'	32:R1:2106:U:H6	1.82	0.43
32:R1:2235:G:H2'	32:R1:2236:U:C6	2.54	0.43
34:R3:1270:G:HO2'	34:R3:1313:U:HO2'	1.67	0.43
34:R3:1308:U:H2'	34:R3:1309:G:H8	1.84	0.43
35:T:15:C:H3'	35:T:16:C:H5"	2.00	0.43
1:1:22:ASP:OD1	1:1:23:ILE:N	2.52	0.43
7:18:4:LYS:HB2	7:18:4:LYS:HE3	1.68	0.43
13:23:38:ALA:HB3	13:23:81:LYS:HD3	2.01	0.43
27:5:53:ALA:HB1	27:5:64:PRO:HG2	2.01	0.43
29:9:18:GLN:NE2	29:9:44:ILE:HD11	2.32	0.43
32:R1:671:C:H2'	32:R1:672:C:H6	1.84	0.43
32:R1:1738:G:O2'	32:R1:1739:A:H8	2.02	0.43
34:R3:142:G:H2'	34:R3:143:A:H8	1.84	0.43
34:R3:1271:A:H2'	34:R3:1272:G:C8	2.54	0.43
5:16:26:VAL:HG13	5:16:104:GLU:OE1	2.18	0.42
21:32:10:SER:O	21:32:14:MET:HG3	2.19	0.42
32:R1:219:A:N3	32:R1:234:U:O2'	2.45	0.42
32:R1:2848:G:H2'	32:R1:2867:G:N2	2.33	0.42
34:R3:528:C:H3'	34:R3:529:G:H5"	2.01	0.42
5:16:47:GLU:HG2	5:16:50:ARG:HH21	1.84	0.42
11:21:32:THR:OG1	11:21:62:GLU:OE1	2.36	0.42
32:R1:593:U:H2'	32:R1:594:U:H6	1.85	0.42
32:R1:724:U:H2'	32:R1:725:G:O4'	2.19	0.42
32:R1:1475:G:H1'	32:R1:1732:C:H41	1.84	0.42
34:R3:575:G:O2'	34:R3:821:G:OP2	2.31	0.42
34:R3:1271:A:C2	34:R3:1272:G:C5	3.07	0.42
34:R3:1305:G:N2	34:R3:1331:G:H2'	2.33	0.42
10:20:50:ARG:NH2	32:R1:993:G:OP2	2.52	0.42
25:36:13:ASN:ND2	25:36:29:ALA:HB2	2.32	0.42
27:5:23:SER:OG	27:5:26:GLN:HB2	2.19	0.42
27:5:87:LYS:HD3	32:R1:2313:C:H5"	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:169:LEU:HD13	27:5:174:PHE:CD2	2.54	0.42
32:R1:172:A:H2'	32:R1:173:A:H8	1.84	0.42
32:R1:1000:A:H2'	32:R1:1001:A:C8	2.54	0.42
32:R1:1383:A:H1'	32:R1:1405:U:O2'	2.19	0.42
32:R1:1443:U:H2'	32:R1:1444:G:C8	2.53	0.42
32:R1:1540:G:H2'	32:R1:1541:C:C6	2.54	0.42
34:R3:625:U:H2'	34:R3:626:G:H8	1.84	0.42
34:R3:1261:A:N6	34:R3:1274:A:HO2'	2.17	0.42
19:3:151:THR:HB	19:3:152:PRO:HD3	2.02	0.42
20:30:2:LYS:HB2	20:30:2:LYS:HE2	1.84	0.42
30:H:411:ARG:HD2	35:T:56:C:O2	2.19	0.42
32:R1:580:U:H2'	32:R1:581:C:C6	2.54	0.42
32:R1:1075:C:H3'	32:R1:1076:C:C6	2.55	0.42
32:R1:2774:C:H2'	32:R1:2775:G:O4'	2.19	0.42
34:R3:91:U:O4	34:R3:92:U:N3	2.52	0.42
34:R3:516:U:H5	34:R3:533:A:N7	2.17	0.42
34:R3:1095:U:OP1	34:R3:1108:G:N1	2.47	0.42
34:R3:1176:A:H2'	34:R3:1177:G:C8	2.54	0.42
34:R3:1237:C:O2'	34:R3:1300:G:N2	2.48	0.42
2:13:110:PRO:O	2:13:115:GLY:HA3	2.19	0.42
6:17:78:LYS:HE2	6:17:83:LEU:HD11	2.02	0.42
21:32:4:GLN:NE2	32:R1:2054:A:H2'	2.35	0.42
30:H:414:LEU:HA	30:H:414:LEU:HD23	1.81	0.42
30:H:463:LEU:HD12	30:H:466:ARG:HH21	1.85	0.42
32:R1:1438:U:H2'	32:R1:1439:A:H8	1.85	0.42
34:R3:465:A:H2'	34:R3:466:A:C8	2.53	0.42
34:R3:501:C:H2'	34:R3:502:A:C8	2.55	0.42
34:R3:935:A:H2'	34:R3:936:C:H6	1.84	0.42
34:R3:1206:G:C4	34:R3:1207:G:C8	3.07	0.42
34:R3:1272:G:H2'	34:R3:1273:C:C6	2.54	0.42
4:15:21:ARG:HA	32:R1:811:U:H2'	2.01	0.42
11:21:58:VAL:O	11:21:102:SER:HB2	2.20	0.42
18:29:56:LEU:O	18:29:60:LYS:HG3	2.20	0.42
19:3:8:LYS:HB2	19:3:201:LEU:HD11	2.00	0.42
21:32:53:VAL:HG23	21:32:54:ILE:N	2.34	0.42
27:5:2:LYS:H	27:5:2:LYS:HG2	1.55	0.42
27:5:70:ARG:NH1	32:R1:2298:A:OP1	2.43	0.42
27:5:101:ARG:NE	27:5:139:GLU:OE2	2.53	0.42
32:R1:729:G:O2'	32:R1:763:G:H4'	2.19	0.42
32:R1:1434:A:H2'	32:R1:1435:G:C8	2.54	0.42
34:R3:709:U:H2'	34:R3:710:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:16:12:MET:HE3	5:16:72:PRO:HD2	2.02	0.42
9:2:120:ASP:HB3	29:9:91:PHE:CE2	2.53	0.42
18:29:1:MET:HB3	18:29:2:LYS:H	1.59	0.42
26:4:128:ALA:HB3	26:4:133:LEU:HD12	2.00	0.42
29:9:83:LYS:HE2	29:9:91:PHE:HE1	1.83	0.42
32:R1:876:C:H2'	32:R1:877:A:O4'	2.19	0.42
34:R3:1328:C:H2'	34:R3:1329:A:H8	1.84	0.42
11:21:51:VAL:HG23	11:21:52:PRO:HD2	2.01	0.42
25:36:36:ARG:HG2	25:36:37:GLN:H	1.83	0.42
27:5:3:LEU:HB3	27:5:172:PHE:CE1	2.52	0.42
32:R1:299:A:N3	32:R1:319:G:O2'	2.37	0.42
32:R1:356:G:H2'	32:R1:357:C:C6	2.55	0.42
32:R1:2273:A:H2'	32:R1:2274:A:C8	2.55	0.42
33:R2:52:A:HO2'	33:R2:53:A:H8	1.64	0.42
34:R3:518:C:H4'	34:R3:519:C:O2	2.19	0.42
6:17:83:LEU:HD22	6:17:115:LEU:HD13	2.02	0.42
7:18:77:ALA:O	7:18:81:ARG:HD2	2.19	0.42
8:19:1:SER:N	32:R1:2875:C:O3'	2.51	0.42
9:2:86:ARG:NH2	32:R1:1817:G:OP1	2.52	0.42
26:4:44:ARG:HH22	32:R1:1248:G:P	2.42	0.42
27:5:33:ILE:HG12	27:5:95:MET:HG3	2.01	0.42
32:R1:272:A:H2'	32:R1:273:G:H8	1.85	0.42
32:R1:2134:A:C6	32:R1:2158:A:H5'	2.54	0.42
33:R2:13:G:C8	33:R2:70:C:H4'	2.55	0.42
34:R3:1179:A:H2'	34:R3:1180:A:O4'	2.20	0.42
34:R3:1405:G:HO2'	34:R3:1518:A:HO2'	1.67	0.42
28:6:120:ILE:N	28:6:120:ILE:HD12	2.35	0.42
30:H:341:ILE:HG22	30:H:496:ASP:CB	2.49	0.42
32:R1:27:G:N2	32:R1:512:G:H1'	2.34	0.42
32:R1:1112:G:H2'	32:R1:1113:U:C6	2.54	0.42
34:R3:200:G:H2'	34:R3:201:G:C8	2.51	0.42
34:R3:1027:C:N3	34:R3:1033:G:N2	2.67	0.42
9:2:244:VAL:HG12	9:2:250:GLN:HA	2.02	0.41
14:24:6:ARG:HB3	32:R1:85:G:OP2	2.20	0.41
14:24:38:ILE:HD13	14:24:38:ILE:HA	1.92	0.41
19:3:97:SER:OG	19:3:98:VAL:N	2.52	0.41
23:34:7:PRO:HB2	32:R1:1309:G:H4'	2.02	0.41
30:H:312:LEU:HG	30:H:337:PRO:HD3	2.01	0.41
32:R1:1069:A:N7	32:R1:1072:C:H3'	2.34	0.41
32:R1:2461:A:H2'	32:R1:2462:C:C6	2.54	0.41
33:R2:39:A:H2'	33:R2:40:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R3:883:C:O2'	34:R3:884:U:H5'	2.20	0.41
2:13:136:GLN:HE21	32:R1:2899:A:H5'	1.85	0.41
5:16:117:PHE:HD2	5:16:130:PHE:HD1	1.68	0.41
13:23:50:LEU:HD23	18:29:26:PHE:CE2	2.54	0.41
14:24:46:LYS:HG2	32:R1:483:A:H5"	2.02	0.41
26:4:8:ALA:C	26:4:9:GLN:HG3	2.40	0.41
27:5:121:PHE:CE2	27:5:166:ARG:HG2	2.55	0.41
32:R1:245:G:O2'	32:R1:384:A:N1	2.41	0.41
32:R1:2097:A:H2'	32:R1:2098:U:C6	2.55	0.41
32:R1:2118:U:O4	32:R1:2149:U:H1'	2.19	0.41
32:R1:2547:A:H2'	32:R1:2548:U:C6	2.55	0.41
34:R3:201:G:O2'	34:R3:469:C:O2'	2.31	0.41
34:R3:1032:G:H3'	34:R3:1032:G:N3	2.35	0.41
8:19:30:TRP:NE1	8:19:81:ASP:OD2	2.53	0.41
10:20:94:LEU:HD23	10:20:94:LEU:HA	1.94	0.41
18:29:17:GLU:HB2	18:29:53:VAL:HG11	2.02	0.41
30:H:56:GLY:O	30:H:57:SER:OG	2.35	0.41
32:R1:287:G:C6	32:R1:354:A:N1	2.88	0.41
32:R1:386:G:H3'	32:R1:387:U:H5'	2.01	0.41
32:R1:570:G:H2'	32:R1:2030:A:N7	2.35	0.41
32:R1:1068:G:H2'	32:R1:1069:A:H5"	2.02	0.41
32:R1:1737:G:O5'	32:R1:1737:G:H8	2.03	0.41
32:R1:1889:A:H2'	32:R1:1890:A:H8	1.85	0.41
32:R1:2212:A:H4'	32:R1:2213:U:H5	1.85	0.41
32:R1:2813:A:C4	32:R1:2814:A:C8	3.08	0.41
34:R3:168:G:H2'	34:R3:169:C:O4'	2.20	0.41
34:R3:204:G:H2'	34:R3:205:A:H8	1.85	0.41
34:R3:441:A:N6	34:R3:492:C:H42	2.19	0.41
34:R3:594:U:H2'	34:R3:595:A:O4'	2.20	0.41
34:R3:678:U:H2'	34:R3:679:C:C6	2.55	0.41
34:R3:1032:G:H21	34:R3:1033:G:H4'	1.85	0.41
34:R3:1112:C:O2	34:R3:1112:C:H2'	2.19	0.41
35:T:66:C:H2'	35:T:67:C:C6	2.54	0.41
17:28:48:LEU:HB3	17:28:50:VAL:HG13	2.02	0.41
20:30:3:THR:HG22	20:30:38:GLU:HA	2.01	0.41
32:R1:227:A:O2'	32:R1:228:C:O5'	2.28	0.41
34:R3:161:A:H2'	34:R3:162:A:C8	2.55	0.41
34:R3:1173:U:H2'	34:R3:1174:G:H8	1.85	0.41
34:R3:1187:G:H2'	34:R3:1188:A:C8	2.55	0.41
4:15:141:LYS:HZ2	4:15:143:GLU:HB3	1.85	0.41
7:18:115:LEU:HD12	7:18:115:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:22:18:ARG:HG3	12:22:76:VAL:HG22	2.02	0.41
24:35:28:LEU:HD13	24:35:43:LEU:HB2	2.02	0.41
28:6:157:LYS:HD2	28:6:159:LYS:HE2	2.03	0.41
30:H:46:LEU:HA	30:H:51:ILE:HG12	2.03	0.41
32:R1:288:U:H2'	32:R1:289:G:H8	1.85	0.41
32:R1:581:C:H2'	32:R1:582:A:H8	1.84	0.41
32:R1:1387:A:H2'	32:R1:1388:G:C8	2.55	0.41
32:R1:1625:C:H2'	32:R1:1626:A:O4'	2.20	0.41
32:R1:2129:C:N4	32:R1:2159:G:O6	2.54	0.41
32:R1:2795:C:H2'	32:R1:2796:U:C6	2.56	0.41
34:R3:35:G:H2'	34:R3:36:C:C6	2.56	0.41
34:R3:154:U:H3'	34:R3:155:A:H8	1.86	0.41
34:R3:351:G:H8	34:R3:351:G:OP2	2.04	0.41
34:R3:665:A:H1'	34:R3:733:G:O4'	2.21	0.41
34:R3:1278:G:OP1	34:R3:1281:C:N4	2.53	0.41
13:23:6:ARG:O	13:23:10:VAL:HG23	2.20	0.41
32:R1:1069:A:O5'	32:R1:1070:A:H5'	2.20	0.41
32:R1:1125:G:OP2	32:R1:1126:A:O2'	2.33	0.41
32:R1:1180:U:H2'	32:R1:1181:U:O4'	2.21	0.41
32:R1:1490:A:H5'	32:R1:1491:G:OP2	2.21	0.41
32:R1:1992:G:N2	32:R1:1996:C:O2'	2.53	0.41
34:R3:1028:C:O2	34:R3:1031:C:O2'	2.30	0.41
34:R3:1206:G:C6	34:R3:1207:G:C5	3.09	0.41
1:1:27:ILE:HD12	1:1:185:LEU:HD12	2.02	0.41
3:14:2:ILE:HD12	3:14:6:THR:HG21	2.01	0.41
27:5:92:GLY:H	27:5:95:MET:HE2	1.85	0.41
27:5:103:ILE:HD12	27:5:175:PRO:HD3	2.03	0.41
28:6:11:PRO:HD2	28:6:14:VAL:CG2	2.43	0.41
28:6:44:HIS:HA	28:6:49:LEU:HD23	2.03	0.41
30:H:461:LEU:HD22	30:H:465:MET:HG3	2.03	0.41
32:R1:52:A:H2'	32:R1:53:A:C8	2.56	0.41
32:R1:1103:A:HO2'	32:R1:1104:C:P	2.44	0.41
32:R1:2127:G:H2'	32:R1:2128:G:C4	2.55	0.41
33:R2:31:C:H2'	33:R2:32:U:C6	2.55	0.41
34:R3:203:G:O2'	34:R3:465:A:N1	2.48	0.41
34:R3:1130:A:C8	34:R3:1146:A:N1	2.88	0.41
20:30:46:MET:O	20:30:50:VAL:HG22	2.20	0.41
21:32:31:LYS:HG2	21:32:50:GLY:HA3	2.01	0.41
27:5:3:LEU:HD11	27:5:100:GLU:HA	2.02	0.41
30:H:48:LYS:HD3	30:H:68:TRP:CD2	2.56	0.41
30:H:502:ASP:O	30:H:504:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:594:U:H2'	32:R1:595:C:C6	2.56	0.41
32:R1:720:U:H2'	32:R1:721:A:C8	2.56	0.41
32:R1:1035:U:H2'	32:R1:1036:G:H8	1.86	0.41
34:R3:231:U:H2'	34:R3:232:G:H8	1.86	0.41
34:R3:455:G:H2'	34:R3:456:A:C8	2.56	0.41
6:17:12:ARG:HG2	6:17:16:HIS:ND1	2.36	0.41
10:20:111:LYS:HB2	10:20:111:LYS:HE3	1.78	0.41
20:30:8:GLN:O	20:30:32:GLY:N	2.43	0.41
26:4:121:VAL:HG21	26:4:124:PHE:HB2	2.02	0.41
27:5:35:LEU:HD11	27:5:151:LEU:CD1	2.39	0.41
28:6:85:LYS:HB2	28:6:164:ALA:HB2	2.03	0.41
30:H:106:ASP:HB3	30:H:109:ALA:HB3	2.01	0.41
30:H:356:LYS:HB2	30:H:356:LYS:HE3	1.94	0.41
32:R1:352:A:H2'	32:R1:353:C:C6	2.56	0.41
32:R1:581:C:H2'	32:R1:582:A:C8	2.56	0.41
32:R1:613:A:H3'	32:R1:613:A:N3	2.36	0.41
32:R1:882:G:H1	32:R1:894:U:H3	1.68	0.41
32:R1:974:G:H8	32:R1:990:A:H62	1.67	0.41
32:R1:1231:U:H2'	32:R1:1232:G:H8	1.86	0.41
32:R1:1301:A:O2'	32:R1:1302:A:H3'	2.21	0.41
32:R1:2133:G:H2'	32:R1:2158:A:C2	2.56	0.41
33:R2:44:G:N2	33:R2:48:U:C2	2.88	0.41
34:R3:645:G:C2	34:R3:646:G:C8	3.09	0.41
34:R3:767:A:H2'	34:R3:768:A:O4'	2.20	0.41
34:R3:925:G:C2	34:R3:927:G:C8	3.09	0.41
34:R3:978:A:C4	34:R3:1319:A:C2	3.08	0.41
34:R3:1312:G:H2'	34:R3:1313:U:C6	2.56	0.41
34:R3:1413:A:H2	34:R3:1487:G:H22	1.69	0.41
7:18:55:GLU:H	7:18:55:GLU:HG3	1.68	0.41
9:2:198:GLU:H	9:2:198:GLU:HG2	1.72	0.41
27:5:25:MET:HB2	27:5:29:ARG:NH2	2.36	0.41
32:R1:154:U:H2'	32:R1:155:A:C8	2.56	0.41
32:R1:1380:G:O2'	32:R1:1569:A:N6	2.53	0.41
32:R1:2537:U:H2'	32:R1:2538:C:H6	1.86	0.41
34:R3:1512:U:H2'	34:R3:1513:A:C8	2.56	0.41
12:22:51:LEU:HD13	12:22:105:VAL:HG11	2.03	0.40
30:H:333:LEU:HD12	30:H:334:ASN:H	1.86	0.40
30:H:405:GLU:CG	30:H:406:LEU:H	2.32	0.40
32:R1:191:A:H2'	32:R1:192:C:H6	1.84	0.40
32:R1:544:C:H2'	32:R1:545:U:O4'	2.21	0.40
32:R1:742:A:H2'	32:R1:743:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:1387:A:H2'	32:R1:1388:G:H8	1.86	0.40
32:R1:2655:G:O2'	32:R1:2664:G:O6	2.30	0.40
34:R3:109:A:H5'	34:R3:110:C:H5	1.86	0.40
34:R3:204:G:H2'	34:R3:205:A:C8	2.56	0.40
34:R3:206:C:H2'	34:R3:207:C:O4'	2.20	0.40
34:R3:553:A:H2'	34:R3:554:A:C8	2.56	0.40
34:R3:908:A:H2'	34:R3:909:A:C8	2.56	0.40
8:19:36:LYS:H	8:19:36:LYS:HG3	1.66	0.40
27:5:144:LYS:HE2	27:5:144:LYS:HB2	1.81	0.40
28:6:117:PRO:CD	28:6:120:ILE:HD13	2.42	0.40
29:9:83:LYS:HA	29:9:149:GLU:HG3	2.03	0.40
30:H:452:LEU:HD23	30:H:452:LEU:HA	1.79	0.40
32:R1:44:A:H2'	32:R1:45:G:O4'	2.21	0.40
32:R1:463:G:N2	32:R1:466:A:OP2	2.38	0.40
32:R1:545:U:H2'	32:R1:548:G:O6	2.21	0.40
32:R1:2109:U:H2'	32:R1:2110:G:C8	2.56	0.40
33:R2:32:U:C2	33:R2:51:G:N2	2.89	0.40
34:R3:321:A:H2'	34:R3:322:C:H6	1.86	0.40
34:R3:1157:A:C2	34:R3:1181:G:C4	3.08	0.40
34:R3:1198:G:H2'	34:R3:1199:U:C6	2.56	0.40
34:R3:1353:G:H2'	34:R3:1354:U:H6	1.86	0.40
5:16:59:ARG:HG3	5:16:60:GLN:HB3	2.03	0.40
12:22:20:VAL:HG21	12:22:43:ALA:HB3	2.04	0.40
29:9:1:MET:HB3	29:9:2:GLN:H	1.76	0.40
32:R1:1254:A:H5"	32:R1:1255:U:H5"	2.03	0.40
32:R1:1689:A:H2'	32:R1:1690:A:C8	2.57	0.40
32:R1:2861:U:H2'	32:R1:2862:G:C8	2.56	0.40
34:R3:779:C:H2'	34:R3:780:A:O4'	2.22	0.40
7:18:26:LEU:HA	7:18:38:GLN:O	2.22	0.40
26:4:141:MET:HE2	26:4:141:MET:HB2	1.94	0.40
29:9:143:ILE:HD13	29:9:143:ILE:HA	1.93	0.40
30:H:149:ASP:HB2	57:H:601:ATP:C5	2.57	0.40
30:H:310:ASN:HD22	30:H:310:ASN:C	2.25	0.40
30:H:486:ASP:OD1	30:H:486:ASP:N	2.55	0.40
32:R1:222:A:N6	32:R1:232:G:H1'	2.36	0.40
32:R1:421:C:O2'	32:R1:422:A:P	2.80	0.40
32:R1:933:A:H5"	32:R1:934:U:OP2	2.22	0.40
32:R1:1103:A:OP2	32:R1:1104:C:N4	2.51	0.40
32:R1:1328:A:H2'	32:R1:1330:C:C5	2.57	0.40
32:R1:1484:U:H2'	32:R1:1485:U:C6	2.57	0.40
32:R1:2350:C:H2'	32:R1:2351:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R1:2430:A:H5'	32:R1:2431:U:OP2	2.22	0.40
34:R3:335:C:H2'	34:R3:336:A:H8	1.86	0.40
34:R3:950:U:H2'	34:R3:951:G:C8	2.56	0.40
34:R3:1027:C:H2'	34:R3:1028:C:H4'	2.03	0.40
34:R3:1143:G:C2	34:R3:1144:G:C5	3.10	0.40
34:R3:1308:U:H2'	34:R3:1309:G:C8	2.56	0.40
2:13:17:VAL:HG22	2:13:55:ILE:HB	2.03	0.40
2:13:19:ASP:OD1	2:13:21:THR:HG23	2.21	0.40
6:17:55:ALA:HA	6:17:80:PHE:CE1	2.57	0.40
9:2:74:PRO:HB2	9:2:114:GLN:HE21	1.87	0.40
12:22:51:LEU:O	12:22:55:ILE:HG12	2.21	0.40
14:24:55:GLY:O	32:R1:483:A:O2'	2.40	0.40
18:29:9:LYS:HE3	18:29:12:GLU:H	1.87	0.40
20:30:23:LEU:HD11	20:30:53:MET:SD	2.62	0.40
21:32:11:LYS:HE3	21:32:11:LYS:HB3	1.78	0.40
28:6:3:VAL:HG12	28:6:68:ARG:HD2	2.02	0.40
32:R1:7:G:H2'	32:R1:8:C:C6	2.56	0.40
32:R1:395:U:H2'	32:R1:396:G:N7	2.36	0.40
32:R1:1409:U:H2'	32:R1:1410:G:H8	1.87	0.40
32:R1:2134:A:H1'	32:R1:2159:G:H1'	2.03	0.40
32:R1:2584:U:H2'	32:R1:2585:U:H2'	2.04	0.40
34:R3:423:G:N2	34:R3:424:G:N3	2.69	0.40
34:R3:455:G:H2'	34:R3:456:A:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	218/220 (99%)	196 (90%)	22 (10%)	0	100	100
2	13	140/142 (99%)	135 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	14	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16 48
4	15	141/143 (99%)	131 (93%)	10 (7%)	0	100 100
5	16	134/136 (98%)	125 (93%)	9 (7%)	0	100 100
6	17	118/120 (98%)	109 (92%)	9 (8%)	0	100 100
7	18	114/116 (98%)	108 (95%)	6 (5%)	0	100 100
8	19	112/114 (98%)	105 (94%)	7 (6%)	0	100 100
9	2	269/271 (99%)	247 (92%)	22 (8%)	0	100 100
10	20	115/117 (98%)	113 (98%)	2 (2%)	0	100 100
11	21	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	13 42
12	22	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14 45
13	23	91/93 (98%)	78 (86%)	13 (14%)	0	100 100
14	24	100/102 (98%)	92 (92%)	7 (7%)	1 (1%)	13 42
15	25	92/94 (98%)	92 (100%)	0	0	100 100
16	27	73/75 (97%)	71 (97%)	2 (3%)	0	100 100
17	28	75/77 (97%)	73 (97%)	2 (3%)	0	100 100
18	29	61/63 (97%)	55 (90%)	6 (10%)	0	100 100
19	3	207/209 (99%)	193 (93%)	14 (7%)	0	100 100
20	30	56/58 (97%)	52 (93%)	4 (7%)	0	100 100
21	32	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	6 27
22	33	48/50 (96%)	43 (90%)	5 (10%)	0	100 100
23	34	44/46 (96%)	44 (100%)	0	0	100 100
24	35	62/64 (97%)	58 (94%)	4 (6%)	0	100 100
25	36	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
26	4	199/201 (99%)	188 (94%)	11 (6%)	0	100 100
27	5	175/177 (99%)	166 (95%)	9 (5%)	0	100 100
28	6	174/176 (99%)	160 (92%)	14 (8%)	0	100 100
29	9	147/149 (99%)	122 (83%)	24 (16%)	1 (1%)	19 51
30	H	524/526 (100%)	454 (87%)	69 (13%)	1 (0%)	44 74
36	sb	216/218 (99%)	194 (90%)	21 (10%)	1 (0%)	25 58
37	sc	204/206 (99%)	195 (96%)	9 (4%)	0	100 100
38	sd	203/205 (99%)	177 (87%)	26 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	se	155/157 (99%)	132 (85%)	21 (14%)	2 (1%)	10 36
40	sf	98/100 (98%)	85 (87%)	13 (13%)	0	100 100
41	sg	149/151 (99%)	138 (93%)	11 (7%)	0	100 100
42	sh	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
43	si	125/127 (98%)	106 (85%)	19 (15%)	0	100 100
44	sj	96/98 (98%)	89 (93%)	7 (7%)	0	100 100
45	sk	114/116 (98%)	102 (90%)	12 (10%)	0	100 100
46	sl	121/123 (98%)	91 (75%)	29 (24%)	1 (1%)	16 48
47	sm	112/114 (98%)	100 (89%)	12 (11%)	0	100 100
48	sn	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	13 42
49	so	86/88 (98%)	80 (93%)	6 (7%)	0	100 100
50	sp	80/82 (98%)	71 (89%)	9 (11%)	0	100 100
51	sq	78/80 (98%)	70 (90%)	8 (10%)	0	100 100
52	sr	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
53	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100 100
54	st	83/85 (98%)	82 (99%)	1 (1%)	0	100 100
55	su	63/65 (97%)	51 (81%)	11 (18%)	1 (2%)	8 31
All	All	6256/6356 (98%)	5688 (91%)	555 (9%)	13 (0%)	45 74

