



Full wwPDB EM Validation Report ⓘ

May 23, 2026 – 04:07 PM EDT

PDB ID : 9PJ8 / pdb_00009pj8
EMDB ID : EMD-71683
Title : C. acnes 70S ribosome bound to Sarecycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-12
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

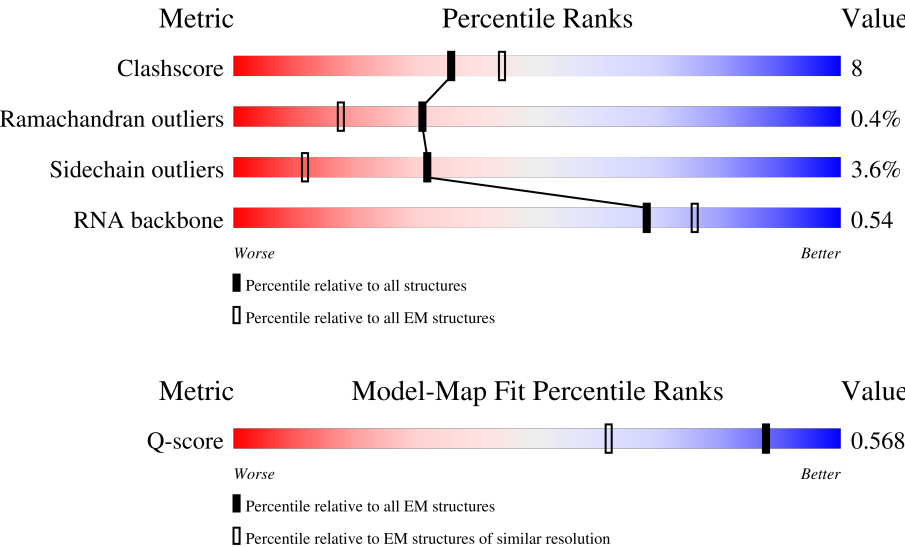
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	44	
3	2	68	

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Mol	Chain	Length	Quality of chain
4	3	37	
5	4	69	
6	A	1537	
7	B	283	
8	C	77	
9	D	201	
10	E	215	
11	F	96	
12	G	269	
13	H	135	
14	I	156	
15	J	173	
16	K	135	
17	L	123	
18	M	103	
19	N	123	
20	O	87	
21	P	147	
22	Q	90	
23	R	79	
24	S	61	
25	T	88	
26	U	93	
27	V	24	
28	X	33	

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Mol	Chain	Length	Quality of chain
29	Y	22	
30	a	3086	
31	b	120	
32	c	278	
33	d	223	
34	e	301	
35	f	210	
36	g	180	
37	i	147	
38	j	122	
39	k	146	
40	l	139	
41	m	187	
42	n	127	
43	o	117	
44	p	123	
45	q	102	
46	r	153	
47	s	102	
48	t	122	
49	u	205	
50	v	89	
51	w	61	
52	x	77	
53	y	60	

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Mol	Chain	Length	Quality of chain
54	z	63	 A horizontal bar chart showing the quality of chain 54 (z). The bar is divided into two segments: a green segment representing 78% and a yellow segment representing 21%. A small red square is at the start of the green segment, and a small grey square is at the end of the yellow segment. A small black dot is at the end of the bar.

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144415 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1505	Total	C	N	O	P	0	0
			32340	14408	5893	10534	1505		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	233	Total	C	N	O	S	0	0
			1836	1163	326	338	9		

- Molecule 8 is a RNA chain called initiator tRNA Met (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	76	Total	C	N	O	P S	0	0
			1625	725	294	529	76 1		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	200	Total	C	N	O	S	0	0
			1632	1021	313	297	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	179	Total	C	N	O	S	0	0
			1309	816	244	245	4		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	96	Total	C	N	O	S	0	0
			785	496	134	149	6		

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	206	Total	C	N	O	S	0	0
			1613	1010	305	294	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	134	Total	C	N	O	S	0	0
			1021	642	182	194	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	155	Total	C	N	O	S	0	0
			1225	764	235	220	6		

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	134	Total	C	N	O	S	0	0
			1012	629	204	177	2		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			858	532	168	154	4		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			948	587	195	164	2		

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	98	Total	C	N	O	S	0	0
			786	496	146	141	3		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	122	Total	C	N	O	S	0	0
			976	598	205	173			

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	87	Total	C	N	O	S	0	0
			708	440	140	125	3		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	128	Total	C	N	O	S	0	0
			994	621	185	187	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	90	Total	C	N	O	S	0	0
			728	446	142	134	6		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	67	Total	C	N	O		0	0
			527	334	103	90			

- Molecule 24 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	60	Total	C	N	O	S	0	0
			474	298	98	73	5		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	87	Total	C	N	O		0	0
			673	408	144	121			

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	84	Total	C	N	O	S	0	0
			658	416	126	113	3		

- Molecule 27 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	23	Total	C	N	O		0	0
			183	106	50	27			

- Molecule 28 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	32	Total	C	N	O	S	0	0
			277	170	71	35	1		

- Molecule 29 is a RNA chain called mRNA 32MF.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2903	Total	C	N	O	P	1	0
			62432	27805	11391	20332	2904		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 32 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	274	Total	C	N	O	S	0	0
			2091	1289	425	372	5		

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	214	Total	C	N	O	S	0	0
			1586	984	304	291	7		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	210	Total	C	N	O	S	0	0
			1577	979	301	295	2		

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	184	Total	C	N	O	S	0	0
			1468	924	269	266	9		

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	177	Total	C	N	O	S	0	0
			1376	867	250	258	1		

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	146	Total	C	N	O	S	0	0
			1139	718	213	205	3		

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	x	69	Total	C	N	O	0	0
			564	348	108	108		

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

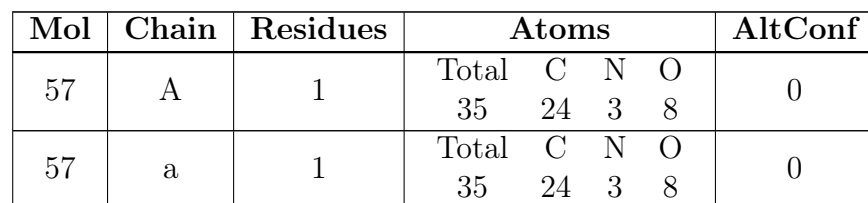
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	S	1	Total	Zn	0
			1	1	
55	w	1	Total	Zn	0
			1	1	
55	z	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	63	Total	Mg	0
			63	63	
56	a	233	Total	Mg	0
			233	233	
56	b	2	Total	Mg	0
			2	2	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	

- Molecule 57 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈) (labeled as "Ligand of Interest" by depositor).

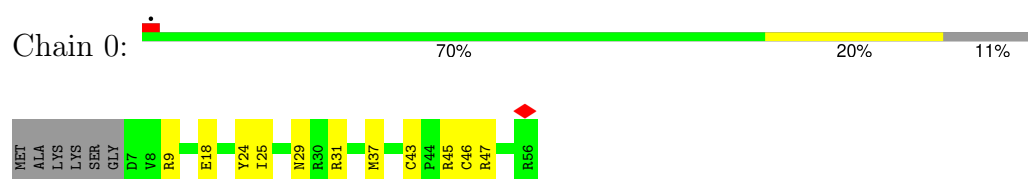


- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|--------------------|---------|
| 58 | A | 11 | Total O
11 11 | 0 |
| 58 | a | 108 | Total O
108 108 | 0 |
| 58 | b | 1 | Total O
1 1 | 0 |
| 58 | c | 1 | Total O
1 1 | 0 |

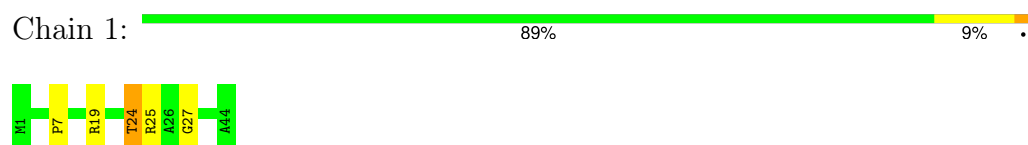
3 Residue-property plots [i](#)

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.

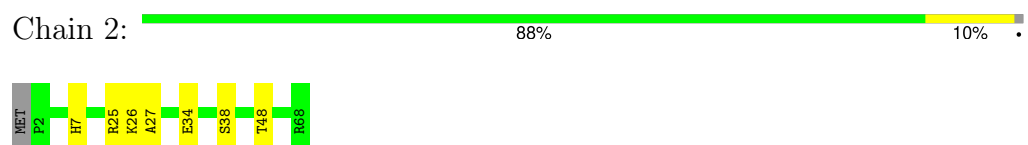
- Molecule 1: 50S ribosomal protein L33



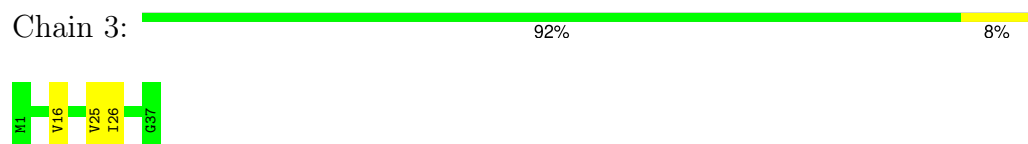
- Molecule 2: 50S ribosomal protein L34



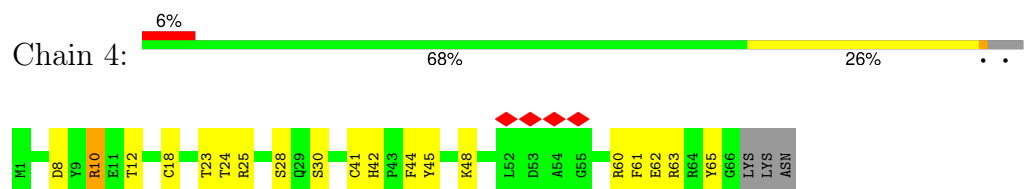
- Molecule 3: Large ribosomal subunit protein bL35



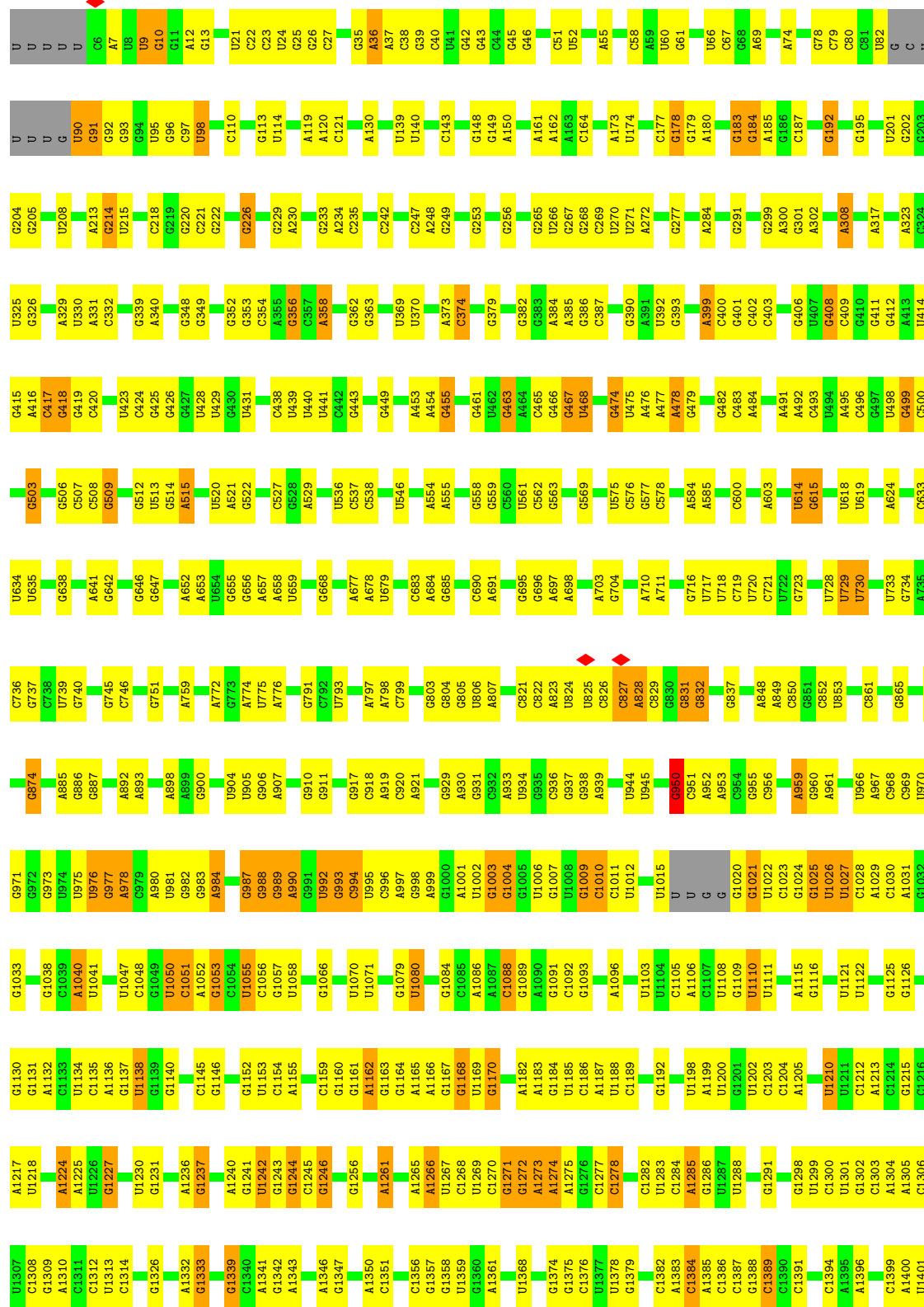
- Molecule 4: 50S ribosomal protein L36

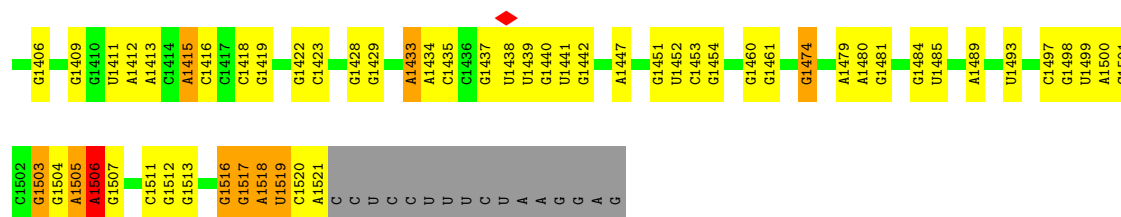


- Molecule 5: 50S ribosomal protein L31

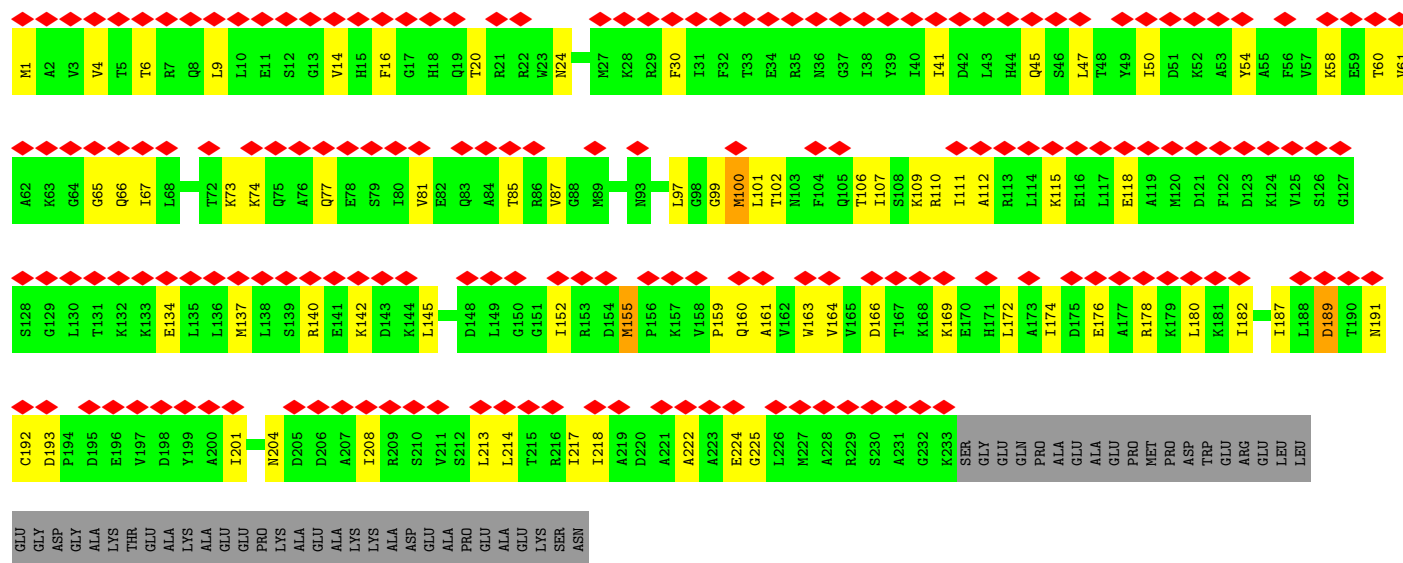


- Molecule 6: 16S rRNA

Chain A: 



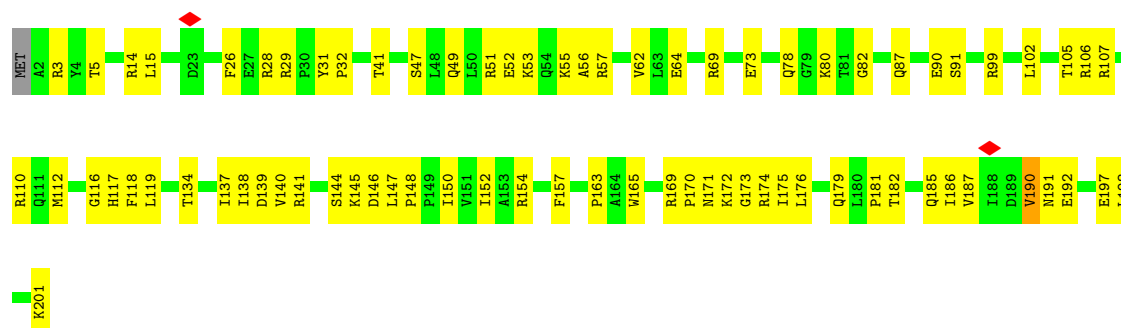
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: initiator tRNA Met (76-MER)

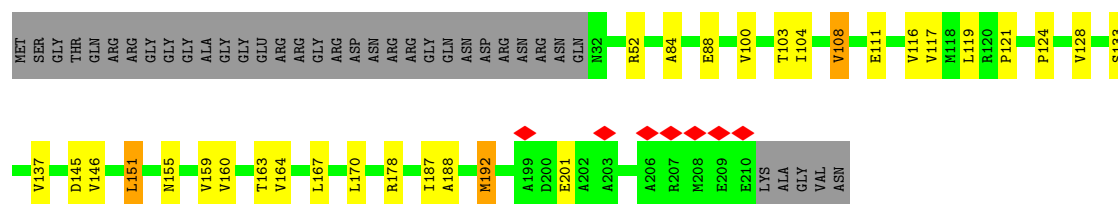


• Molecule 9: 30S ribosomal protein S4



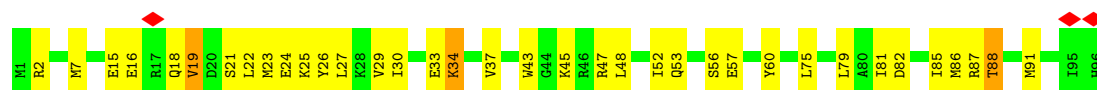
• Molecule 10: Small ribosomal subunit protein uS5

Chain E: 



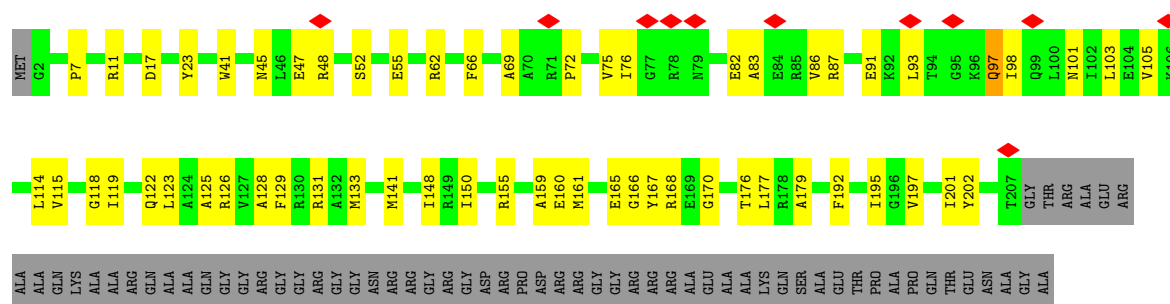
- Molecule 11: 30S ribosomal protein S6

Chain F: 



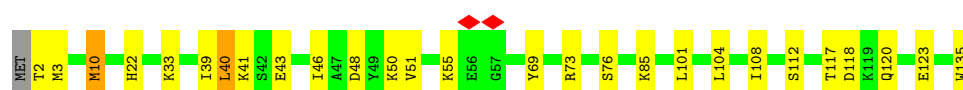
- Molecule 12: 30S ribosomal protein S3

Chain G: 



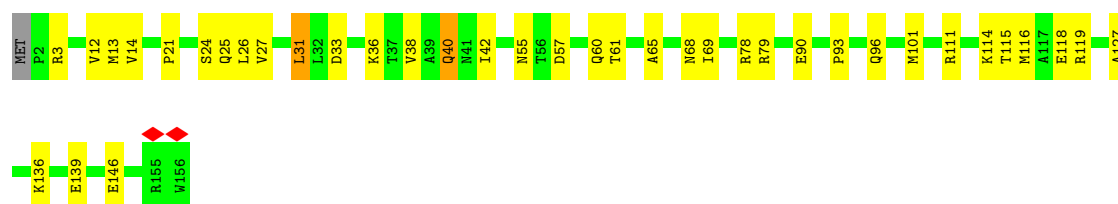
- Molecule 13: 30S ribosomal protein S8

Chain H: 

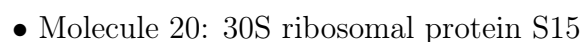


- Molecule 14: 30S ribosomal protein S7

Chain I: 



- Molecule 15: 30S ribosomal protein S9

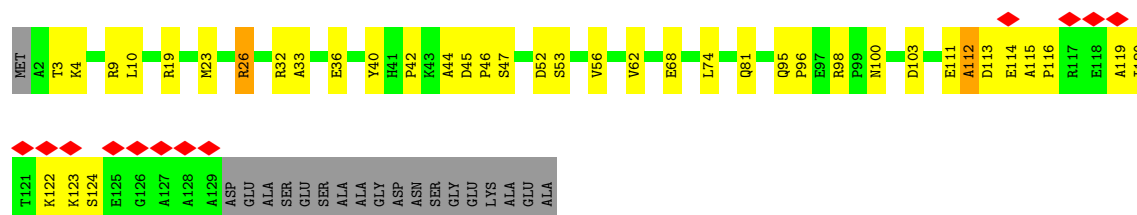


Chain O:  75% 25%



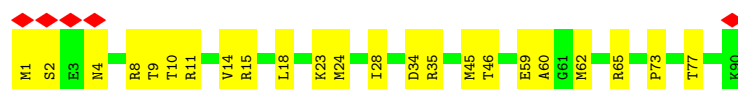
- Molecule 21: 30S ribosomal protein S16

Chain P:  8% 61% 25% 13%



- Molecule 22: 30S ribosomal protein S17

Chain Q:  6% 74% 26%



- Molecule 23: 30S ribosomal protein S18

Chain R:  9% 63% 19% 15%



- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:  74% 23% 3%



- Molecule 25: 30S ribosomal protein S20

Chain T:  74% 25% 1%



- Molecule 26: 30S ribosomal protein S19

Chain U:  68% 22% 10%



- Molecule 27: 50S ribosomal protein bL37

Chain V: 75% 21% .



- Molecule 28: AURKAIP1/COX24 domain-containing protein

Chain X: 70% 27% .



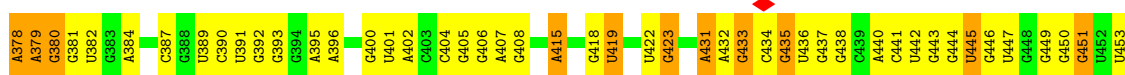
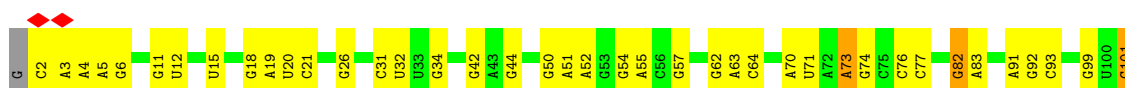
- Molecule 29: mRNA 32MF