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	14	110	GLU
55	su	36	PHE
36	sb	18	GLN
39	se	121	ASN
39	se	122	VAL
48	sn	2	LYS
21	32	25	THR
12	22	6	LYS
14	24	88	ASP
30	H	122	ALA
29	9	9	VAL
11	21	51	VAL
46	sl	86	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	106/171 (62%)	103 (97%)	3 (3%)	38	66
2	13	116/116 (100%)	115 (99%)	1 (1%)	75	88
3	14	103/103 (100%)	102 (99%)	1 (1%)	73	86
4	15	102/102 (100%)	99 (97%)	3 (3%)	37	65
5	16	109/109 (100%)	104 (95%)	5 (5%)	23	52
6	17	100/100 (100%)	99 (99%)	1 (1%)	73	86
7	18	86/86 (100%)	85 (99%)	1 (1%)	67	83
8	19	99/99 (100%)	95 (96%)	4 (4%)	27	58
9	2	216/216 (100%)	208 (96%)	8 (4%)	29	59
10	20	89/89 (100%)	87 (98%)	2 (2%)	47	71
11	21	84/84 (100%)	81 (96%)	3 (4%)	30	60
12	22	93/93 (100%)	91 (98%)	2 (2%)	47	71
13	23	80/80 (100%)	78 (98%)	2 (2%)	42	69
14	24	83/83 (100%)	80 (96%)	3 (4%)	30	60
15	25	78/78 (100%)	75 (96%)	3 (4%)	28	59
16	27	57/57 (100%)	55 (96%)	2 (4%)	31	61
17	28	67/67 (100%)	66 (98%)	1 (2%)	60	80
18	29	55/55 (100%)	53 (96%)	2 (4%)	30	60
19	3	164/164 (100%)	160 (98%)	4 (2%)	44	70
20	30	48/48 (100%)	48 (100%)	0	100	100
21	32	47/47 (100%)	46 (98%)	1 (2%)	48	72
22	33	45/45 (100%)	42 (93%)	3 (7%)	13	40
23	34	38/38 (100%)	36 (95%)	2 (5%)	19	48
24	35	51/51 (100%)	50 (98%)	1 (2%)	50	74
25	36	34/34 (100%)	32 (94%)	2 (6%)	16	44
26	4	165/165 (100%)	163 (99%)	2 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	5	148/148 (100%)	142 (96%)	6 (4%)	26 57
28	6	137/137 (100%)	134 (98%)	3 (2%)	47 71
29	9	114/114 (100%)	112 (98%)	2 (2%)	54 76
30	H	443/443 (100%)	428 (97%)	15 (3%)	32 62
36	sb	180/180 (100%)	175 (97%)	5 (3%)	38 66
37	sc	170/170 (100%)	167 (98%)	3 (2%)	54 76
38	sd	172/172 (100%)	168 (98%)	4 (2%)	45 70
39	se	119/119 (100%)	118 (99%)	1 (1%)	79 89
40	sf	87/87 (100%)	86 (99%)	1 (1%)	70 84
41	sg	124/124 (100%)	121 (98%)	3 (2%)	44 70
42	sh	104/104 (100%)	101 (97%)	3 (3%)	37 65
43	si	105/105 (100%)	99 (94%)	6 (6%)	17 46
44	sj	86/86 (100%)	86 (100%)	0	100 100
45	sk	89/89 (100%)	89 (100%)	0	100 100
46	sl	103/103 (100%)	100 (97%)	3 (3%)	37 65
47	sm	92/92 (100%)	91 (99%)	1 (1%)	70 84
48	sn	83/83 (100%)	81 (98%)	2 (2%)	44 70
49	so	76/76 (100%)	71 (93%)	5 (7%)	14 41
50	sp	65/65 (100%)	65 (100%)	0	100 100
51	sq	74/74 (100%)	73 (99%)	1 (1%)	62 81
52	sr	56/56 (100%)	56 (100%)	0	100 100
53	ss	70/70 (100%)	69 (99%)	1 (1%)	62 81
54	st	65/65 (100%)	65 (100%)	0	100 100
55	su	55/55 (100%)	49 (89%)	6 (11%)	5 21
All	All	5132/5197 (99%)	4999 (97%)	133 (3%)	42 68