Chain Y: 5% 23% 14% 9% 55%

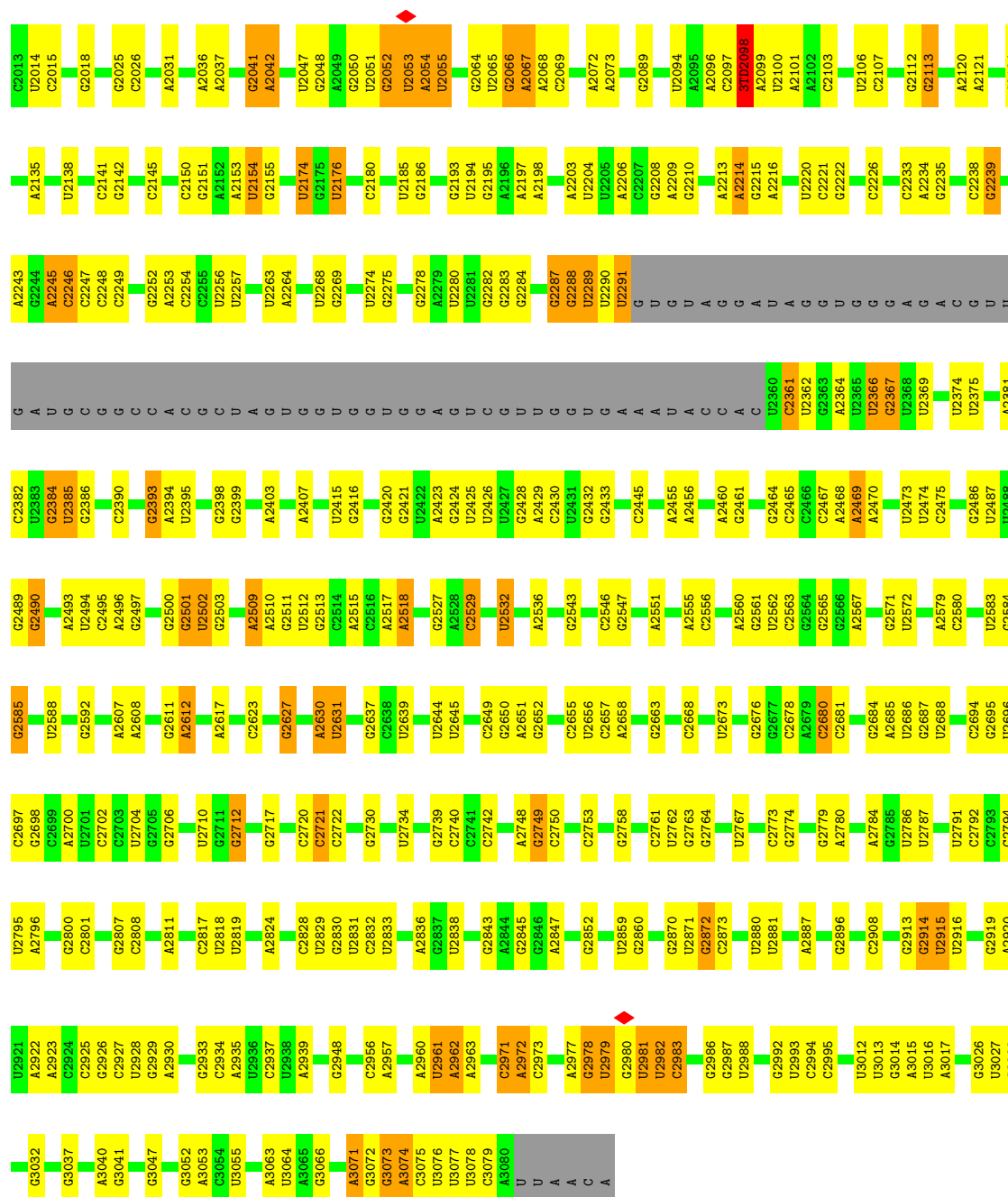


- Molecule 30: 23S rRNA

Chain a: 57% 31% 6% 6%

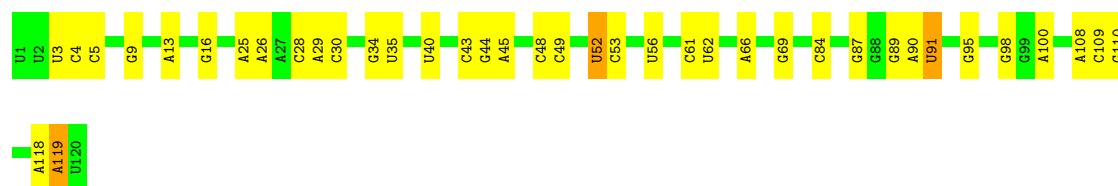


U1904	G1761	A1675	G	C	A1441	G1318	G1190	U1124	A1010	A904	G794	U682	G581
G1905	U1762	A1676	U	U	U1455	G1327	U1191	U1128	A1011	A905	G797	G683	U587
C1906	G1763	G1685	A	G	G1460	A1328	A1192	A1129	G1014	U911	G798	G686	G588
C1908	C1686	C1687	G	U	A1461	A1331	G1195	G1130	U1015	U912	G799	A687	A589
C1909	G1767	G1688	U	C	C1462	U1332	U1196	C1135	A1028	U913	A800	G592	G592
A1910	A1768	U1689	U	U	C1463	G1333	U1199	C1136	G1029	G916	A801	A692	A593
G1911	G1769	G1690	G	G	C1464	G1337	U1200	A1137	A1030	U917	G802	A693	A593
G1912	U1770	A1691	G	U	U1465	G1338	U1201	G1138	C1031	G918	U806	U698	U596
G1913	G1771	G1692	G	G	U1466	G1339	A1211	A1139	U1038	G921	C807	G699	U599
G1914	G1772	G1693	G	G	A1471	U1340	U1215	G1140	U1039	U921	G814	G700	G600
G1915	G1773	A1694	A	A	U1472	G1349	U1216	G1141	A1042	G930	U815	U701	U608
G1916	G1774	C1695	U	U	U1473	U1350	A1217	G1142	A1043	G931	C816	G704	C609
G1917	G1775	G1696	U	U	C1481	U1351	U1218	U1143	G1044	U935	G817	U709	G618
G1918	G1776	G1697	G	G	U1482	U1358	U1219	U1144	U1045	U936	G818	C710	C619
G1919	C1780	G1698	U	U	U1483	G1359	U1220	U1145	U1046	U937	A824	G711	C620
G1920	G1781	G1703	U	U	U1484	G1360	U1221	G1146	G1052	U938	C825	U712	G621
G1921	U1782	U1704	U	U	U1485	G1361	U1222	C1147	U1053	U939	U826	A713	G622
G1922	A1792	U1705	U	U	C1486	G1362	U1223	U1148	G1054	G940	U827	G714	C623
G1923	A1793	G1706	G	G	U1487	G1363	U1224	U1149	G1055	G941	C828	C715	
A1924	A1794	G1707	A	A	C1488	U1364	U1225	U1150	U1056	G942	U832	A718	C629
G1925	G1797	G1708	U	U	U1489	U1365	A1226	G1151	A1063	G943	U833	A719	U630
G1926	G1798	G1709	U	U	C1490	U1366	U1227	C1152	C1065	G944	U834	G720	G631
G1927	G1799	U1710	G	G	C1491	U1367	U1228	U1153	A1066	G945	G839	U632	U632
G1928	U1812	A1710	C	C	C1492	A1376	U1229	C1154	C1067	G946	G848	G721	U633
G1929	U1813	G1711	U	U	U1493	U1377	U1230	U1155	C1068	G947	A849	G722	U634
G1930	U1814	G1712	U	U	U1494	U1378	U1231	C1156	C1069	G948	U852	G723	G635
G1931	U1815	C1713	U	U	U1495	U1379	U1232	U1157	C1070	G949	U853	G724	G636
G1932	U1816	C1714	U	U	U1496	U1380	U1233	C1158	C1071	G950	U854	U725	U637
G1933	U1817	A1715	U	U	U1497	U1381	U1234	U1159	A1072	G951	U855	C726	G638
G1934	U1818	G1716	G	G	U1498	U1382	U1235	U1160	C1073	U960	U856	C727	U639
G1935	U1819	G1717	G	G	U1499	C1391	U1236	U1161	C1074	G966	U857	G728	G646
G1936	U1820	U1718	U	U	U1500	A1392	U1237	U1162	C1075	U967	U858	U729	U640
G1937	U1821	G1719	G	G	U1501	U1393	U1238	U1163	C1076	U968	U859	U730	U641
G1938	U1822	U1720	G	G	U1502	U1394	U1239	U1164	C1077	U969	U860	A731	U642
G1939	U1823	G1721	U	U	U1503	C1395	U1240	U1165	C1078	U970	U861	G734	U643
G1940	U1824	U1722	U	U	U1504	U1396	U1241	U1166	C1079	U971	U862	G735	G653
G1941	U1825	G1723	G	G	U1505	U1397	U1242	U1167	C1080	U972	U863	A654	A654
G1942	U1826	U1724	U	U	U1506	U1400	U1243	U1168	C1081	U973	U864	G655	G655
G1943	U1827	G1725	G	G	U1507	U1401	U1244	U1169	C1082	U974	U865	A656	A656
G1944	U1828	U1726	U	U	U1508	U1402	U1245	U1170	C1083	U975	U866	A657	A657
G1945	U1829	G1727	G	G	U1509	U1403	U1246	U1171	C1084	U976	U867	A658	U659
G1946	U1830	U1728	U	U	U1510	U1404	U1247	U1172	C1085	U977	U868	G660	G660
G1947	U1831	G1729	G	G	U1511	U1405	U1248	U1173	C1086	U978	U869	C751	C663
G1948	U1832	U1730	U	U	U1512	U1406	U1249	U1174	C1087	U979	U870	U752	C664
G1949	U1833	G1731	G	G	U1513	U1407	U1250	U1175	C1088	U980	U871	A753	A669
G1950	U1834	U1732	U	U	U1514	U1408	U1251	U1176	C1089	U981	U872	G764	G670
G1951	U1835	G1733	G	G	U1515	U1409	U1252	U1177	C1090	U982	U873	G765	U671
G1952	U1836	U1734	U	U	U1516	U1410	U1253	U1178	C1091	U983	U874	A770	U672
G1953	U1837	G1735	G	G	U1517	U1411	U1254	U1179	C1092	U984	U875	U771	A673
G1954	U1838	U1736	U	U	U1518	U1412	U1255	U1180	C1093	U985	U876	G789	G674
G1955	U1839	G1737	G	G	U1519	U1413	U1256	U1181	C1094	U986	U877	U788	U675
G1956	U1840	U1738	U	U	U1520	U1414	U1257	U1182	C1095	U987	U878	U789	G676
G1957	U1841	G1739	G	G	U1521	U1415	U1258	U1183	C1096	U988	U879		
G1958	U1842	U1740	U	U	U1522	U1416	U1259	U1184	C1097	U989	U880		
G1959	U1843	G1741	G	G	U1523	U1417	U1260	U1185	C1098	U990	U881		
G1960	U1844	U1742	U	U	U1524	U1418	U1261	U1186	C1099	U991	U882		
G1961	U1845	G1743	G	G	U1525	U1419	U1262	U1187	C1100	U992	U883		
G1962	U1846	U1744	U	U	U1526	U1420	U1263	U1188	C1101	U993	U884		
G1963	U1847	G1745	G	G	U1527	U1421	U1264	U1189	C1102	U994	U885		
G1964	U1848	U1746	U	U	U1528	U1422	U1265	U1190	C1103	U995	U886		
G1965	U1849	G1747	G	G	U1529	U1423	U1266	U1191	C1104	U996	U887		
G1966	U1850	U1748	U	U	U1530	U1424	U1267	U1192	C1105	U997	U888		
G1967	U1851	G1749	G	G	U1531	U1425	U1268	U1193	C1106	U998	U889		
G1968	U1852	U1750	U	U	U1532	U1426	U1269	U1194	C1107	U999	U890		
G1969	U1853	G1751	G	G	U1533	U1427	U1270	U1195	C1108	U1000	U891		
G1970	U1854	U1752	U	U	U1534	U1428	U1271	U1196	C1109	U1001	U892		
G1971	U1855	G1753	G	G	U1535	U1429	U1272	U1197	C1110	U1002	U893		
G1972	U1856	U1754	U	U	U1536	U1430	U1273	U1198	C1111	U1003	U894		
G1973	U1857	G1755	G	G	U1537	U1431	U1274	U1199	C1112	U1004	U895		
G1974	U1858	U1756	U	U	U1538	U1432	U1275	U1200	C1113	U1005	U896		
G1975	U1859	G1757	G	G	U1539	U1433	U1276	U1201	C1114	U1006	U897		
G1976	U1860	U1758	U	U	U1540	U1434	U1277	U1202	C1115	U1007	U898		
G1977	U1861	G1759	G	G	U1541	U1435	U1278	U1203	C1116	U1008	U899		
G1978	U1862	U1760	U	U	U1542	U1436	U1279	U1204	C1117	U1009	U900		
G1979	U1863	G1761	G	G	U1543	U1437	U1280	U1205	C1118	U1010	U901		
G1980	U1864	U1762	U	U	U1544	U1438	U1281	U1206	C1119	U1011	U902		
G1981	U1865	G1763	G	G	U1545	U1439	U1282	U1207	C1120	U1012	U903		
G1982	U1866	U1764	U	U	U1546	U1440	U1283	U1208	C1121	U1013	U904		
G1983	U1867	G1765	G	G	U1547	U1441	U1284	U1209	C1122	U1014	U905		
G1984	U1868	U1766	U	U	U1548	U1442	U1285	U1210	C1123	U1015	U906		
G1985	U1869	G1767	G	G	U1549	U1443	U1286	U1211	C1124	U1016	U907		
G1986	U1870	U1768	U	U	U1550	U1444	U1287	U1212	C1125	U1017	U908		
G1987	U1871	G1769	G	G	U1551	U1445	U1288	U1213	C1126	U1018	U909		
G1988	U1872	U1770	U	U	U1552	U1446	U1289	U1214	C1127	U1019	U910		
G1989	U1873	G1771	G	G	U1553	U1447	U1290	U1215	C1128	U1020	U911		
G1990	U1874	U1772	U	U	U1554	U1448	U1291	U1216	C1129	U1021	U912		
G1991	U1875	G1773	G	G	U1555	U1449	U1292	U1217	C1130	U1022	U913		
G1992	U1876	U1774	U	U	U1556	U1450	U1293	U1218	C1131	U1023	U914		
G1993	U1877	G1775	G	G	U1557	U1451	U1294	U1219	C1132	U1024	U915		
G1994	U1878	U1776	U	U	U1558	U1452	U1295	U1220	C1133	U1025	U916		
G1995	U1879	G1777	G	G	U1559	U1453	U1296	U1221	C1134	U1026	U917		
G1996	U1880	U1778	U	U	U1560	U1454	U1297	U1222	C1135	U1027	U918		
G1997	U1881	G1779	G	G	U1561	U1455	U1298	U1223	C1136	U1028	U919		
G1998	U1882	U1780	U	U	U1562	U1456	U1299	U1224	C1137	U1029	U920		
G1999	U1883	G1781	G	G	U1563	U1457	U1300	U1225	C1138	U1030	U921		
G2000	U1884	U1782	U	U	U1564	U1458	U1301	U1226	C1139	U1031	U922		
G2001	U1885	G1783	G	G	U1565	U1459	U1302	U1227	C1140	U1032	U923		
G2002	U1886	U1784	U	U	U1566	U1460	U1303	U1228	C1141	U1033	U924		
G2003	U1887	G1785	G	G	U1567	U1461	U1304	U1229	C1142	U1034	U925		
G2004	U1888	U1786	U	U	U1568	U1462	U1305	U1230	C1143	U1035	U926		
G2005	U1889	G1787											



Molecule 31: 5S rRNA

Chain b: 68% 30%



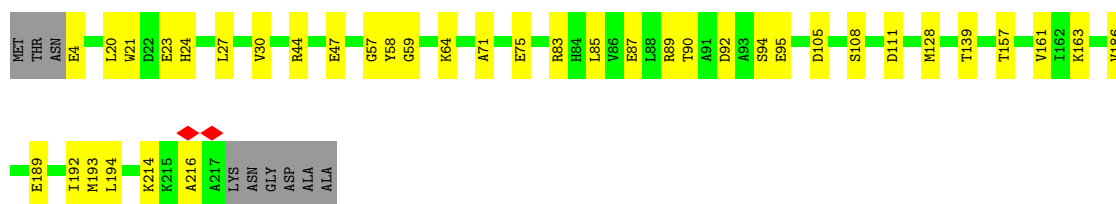
Molecule 32: 50S ribosomal protein L2

Chain c:  85% 13% ..



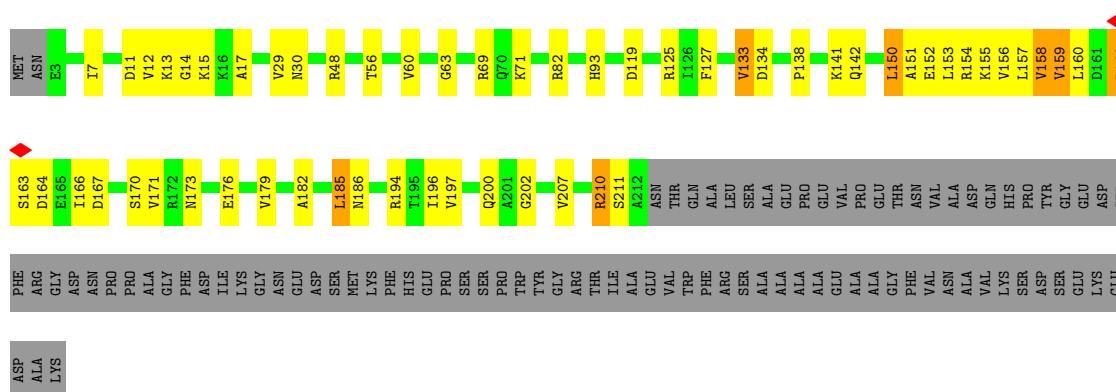
- Molecule 33: 50S ribosomal protein L3

Chain d:  79% 17% .



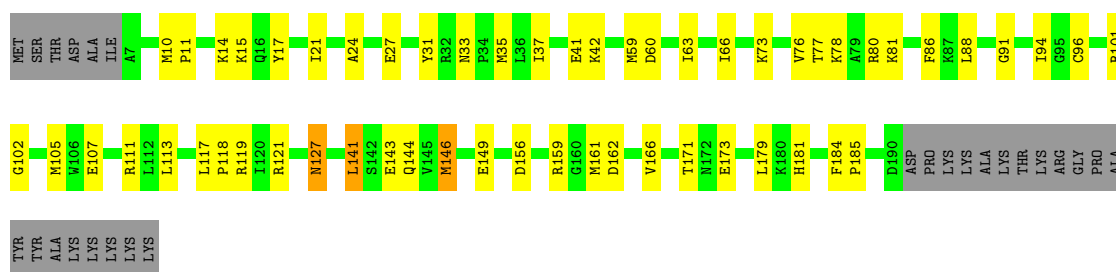
- Molecule 34: 50S ribosomal protein L4

Chain e:  51% 17% . 30%

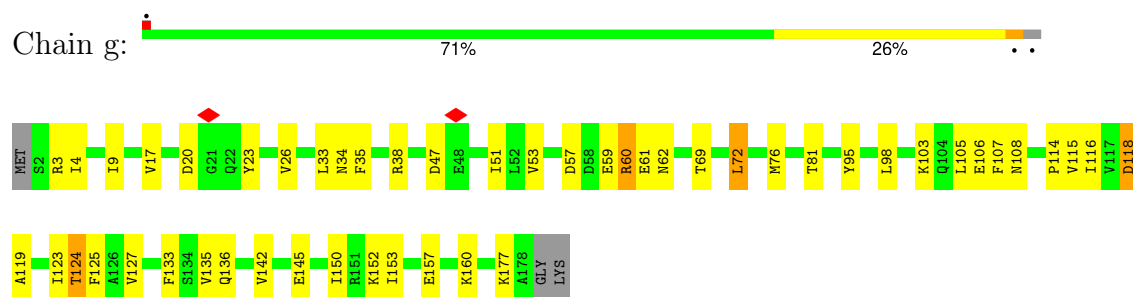


- Molecule 35: 50S ribosomal protein L5

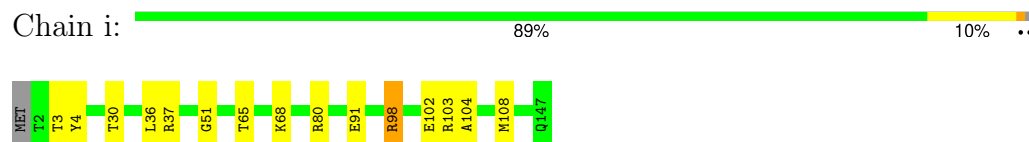
Chain f:  61% 25% . 12%



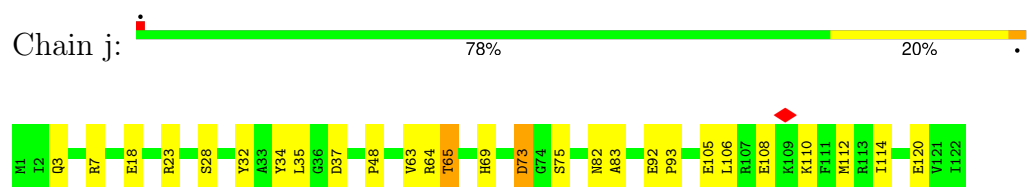
- Molecule 36: 50S ribosomal protein L6



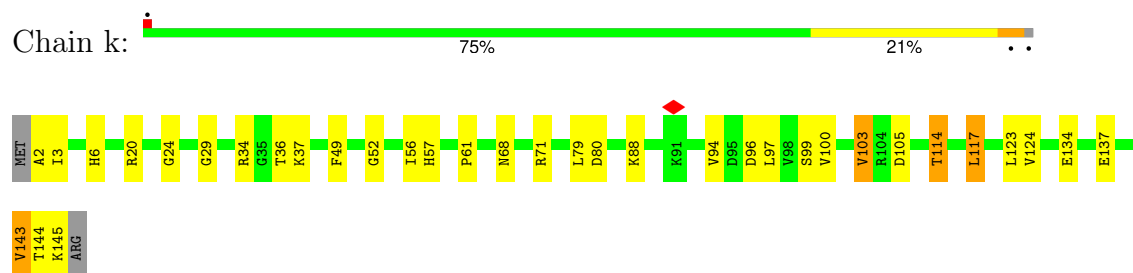
- Molecule 37: 50S ribosomal protein L13



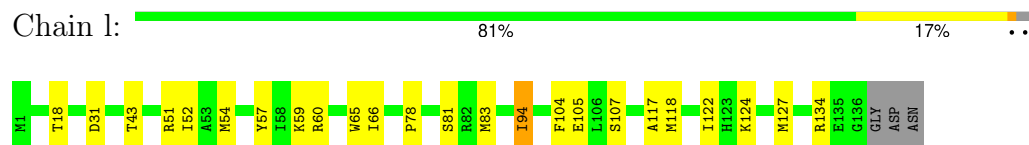
- Molecule 38: 50S ribosomal protein L14



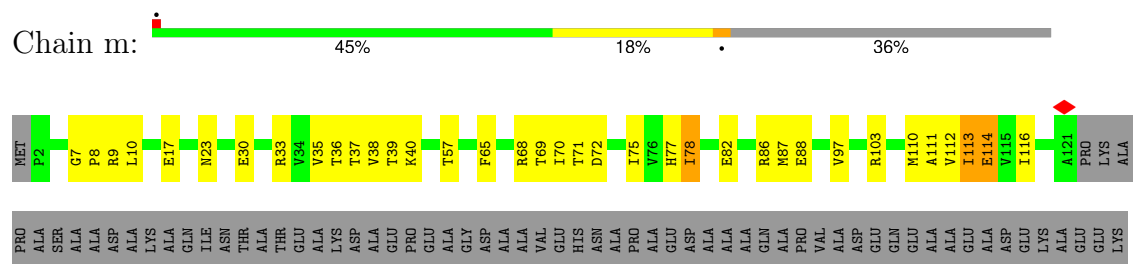
- Molecule 39: 50S ribosomal protein L15



- Molecule 40: 50S ribosomal protein L16



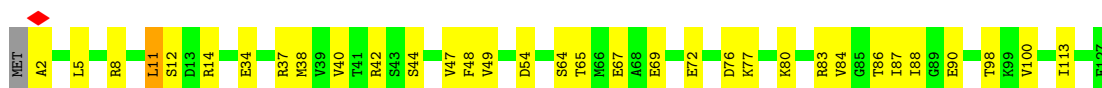
- Molecule 41: Large ribosomal subunit protein bL17



PRO
GLU
ALA

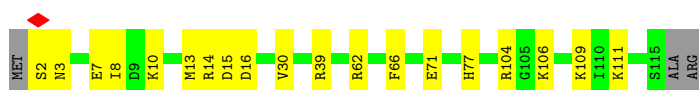
- Molecule 42: 50S ribosomal protein L18

Chain n:  73% 25% ..



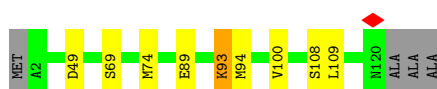
- Molecule 43: 50S ribosomal protein L19

Chain o:  81% 16% .



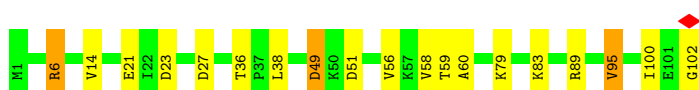
- Molecule 44: 50S ribosomal protein L20

Chain p:  89% 7% ..



- Molecule 45: Large ribosomal subunit protein bL21

Chain q:  81% 16% .



- Molecule 46: 50S ribosomal protein L22

Chain r:  69% 17% 14%



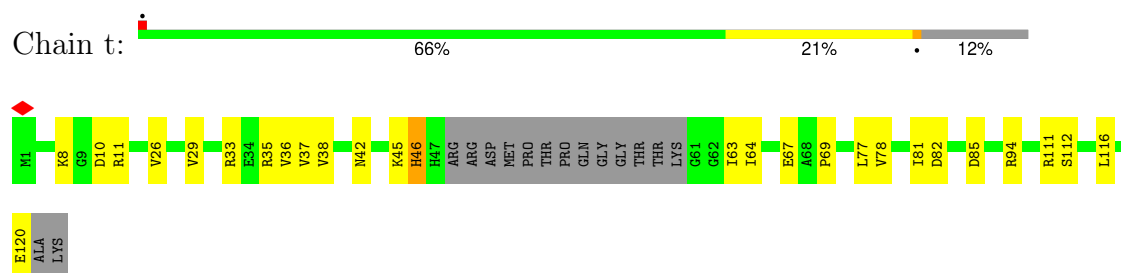
ALA
ALA
LYS
SER
GLU
THR
GLY
LYS
GLY
ALA

- Molecule 47: 50S ribosomal protein L23

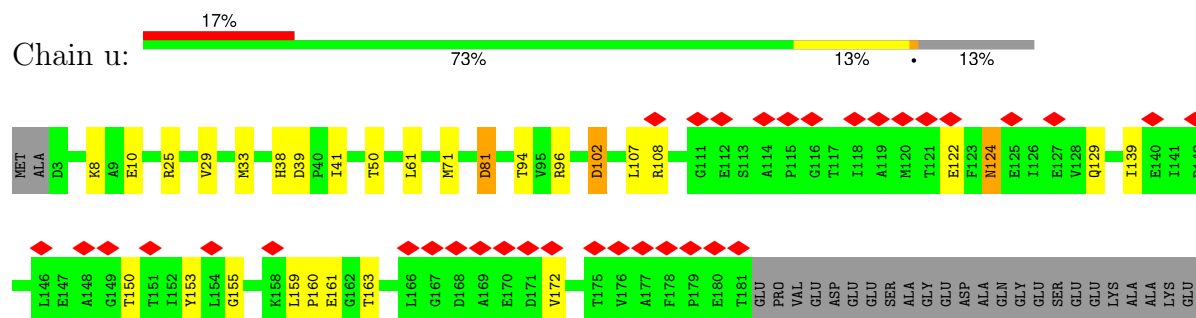
Chain s:  67% 26% 7%



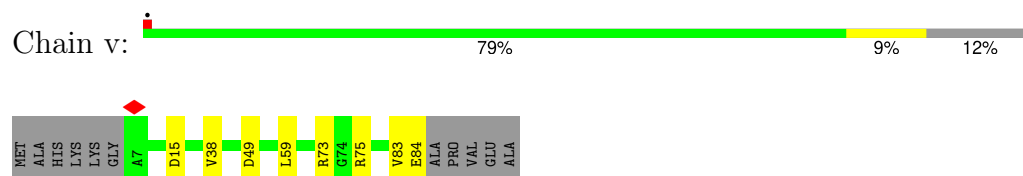
- Molecule 48: Large ribosomal subunit protein uL24



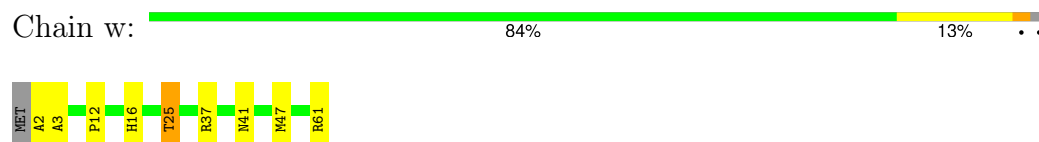
- Molecule 49: 50S ribosomal protein L25



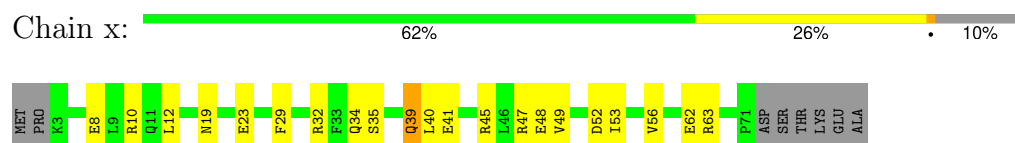
- Molecule 50: 50S ribosomal protein L27



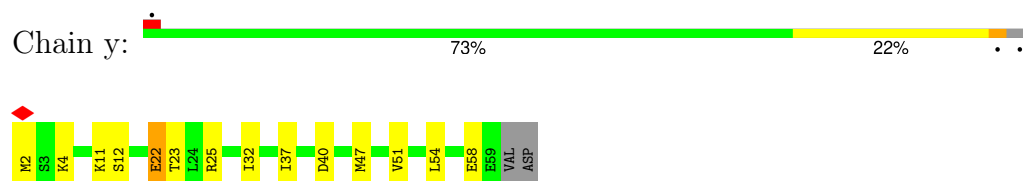
- Molecule 51: 50S ribosomal protein L28



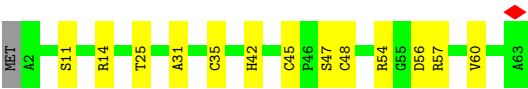
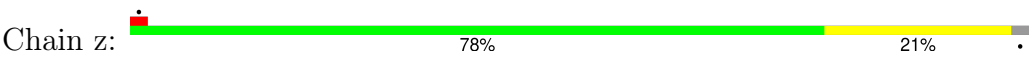
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L30



● Molecule 54: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.654	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, OMC, PSU, UR3, OMG, H2U, 3TD, 5MC, 2MA, G7M, 4SU, OMU, V7A, 2MG, 5MU, ZN, MA6, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.21	0/429	0.42	0/569
2	1	0.20	0/365	0.26	0/478
3	2	0.20	0/519	0.30	0/682
4	3	0.18	0/305	0.31	0/401
5	4	0.28	0/521	0.46	0/700
6	A	0.21	0/35898	0.30	0/56012
7	B	0.14	0/1864	0.40	1/2509 (0.0%)
8	C	0.27	0/1725	0.35	0/2689
9	D	0.25	0/1662	0.45	0/2239
10	E	0.16	0/1325	0.34	0/1789
11	F	0.20	0/794	0.56	1/1069 (0.1%)
12	G	0.17	0/1638	0.41	0/2201
13	H	0.20	0/1036	0.44	0/1395
14	I	0.17	0/1246	0.43	0/1679
15	J	0.19	0/1027	0.45	0/1376
16	K	0.20	0/874	0.46	0/1177
17	L	0.26	0/960	0.44	0/1283
18	M	0.20	0/800	0.55	0/1080
19	N	0.17	0/985	0.39	0/1317
20	O	0.20	0/718	0.44	0/959
21	P	0.38	0/1013	0.59	0/1370
22	Q	0.18	0/734	0.41	0/978
23	R	0.21	0/532	0.41	0/713
24	S	0.62	0/484	0.88	1/644 (0.2%)
25	T	0.19	0/676	0.30	0/897
26	U	0.19	0/675	0.47	0/908
27	V	0.21	0/184	0.30	0/236
28	X	0.19	0/277	0.36	0/355
29	Y	0.50	0/235	0.64	0/363
30	a	0.26	0/69472	0.35	3/108408 (0.0%)
31	b	0.22	0/2871	0.29	0/4475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.22	0/2132	0.38	1/2871 (0.0%)
33	d	0.22	0/1611	0.41	0/2172
34	e	0.30	0/1600	0.56	0/2165
35	f	0.20	0/1493	0.44	0/2001
36	g	0.16	0/1398	0.38	0/1884
37	i	0.29	0/1164	0.48	0/1574
38	j	0.21	0/957	0.37	0/1282
39	k	0.31	0/1090	0.57	0/1465
40	l	0.22	0/1108	0.40	0/1488
41	m	0.42	0/949	0.63	1/1277 (0.1%)
42	n	0.21	0/959	0.44	0/1281
43	o	0.20	0/909	0.31	0/1216
44	p	0.22	0/969	0.28	0/1292
45	q	0.20	0/785	0.42	0/1050
46	r	0.20	0/1028	0.33	0/1379
47	s	0.22	0/759	0.42	0/1022
48	t	0.19	0/840	0.43	0/1123
49	u	0.17	0/1396	0.39	0/1896
50	v	0.20	0/598	0.35	0/800
51	w	0.22	0/483	0.34	0/648
52	x	0.20	0/567	0.38	0/759
53	y	0.18	0/471	0.31	0/627
54	z	0.20	0/487	0.29	0/654
All	All	0.24	0/155597	0.36	8/232877 (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
21	P	0	1
24	S	0	2
34	e	0	1
37	i	0	2
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	152	ILE	N-CA-C	-6.23	106.70	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1898	C	O3'-P-O5'	-6.21	94.69	104.00
32	c	274	SER	CB-CA-C	-5.51	110.20	116.54
30	a	739	G	C4'-C3'-O3'	5.20	117.19	109.40
30	a	2961	U	O3'-P-O5'	5.18	111.78	104.00
24	S	26	ARG	CA-C-O	-5.17	115.54	120.92
41	m	78	ILE	CA-C-O	-5.06	116.14	121.41
11	F	34	LYS	CA-CB-CG	5.04	124.19	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	P	26	ARG	Sidechain
24	S	23	ARG	Sidechain
24	S	45	ARG	Sidechain
34	e	162	ARG	Sidechain
37	i	103	ARG	Sidechain
37	i	98	ARG	Sidechain

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	0	423	0	429	9	0
2	1	362	0	388	4	0
3	2	513	0	565	5	0
4	3	302	0	330	2	0
5	4	512	0	499	14	0
6	A	32340	0	16267	392	0
7	B	1836	0	1902	46	0
8	C	1625	0	829	8	0
9	D	1632	0	1663	55	0
10	E	1309	0	1349	22	0
11	F	785	0	818	27	0
12	G	1613	0	1626	41	0
13	H	1021	0	1059	17	0
14	I	1225	0	1275	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1012	0	1069	34	0
16	K	858	0	884	27	0
17	L	948	0	1031	14	0
18	M	786	0	823	37	0
19	N	976	0	1031	26	0
20	O	708	0	737	23	0
21	P	994	0	1008	29	0
22	Q	728	0	772	14	0
23	R	527	0	580	11	0
24	S	474	0	499	11	0
25	T	673	0	726	14	0
26	U	658	0	671	15	0
27	V	183	0	202	5	0
28	X	277	0	338	5	0
29	Y	211	0	106	4	0
30	a	62432	0	31308	621	0
31	b	2567	0	1297	23	0
32	c	2091	0	2150	24	0
33	d	1586	0	1634	31	0
34	e	1577	0	1619	51	0
35	f	1468	0	1487	43	0
36	g	1376	0	1421	34	0
37	i	1139	0	1163	8	0
38	j	946	0	1011	16	0
39	k	1072	0	1106	30	0
40	l	1082	0	1117	16	0
41	m	936	0	997	22	0
42	n	952	0	995	21	0
43	o	896	0	928	15	0
44	p	958	0	986	6	0
45	q	778	0	824	9	0
46	r	1017	0	1070	14	0
47	s	751	0	803	20	0
48	t	833	0	883	15	0
49	u	1376	0	1397	19	0
50	v	591	0	581	4	0
51	w	474	0	487	5	0
52	x	564	0	582	15	0
53	y	467	0	504	8	0
54	z	477	0	479	11	0
55	0	1	0	0	0	0
55	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	4	1	0	0	0	0
55	S	1	0	0	0	0
55	w	1	0	0	0	0
55	z	1	0	0	0	0
56	A	63	0	0	0	0
56	a	233	0	0	0	0
56	b	2	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
57	A	35	0	0	0	0
57	a	35	0	0	0	0
58	A	11	0	0	0	0
58	a	108	0	0	0	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
All	All	144415	0	96305	1820	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 8.