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	38	PHE
1	1	183	ASP
1	1	208	TYR
2	13	96	ARG
3	14	73	ASP

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Mol	Chain	Res	Type
4	15	59	ARG
4	15	78	ARG
4	15	84	LYS
5	16	1	MET
5	16	6	ARG
5	16	25	ASP
5	16	106	ASP
5	16	123	LYS
6	17	118	ARG
7	18	102	ARG
8	19	36	LYS
8	19	65	ASN
8	19	81	ASP
8	19	110	LYS
9	2	113	ASP
9	2	116	GLN
9	2	166	ARG
9	2	167	ASP
9	2	212	TRP
9	2	252	LYS
9	2	259	ASN
9	2	268	ARG
10	20	27	ARG
10	20	29	ARG
11	21	68	ARG
11	21	95	ASP
11	21	102	SER
12	22	62	ASP
12	22	86	MET
13	23	37	ASP
13	23	77	ARG
14	24	7	ASP
14	24	20	LYS
14	24	80	ASP
15	25	50	MET
15	25	51	GLN
15	25	53	LYS
16	27	35	SER
16	27	55	ARG
17	28	71	ARG
18	29	1	MET
18	29	25	GLN

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Mol	Chain	Res	Type
19	3	1	MET
19	3	18	ASP
19	3	55	LYS
19	3	114	LYS
21	32	39	ARG
22	33	10	LEU
22	33	25	ASN
22	33	36	LYS
23	34	15	SER
23	34	25	LYS
24	35	30	HIS
25	36	6	SER
25	36	30	GLU
26	4	21	ARG
26	4	139	LYS
27	5	13	LYS
27	5	37	MET
27	5	76	PHE
27	5	86	CYS
27	5	160	LYS
27	5	172	PHE
28	6	72	ASN
28	6	132	LEU
28	6	151	ARG
29	9	42	LYS
29	9	50	ARG
30	H	70	ASN
30	H	100	ASP
30	H	150	PHE
30	H	156	MET
30	H	167	ARG
30	H	190	LYS
30	H	232	SER
30	H	254	GLU
30	H	310	ASN
30	H	322	TYR
30	H	332	LYS
30	H	340	ARG
30	H	380	PHE
30	H	430	ARG
30	H	480	LEU
36	sb	22	TRP

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Mol	Chain	Res	Type
36	sb	31	PHE
36	sb	49	PHE
36	sb	62	ARG
36	sb	222	GLU
37	sc	17	TRP
37	sc	79	LYS
37	sc	168	ARG
38	sd	30	LYS
38	sd	62	ARG
38	sd	80	ARG
38	sd	145	ARG
39	se	137	ARG
40	sf	93	LYS
41	sg	4	ARG
41	sg	24	LYS
41	sg	73	GLU
42	sh	3	GLN
42	sh	46	GLU
42	sh	126	CYS
43	si	33	SER
43	si	38	PHE
43	si	45	MET
43	si	56	MET
43	si	94	ARG
43	si	96	GLU
46	sl	11	ARG
46	sl	49	ARG
46	sl	103	CYS
47	sm	106	ARG
48	sn	37	ASP
48	sn	60	ARG
49	so	19	ASN
49	so	20	ASP
49	so	34	GLN
49	so	86	LEU
49	so	88	ARG
51	sq	26	ARG
53	ss	54	ARG
55	su	11	PHE
55	su	16	ARG
55	su	24	LYS
55	su	32	ARG

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Mol	Chain	Res	Type
55	su	36	PHE
55	su	37	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	168	ASN
30	H	347	ASN
30	H	459	ASN
47	sm	99	GLN
54	st	20	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	M	8/9 (88%)	0	0
32	R1	2902/2903 (99%)	454 (15%)	13 (0%)
33	R2	118/119 (99%)	17 (14%)	1 (0%)
34	R3	1538/1539 (99%)	272 (17%)	5 (0%)
35	T	75/78 (96%)	21 (28%)	4 (5%)
All	All	4641/4648 (99%)	764 (16%)	23 (0%)

All (764) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	R1	10	A
32	R1	14	A
32	R1	15	G
32	R1	35	G
32	R1	36	G
32	R1	46	G
32	R1	51	G
32	R1	63	A
32	R1	71	A
32	R1	74	A
32	R1	75	G
32	R1	100	U
32	R1	102	U
32	R1	118	A
32	R1	119	A

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Mol	Chain	Res	Type
32	R1	120	U
32	R1	138	U
32	R1	139	U
32	R1	140	C
32	R1	153	U
32	R1	162	U
32	R1	163	C
32	R1	181	A
32	R1	196	A
32	R1	199	A
32	R1	215	G
32	R1	216	A
32	R1	218	A
32	R1	219	A
32	R1	222	A
32	R1	224	U
32	R1	228	C
32	R1	230	G
32	R1	233	A
32	R1	248	G
32	R1	255	A
32	R1	266	G
32	R1	276	U
32	R1	323	C
32	R1	324	A
32	R1	329	G
32	R1	330	A
32	R1	353	C
32	R1	361	G
32	R1	362	A
32	R1	363	G
32	R1	369	U
32	R1	371	A
32	R1	372	G
32	R1	373	U
32	R1	386	G
32	R1	387	U
32	R1	395	U
32	R1	396	G
32	R1	404	A
32	R1	405	U
32	R1	406	G

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Mol	Chain	Res	Type
32	R1	411	G
32	R1	417	C
32	R1	422	A
32	R1	424	G
32	R1	443	A
32	R1	448	U
32	R1	457	A
32	R1	473	G
32	R1	481	G
32	R1	490	C
32	R1	491	G
32	R1	504	A
32	R1	505	A
32	R1	509	C
32	R1	510	C
32	R1	530	G
32	R1	531	C
32	R1	532	A
32	R1	545	U
32	R1	546	U
32	R1	548	G
32	R1	562	U
32	R1	563	A
32	R1	573	U
32	R1	575	A
32	R1	586	A
32	R1	603	A
32	R1	614	A
32	R1	627	A
32	R1	637	A
32	R1	645	C
32	R1	647	G
32	R1	654	A
32	R1	655	A
32	R1	669	G
32	R1	685	A
32	R1	686	U
32	R1	696	G
32	R1	705	A
32	R1	710	U
32	R1	711	G
32	R1	722	A

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Mol	Chain	Res	Type
32	R1	729	G
32	R1	730	A
32	R1	738	G
32	R1	747	U
32	R1	748	G
32	R1	752	A
32	R1	764	A
32	R1	765	C
32	R1	775	G
32	R1	776	G
32	R1	782	A
32	R1	784	G
32	R1	785	G
32	R1	805	G
32	R1	812	C
32	R1	819	A
32	R1	827	U
32	R1	828	U
32	R1	830	G
32	R1	845	A
32	R1	846	U
32	R1	847	U
32	R1	858	G
32	R1	859	G
32	R1	866	A
32	R1	879	G
32	R1	886	A
32	R1	887	U
32	R1	888	C
32	R1	891	G
32	R1	893	C
32	R1	894	U
32	R1	896	A
32	R1	897	C
32	R1	910	A
32	R1	931	U
32	R1	941	A
32	R1	945	A
32	R1	946	C
32	R1	961	C
32	R1	974	G
32	R1	983	A

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Mol	Chain	Res	Type
32	R1	990	A
32	R1	995	C
32	R1	996	A
32	R1	1005	C
32	R1	1008	A
32	R1	1009	A
32	R1	1012	U
32	R1	1013	C
32	R1	1021	A
32	R1	1022	G
32	R1	1026	G
32	R1	1033	U
32	R1	1040	A
32	R1	1046	A
32	R1	1047	G
32	R1	1048	A
32	R1	1049	C
32	R1	1055	G
32	R1	1059	G
32	R1	1060	U
32	R1	1061	U
32	R1	1062	G
32	R1	1063	G
32	R1	1064	C
32	R1	1065	U
32	R1	1066	U
32	R1	1069	A
32	R1	1070	A
32	R1	1071	G
32	R1	1072	C
32	R1	1076	C
32	R1	1077	A
32	R1	1078	U
32	R1	1079	C
32	R1	1080	A
32	R1	1081	U
32	R1	1082	U
32	R1	1083	U
32	R1	1085	A
32	R1	1088	A
32	R1	1089	A
32	R1	1090	A

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Mol	Chain	Res	Type
32	R1	1095	A
32	R1	1096	A
32	R1	1097	U
32	R1	1104	C
32	R1	1106	G
32	R1	1110	G
32	R1	1111	A
32	R1	1112	G
32	R1	1132	U
32	R1	1133	A
32	R1	1135	C
32	R1	1139	G
32	R1	1142	A
32	R1	1174	U
32	R1	1175	A
32	R1	1176	U
32	R1	1178	C
32	R1	1180	U
32	R1	1206	G
32	R1	1212	G
32	R1	1237	A
32	R1	1250	G
32	R1	1253	A
32	R1	1256	G
32	R1	1258	U
32	R1	1271	G
32	R1	1272	A
32	R1	1300	G
32	R1	1301	A
32	R1	1311	G
32	R1	1345	C
32	R1	1352	U
32	R1	1365	A
32	R1	1368	G
32	R1	1378	A
32	R1	1379	U
32	R1	1383	A
32	R1	1395	A
32	R1	1416	G
32	R1	1417	C
32	R1	1427	A
32	R1	1428	C