All (1820) 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)
11:F:22:LEU:HA	11:F:25:LYS:HE3	1.52	0.90
35:f:21:ILE:HD12	35:f:181:HIS:HB3	1.58	0.86
30:a:669:A:H62	30:a:1328:A:H2	1.23	0.84
34:e:133:VAL:HG23	34:e:141:LYS:HD3	1.60	0.81
9:D:90:GLU:HG3	9:D:186:ILE:HG12	1.65	0.79
30:a:1710:A:H61	30:a:1726:U:H5'	1.48	0.79
30:a:6:G:H1	30:a:3076:U:H3	1.30	0.78
30:a:2239:G:H1	30:a:2794:C:H5	1.31	0.78
38:j:108:GLU:HB3	38:j:110:LYS:HE2	1.66	0.78
30:a:1327:G:N7	39:k:20:ARG:NH2	2.33	0.76
18:M:36:VAL:HG12	18:M:76:ILE:HD13	1.66	0.76
9:D:172:LYS:HD2	21:P:115:ALA:HB1	1.68	0.75
6:A:78:G:H22	6:A:95:U:H3	1.32	0.75
6:A:1023:C:H2'	6:A:1024:G:H8	1.50	0.75
30:a:1638:U:O2'	30:a:1640:G:N2	2.20	0.74
33:d:4:GLU:OE1	33:d:4:GLU:N	2.21	0.74
13:H:101:LEU:HD22	13:H:104:LEU:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1166:G:N2	30:a:1169:A:OP2	2.20	0.74
6:A:1428:G:H8	6:A:1447:A:H62	1.36	0.73
13:H:41:LYS:NZ	13:H:48:ASP:OD1	2.22	0.73
34:e:153:LEU:H	34:e:154:ARG:NE	1.85	0.73
6:A:1089:G:O2'	7:B:109:LYS:NZ	2.20	0.73
22:Q:59:GLU:OE1	22:Q:59:GLU:N	2.20	0.73
27:V:3:LYS:NZ	30:a:1217:G:OP2	2.21	0.73
9:D:102:LEU:HD11	9:D:173:GLY:HA2	1.70	0.73
49:u:10:GLU:N	49:u:10:GLU:OE2	2.22	0.73
6:A:1215:G:OP2	19:N:114:ARG:NH2	2.22	0.73
40:l:60:ARG:HD3	40:l:60:ARG:H	1.52	0.73
30:a:1617:G:HO2'	30:a:1698:G:HO2'	1.32	0.72
30:a:1647:G:H5''	30:a:1648:C:H5'	1.71	0.72
30:a:2042:A:H61	30:a:2066:G:H1	1.37	0.72
30:a:1775:G:N2	30:a:1776:G:N7	2.36	0.72
34:e:176:GLU:N	34:e:176:GLU:OE2	2.23	0.72
6:A:1105:C:H2'	6:A:1106:A:H8	1.55	0.72
30:a:2495:C:OP2	35:f:80:ARG:NH2	2.21	0.71
30:a:225:G:H22	30:a:242:U:H4'	1.55	0.71
30:a:1281:C:H5	30:a:1318:G:H1	1.38	0.71
12:G:129:PHE:O	12:G:133:MET:HG3	1.89	0.71
30:a:712:U:H4'	30:a:739:G:N7	2.06	0.71
6:A:655:G:H2'	6:A:656:G:C8	2.26	0.70
6:A:1409:G:H5'	38:j:48:PRO:HB3	1.72	0.70
30:a:1254:G:N1	30:a:1257:U:OP2	2.24	0.70
46:r:42:ARG:NH1	46:r:91:ALA:O	2.23	0.70
30:a:130:G:H22	30:a:154:G:H22	1.40	0.70
39:k:36:THR:HG22	39:k:37:LYS:HG2	1.72	0.70
47:s:68:VAL:HG22	47:s:77:LYS:HG3	1.72	0.70
41:m:88:GLU:OE1	41:m:88:GLU:N	2.24	0.70
6:A:1272:G:H2'	6:A:1273:A:H4'	1.74	0.69
30:a:1138:G:H21	30:a:1168:A:H1'	1.57	0.69
15:J:135:GLU:N	15:J:135:GLU:OE2	2.25	0.69
30:a:73:A:OP1	52:x:47:ARG:NH2	2.25	0.69
42:n:67:GLU:OE1	42:n:67:GLU:N	2.23	0.69
45:q:6:ARG:HB3	45:q:38:LEU:HD21	1.73	0.69
7:B:24:ASN:ND2	7:B:192:CYS:O	2.25	0.69
30:a:1148:U:O2	30:a:1156:A:N6	2.25	0.69
33:d:189:GLU:OE1	33:d:189:GLU:N	2.25	0.69
4:3:16:VAL:HG12	4:3:25:VAL:HG22	1.74	0.69
11:F:30:ILE:HD11	11:F:75:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:9:G:N7	42:n:2:ALA:N	2.40	0.69
31:b:43:C:O2	35:f:101:ARG:NH1	2.25	0.69
34:e:155:LYS:HZ2	34:e:196:ILE:HG12	1.56	0.69
12:G:41:TRP:O	12:G:45:ASN:ND2	2.26	0.69
30:a:2706:G:H1	30:a:2721:C:H5	1.38	0.69
19:N:49:THR:H	19:N:52:GLN:HE21	1.41	0.69
30:a:2510:A:H2'	30:a:2511:G:C8	2.28	0.68
39:k:94:VAL:HG22	39:k:97:LEU:HD22	1.75	0.68
6:A:656:G:H2'	6:A:657:A:H8	1.58	0.68
6:A:1246:G:H8	6:A:1261:A:H62	1.41	0.68
34:e:153:LEU:H	34:e:154:ARG:HE	1.42	0.68
9:D:145:LYS:HE2	21:P:122:LYS:HD3	1.75	0.68
21:P:19:ARG:NH1	21:P:36:GLU:OE2	2.27	0.68
36:g:118:ASP:N	36:g:118:ASP:OD1	2.26	0.68
21:P:95:GLN:HB2	21:P:98:ARG:HH12	1.58	0.68
2:1:19:ARG:NH1	30:a:124:A:OP2	2.26	0.68
6:A:1237:G:H21	6:A:1356:C:H1'	1.58	0.68
40:l:65:TRP:HB2	40:l:105:GLU:HB2	1.75	0.68
48:t:11:ARG:NH2	48:t:85:ASP:OD2	2.27	0.68
6:A:1096:A:N1	12:G:176:THR:OG1	2.26	0.68
6:A:1243:G:OP1	6:A:1243:G:N2	2.27	0.68
30:a:1688:U:H2'	30:a:1689:G:O4'	1.93	0.67
6:A:874:G:OP2	28:X:10:LYS:NZ	2.27	0.67
13:H:55:LYS:HA	13:H:55:LYS:HE3	1.75	0.67
30:a:670:G:H1	39:k:34:ARG:HD2	1.59	0.67
30:a:2824:A:H5''	37:i:80:ARG:HD2	1.76	0.67
7:B:99:GLY:O	7:B:101:LEU:N	2.28	0.67
18:M:5:LYS:HB3	18:M:6:ILE:HD12	1.76	0.67
30:a:1698:G:H1	30:a:1915:G:H22	1.41	0.67
12:G:52:SER:HB2	12:G:114:LEU:HD11	1.77	0.67
41:m:35:VAL:HG22	41:m:112:VAL:HG22	1.75	0.67
31:b:87:G:H21	31:b:90:A:H2	1.41	0.67
30:a:392:G:H21	30:a:415:A:H62	1.41	0.67
41:m:30:GLU:HG3	41:m:75:ILE:HD11	1.76	0.67
3:2:25:ARG:HB3	39:k:61:PRO:HG2	1.77	0.67
30:a:291:U:H5'	30:a:308:U:C5	2.30	0.67
11:F:23:MET:HA	11:F:23:MET:HE3	1.77	0.66
17:L:74:LEU:HD23	17:L:104:THR:HB	1.77	0.66
18:M:85:ASP:O	18:M:89:ARG:HD2	1.95	0.66
33:d:47:GLU:N	33:d:47:GLU:OE2	2.28	0.66
19:N:47:GLU:N	19:N:47:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:159:VAL:HB	34:e:202:GLY:HA2	1.77	0.66
30:a:2649:C:O2	40:l:124:LYS:NZ	2.27	0.66
18:M:5:LYS:HB2	18:M:77:LEU:HA	1.77	0.66
18:M:78:GLU:HG2	18:M:80:THR:HB	1.76	0.66
25:T:28:LEU:HD22	25:T:58:LEU:HD23	1.77	0.66
30:a:142:G:H21	30:a:147:G:H1	1.44	0.66
42:n:69:GLU:OE1	42:n:69:GLU:N	2.26	0.66
33:d:108:SER:N	33:d:111:ASP:OD2	2.28	0.66
6:A:917:G:O6	14:I:3:ARG:NH2	2.29	0.66
30:a:2584:G:OP2	30:a:2584:G:N2	2.22	0.66
52:x:10:ARG:NH1	52:x:62:GLU:OE2	2.29	0.66
1:0:9:ARG:NH1	30:a:2467:C:OP2	2.29	0.66
30:a:1687:G:H2'	30:a:1688:U:H5	1.61	0.66
42:n:83:ARG:O	42:n:87:ILE:HG13	1.95	0.66
33:d:95:GLU:OE2	33:d:95:GLU:N	2.29	0.66
41:m:103:ARG:HG3	41:m:110:MET:HE3	1.77	0.65
53:y:2:MET:HE1	53:y:4:LYS:HG3	1.78	0.65
6:A:271:U:H2'	6:A:272:A:C8	2.30	0.65
35:f:10:MET:HE3	35:f:14:LYS:HB3	1.78	0.65
34:e:142:GLN:NE2	34:e:170:SER:O	2.28	0.65
30:a:71:U:OP1	47:s:5:LYS:NZ	2.28	0.65
36:g:127:VAL:HG23	36:g:133:PHE:HB3	1.78	0.65
16:K:87:ARG:HB2	16:K:112:GLU:HB2	1.79	0.65
30:a:1698:G:H22	30:a:1915:G:N2	1.95	0.65
6:A:728:U:H2'	6:A:729:U:C2	2.32	0.65
7:B:58:LYS:HE3	7:B:224:GLU:HG2	1.79	0.65
18:M:10:LEU:HD23	18:M:98:ILE:HD11	1.77	0.65
30:a:941:G:H2'	30:a:942:A:C8	2.32	0.65
14:I:27:VAL:O	14:I:31:LEU:HB2	1.97	0.65
39:k:94:VAL:HG23	39:k:96:ASP:H	1.62	0.65
30:a:379:A:O2'	30:a:380:G:O4'	2.14	0.65
30:a:1831:U:H5'	30:a:1832:C:H5'	1.77	0.65
8:C:21:A:H61	8:C:46:G:H2'	1.62	0.64
34:e:150:LEU:O	34:e:154:ARG:NH1	2.31	0.64
34:e:207:VAL:O	34:e:211:SER:HB3	1.97	0.64
6:A:696:G:H2'	6:A:697:A:C8	2.32	0.64
30:a:1623:C:H5	30:a:1731:G:H1	1.45	0.64
6:A:271:U:H2'	6:A:272:A:H8	1.62	0.64
6:A:659:U:H3	6:A:695:G:H22	1.45	0.64
6:A:984:A:N1	6:A:1025:G:O6	2.31	0.64
6:A:406:G:OP2	9:D:110:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:695:G:H2'	6:A:696:G:C8	2.32	0.64
21:P:46:PRO:HG2	21:P:96:PRO:HA	1.78	0.64
6:A:805:G:HO2'	13:H:2:THR:N	1.94	0.64
11:F:23:MET:O	11:F:27:LEU:HG	1.98	0.64
30:a:332:U:H3	30:a:449:G:H1	1.44	0.64
6:A:1204:C:H2'	6:A:1205:A:C8	2.33	0.64
18:M:34:ALA:HB1	18:M:76:ILE:HD11	1.80	0.64
26:U:11:VAL:HA	26:U:38:SER:HB2	1.79	0.64
21:P:45:ASP:HB3	21:P:46:PRO:HD3	1.80	0.64
41:m:33:ARG:NH1	54:z:60:VAL:O	2.31	0.64
49:u:107:LEU:O	49:u:108:ARG:NH1	2.29	0.64
30:a:2287:G:H1	30:a:2366:U:H3	1.46	0.64
30:a:970:U:H3	30:a:975:G:H1	1.44	0.63
30:a:1143:U:H3	30:a:1171:A:H8	1.42	0.63
12:G:119:ILE:O	12:G:123:LEU:HG	1.97	0.63
9:D:169:ARG:HD2	21:P:116:PRO:HD3	1.80	0.63
31:b:16:G:OP1	42:n:8:ARG:NH2	2.30	0.63
14:I:36:LYS:O	14:I:40:GLN:HG2	1.97	0.63
30:a:179:G:N2	30:a:180:U:O4	2.29	0.63
36:g:9:ILE:HB	36:g:51:ILE:HB	1.81	0.63
21:P:68:GLU:N	21:P:68:GLU:OE2	2.32	0.63
30:a:875:U:O4	34:e:69:ARG:NH1	2.31	0.63
34:e:127:PHE:HB2	34:e:197:VAL:HG12	1.79	0.63
36:g:17:VAL:HG12	36:g:26:VAL:HG22	1.79	0.63
11:F:27:LEU:HB3	11:F:37:VAL:HG21	1.79	0.63
6:A:988:G:N2	6:A:1022:U:O2	2.32	0.63
6:A:1270:C:OP2	6:A:1271:G:O2'	2.16	0.63
11:F:33:GLU:OE1	11:F:33:GLU:N	2.32	0.63
6:A:60:U:H2'	6:A:61:G:H8	1.64	0.63
6:A:195:G:O2'	22:Q:8:ARG:NH2	2.32	0.63
6:A:438:C:H4'	9:D:148:PRO:HG2	1.80	0.63
30:a:1489:C:H2'	30:a:1490:A:C8	2.34	0.63
6:A:1342:G:H2'	6:A:1343:A:C8	2.33	0.62
19:N:88:GLN:HG2	19:N:98:VAL:HB	1.81	0.62
30:a:2288:G:O2'	30:a:2289:U:OP1	2.17	0.62
33:d:71:ALA:O	33:d:75:GLU:HG3	1.98	0.62
30:a:1105:G:N2	30:a:1106:U:O4	2.30	0.62
18:M:77:LEU:HD23	18:M:77:LEU:H	1.62	0.62
30:a:1981:U:OP2	32:c:270:ARG:NH2	2.31	0.62
30:a:3073:G:H4'	30:a:3074:A:H5'	1.80	0.62
30:a:1687:G:H2'	30:a:1688:U:C5	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2720:C:O2'	30:a:2721:C:O2	2.10	0.62
34:e:160:LEU:HB2	34:e:164:ASP:HB2	1.80	0.62
6:A:822:C:H2'	6:A:823:A:C8	2.34	0.62
32:c:223:GLY:HA2	32:c:226:MET:HG3	1.81	0.62
47:s:7:ARG:NH2	47:s:43:GLU:OE2	2.33	0.62
52:x:34:GLN:HG2	52:x:39:GLN:HB2	1.81	0.62
30:a:2291:U:O2	30:a:2361:C:N4	2.33	0.62
14:I:118:GLU:OE1	14:I:118:GLU:N	2.32	0.61
25:T:48:THR:O	25:T:52:ARG:HG2	1.99	0.61
35:f:59:MET:HE2	35:f:76:VAL:HG13	1.82	0.61
36:g:98:LEU:HG	36:g:106:GLU:HB3	1.81	0.61
49:u:102:ASP:HA	49:u:129:GLN:HA	1.82	0.61
5:4:10:ARG:HH12	5:4:30:SER:HA	1.63	0.61
11:F:34:LYS:HD2	11:F:34:LYS:O	2.00	0.61
7:B:214:LEU:O	7:B:218:ILE:HG12	2.00	0.61
41:m:69:THR:HG22	41:m:70:ILE:H	1.66	0.61
41:m:69:THR:O	41:m:71:THR:N	2.33	0.61
22:Q:35:ARG:NH2	22:Q:46:THR:OG1	2.34	0.61
30:a:153:U:H2'	30:a:154:G:C8	2.36	0.61
33:d:186:VAL:HG22	33:d:193:MET:HG2	1.83	0.61
53:y:22:GLU:HG3	53:y:25:ARG:HH21	1.65	0.61
30:a:1092:A:N3	30:a:1237:C:O2'	2.34	0.61
34:e:159:VAL:HG22	34:e:160:LEU:H	1.64	0.61
53:y:23:THR:HG23	53:y:47:MET:HG2	1.81	0.61
6:A:1204:C:H2'	6:A:1205:A:H8	1.65	0.61
12:G:76:ILE:HA	12:G:83:ALA:HB2	1.83	0.61
36:g:33:LEU:HB3	36:g:76:MET:HE2	1.82	0.61
40:l:43:THR:HG22	40:l:94:ILE:HG22	1.82	0.61
6:A:348:G:OP1	43:o:39:ARG:NH1	2.33	0.61
6:A:358:A:N3	6:A:370:U:O2'	2.33	0.61
22:Q:18:LEU:HD13	22:Q:65:ARG:HH21	1.66	0.60
30:a:1716:U:O2'	30:a:1721:G:N2	2.34	0.60
46:r:23:ILE:HG12	46:r:121:THR:HG23	1.82	0.60
49:u:161:GLU:N	49:u:161:GLU:OE2	2.33	0.60
15:J:71:LYS:HA	15:J:71:LYS:HE3	1.82	0.60
23:R:29:LEU:O	23:R:33:ILE:HG13	2.01	0.60
30:a:198:A:H2'	30:a:199:G:C8	2.36	0.60
6:A:1384:C:OP2	10:E:52:ARG:NH2	2.34	0.60
18:M:11:ARG:HE	18:M:71:LYS:HG3	1.66	0.60
30:a:1982:G:OP1	32:c:258:ARG:NH1	2.34	0.60
39:k:24:GLY:O	39:k:29:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:95:G:OP1	49:u:25:ARG:NH2	2.30	0.60
20:O:5:GLU:H	20:O:5:GLU:CD	2.09	0.60
30:a:130:G:N2	30:a:154:G:H22	1.99	0.60
18:M:52:ILE:HB	24:S:41:ARG:HD2	1.84	0.60
34:e:152:GLU:HB3	34:e:176:GLU:HG3	1.82	0.60
30:a:949:G:H21	30:a:951:A:H62	1.49	0.60
6:A:148:G:H2'	6:A:149:G:C8	2.36	0.60
6:A:930:A:H2'	6:A:931:G:C8	2.37	0.60
24:S:27:CYS:SG	24:S:28:GLY:N	2.74	0.60
30:a:1647:G:H4'	30:a:1729:G:H21	1.67	0.60
40:l:59:LYS:HB3	40:l:60:ARG:HD3	1.83	0.60
6:A:1341:A:H2'	6:A:1342:G:H8	1.65	0.60
7:B:67:ILE:HD12	7:B:161:ALA:HB3	1.82	0.60
30:a:132:A:N3	30:a:1598:U:O2'	2.33	0.60
30:a:288:G:N3	30:a:310:C:N4	2.49	0.60
6:A:25:G:H2'	6:A:26:G:C8	2.36	0.59
19:N:108:ARG:NH2	19:N:113:LYS:O	2.35	0.59
30:a:384:A:N3	30:a:404:C:O2'	2.32	0.59
6:A:183:G:H2'	6:A:184:G:H2'	1.84	0.59
6:A:1006:U:H2'	6:A:1007:G:H8	1.67	0.59
6:A:1359:U:OP1	15:J:115:THR:OG1	2.20	0.59
12:G:168:ARG:NH2	12:G:170:GLY:O	2.35	0.59
30:a:1695:U:H3'	30:a:1696:G:C8	2.37	0.59
6:A:656:G:H2'	6:A:657:A:C8	2.37	0.59
15:J:84:LYS:O	15:J:84:LYS:NZ	2.27	0.59
19:N:106:ASN:O	19:N:108:ARG:HD2	2.02	0.59
21:P:56:VAL:HG21	21:P:74:LEU:HD21	1.83	0.59
9:D:3:ARG:HD2	9:D:110:ARG:HE	1.66	0.59
16:K:23:VAL:O	16:K:86:LYS:N	2.35	0.59
30:a:1047:U:O2'	30:a:2455:A:N3	2.34	0.59
30:a:1440:G:OP1	51:w:2:ALA:N	2.36	0.59
14:I:38:VAL:O	14:I:42:ILE:HG13	2.01	0.59
30:a:3016:U:H2'	30:a:3017:A:C8	2.38	0.59
47:s:72:ARG:O	47:s:73:THR:OG1	2.17	0.59
6:A:1115:A:H2'	6:A:1116:G:H8	1.68	0.59
11:F:47:ARG:NH1	11:F:56:SER:OG	2.36	0.59
30:a:2801:C:OP1	33:d:163:LYS:NZ	2.35	0.59
52:x:41:GLU:H	52:x:41:GLU:CD	2.09	0.59
7:B:61:VAL:HG11	7:B:225:GLY:HA3	1.85	0.59
30:a:287:U:O2'	30:a:311:A:N6	2.34	0.59
31:b:30:C:OP1	42:n:14:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:m:30:GLU:HG3	41:m:75:ILE:CD1	2.32	0.59
49:u:102:ASP:OD1	49:u:102:ASP:N	2.26	0.59
5:4:42:HIS:HB3	5:4:45:TYR:HD2	1.68	0.59
48:t:67:GLU:OE1	48:t:67:GLU:N	2.35	0.59
1:0:45:ARG:HH22	30:a:2583:U:H5'	1.66	0.58
9:D:53:LYS:NZ	9:D:64:GLU:OE1	2.35	0.58
6:A:1422:G:H2'	6:A:1423:C:C6	2.37	0.58
9:D:49:GLN:HB3	9:D:198:LEU:HB2	1.85	0.58
10:E:108:VAL:HG23	10:E:119:LEU:HB2	1.85	0.58
30:a:660:G:O2'	30:a:1331:A:OP1	2.21	0.58
30:a:799:U:O2'	30:a:801:A:N7	2.29	0.58
32:c:166:VAL:HG21	32:c:182:MET:HE1	1.85	0.58
35:f:127:ASN:HD22	35:f:127:ASN:H	1.51	0.58
6:A:977:G:O2'	6:A:978:A:N7	2.36	0.58
9:D:87:GLN:O	9:D:91:SER:OG	2.21	0.58
34:e:157:LEU:HD11	34:e:185:LEU:HD13	1.85	0.58
30:a:838:U:H2'	30:a:839:G:H8	1.67	0.58
23:R:47:LEU:HD22	23:R:51:ASP:HB3	1.84	0.58
30:a:480:A:H1'	30:a:500:G:O4'	2.03	0.58
35:f:119:ARG:NH1	35:f:146:MET:O	2.31	0.58
36:g:107:PHE:HB2	36:g:115:VAL:HG13	1.86	0.58
6:A:183:G:H21	6:A:226:G:H4'	1.67	0.58
6:A:1024:G:H2'	6:A:1025:G:C8	2.38	0.58
34:e:15:LYS:H	34:e:15:LYS:HE2	1.68	0.58
44:p:93:LYS:HG2	44:p:94:MET:HE2	1.84	0.58
6:A:646:G:H22	6:A:723:G:H1	1.51	0.58
6:A:718:U:H2'	6:A:719:C:C6	2.39	0.58
6:A:1274:A:H2'	6:A:1275:A:C8	2.38	0.58
49:u:71:MET:HE2	49:u:94:THR:HG21	1.86	0.58
6:A:980:A:H2'	6:A:981:U:C6	2.39	0.58
6:A:1341:A:H2'	6:A:1342:G:C8	2.38	0.58
30:a:279:A:HO2'	30:a:456:C:HO2'	1.50	0.58
41:m:7:GLY:O	41:m:9:ARG:NH1	2.36	0.58
15:J:97:ALA:HB2	15:J:141:LEU:HD11	1.84	0.58
20:O:87:ARG:HH21	30:a:799:U:H3'	1.69	0.58
30:a:204:A:N6	30:a:2612:A:O2'	2.36	0.58
30:a:1489:C:H2'	30:a:1490:A:H8	1.66	0.58
30:a:2052:G:N2	30:a:2055:U:OP2	2.36	0.58
50:v:38:VAL:HG12	50:v:59:LEU:HB2	1.86	0.58
22:Q:8:ARG:O	22:Q:10:THR:N	2.37	0.57
36:g:124:THR:HG23	36:g:136:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:150:ILE:HA	36:g:153:ILE:HD12	1.86	0.57
9:D:139:ASP:OD2	9:D:140:VAL:N	2.37	0.57
30:a:2036:A:H2'	30:a:2037:A:C8	2.39	0.57
6:A:265:G:OP1	25:T:74:ASN:ND2	2.26	0.57
6:A:384:A:H2'	6:A:385:A:H8	1.69	0.57
11:F:16:GLU:O	11:F:19:VAL:HG22	2.05	0.57
25:T:15:GLU:OE2	25:T:18:ARG:NH2	2.36	0.57
30:a:2288:G:N2	30:a:2366:U:O2	2.36	0.57
34:e:155:LYS:NZ	34:e:196:ILE:HG12	2.19	0.57
44:p:89:GLU:OE2	45:q:6:ARG:NH2	2.36	0.57
6:A:1309:G:H2'	6:A:1310:A:C8	2.39	0.57
20:O:76:TYR:O	20:O:80:ILE:HG12	2.03	0.57
30:a:82:G:N2	30:a:102:A:OP2	2.35	0.57
30:a:1118:U:H5''	36:g:60:ARG:HE	1.69	0.57
38:j:69:HIS:ND1	38:j:105:GLU:OE1	2.37	0.57
7:B:66:GLN:HB2	7:B:160:GLN:HG2	1.86	0.57
12:G:179:ALA:HB1	12:G:202:TYR:HE1	1.69	0.57
30:a:903:G:N1	30:a:1265:U:OP2	2.30	0.57
44:p:69:SER:OG	44:p:74:MET:O	2.21	0.57
6:A:1057:G:H21	7:B:106:THR:HG21	1.69	0.57
30:a:106:G:H4'	30:a:379:A:H5''	1.86	0.57
30:a:1727:G:H2'	30:a:1728:A:C8	2.39	0.57
35:f:113:LEU:HA	35:f:117:LEU:HD21	1.87	0.57
6:A:618:U:O3'	22:Q:11:ARG:NH2	2.37	0.57
30:a:1224:U:OP2	37:i:68:LYS:NZ	2.37	0.57
30:a:2843:G:O6	36:g:177:LYS:NZ	2.31	0.57
32:c:147:LEU:HD13	32:c:155:MET:HE2	1.87	0.57
6:A:1023:C:H2'	6:A:1024:G:C8	2.36	0.57
11:F:21:SER:HA	11:F:24:GLU:HG3	1.86	0.57
18:M:80:THR:HG23	18:M:83:THR:OG1	2.04	0.57
5:4:44:PHE:HE2	35:f:185:PRO:HB3	1.70	0.57
6:A:668:G:O2'	6:A:685:G:N2	2.38	0.57
6:A:1056:C:H2'	6:A:1057:G:H8	1.70	0.57
30:a:392:G:N1	30:a:395:A:OP2	2.35	0.57
30:a:2208:G:H2'	30:a:2209:A:C8	2.40	0.57
52:x:19:ASN:O	52:x:23:GLU:HG3	2.04	0.57
6:A:21:U:H2'	6:A:22:C:C6	2.40	0.56
34:e:160:LEU:C	34:e:162:ARG:H	2.13	0.56
43:o:3:ASN:O	43:o:7:GLU:HG3	2.04	0.56
9:D:26:PHE:O	9:D:29:ARG:NE	2.28	0.56
34:e:153:LEU:HB3	34:e:194:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:521:A:H2'	6:A:522:G:H8	1.70	0.56
6:A:739:U:H2'	6:A:740:G:O4'	2.06	0.56
6:A:1154:C:H3'	6:A:1155:A:H8	1.69	0.56
6:A:1441:U:H2'	6:A:1442:G:C8	2.40	0.56
9:D:69:ARG:O	9:D:73:GLU:HG3	2.06	0.56
9:D:148:PRO:O	9:D:152:ILE:HG12	2.05	0.56
30:a:63:A:H2'	30:a:64:C:C6	2.40	0.56
30:a:142:G:H22	30:a:147:G:H22	1.53	0.56
7:B:174:ILE:O	7:B:178:ARG:HG2	2.06	0.56
30:a:1481:C:H2'	30:a:1482:G:H8	1.70	0.56
30:a:1711:G:N1	30:a:1725:G:O2'	2.30	0.56
32:c:133:LEU:HD12	32:c:136:ILE:HD12	1.88	0.56
6:A:12:A:N6	9:D:197:GLU:O	2.39	0.56
15:J:69:GLN:NE2	15:J:104:ASP:OD1	2.39	0.56
52:x:35:SER:HB2	52:x:40:LEU:HD22	1.87	0.56
6:A:454:A:H5''	6:A:455:G:H21	1.70	0.56
6:A:751:G:H4'	6:A:1500:A:H4'	1.87	0.56
31:b:40:U:N3	31:b:44:G:OP2	2.32	0.56
46:r:54:LYS:HE3	46:r:65:ARG:HD2	1.88	0.56
6:A:317:A:N7	6:A:330:U:H5	2.03	0.56
34:e:153:LEU:H	34:e:154:ARG:CZ	2.19	0.56
43:o:2:SER:OG	43:o:3:ASN:N	2.39	0.56
6:A:1189:C:OP1	24:S:2:ALA:N	2.38	0.56
6:A:1500:A:H2'	6:A:1501:C:C6	2.41	0.56
6:A:1507:G:N7	28:X:15:LYS:NZ	2.44	0.56
7:B:213:LEU:O	7:B:217:ILE:HG23	2.06	0.56
27:V:21:ARG:NH2	30:a:1065:C:N3	2.54	0.56
30:a:1255:U:H4'	30:a:1256:G:N2	2.21	0.56
35:f:10:MET:HE1	35:f:15:LYS:HB3	1.87	0.56
6:A:697:A:H2'	6:A:698:A:C8	2.40	0.56
30:a:917:U:H2'	30:a:918:G:H8	1.70	0.56
6:A:1383:A:H4'	6:A:1384:C:H5''	1.88	0.55
19:N:12:ASP:O	19:N:44:ARG:NH2	2.38	0.55
30:a:1175:C:H2'	30:a:1176:G:O4'	2.07	0.55
36:g:57:ASP:OD2	36:g:59:GLU:N	2.39	0.55
38:j:35:LEU:HD21	38:j:65:THR:H	1.71	0.55
48:t:120:GLU:OE1	48:t:120:GLU:N	2.39	0.55
9:D:182:THR:O	9:D:186:ILE:HD12	2.05	0.55
30:a:1835:G:H5'	41:m:39:THR:HG21	1.88	0.55
6:A:1040:A:O2'	12:G:160:GLU:O	2.24	0.55
6:A:1309:G:H2'	6:A:1310:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:60:THR:HG22	7:B:65:GLY:HA2	1.89	0.55
30:a:2428:G:H2'	30:a:2429:A:C8	2.42	0.55
6:A:1342:G:H2'	6:A:1343:A:H8	1.69	0.55
9:D:14:ARG:HA	9:D:32:PRO:HB3	1.88	0.55
10:E:133:SER:HB3	10:E:160:VAL:HG23	1.88	0.55
14:I:90:GLU:H	14:I:90:GLU:CD	2.15	0.55
19:N:7:VAL:HG11	19:N:22:ILE:HG12	1.89	0.55
30:a:1901:U:H2'	30:a:1902:C:C6	2.41	0.55
30:a:2042:A:N6	30:a:2066:G:H1	2.03	0.55
34:e:11:ASP:HB2	34:e:17:ALA:HB3	1.87	0.55
39:k:56:ILE:HD12	39:k:57:HIS:N	2.21	0.55
54:z:31:ALA:O	54:z:54:ARG:NH1	2.39	0.55
7:B:100:MET:HA	7:B:107:ILE:HG13	1.88	0.55
7:B:191:ASN:ND2	7:B:191:ASN:O	2.40	0.55
9:D:80:LYS:HE2	10:E:124:PRO:HB2	1.89	0.55
12:G:11:ARG:NH1	12:G:176:THR:O	2.39	0.55
30:a:83:A:H62	30:a:101:G:H8	1.53	0.55
30:a:373:G:N3	30:a:438:G:N2	2.55	0.55
6:A:521:A:H2'	6:A:522:G:C8	2.40	0.55
6:A:829:C:H5'	23:R:17:HIS:CE1	2.42	0.55
30:a:994:A:H2'	30:a:995:A:C8	2.42	0.55
30:a:2425:U:H2'	30:a:2426:U:C6	2.41	0.55
30:a:2612:A:H2'	30:a:2612:A:N3	2.21	0.55
6:A:1080:U:OP1	6:A:1093:G:N2	2.33	0.55
25:T:36:ARG:O	25:T:40:GLU:HG3	2.07	0.55
6:A:208:U:H5''	25:T:52:ARG:NH2	2.21	0.55