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Mol	Chain	Res	Type
32	R1	1452	G
32	R1	1455	G
32	R1	1460	U
32	R1	1461	C
32	R1	1482	G
32	R1	1490	A
32	R1	1494	A
32	R1	1507	C
32	R1	1508	A
32	R1	1515	A
32	R1	1519	G
32	R1	1522	A
32	R1	1523	U
32	R1	1524	G
32	R1	1535	A
32	R1	1536	C
32	R1	1537	G
32	R1	1542	U
32	R1	1554	U
32	R1	1559	U
32	R1	1560	G
32	R1	1569	A
32	R1	1578	U
32	R1	1583	A
32	R1	1584	U
32	R1	1608	A
32	R1	1610	A
32	R1	1647	U
32	R1	1648	U
32	R1	1649	G
32	R1	1654	A
32	R1	1674	G
32	R1	1675	C
32	R1	1694	C
32	R1	1715	G
32	R1	1729	U
32	R1	1730	C
32	R1	1733	G
32	R1	1735	A
32	R1	1738	G
32	R1	1744	A
32	R1	1758	U

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Mol	Chain	Res	Type
32	R1	1764	C
32	R1	1773	A
32	R1	1776	G
32	R1	1800	C
32	R1	1801	A
32	R1	1802	A
32	R1	1808	A
32	R1	1811	G
32	R1	1816	C
32	R1	1829	A
32	R1	1870	C
32	R1	1871	A
32	R1	1873	G
32	R1	1884	G
32	R1	1890	A
32	R1	1896	G
32	R1	1906	G
32	R1	1910	G
32	R1	1914	C
32	R1	1929	G
32	R1	1930	G
32	R1	1936	A
32	R1	1937	A
32	R1	1938	A
32	R1	1955	U
32	R1	1966	A
32	R1	1967	C
32	R1	1970	A
32	R1	1971	U
32	R1	1972	G
32	R1	1975	G
32	R1	1991	U
32	R1	1993	U
32	R1	1996	C
32	R1	1997	C
32	R1	2022	U
32	R1	2023	C
32	R1	2031	A
32	R1	2033	A
32	R1	2036	C
32	R1	2043	C
32	R1	2055	C

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Mol	Chain	Res	Type
32	R1	2056	G
32	R1	2060	A
32	R1	2061	G
32	R1	2063	C
32	R1	2069	G
32	R1	2093	G
32	R1	2110	G
32	R1	2111	U
32	R1	2112	G
32	R1	2113	U
32	R1	2114	A
32	R1	2115	G
32	R1	2117	A
32	R1	2118	U
32	R1	2119	A
32	R1	2120	G
32	R1	2121	G
32	R1	2122	U
32	R1	2123	G
32	R1	2124	G
32	R1	2126	A
32	R1	2128	G
32	R1	2131	U
32	R1	2132	U
32	R1	2133	G
32	R1	2136	G
32	R1	2139	U
32	R1	2145	C
32	R1	2146	C
32	R1	2148	G
32	R1	2149	U
32	R1	2151	U
32	R1	2157	G
32	R1	2160	C
32	R1	2165	C
32	R1	2166	U
32	R1	2170	A
32	R1	2171	A
32	R1	2172	U
32	R1	2173	A
32	R1	2176	A
32	R1	2177	C

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Mol	Chain	Res	Type
32	R1	2178	C
32	R1	2182	U
32	R1	2188	U
32	R1	2189	U
32	R1	2198	A
32	R1	2204	G
32	R1	2211	A
32	R1	2213	U
32	R1	2225	A
32	R1	2226	C
32	R1	2238	G
32	R1	2239	G
32	R1	2246	G
32	R1	2250	G
32	R1	2266	A
32	R1	2283	C
32	R1	2286	G
32	R1	2287	A
32	R1	2288	A
32	R1	2301	C
32	R1	2304	G
32	R1	2305	U
32	R1	2307	G
32	R1	2309	A
32	R1	2320	U
32	R1	2322	A
32	R1	2325	G
32	R1	2327	A
32	R1	2333	A
32	R1	2335	A
32	R1	2345	G
32	R1	2347	C
32	R1	2350	C
32	R1	2361	G
32	R1	2383	G
32	R1	2385	C
32	R1	2396	G
32	R1	2402	U
32	R1	2406	A
32	R1	2423	U
32	R1	2429	G
32	R1	2430	A

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Mol	Chain	Res	Type
32	R1	2441	U
32	R1	2448	A
32	R1	2470	G
32	R1	2475	C
32	R1	2476	A
32	R1	2491	U
32	R1	2498	C
32	R1	2502	G
32	R1	2503	A
32	R1	2504	U
32	R1	2505	G
32	R1	2506	U
32	R1	2507	C
32	R1	2518	A
32	R1	2520	C
32	R1	2529	G
32	R1	2547	A
32	R1	2554	U
32	R1	2566	A
32	R1	2567	G
32	R1	2572	A
32	R1	2573	C
32	R1	2574	G
32	R1	2585	U
32	R1	2602	A
32	R1	2609	U
32	R1	2613	U
32	R1	2615	U
32	R1	2629	U
32	R1	2646	C
32	R1	2661	G
32	R1	2682	A
32	R1	2689	U
32	R1	2690	U
32	R1	2732	G
32	R1	2733	A
32	R1	2744	G
32	R1	2748	A
32	R1	2760	C
32	R1	2764	A
32	R1	2765	A
32	R1	2776	A

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Mol	Chain	Res	Type
32	R1	2778	A
32	R1	2779	U
32	R1	2791	G
32	R1	2798	U
32	R1	2799	A
32	R1	2800	A
32	R1	2807	U
32	R1	2808	G
32	R1	2820	A
32	R1	2833	U
32	R1	2849	U
32	R1	2861	U
32	R1	2867	G
32	R1	2873	A
32	R1	2880	C
32	R1	2883	A
32	R1	2884	U
32	R1	2891	U
32	R1	2901	C
33	R2	9	G
33	R2	12	C
33	R2	13	G
33	R2	30	C
33	R2	35	C
33	R2	38	C
33	R2	44	G
33	R2	45	A
33	R2	52	A
33	R2	66	A
33	R2	67	G
33	R2	87	U
33	R2	89	U
33	R2	90	C
33	R2	108	A
33	R2	109	A
33	R2	119	A
34	R3	4	U
34	R3	6	G
34	R3	7	A
34	R3	9	G
34	R3	13	U
34	R3	32	A

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Mol	Chain	Res	Type
34	R3	39	G
34	R3	47	C
34	R3	48	C
34	R3	51	A
34	R3	64	G
34	R3	70	U
34	R3	71	A
34	R3	72	A
34	R3	73	C
34	R3	80	A
34	R3	81	A
34	R3	82	G
34	R3	83	C
34	R3	84	U
34	R3	85	U
34	R3	86	G
34	R3	88	U
34	R3	89	U
34	R3	91	U
34	R3	94	G
34	R3	95	C
34	R3	98	A
34	R3	121	U
34	R3	130	A
34	R3	131	A
34	R3	135	C
34	R3	141	G
34	R3	153	C
34	R3	155	A
34	R3	156	C
34	R3	164	G
34	R3	170	U
34	R3	173	U
34	R3	188	C
34	R3	190	A
34	R3	197	A
34	R3	199	A
34	R3	208	U
34	R3	209	U
34	R3	210	C
34	R3	211	G
34	R3	212	G

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Mol	Chain	Res	Type
34	R3	214	C
34	R3	216	U
34	R3	226	G
34	R3	240	G
34	R3	245	U
34	R3	247	G
34	R3	251	G
34	R3	265	G
34	R3	266	G
34	R3	267	C
34	R3	281	G
34	R3	289	G
34	R3	292	G
34	R3	306	A
34	R3	321	A
34	R3	328	C
34	R3	330	C
34	R3	341	C
34	R3	344	A
34	R3	347	G
34	R3	351	G
34	R3	352	C
34	R3	354	G
34	R3	367	U
34	R3	372	C
34	R3	382	A
34	R3	391	G
34	R3	392	C
34	R3	394	G
34	R3	398	U
34	R3	404	G
34	R3	406	G
34	R3	411	A
34	R3	412	A
34	R3	413	G
34	R3	414	A
34	R3	415	A
34	R3	420	U
34	R3	421	U
34	R3	422	C
34	R3	423	G
34	R3	425	G

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Mol	Chain	Res	Type
34	R3	429	U
34	R3	438	U
34	R3	442	G
34	R3	448	A
34	R3	457	G
34	R3	458	U
34	R3	459	A
34	R3	460	A
34	R3	463	U
34	R3	464	U
34	R3	465	A
34	R3	466	A
34	R3	467	U
34	R3	468	A
34	R3	472	U
34	R3	475	C
34	R3	476	U
34	R3	479	U
34	R3	480	U
34	R3	482	A
34	R3	484	G
34	R3	485	U
34	R3	486	U
34	R3	491	G
34	R3	492	C
34	R3	495	A
34	R3	497	G
34	R3	500	G
34	R3	511	C
34	R3	518	C
34	R3	521	G
34	R3	524	G
34	R3	527	G
34	R3	529	G
34	R3	531	U
34	R3	532	A
34	R3	535	A
34	R3	547	A
34	R3	549	C
34	R3	561	U
34	R3	564	C
34	R3	566	G

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Mol	Chain	Res	Type
34	R3	572	A
34	R3	573	A
34	R3	575	G
34	R3	576	C
34	R3	577	G
34	R3	579	A
34	R3	614	C
34	R3	615	G
34	R3	616	G
34	R3	621	A
34	R3	633	G
34	R3	654	G
34	R3	665	A
34	R3	682	G
34	R3	695	A
34	R3	703	G
34	R3	721	G
34	R3	723	U
34	R3	724	G
34	R3	731	G
34	R3	755	G
34	R3	760	G
34	R3	777	A
34	R3	781	A
34	R3	794	A
34	R3	815	A
34	R3	817	C
34	R3	818	G
34	R3	819	A
34	R3	821	G
34	R3	829	G
34	R3	832	G
34	R3	842	U
34	R3	843	U
34	R3	846	G
34	R3	851	G
34	R3	858	G
34	R3	872	A
34	R3	902	G
34	R3	914	A
34	R3	934	C
34	R3	935	A

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Mol	Chain	Res	Type
34	R3	945	G
34	R3	946	A
34	R3	947	G
34	R3	953	G
34	R3	960	U
34	R3	961	U
34	R3	965	U
34	R3	966	G
34	R3	969	A
34	R3	971	G
34	R3	975	A
34	R3	976	G
34	R3	977	A
34	R3	992	U
34	R3	993	G
34	R3	998	C
34	R3	1004	A
34	R3	1012	A
34	R3	1020	G
34	R3	1025	U
34	R3	1028	C
34	R3	1029	U
34	R3	1031	C
34	R3	1032	G
34	R3	1033	G
34	R3	1034	G
34	R3	1036	A
34	R3	1038	C
34	R3	1045	C
34	R3	1053	G
34	R3	1064	G
34	R3	1065	U
34	R3	1066	C
34	R3	1094	G
34	R3	1101	A
34	R3	1136	C
34	R3	1137	C
34	R3	1138	G
34	R3	1139	G
34	R3	1143	G
34	R3	1152	A
34	R3	1158	C

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Mol	Chain	Res	Type
34	R3	1159	U
34	R3	1168	U
34	R3	1169	A
34	R3	1182	G
34	R3	1184	G
34	R3	1196	A
34	R3	1212	U
34	R3	1225	A
34	R3	1227	A
34	R3	1238	A
34	R3	1241	G
34	R3	1250	A
34	R3	1256	A
34	R3	1258	G
34	R3	1261	A
34	R3	1270	G
34	R3	1275	A
34	R3	1278	G
34	R3	1279	G
34	R3	1280	A
34	R3	1282	C
34	R3	1285	A
34	R3	1286	U
34	R3	1287	A
34	R3	1290	G
34	R3	1298	U
34	R3	1300	G
34	R3	1302	C
34	R3	1315	U
34	R3	1317	C
34	R3	1340	A
34	R3	1346	A
34	R3	1363	A
34	R3	1370	G
34	R3	1378	C
34	R3	1379	G
34	R3	1381	U
34	R3	1405	G
34	R3	1419	G
34	R3	1441	A
34	R3	1446	A
34	R3	1448	C

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Mol	Chain	Res	Type
34	R3	1451	U
34	R3	1452	C
34	R3	1453	G
34	R3	1487	G
34	R3	1497	G
34	R3	1499	A
34	R3	1502	A
34	R3	1506	U
34	R3	1517	G
34	R3	1529	G
34	R3	1530	G
34	R3	1533	C
34	R3	1535	C
34	R3	1536	C
35	T	1	G
35	T	5	G
35	T	8	4SU
35	T	9	G
35	T	10	A
35	T	12	C
35	T	15	C
35	T	16	C
35	T	17	U
35	T	18	G
35	T	19	G
35	T	20	H2U
35	T	21	A
35	T	31	G
35	T	33	U
35	T	45	G
35	T	47	U
35	T	54	5MU
35	T	55	PSU
35	T	56	C
35	T	60	U

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	R1	227	A
32	R1	372	G
32	R1	421	C

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Mol	Chain	Res	Type
32	R1	704	G
32	R1	774	G
32	R1	784	G
32	R1	1020	A
32	R1	1103	A
32	R1	1173	U
32	R1	1236	G
32	R1	2164	C
32	R1	2326	C
32	R1	2503	A
33	R2	66	A
34	R3	391	G
34	R3	945	G
34	R3	1168	U
34	R3	1183	U
34	R3	1297	G
35	T	8	4SU
35	T	17	U
35	T	20	H2U
35	T	55	PSU