6:A:1460:G:H2'	6:A:1461:G:C8	2.41	0.55
24:S:47:MET:HG2	24:S:52:GLN:HB2	1.89	0.55
30:a:263:A:H2'	30:a:264:A:C8	2.42	0.55
33:d:105:ASP:N	33:d:105:ASP:OD2	2.38	0.55
40:l:60:ARG:HD3	40:l:60:ARG:N	2.19	0.55
6:A:326:G:N1	6:A:329:A:OP2	2.40	0.55
6:A:1162:A:H2'	6:A:1163:G:C8	2.42	0.55
30:a:827:U:H2'	30:a:828:C:C6	2.42	0.55
39:k:56:ILE:HD12	39:k:57:HIS:H	1.72	0.55
11:F:18:GLN:O	11:F:22:LEU:HG	2.06	0.54
30:a:63:A:H2'	30:a:64:C:H6	1.72	0.54
30:a:130:G:H22	30:a:154:G:N2	2.04	0.54
30:a:1143:U:H4'	30:a:1144:U:H5'	1.89	0.54
30:a:2382:C:OP2	51:w:37:ARG:NH1	2.40	0.54
6:A:9:U:O2'	6:A:10:G:O5'	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:208:U:H4'	25:T:52:ARG:HE	1.72	0.54
6:A:527:C:H5'	9:D:64:GLU:HB2	1.90	0.54
6:A:728:U:H2'	6:A:729:U:N3	2.21	0.54
17:L:33:VAL:HG22	17:L:79:MET:HE1	1.89	0.54
18:M:40:VAL:HG23	18:M:73:LEU:HB3	1.88	0.54
30:a:1078:C:O2	37:i:3:THR:OG1	2.25	0.54
33:d:23:GLU:OE2	33:d:24:HIS:ND1	2.40	0.54
6:A:140:U:O2	6:A:226:G:O6	2.26	0.54
30:a:1985:A:H2'	30:a:1986:A:C8	2.41	0.54
30:a:2445:C:N4	50:v:15:ASP:OD1	2.40	0.54
34:e:11:ASP:OD2	34:e:200:GLN:NE2	2.39	0.54
6:A:495:A:H2'	6:A:496:C:C6	2.42	0.54
30:a:1159:C:H2'	30:a:1160:A:C4	2.42	0.54
30:a:1490:A:H2	30:a:1772:G:H22	1.56	0.54
30:a:1708:G:H22	30:a:1729:G:H1	1.55	0.54
6:A:1091:G:O2'	12:G:168:ARG:NH2	2.40	0.54
15:J:84:LYS:HZ3	15:J:88:GLN:H	1.55	0.54
30:a:1418:A:O2'	30:a:1420:U:OP1	2.26	0.54
35:f:144:GLN:HG2	35:f:159:ARG:HG3	1.88	0.54
49:u:38:HIS:ND1	49:u:39:ASP:O	2.41	0.54
6:A:987:G:H1	6:A:1022:U:H3	1.56	0.54
30:a:1698:G:H1	30:a:1915:G:N2	2.05	0.54
30:a:2650:G:O2'	30:a:2663:G:N2	2.39	0.54
45:q:49:ASP:OD1	45:q:49:ASP:N	2.39	0.54
6:A:277:G:H5'	22:Q:23:LYS:HD3	1.89	0.54
6:A:418:G:H2'	6:A:419:G:H8	1.73	0.54
6:A:996:C:H2'	6:A:997:A:C8	2.43	0.54
30:a:374:C:H2'	30:a:375:G:C8	2.42	0.54
30:a:565:G:N1	30:a:568:A:OP2	2.37	0.54
1:O:24:TYR:OH	30:a:2529:C:O2'	2.24	0.54
23:R:73:THR:OG1	23:R:74:ALA:N	2.36	0.54
15:J:84:LYS:HZ3	15:J:88:GLN:N	2.05	0.54
30:a:2773:C:H2'	30:a:2774:G:C8	2.43	0.54
40:l:54:MET:SD	40:l:118:MET:HG2	2.48	0.54
42:n:86:THR:O	42:n:90:GLU:HG2	2.07	0.54
6:A:506:G:H2'	6:A:507:C:C6	2.43	0.54
9:D:171:ASN:C	21:P:119:ALA:HB1	2.32	0.54
30:a:1156:A:H2'	30:a:1157:G:C8	2.41	0.54
30:a:1350:G:N2	30:a:1378:U:O4	2.41	0.54
32:c:119:SER:HB2	32:c:130:ASN:HB3	1.90	0.54
34:e:167:ASP:O	34:e:171:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:61:GLU:OE1	36:g:62:ASN:ND2	2.41	0.54
6:A:721:C:OP1	11:F:2:ARG:NH2	2.41	0.53
6:A:1040:A:H2	6:A:1186:C:H42	1.56	0.53
13:H:118:ASP:OD2	13:H:118:ASP:N	2.41	0.53
30:a:1090:C:OP1	37:i:37:ARG:NH1	2.39	0.53
36:g:3:ARG:NH1	36:g:3:ARG:O	2.42	0.53
11:F:82:ASP:HB3	11:F:85:ILE:HD12	1.90	0.53
16:K:94:GLY:O	16:K:99:ARG:NH2	2.40	0.53
20:O:45:LYS:O	20:O:51:ARG:NH2	2.35	0.53
33:d:90:THR:OG1	33:d:92:ASP:OD2	2.27	0.53
34:e:154:ARG:HE	34:e:154:ARG:N	2.06	0.53
17:L:50:ARG:NH1	17:L:89:ASP:OD2	2.40	0.53
30:a:1042:A:H2'	30:a:1043:A:C8	2.43	0.53
30:a:1253:U:H2'	30:a:1254:G:C8	2.43	0.53
30:a:2291:U:O2'	30:a:2362:U:O4	2.23	0.53
30:a:2486:G:O2'	35:f:162:ASP:OD1	2.26	0.53
30:a:2961:U:H4'	30:a:2962:A:O5'	2.07	0.53
6:A:183:G:N2	6:A:226:G:O5'	2.41	0.53
6:A:463:G:O2'	6:A:465:C:N4	2.41	0.53
30:a:960:U:H4'	49:u:172:VAL:HG11	1.90	0.53
30:a:1152:A:H4'	30:a:1153:A:H8	1.73	0.53
6:A:9:U:O4	9:D:78:GLN:NE2	2.42	0.53
6:A:483:C:H2'	6:A:484:A:H8	1.73	0.53
6:A:1047:U:H2'	6:A:1048:C:C6	2.43	0.53
6:A:1503:2MG:N1	6:A:1506:MA6:OP2	2.41	0.53
18:M:11:ARG:NE	18:M:71:LYS:HG3	2.23	0.53
30:a:622:U:H2'	30:a:623:C:C6	2.44	0.53
30:a:1111:A:N3	30:a:2668:C:O2'	2.36	0.53
30:a:2473:U:H2'	30:a:2474:U:C6	2.43	0.53
6:A:989:G:O6	6:A:1009:G:O2'	2.23	0.53
14:I:114:LYS:O	14:I:119:ARG:NH1	2.41	0.53
18:M:63:GLU:OE2	24:S:58:LYS:NZ	2.37	0.53
6:A:42:G:H22	6:A:399:A:H5'	1.73	0.53
18:M:30:THR:HA	18:M:33:GLY:O	2.09	0.53
30:a:898:U:H2'	30:a:899:C:C6	2.44	0.53
34:e:133:VAL:HG21	34:e:138:PRO:HD2	1.89	0.53
40:l:31:ASP:H	40:l:107:SER:HB3	1.74	0.53
6:A:537:C:H2'	6:A:538:C:C6	2.44	0.53
6:A:537:C:H2'	6:A:538:C:H6	1.74	0.53
6:A:1412:A:H2'	6:A:1413:A:O4'	2.08	0.53
12:G:148:ILE:HD12	12:G:201:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:87:ARG:NH2	30:a:799:U:O5'	2.42	0.53
30:a:552:G:N2	30:a:555:A:OP2	2.32	0.53
30:a:1903:G:H22	30:a:1922:U:H5	1.57	0.53
30:a:2197:A:H2'	30:a:2198:A:C8	2.43	0.53
31:b:48:C:H2'	31:b:49:C:H6	1.73	0.53
48:t:29:VAL:HG13	48:t:36:VAL:HG12	1.91	0.53
46:r:78:THR:OG1	46:r:79:GLU:OE1	2.23	0.53
6:A:1283:U:H1'	6:A:1284:C:H5	1.73	0.53
30:a:2290:U:H3'	30:a:2291:U:C6	2.44	0.53
38:j:3:GLN:HE21	38:j:32:TYR:HE1	1.54	0.53
45:q:60:ALA:HB1	45:q:95:VAL:HG13	1.91	0.53
6:A:483:C:H2'	6:A:484:A:C8	2.43	0.52
6:A:1026:U:H2'	6:A:1027:U:C6	2.44	0.52
9:D:197:GLU:OE1	10:E:128:VAL:N	2.33	0.52
26:U:41:THR:O	26:U:44:MET:HG2	2.09	0.52
30:a:1142:G:N2	30:a:1163:C:O2	2.43	0.52
48:t:94:ARG:NH1	48:t:112:SER:OG	2.36	0.52
6:A:384:A:H2'	6:A:385:A:C8	2.44	0.52
6:A:512:G:C2	29:Y:22:U:H5''	2.44	0.52
6:A:1300:C:H2'	6:A:1301:U:C6	2.44	0.52
20:O:68:ILE:HG22	20:O:76:TYR:HB2	1.91	0.52
30:a:2180:C:H5'	33:d:128:MET:HE1	1.91	0.52
12:G:118:GLY:O	12:G:122:GLN:HG3	2.10	0.52
30:a:374:C:O2'	30:a:375:G:O4'	2.19	0.52
30:a:1145:G:N2	30:a:1160:A:N1	2.56	0.52
30:a:2509:A:H2'	30:a:2510:A:C8	2.44	0.52
42:n:38:MET:HE2	42:n:100:VAL:HG21	1.92	0.52
6:A:382:G:N2	6:A:385:A:OP2	2.39	0.52
30:a:130:G:H1	30:a:154:G:H1	1.56	0.52
30:a:1391:C:H2'	30:a:1392:A:H8	1.74	0.52
30:a:2502:U:O4	30:a:2515:A:O2'	2.22	0.52
35:f:127:ASN:H	35:f:127:ASN:ND2	2.07	0.52
6:A:1242:U:OP2	6:A:1265:A:N6	2.43	0.52
9:D:163:PRO:HB2	9:D:165:TRP:CD1	2.45	0.52
9:D:179:GLN:OE1	9:D:179:GLN:N	2.43	0.52
21:P:112:ALA:O	21:P:116:PRO:HD2	2.10	0.52
30:a:1491:C:H2'	30:a:1492:C:H6	1.74	0.52
2:l:7:PRO:HB2	30:a:1385:G:H4'	1.92	0.52
6:A:1517:G:H2'	6:A:1518:A:O4'	2.10	0.52
30:a:4:A:H2'	30:a:5:A:C8	2.45	0.52
30:a:2256:U:H2'	30:a:2257:U:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2982:U:OP2	30:a:2983:C:N4	2.43	0.52
51:w:3:ALA:HB1	51:w:12:PRO:HG3	1.90	0.52
25:T:31:TYR:CE2	25:T:57:GLN:HG3	2.45	0.52
30:a:917:U:H2'	30:a:918:G:C8	2.45	0.52
30:a:1147:C:H2'	30:a:1148:U:O4'	2.10	0.52
39:k:68:ASN:HB3	39:k:71:ARG:HB2	1.92	0.52
9:D:147:LEU:HB2	9:D:150:ILE:HG22	1.92	0.52
16:K:112:GLU:H	16:K:112:GLU:CD	2.15	0.52
17:L:54:ARG:HH21	17:L:62:GLU:HB3	1.74	0.52
27:V:12:ARG:NH2	31:b:89:G:OP1	2.39	0.52
30:a:3016:U:H2'	30:a:3017:A:H8	1.75	0.52
21:P:113:ASP:OD1	21:P:114:GLU:N	2.43	0.52
30:a:3055:U:H4'	43:o:2:SER:HA	1.91	0.52
52:x:49:VAL:O	52:x:53:ILE:HG13	2.10	0.52
11:F:15:GLU:OE1	11:F:15:GLU:N	2.43	0.51
30:a:26:G:N2	30:a:600:G:H1'	2.26	0.51
30:a:1043:A:H61	40:l:83:MET:HE2	1.76	0.51
30:a:1095:U:H5'	30:a:1096:G:H5''	1.92	0.51
30:a:1492:C:H2'	30:a:1493:G:C8	2.45	0.51
30:a:2915:U:H2'	30:a:2916:U:C6	2.44	0.51
33:d:192:ILE:HG21	43:o:8:ILE:HD11	1.93	0.51
7:B:110:ARG:HH21	7:B:145:LEU:HD11	1.75	0.51
54:z:35:CYS:HB2	54:z:48:CYS:HB3	1.91	0.51
30:a:1145:G:H2'	30:a:1146:G:H8	1.76	0.51
30:a:2252:G:H2'	30:a:2253:A:C8	2.46	0.51
6:A:1236:A:H4'	15:J:111:GLY:HA2	1.91	0.51
17:L:54:ARG:NH1	17:L:64:THR:OG1	2.44	0.51
30:a:599:U:H4'	30:a:1312:G:H4'	1.91	0.51
30:a:881:A:H2'	30:a:882:C:C6	2.46	0.51
30:a:1156:A:H1'	30:a:2656:U:H4'	1.92	0.51
30:a:1862:A:H2'	30:a:1863:A:C8	2.45	0.51
30:a:2053:U:H3'	30:a:2054:A:H8	1.74	0.51
30:a:3037:G:N2	30:a:3040:A:OP2	2.31	0.51
39:k:94:VAL:HG22	39:k:97:LEU:CD2	2.41	0.51
6:A:339:G:H2'	6:A:340:A:C8	2.46	0.51
6:A:936:C:H2'	6:A:937:G:H8	1.76	0.51
12:G:47:GLU:OE1	12:G:47:GLU:HA	2.09	0.51
12:G:133:MET:HE2	12:G:167:TYR:HD1	1.75	0.51
14:I:65:ALA:O	14:I:69:ILE:HD12	2.11	0.51
30:a:503:C:H2'	30:a:504:A:H8	1.75	0.51
30:a:1404:G:H2'	30:a:1406:C:C5	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:60:U:H2'	6:A:61:G:C8	2.45	0.51
30:a:336:G:O2'	30:a:357:G:N7	2.44	0.51
30:a:503:C:H2'	30:a:504:A:C8	2.45	0.51
30:a:725:U:H2'	30:a:726:C:C6	2.45	0.51
30:a:1189:G:H2'	30:a:1190:G:H8	1.75	0.51
30:a:1851:G:O2'	30:a:2174:U:O4	2.26	0.51
32:c:172:TYR:HB3	32:c:184:MET:HG2	1.92	0.51
40:l:51:ARG:HD3	40:l:66:ILE:HD11	1.91	0.51
6:A:110:C:O2'	21:P:26:ARG:O	2.28	0.51
15:J:44:MET:H	15:J:44:MET:HE3	1.75	0.51
30:a:263:A:H2'	30:a:264:A:H8	1.74	0.51
30:a:1083:A:H2'	30:a:1084:A:C8	2.45	0.51
30:a:2880:U:H2'	30:a:2881:U:C6	2.45	0.51
43:o:16:ASP:OD1	43:o:16:ASP:N	2.34	0.51
54:z:45:CYS:HB3	54:z:48:CYS:SG	2.51	0.51
6:A:443:G:H1'	6:A:479:G:N2	2.26	0.51
6:A:930:A:H2'	6:A:931:G:H8	1.75	0.51
21:P:81:GLN:OE1	21:P:81:GLN:N	2.44	0.51
30:a:1224:U:OP2	37:i:65:THR:OG1	2.27	0.51
30:a:1861:A:H2'	30:a:1862:A:H8	1.75	0.51
30:a:2253:A:H2'	30:a:2254:C:C6	2.46	0.51
40:l:57:TYR:HD1	40:l:117:ALA:HB2	1.76	0.51
3:2:7:HIS:NE2	30:a:258:A:OP1	2.40	0.51
6:A:1137:G:O2'	6:A:1138:U:H5''	2.11	0.51
6:A:1378:U:H2'	6:A:1379:G:C8	2.46	0.51
14:I:115:THR:O	14:I:119:ARG:HB2	2.11	0.51
30:a:279:A:H62	30:a:319:G:H21	1.58	0.51
30:a:2247:C:H2'	30:a:2248:C:C6	2.46	0.51