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

6 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	$\#\|Z\| > 2$
35	H2U	T	20	35	18,21,22	4.46	5 (27%)	19,30,33	3.90	6 (31%)
35	4OC	T	32	35	20,23,24	2.59	5 (25%)	25,32,35	1.69	6 (24%)
35	FME	T	101	35	8,9,10	0.97	0	8,9,11	0.85	0
35	PSU	T	55	35	18,21,22	2.27	7 (38%)	21,30,33	1.75	4 (19%)
35	5MU	T	54	35	19,22,23	2.18	8 (42%)	27,32,35	2.26	6 (22%)
35	4SU	T	8	35	18,21,22	3.89	6 (33%)	25,30,33	2.31	7 (28%)

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
35	H2U	T	20	35	2/2/8/9	3/7/38/39	0/2/2/2
35	4OC	T	32	35	2/2/5/6	4/9/29/30	0/2/2/2
35	FME	T	101	35	-	3/7/9/11	-
35	PSU	T	55	35	1/1/5/5	1/7/25/26	0/2/2/2
35	5MU	T	54	35	1/1/5/5	3/7/25/26	0/2/2/2
35	4SU	T	8	35	2/2/5/5	3/7/25/26	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	20	H2U	O4-C4	10.35	1.43	1.23
35	T	8	4SU	O2-C2	10.20	1.41	1.23
35	T	8	4SU	C4-S4	9.62	1.86	1.68
35	T	20	H2U	C2-N1	9.50	1.48	1.35
35	T	32	4OC	O2-C2	8.87	1.40	1.23
35	T	20	H2U	O2-C2	8.69	1.38	1.23
35	T	20	H2U	C2-N3	7.11	1.50	1.38
35	T	20	H2U	C4-N3	5.51	1.46	1.37
35	T	8	4SU	C2-N1	-5.44	1.29	1.38
35	T	55	PSU	C6-C5	4.86	1.40	1.35
35	T	32	4OC	C4-N4	4.49	1.45	1.36
35	T	8	4SU	C4-N3	-4.42	1.33	1.37
35	T	32	4OC	C2-N1	-4.34	1.31	1.40
35	T	54	5MU	C2-N1	-4.31	1.31	1.38
35	T	55	PSU	C2-N1	-4.05	1.31	1.36
35	T	54	5MU	C4-C5	-3.86	1.38	1.44
35	T	54	5MU	C4-N3	-3.62	1.32	1.38
35	T	54	5MU	C2-N3	-3.45	1.32	1.38
35	T	55	PSU	C1'-C5	3.44	1.58	1.50
35	T	55	PSU	C4-N3	-3.41	1.32	1.38
35	T	8	4SU	C5-C4	-3.41	1.38	1.42
35	T	8	4SU	C2-N3	-3.34	1.32	1.38
35	T	54	5MU	C6-N1	-3.25	1.32	1.38
35	T	55	PSU	O2-C2	-2.92	1.17	1.23
35	T	54	5MU	O4-C4	-2.57	1.18	1.23
35	T	54	5MU	O2-C2	-2.52	1.18	1.23
35	T	32	4OC	C6-N1	-2.50	1.32	1.38
35	T	55	PSU	O4'-C1'	-2.46	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	T	55	PSU	C6-N1	-2.37	1.32	1.36
35	T	54	5MU	C6-C5	2.31	1.38	1.34
35	T	32	4OC	C2-N3	-2.07	1.32	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	T	20	H2U	O2-C2-N1	-10.88	110.02	123.10
35	T	20	H2U	O4-C4-N3	-7.66	108.49	120.30
35	T	20	H2U	O4-C4-C5	-6.61	108.67	122.20
35	T	8	4SU	C4-N3-C2	-6.04	121.52	127.31
35	T	20	H2U	O2-C2-N3	-6.04	110.35	121.49
35	T	8	4SU	N3-C2-N1	5.45	121.98	114.89
35	T	54	5MU	N3-C2-N1	5.42	121.94	114.89
35	T	54	5MU	C4-N3-C2	-5.28	120.42	127.34
35	T	8	4SU	C5-C4-N3	4.82	119.23	114.75
35	T	55	PSU	N1-C2-N3	4.56	119.98	115.17
35	T	54	5MU	C5-C4-N3	4.55	119.28	115.32
35	T	54	5MU	C5-C6-N1	-4.33	118.61	123.31
35	T	54	5MU	O4-C4-C5	-4.31	119.99	124.92
35	T	20	H2U	N3-C2-N1	-3.78	112.85	116.65
35	T	32	4OC	C1'-N1-C6	-3.41	113.50	120.78
35	T	55	PSU	C4-N3-C2	-3.37	121.73	126.37
35	T	8	4SU	C5-C4-S4	-3.23	120.62	124.31
35	T	55	PSU	O2-C2-N1	-3.18	119.51	122.79
35	T	54	5MU	O2-C2-N1	-3.03	118.85	122.80
35	T	20	H2U	C5-C4-N3	-2.99	113.51	116.69
35	T	55	PSU	C6-C5-C4	-2.97	116.17	118.17
35	T	8	4SU	C6-C5-C4	-2.90	117.44	119.95
35	T	32	4OC	C3'-C2'-C1'	-2.86	97.34	102.81
35	T	32	4OC	C1'-N1-C2	2.84	124.72	118.44
35	T	8	4SU	O2-C2-N1	-2.80	119.15	122.80
35	T	32	4OC	O2'-C2'-C1'	2.68	114.07	108.99
35	T	8	4SU	C1'-N1-C2	2.63	122.31	117.59
35	T	32	4OC	O4'-C1'-N1	2.53	114.09	108.36
35	T	32	4OC	CM2-O2'-C2'	-2.35	108.44	114.47

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	T	8	4SU	C2'
35	T	8	4SU	C3'

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Mol	Chain	Res	Type	Atom
35	T	20	H2U	C2'
35	T	20	H2U	C3'
35	T	32	4OC	C1'
35	T	32	4OC	C2'
35	T	54	5MU	C4'
35	T	55	PSU	C4'

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	T	20	H2U	O4'-C1'-N1-C2
35	T	20	H2U	O4'-C1'-N1-C6
35	T	54	5MU	C4'-C5'-O5'-P
35	T	101	FME	O1-CN-N-CA
35	T	101	FME	O-C-CA-CB
35	T	54	5MU	O4'-C4'-C5'-O5'
35	T	54	5MU	C3'-C4'-C5'-O5'
35	T	55	PSU	C4'-C5'-O5'-P
35	T	101	FME	CB-CG-SD-CE
35	T	8	4SU	O4'-C1'-N1-C6
35	T	20	H2U	C4'-C5'-O5'-P
35	T	8	4SU	O4'-C1'-N1-C2
35	T	32	4OC	O4'-C1'-N1-C2
35	T	32	4OC	O4'-C1'-N1-C6
35	T	32	4OC	C2'-C1'-N1-C2
35	T	32	4OC	C2'-C1'-N1-C6
35	T	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	T	20	H2U	2	0
35	T	55	PSU	1	0
35	T	54	5MU	2	0
35	T	8	4SU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 267 ligands modelled in this entry, 265 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	ATP	H	602	58	28,33,33	0.80	0	34,52,52	0.60	1 (2%)
57	ATP	H	601	58	28,33,33	0.73	0	34,52,52	0.61	1 (2%)

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
57	ATP	H	602	58	-	1/18/38/38	0/3/3/3
57	ATP	H	601	58	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	H	601	ATP	C5-C6-N6	2.32	123.85	120.31
57	H	602	ATP	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

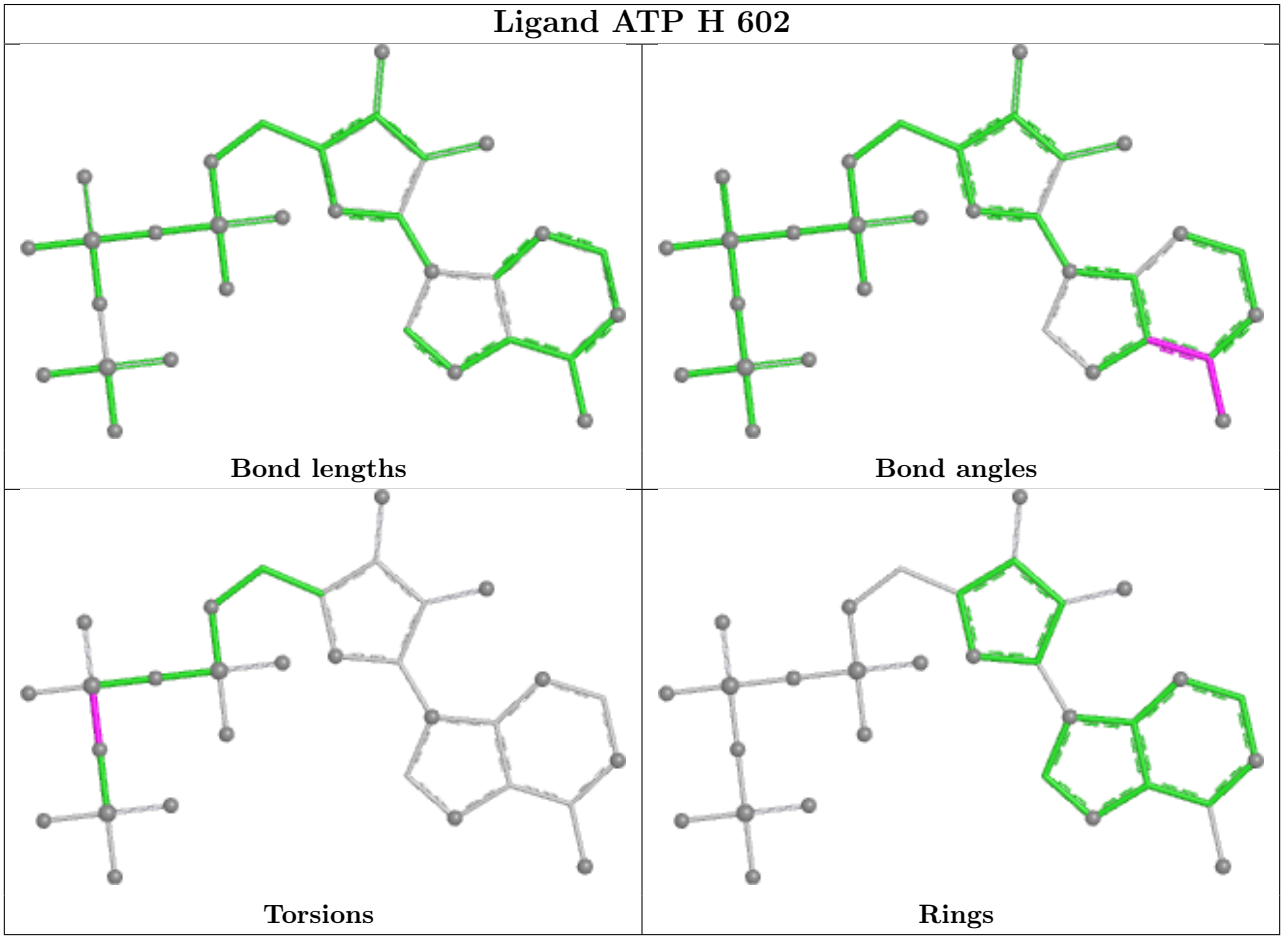
Mol	Chain	Res	Type	Atoms
57	H	601	ATP	PB-O3B-PG-O2G
57	H	602	ATP	PG-O3B-PB-O2B
57	H	601	ATP	PB-O3B-PG-O3G
57	H	601	ATP	PA-O3A-PB-O2B

There are no ring outliers.

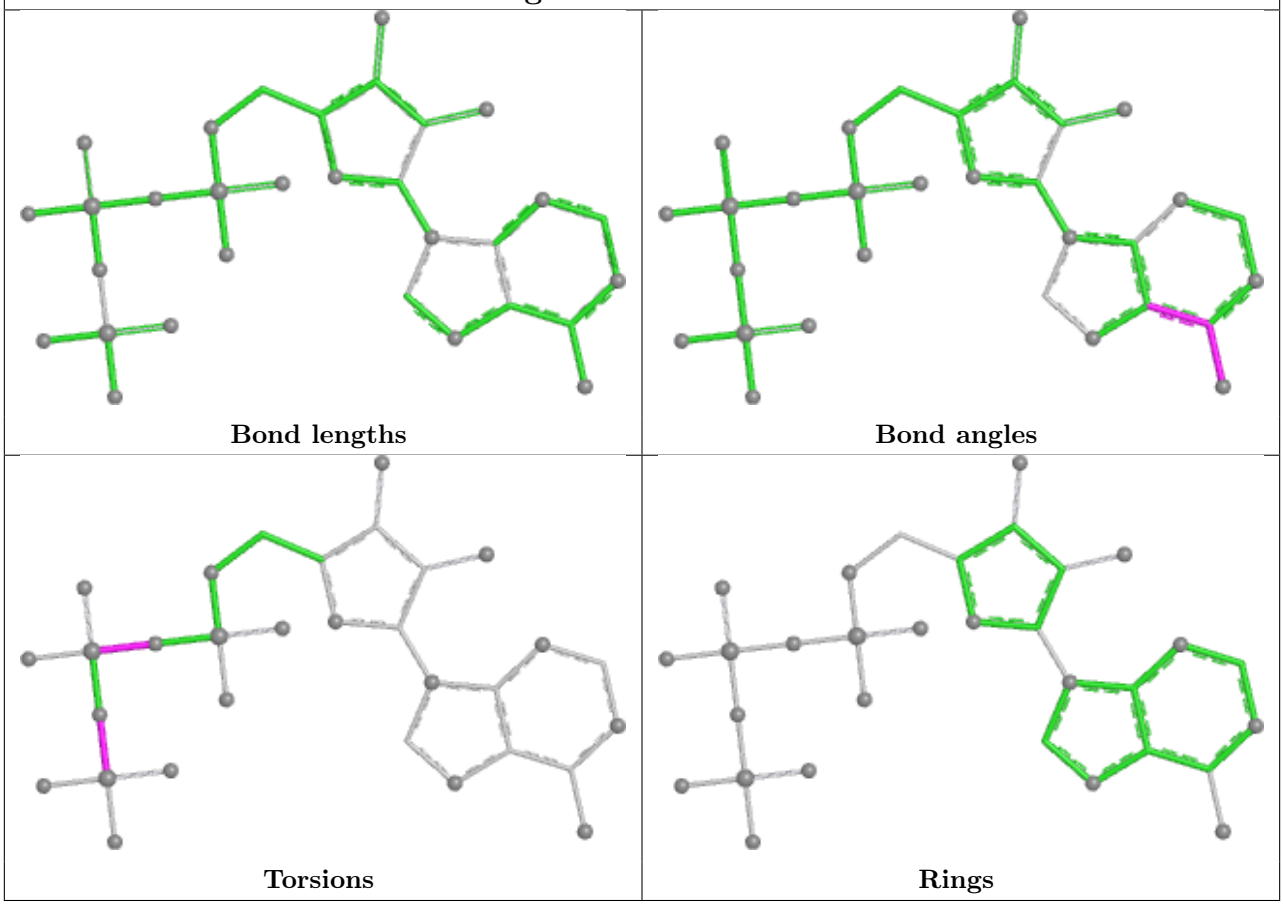
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	H	602	ATP	1	0
57	H	601	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand ATP H 601



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.

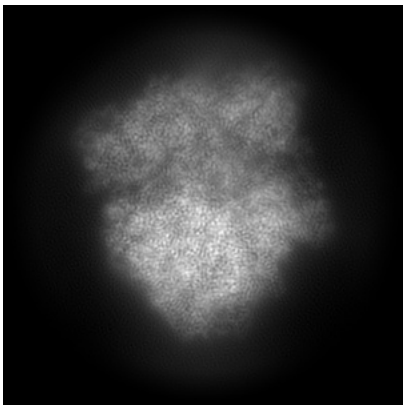
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29405. These allow visual inspection of the internal detail of the map and identification of artifacts.

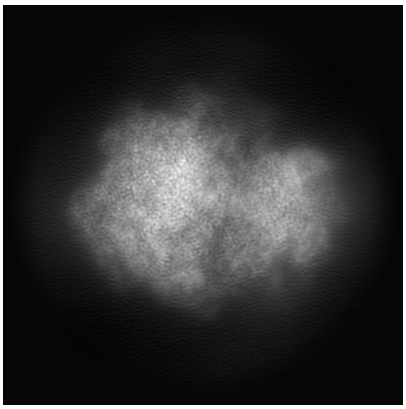
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

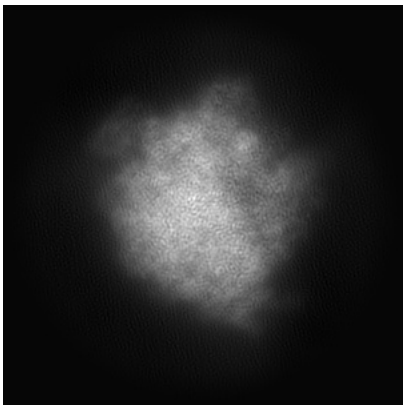
6.1.1 Primary map



X

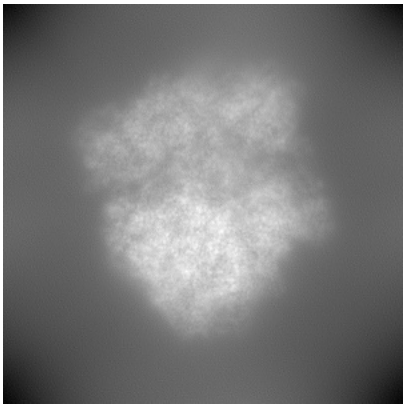


Y

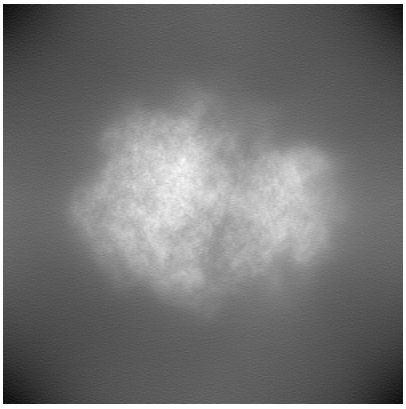


Z

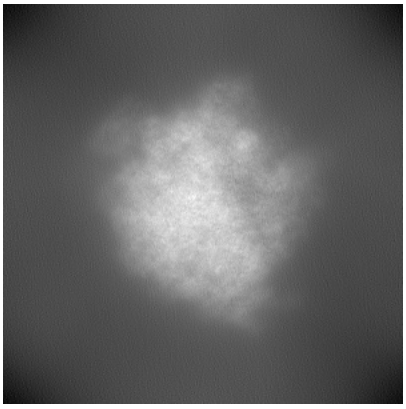
6.1.2 Raw map



X



Y

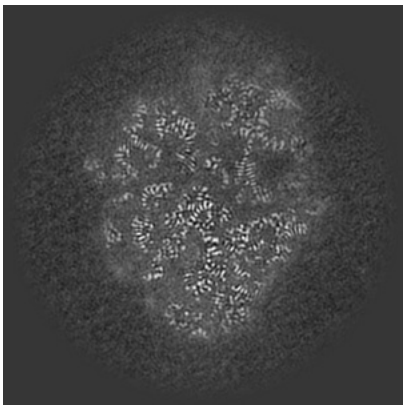


Z

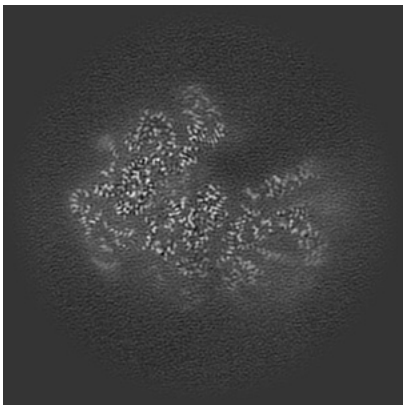
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

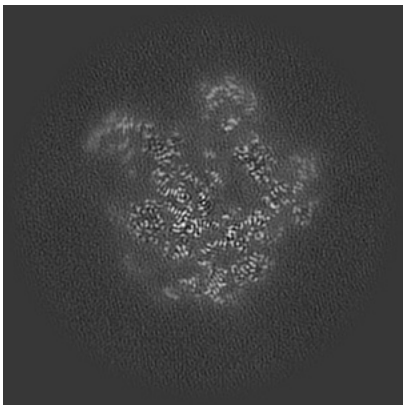
6.2.1 Primary map



X Index: 200

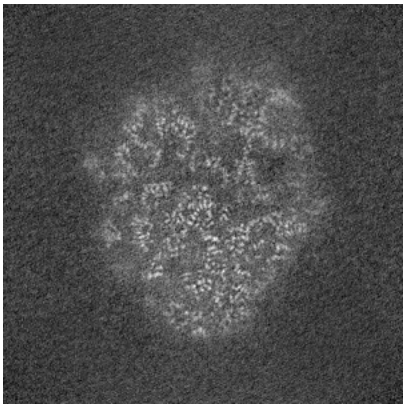


Y Index: 200



Z Index: 200

6.2.2 Raw map



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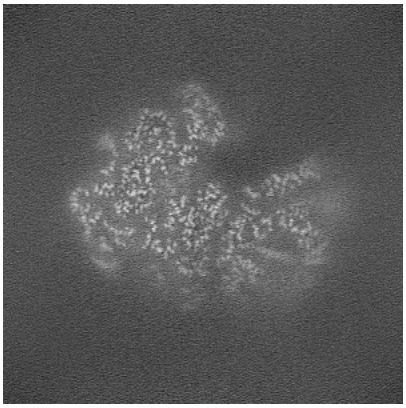
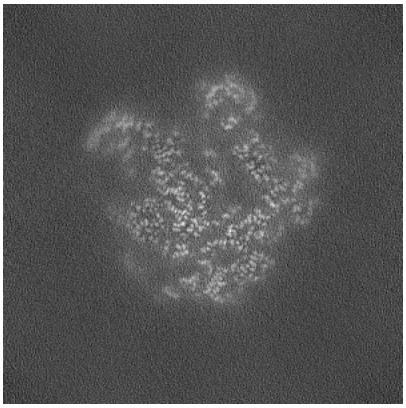


Y Index: 200

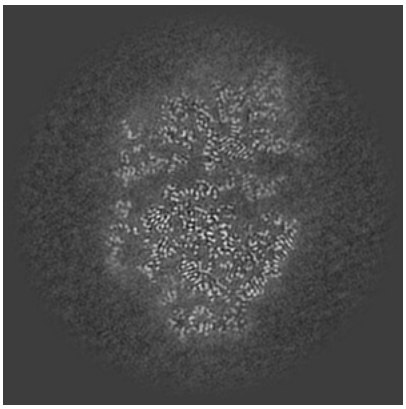


Z Index: 200

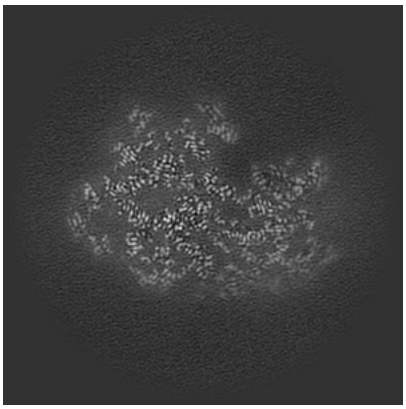
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

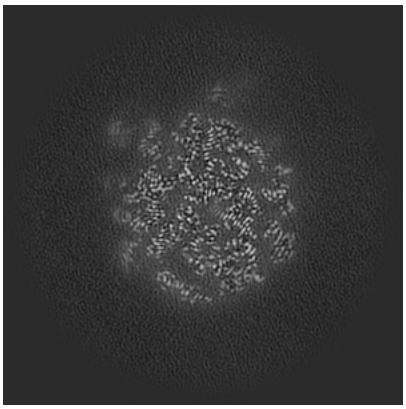
6.3.1 Primary map



X Index: 190

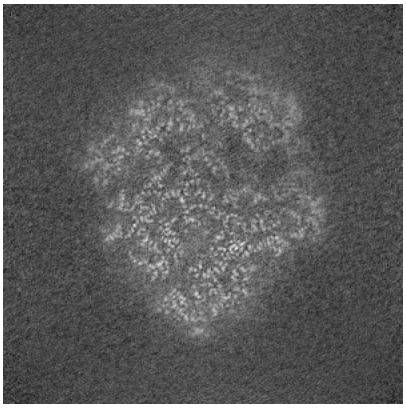


Y Index: 185

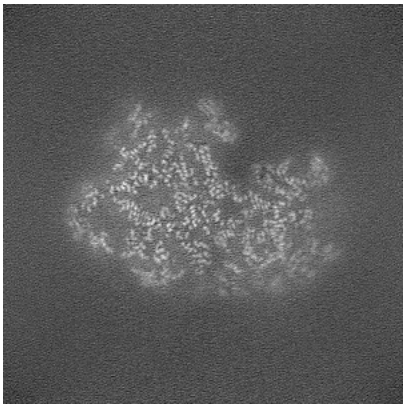


Z Index: 161

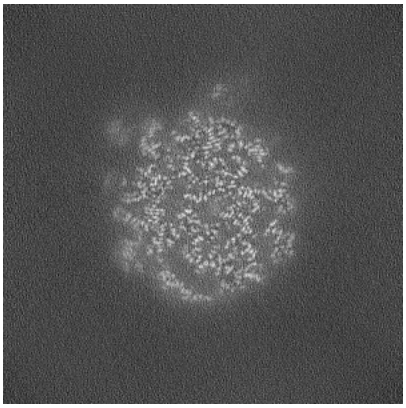
6.3.2 Raw map



X Index: 208



Y Index: 183

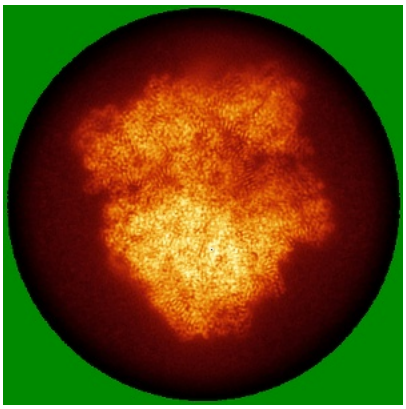


Z Index: 160

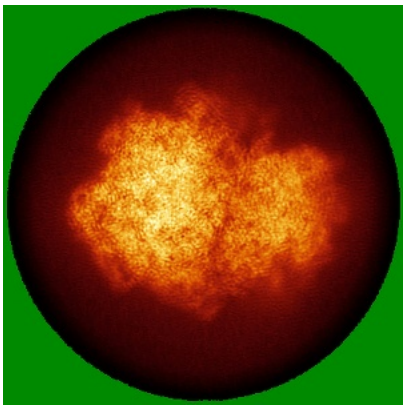
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

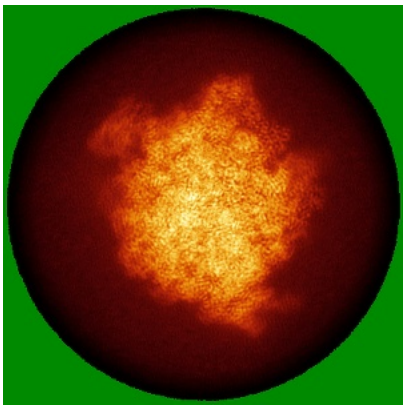
6.4.1 Primary map



X

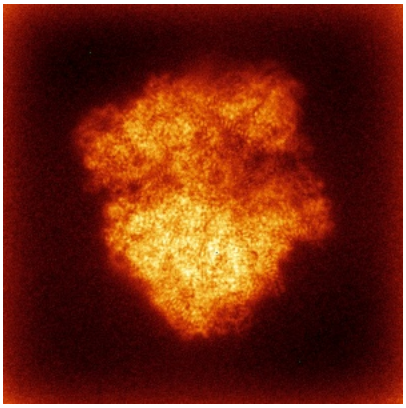


Y



Z

6.4.2 Raw map



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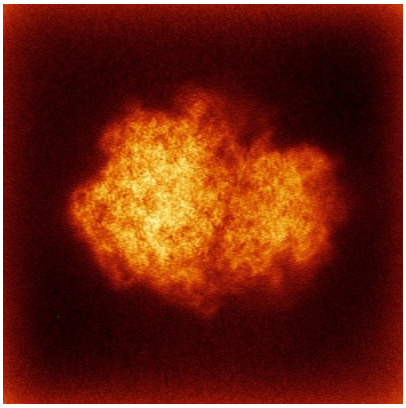
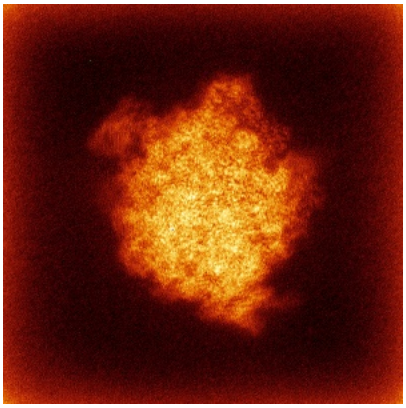


Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

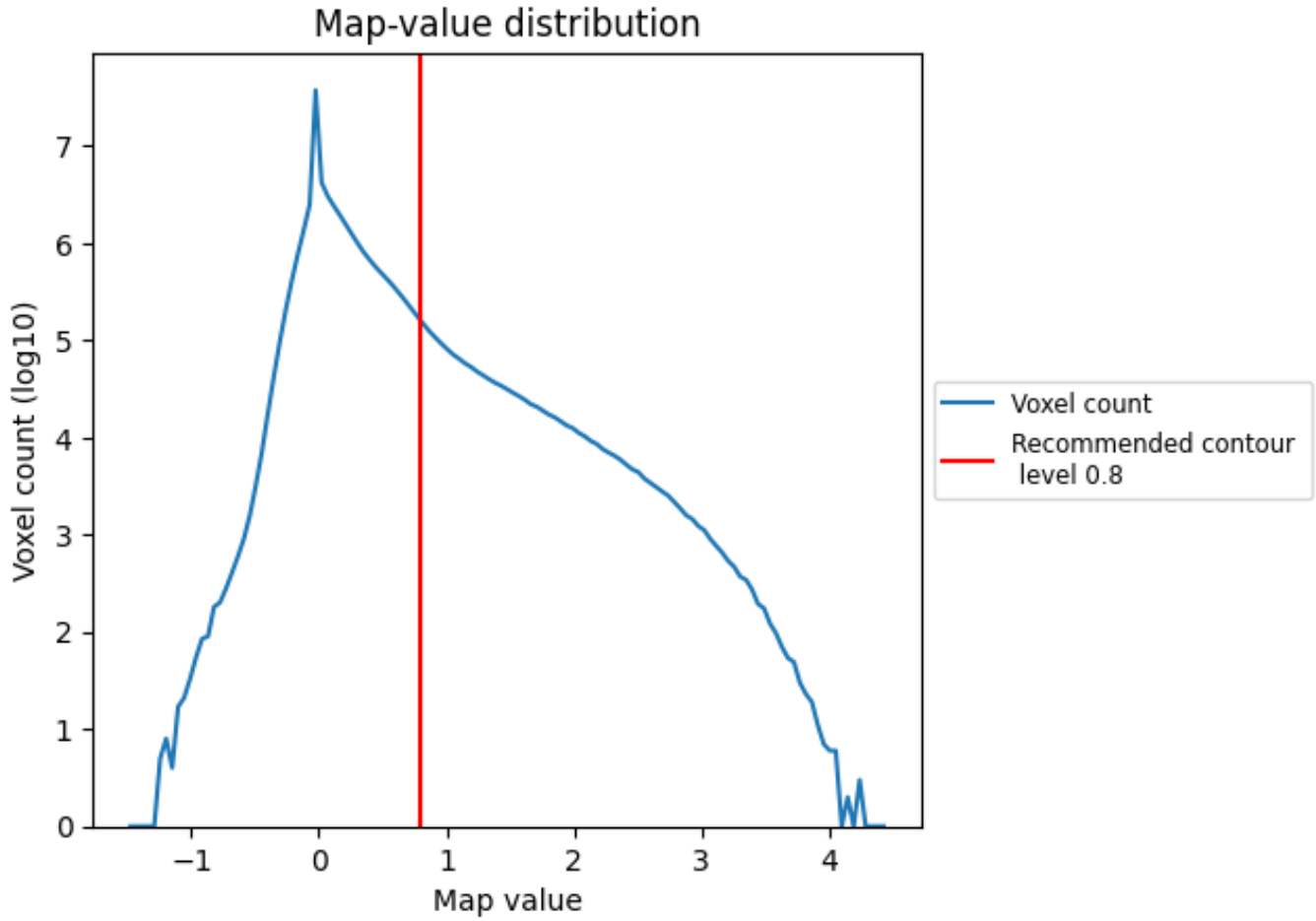
6.6 Mask visualisation (i)

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

7 Map analysis

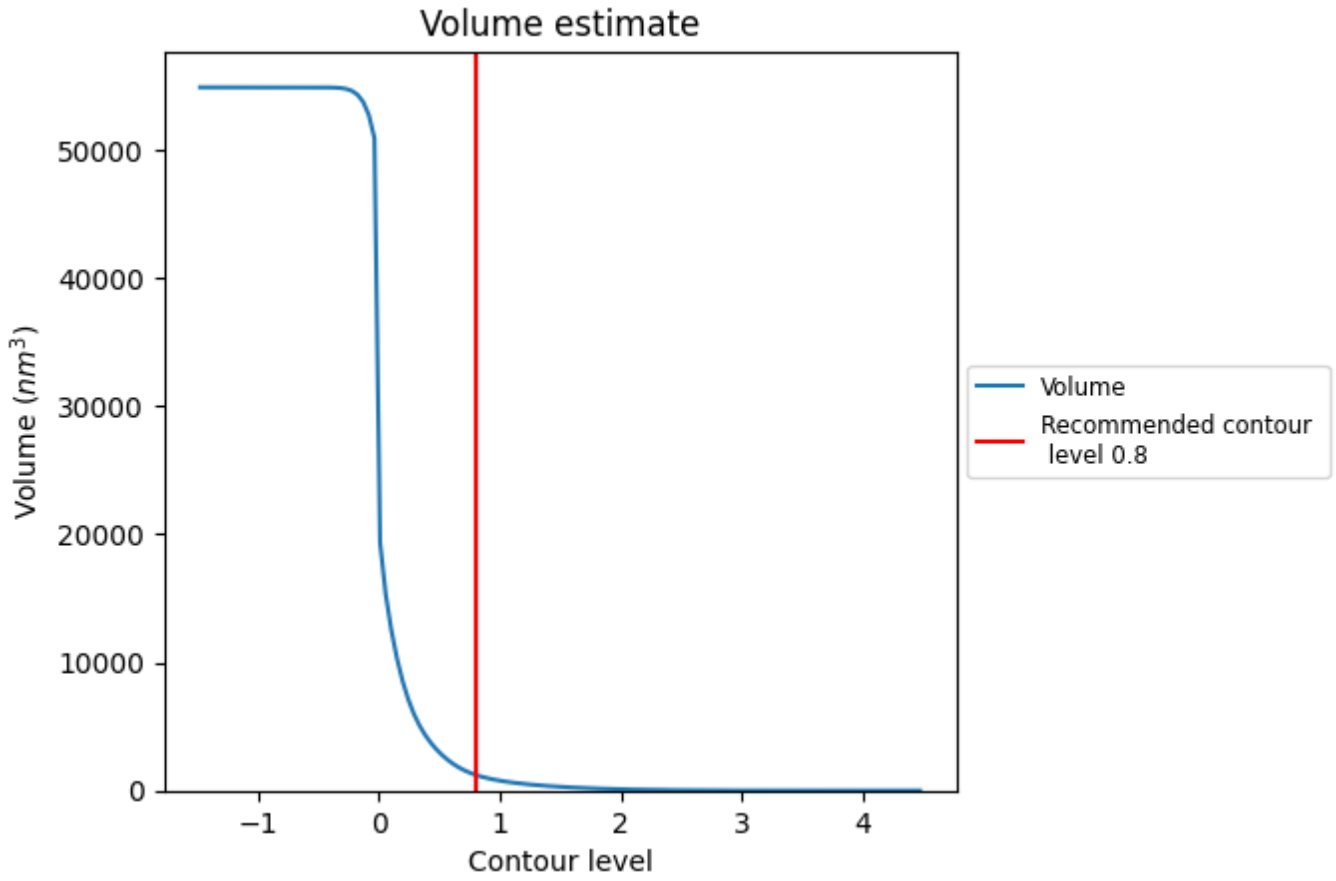
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

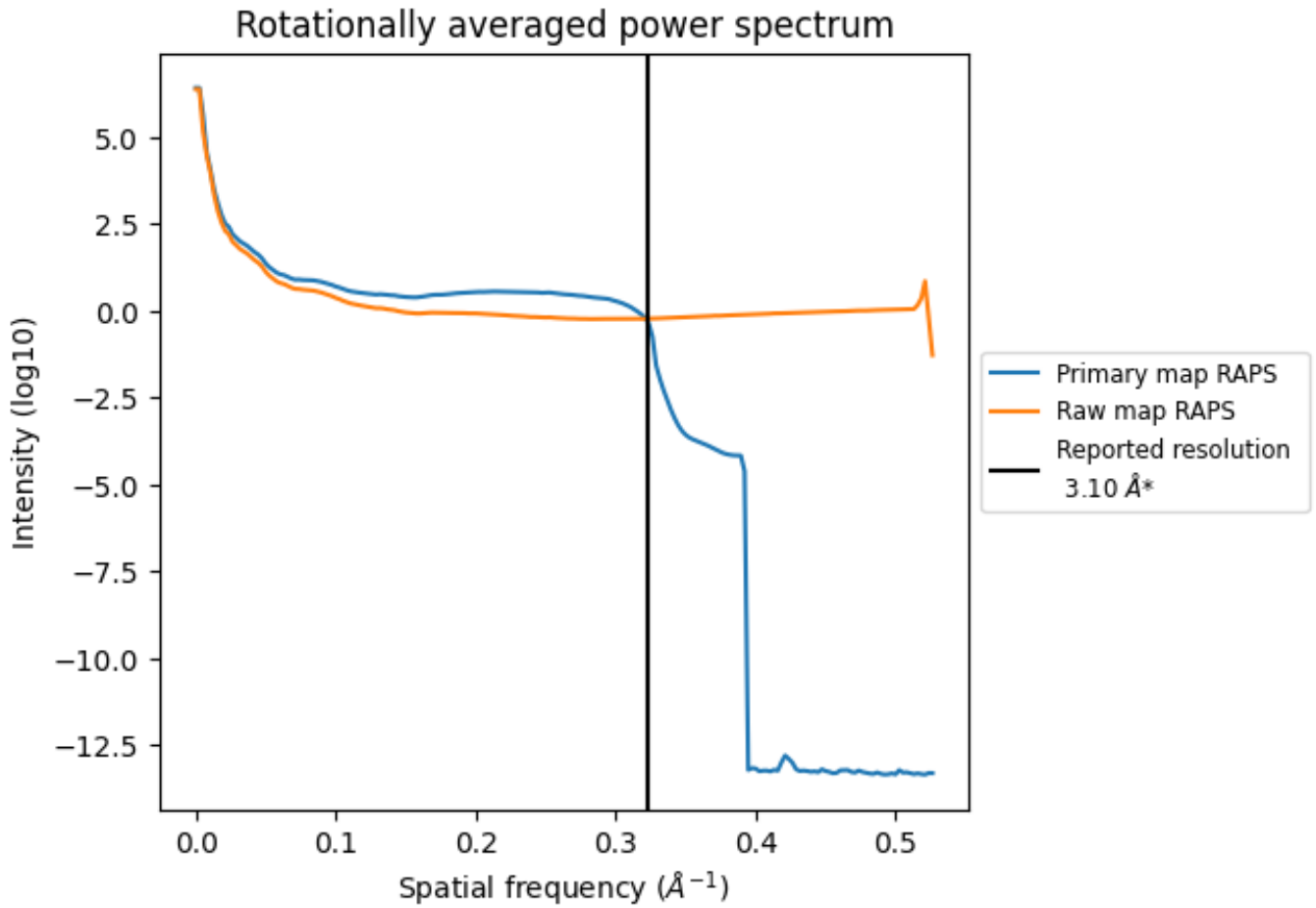
7.2 Volume estimate



The volume at the recommended contour level is 1223 nm^3; this corresponds to an approximate mass of 1105 kDa.

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

7.3 Rotationally averaged power spectrum (i)

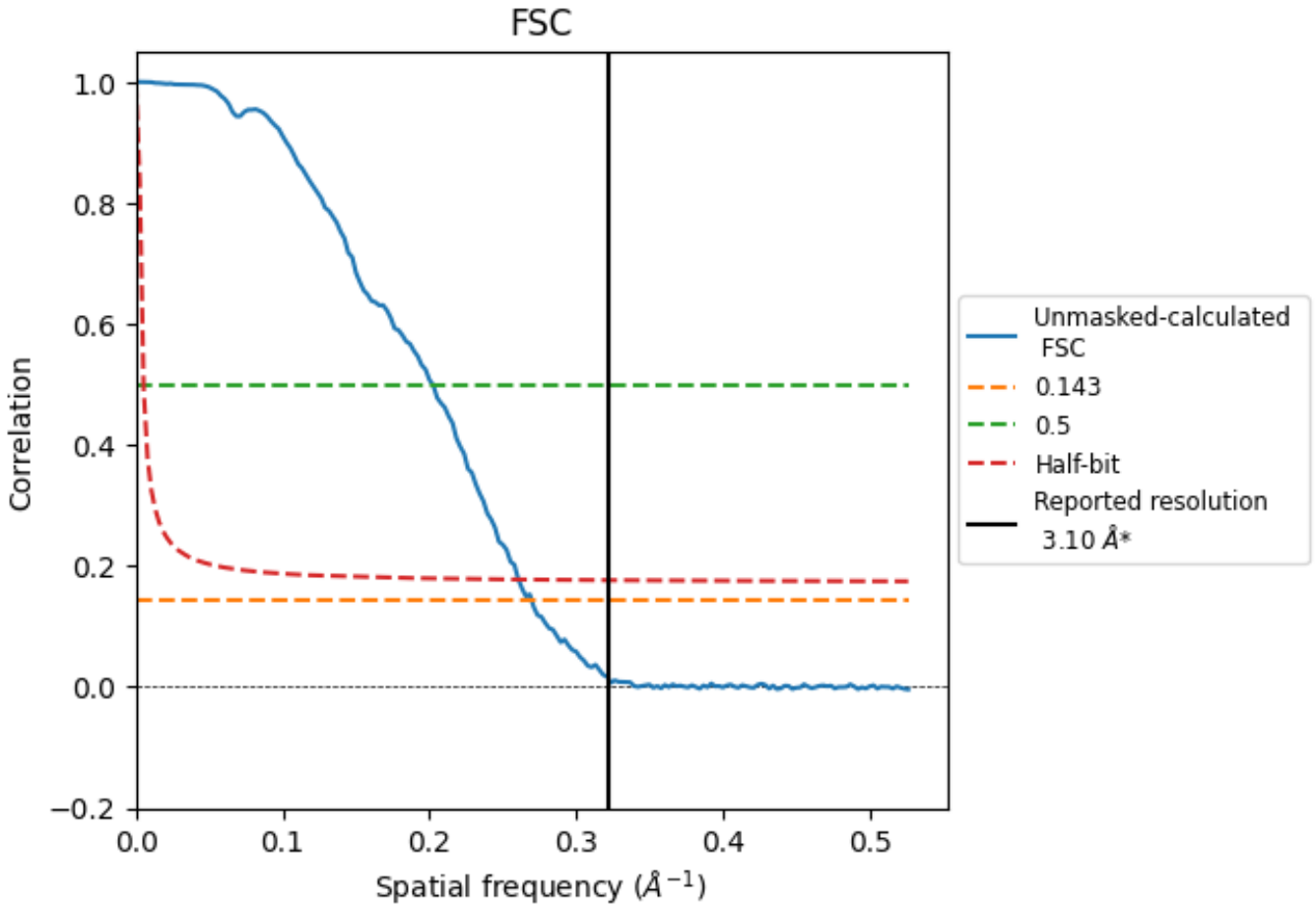


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

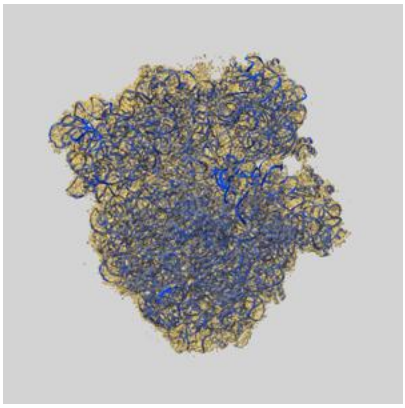
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	4.94	3.84

*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 3.71 differs from the reported value 3.1 by more than 10 %

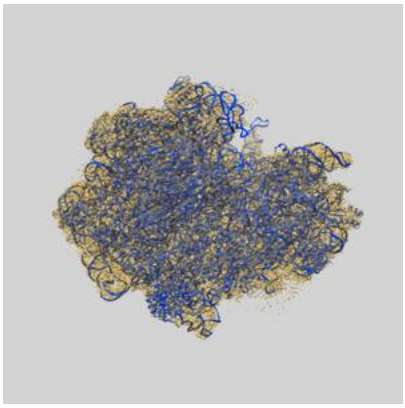
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29405 and PDB model 9NLH. Per-residue inclusion information can be found in section 3 on page 15.

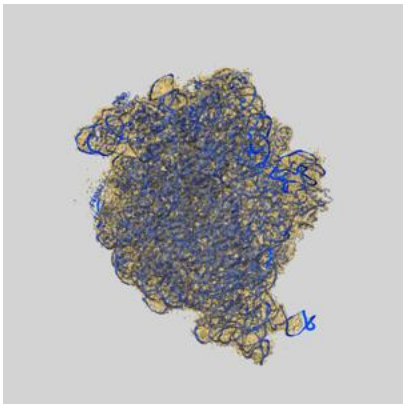
9.1 Map-model overlay



X



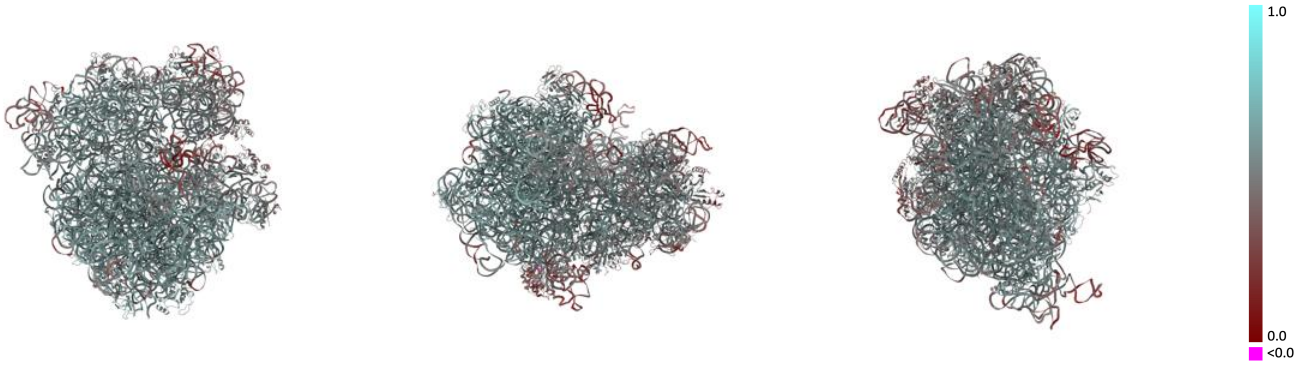
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

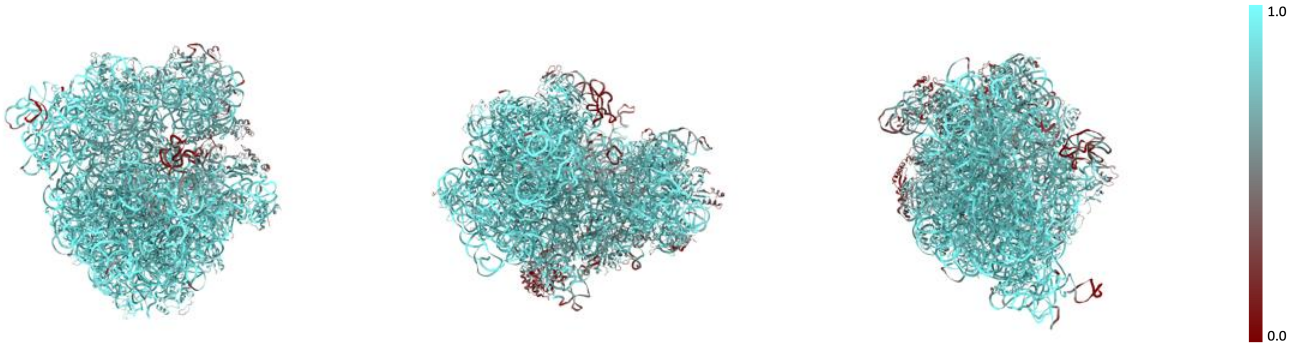
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

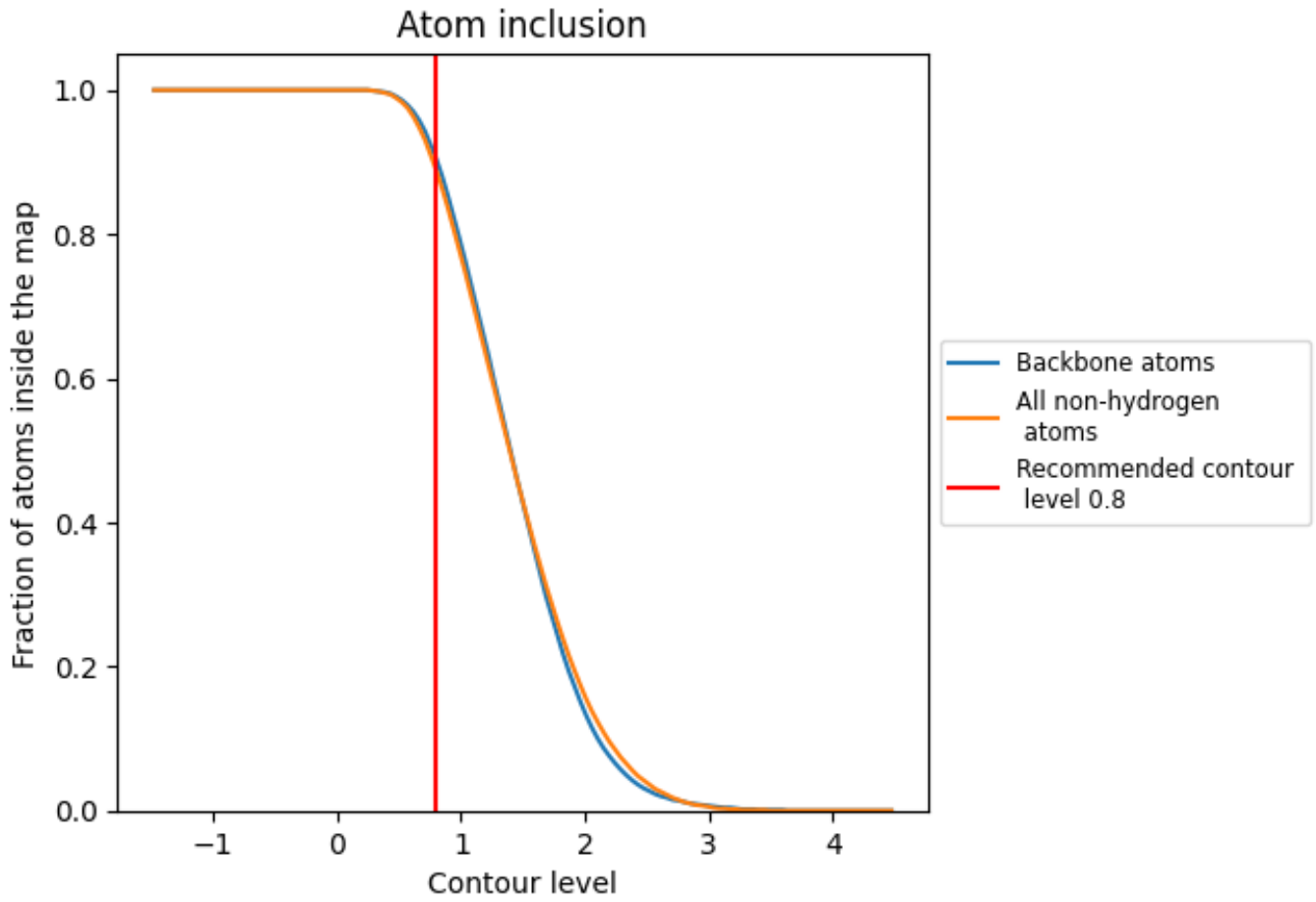
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.5360
1	0.4490	0.3840
13	0.9300	0.5790
14	0.8690	0.5810
15	0.9260	0.5880
16	0.8940	0.5810
17	0.9560	0.5740
18	0.8150	0.5170
19	0.8750	0.5720
2	0.9190	0.5890
20	0.9440	0.5900
21	0.8700	0.5650
22	0.9350	0.5760
23	0.9070	0.5490
24	0.9000	0.5480
25	0.7940	0.5430
27	0.9500	0.5900
28	0.9350	0.5860
29	0.8550	0.5280
3	0.9080	0.5780
30	0.8860	0.5650
32	0.9440	0.5840
33	0.9180	0.5820
34	0.9940	0.6130
35	0.9780	0.6050
36	0.9010	0.5860
4	0.8930	0.5600
5	0.6320	0.4620
6	0.6550	0.4870
9	0.2370	0.3890
H	0.7200	0.5220
M	0.9080	0.5260
R1	0.9400	0.5540
R2	0.9350	0.5210
R3	0.9250	0.5200

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Chain	Atom inclusion	Q-score
T	0.9020	0.5370
sb	0.7040	0.4240
sc	0.8000	0.5070
sd	0.8320	0.5160
se	0.8910	0.5350
sf	0.6180	0.4620
sg	0.6700	0.4810
sh	0.8910	0.5440
si	0.7370	0.4750
sj	0.6730	0.4420
sk	0.7470	0.5220
sl	0.8000	0.5480
sm	0.6060	0.4630
sn	0.8190	0.4810
so	0.8010	0.5160
sp	0.8660	0.5300
sq	0.8480	0.5230
sr	0.7300	0.4940
ss	0.6220	0.4410
st	0.8370	0.5290
su	0.6360	0.4330