36:g:95:TYR:HA	36:g:108:ASN:O	2.11	0.51
38:j:92:GLU:HG3	38:j:93:PRO:HD2	1.92	0.51
49:u:160:PRO:O	49:u:163:THR:OG1	2.25	0.51
6:A:1418:C:H2'	6:A:1419:G:O4'	2.10	0.51
14:I:136:LYS:HA	14:I:139:GLU:OE1	2.11	0.51
19:N:69:ASP:OD2	19:N:70:LEU:N	2.44	0.51
24:S:24:CYS:HB3	24:S:29:ARG:H	1.76	0.51
26:U:44:MET:C	26:U:47:HIS:HD1	2.19	0.51
30:a:669:A:N1	30:a:894:G:O2'	2.38	0.51
30:a:1612:G:H2'	30:a:1613:U:C6	2.46	0.51
6:A:561:U:H2'	6:A:562:C:C6	2.46	0.50
6:A:938:G:H2'	6:A:939:A:C8	2.45	0.50
30:a:723:A:H5''	39:k:114:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:806:U:H2'	30:a:807:C:C6	2.47	0.50
36:g:106:GLU:OE1	36:g:114:PRO:HB2	2.10	0.50
38:j:63:VAL:HG12	38:j:106:LEU:HD21	1.93	0.50
22:Q:14:VAL:O	22:Q:15:ARG:NH1	2.43	0.50
30:a:1491:C:H2'	30:a:1492:C:C6	2.45	0.50
32:c:9:THR:HG22	32:c:10:THR:HG23	1.93	0.50
47:s:20:GLU:H	47:s:20:GLU:CD	2.18	0.50
6:A:1356:C:H2'	6:A:1357:G:C8	2.45	0.50
6:A:1399:C:H2'	6:A:1400:A:C8	2.47	0.50
9:D:99:ARG:HH22	9:D:187:VAL:HG22	1.77	0.50
18:M:42:LEU:HG	18:M:71:LYS:HD3	1.92	0.50
30:a:303:G:H2'	30:a:304:G:O4'	2.11	0.50
30:a:788:U:H2'	30:a:789:G:O4'	2.12	0.50
30:a:1199:U:H2'	30:a:1200:U:C6	2.46	0.50
30:a:1754:A:H2'	30:a:1755:A:C8	2.46	0.50
30:a:2651:A:H2'	30:a:2652:G:O4'	2.12	0.50
43:o:15:ASP:OD2	43:o:15:ASP:N	2.43	0.50
43:o:62:ARG:HG3	43:o:71:GLU:HG3	1.93	0.50
6:A:79:C:H2'	6:A:80:C:C6	2.46	0.50
30:a:339:U:H3'	30:a:340:C:H6	1.76	0.50
30:a:670:G:H5'	34:e:93:HIS:CD2	2.47	0.50
30:a:729:A:N1	30:a:2551:A:O2'	2.44	0.50
30:a:2009:C:O2'	30:a:2154:U:OP2	2.29	0.50
30:a:2473:U:OP1	30:a:2562:U:O2'	2.30	0.50
48:t:35:ARG:HB3	48:t:69:PRO:HB2	1.93	0.50
6:A:208:U:H5''	25:T:52:ARG:HH21	1.76	0.50
6:A:718:U:H2'	6:A:719:C:H6	1.76	0.50
6:A:1241:G:O2'	6:A:1244:G:N3	2.38	0.50
20:O:87:ARG:HH11	20:O:87:ARG:C	2.20	0.50
25:T:8:ILE:O	25:T:11:VAL:HG22	2.11	0.50
26:U:3:ARG:HH11	26:U:10:PHE:HB2	1.76	0.50
29:Y:21:U:H2'	29:Y:22:U:H4'	1.93	0.50
30:a:453:U:O2	30:a:455:C:N4	2.40	0.50
31:b:25:A:H2'	31:b:26:A:C8	2.46	0.50
6:A:1138:U:OP1	18:M:70:HIS:ND1	2.37	0.50
11:F:45:LYS:HG2	11:F:57:GLU:HG2	1.94	0.50
30:a:1174:G:H2'	30:a:1175:C:C6	2.47	0.50
30:a:2579:A:H2'	30:a:2580:C:C6	2.47	0.50
50:v:84:GLU:OE1	50:v:84:GLU:N	2.33	0.50
10:E:155:ASN:O	10:E:159:VAL:HG23	2.11	0.50
30:a:291:U:H5'	30:a:308:U:H5	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2268:U:H2'	30:a:2269:G:C8	2.47	0.50
35:f:117:LEU:H	35:f:117:LEU:HD23	1.77	0.50
5:4:65:TYR:HE2	26:U:5:LEU:HD12	1.76	0.50
6:A:1169:U:O2'	6:A:1170:G:OP1	2.28	0.50
12:G:55:GLU:HB3	12:G:66:PHE:HB2	1.94	0.50
12:G:125:ALA:O	12:G:126:ARG:HG2	2.11	0.50
38:j:7:ARG:HD3	38:j:18:GLU:OE2	2.12	0.50
2:1:25:ARG:NH2	30:a:218:G:OP1	2.42	0.50
6:A:996:C:H2'	6:A:997:A:H8	1.75	0.50
6:A:1282:C:H4'	6:A:1288:U:O4	2.12	0.50
7:B:30:PHE:CZ	7:B:41:ILE:HG23	2.47	0.50
30:a:1912:U:H3'	30:a:1913:G:H3'	1.93	0.50
30:a:1980:G:HO2'	32:c:257:THR:HG1	1.60	0.50
30:a:2971:C:H1'	30:a:3071:A:H2	1.77	0.50
36:g:157:GLU:OE2	36:g:160:LYS:N	2.45	0.50
6:A:992:U:H2'	6:A:993:G:C8	2.46	0.49
30:a:1165:U:H3'	30:a:1166:G:H8	1.76	0.49
14:I:31:LEU:O	14:I:31:LEU:HD13	2.11	0.49
15:J:109:ILE:HD12	15:J:121:LEU:HD21	1.94	0.49
20:O:10:ILE:HG21	20:O:20:THR:HG22	1.95	0.49
25:T:15:GLU:O	25:T:19:GLN:HG2	2.12	0.49
30:a:2403:A:O2'	32:c:188:ARG:NH2	2.44	0.49
30:a:2773:C:H2'	30:a:2774:G:H8	1.76	0.49
47:s:54:VAL:HG13	47:s:92:ASP:HB3	1.94	0.49
51:w:16:HIS:HA	51:w:25:THR:O	2.11	0.49
6:A:503:G:H4'	17:L:70:VAL:HG22	1.93	0.49
6:A:1271:G:H4'	6:A:1272:G:O5'	2.12	0.49
20:O:6:LYS:O	20:O:10:ILE:HG13	2.12	0.49
20:O:38:THR:O	20:O:42:LYS:HG2	2.12	0.49
26:U:3:ARG:HH21	26:U:7:LYS:HG2	1.78	0.49
30:a:2977:A:H2'	30:a:2978:G:O4'	2.11	0.49
30:a:2986:G:H2'	30:a:2987:G:C8	2.47	0.49
10:E:116:VAL:HB	10:E:151:LEU:O	2.12	0.49
30:a:709:U:H2'	30:a:710:C:C6	2.47	0.49
30:a:1650:A:H2'	30:a:1651:A:C8	2.47	0.49
42:n:64:SER:OG	42:n:65:THR:N	2.45	0.49
6:A:299:G:N2	6:A:302:A:OP2	2.32	0.49
6:A:827:C:H3'	6:A:828:A:C8	2.47	0.49
6:A:1202:U:H2'	6:A:1203:C:H6	1.76	0.49
6:A:1225:A:H62	6:A:1285:A:N6	2.11	0.49
10:E:117:VAL:HG11	10:E:163:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:71:LYS:HB3	15:J:106:ILE:HD13	1.94	0.49
18:M:10:LEU:HD12	18:M:72:ARG:HB3	1.94	0.49
30:a:373:G:N2	30:a:374:C:O4'	2.45	0.49
30:a:692:A:H2'	30:a:693:A:C8	2.48	0.49
30:a:1995:A:H2'	30:a:1996:C:C6	2.48	0.49
30:a:2494:U:H5'	35:f:94:ILE:HD11	1.94	0.49
30:a:2513:G:O2'	30:a:2518:A:N1	2.42	0.49
7:B:73:LYS:HZ3	7:B:166:ASP:HB2	1.77	0.49
9:D:56:ALA:HB2	9:D:190:VAL:HG21	1.94	0.49
25:T:7:GLN:O	25:T:11:VAL:HG13	2.13	0.49
30:a:2527:G:N3	30:a:2563:C:H2'	2.27	0.49
30:a:2800:G:H21	33:d:161:VAL:HG21	1.77	0.49
30:a:2859:U:H2'	30:a:2860:G:C8	2.48	0.49
6:A:678:A:H2'	6:A:679:U:H6	1.76	0.49
6:A:821:C:H2'	6:A:822:C:H6	1.78	0.49
20:O:5:GLU:CD	20:O:5:GLU:N	2.70	0.49
30:a:115:C:O2'	30:a:125:A:N3	2.41	0.49
30:a:1716:U:H2'	30:a:1717:G:C8	2.48	0.49
35:f:171:THR:HG22	35:f:173:GLU:H	1.76	0.49
1:0:43:CYS:HB3	1:0:46:CYS:HB2	1.94	0.49
6:A:710:A:H2'	6:A:711:A:C8	2.48	0.49
3:2:26:LYS:HD3	3:2:48:THR:HB	1.93	0.49
12:G:82:GLU:O	12:G:86:VAL:HG13	2.13	0.49
18:M:51:VAL:CG1	24:S:41:ARG:HG3	2.43	0.49
30:a:450:G:C2	30:a:451:G:C8	3.01	0.49
30:a:2630:A:O2'	30:a:2631:H2U:H52	2.13	0.49
31:b:48:C:H2'	31:b:49:C:C6	2.47	0.49
6:A:1304:A:H1'	26:U:37:ARG:HH11	1.78	0.49
22:Q:1:MET:SD	22:Q:2:SER:N	2.85	0.49
30:a:203:A:C2	39:k:49:PHE:HZ	2.31	0.49
30:a:373:G:N2	30:a:437:G:H1	2.11	0.49
52:x:52:ASP:O	52:x:56:VAL:HG23	2.13	0.49
6:A:998:G:N2	6:A:1001:A:OP2	2.35	0.48
6:A:1346:A:H2'	6:A:1347:G:C8	2.48	0.48
30:a:682:U:H2'	30:a:683:G:C8	2.48	0.48
30:a:1628:C:O2'	30:a:1727:G:N3	2.38	0.48
49:u:122:GLU:HG3	49:u:172:VAL:HG23	1.94	0.48
53:y:12:SER:HB3	53:y:32:ILE:HD11	1.95	0.48
6:A:12:A:N6	9:D:201:LYS:HB3	2.28	0.48
6:A:821:C:H2'	6:A:822:C:C6	2.48	0.48
6:A:982:G:H2'	6:A:983:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1003:G:H2'	6:A:1004:G:H5'	1.95	0.48
6:A:1503:2MG:HM21	6:A:1506:MA6:N7	2.28	0.48
7:B:176:GLU:O	7:B:180:LEU:HG	2.13	0.48
10:E:178:ARG:HG2	10:E:178:ARG:HH11	1.78	0.48
14:I:21:PRO:O	14:I:24:SER:OG	2.26	0.48
40:l:54:MET:HE1	40:l:104:PHE:HB3	1.95	0.48
5:4:44:PHE:CE2	35:f:185:PRO:HB3	2.48	0.48
6:A:78:G:H2'	6:A:79:C:C6	2.49	0.48
30:a:272:A:N6	30:a:516:U:O2'	2.37	0.48
30:a:445:U:H2'	30:a:446:G:C8	2.48	0.48
30:a:2474:U:H2'	30:a:2475:C:C6	2.47	0.48
48:t:81:ILE:HD12	48:t:82:ASP:N	2.27	0.48
53:y:2:MET:HA	53:y:40:ASP:HB3	1.95	0.48
5:4:61:PHE:O	5:4:65:TYR:HB2	2.12	0.48
6:A:1333:G:N7	15:J:55:LYS:HE2	2.29	0.48
30:a:491:A:H2'	30:a:492:U:O4'	2.13	0.48
30:a:1624:A:H2'	30:a:1626:C:C5	2.48	0.48
30:a:1686:C:H2'	30:a:1687:G:O4'	2.13	0.48
30:a:1973:C:H2'	30:a:1974:A:C5	2.49	0.48
30:a:2644:U:H2'	30:a:2645:U:C6	2.48	0.48
30:a:2779:G:H2'	30:a:2780:A:C8	2.48	0.48
33:d:23:GLU:OE1	33:d:23:GLU:N	2.45	0.48
6:A:508:C:OP2	17:L:88:LYS:NZ	2.43	0.48
6:A:904:U:H2'	6:A:905:U:C6	2.49	0.48
6:A:1105:C:H2'	6:A:1106:A:C8	2.42	0.48
7:B:155:MET:HE1	7:B:159:PRO:HG3	1.96	0.48
13:H:101:LEU:HD12	13:H:135:TRP:CD1	2.48	0.48
30:a:663:C:H2'	30:a:664:C:C6	2.48	0.48
30:a:1418:A:OP1	47:s:41:LYS:NZ	2.27	0.48
30:a:1894:U:H2'	30:a:1895:G:O4'	2.13	0.48
30:a:2571:G:H5''	30:a:2572:U:O4'	2.13	0.48
30:a:2838:U:O2	30:a:2847:A:N7	2.47	0.48
30:a:2980:G:H2'	30:a:2981:U:C2	2.49	0.48
34:e:155:LYS:HZ2	34:e:155:LYS:HB3	1.78	0.48
38:j:73:ASP:OD1	38:j:75:SER:OG	2.22	0.48
6:A:113:G:H1'	6:A:356:G:H5'	1.96	0.48
6:A:148:G:H2'	6:A:149:G:H8	1.78	0.48
30:a:714:G:H2'	30:a:715:C:C6	2.48	0.48
30:a:1615:A:H2'	30:a:1616:G:C8	2.48	0.48
39:k:99:SER:OG	39:k:105:ASP:HB3	2.14	0.48
6:A:266:U:O2'	22:Q:73:PRO:O	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:116:PRO:HA	21:P:119:ALA:HB3	1.94	0.48
30:a:1111:A:H2'	30:a:1112:A:C8	2.49	0.48
30:a:1306:U:O2'	30:a:1307:G:OP1	2.24	0.48
30:a:1337:G:OP1	46:r:100:ARG:NH1	2.47	0.48
30:a:1812:G:H2'	30:a:1813:U:C6	2.48	0.48
30:a:2455:A:H2'	30:a:2456:A:C8	2.48	0.48
34:e:119:ASP:OD2	39:k:2:ALA:N	2.47	0.48
16:K:56:VAL:HG21	16:K:71:MET:HB3	1.96	0.48
19:N:15:LEU:HD23	19:N:34:LEU:HD11	1.95	0.48
26:U:84:VAL:C	26:U:85:LYS:HE2	2.39	0.48
30:a:2263:U:H2'	30:a:2264:A:H8	1.79	0.48
35:f:156:ASP:OD1	35:f:156:ASP:N	2.41	0.48
41:m:36:THR:O	41:m:40:LYS:HB2	2.14	0.48
1:0:47:ARG:HG2	1:0:47:ARG:HH11	1.78	0.48
6:A:1265:A:O2'	6:A:1268:C:N4	2.46	0.48
23:R:68:LEU:HD23	23:R:69:PRO:HD2	1.96	0.48
30:a:286:G:N7	30:a:313:G:N2	2.61	0.48
30:a:727:C:O2'	30:a:2532:U:OP1	2.25	0.48
30:a:1600:C:O2'	30:a:2393:G:N1	2.46	0.48
30:a:2366:U:H2'	30:a:2367:G:C8	2.49	0.48
35:f:143:GLU:OE2	35:f:146:MET:N	2.46	0.48
6:A:392:U:H2'	6:A:393:G:C8	2.48	0.48
6:A:772:A:OP1	8:C:38:A:O2'	2.32	0.48
6:A:1434:A:P	6:A:1435:C:H41	2.37	0.48
12:G:69:ALA:O	12:G:105:VAL:HG23	2.14	0.48
30:a:2423:A:H2'	30:a:2424:G:C8	2.49	0.48
30:a:2710:U:H2'	30:a:2712:G:H5''	1.95	0.48
34:e:156:VAL:HG12	34:e:158:VAL:HG13	1.96	0.48
45:q:89:ARG:HA	45:q:89:ARG:HD2	1.70	0.48
47:s:8:ASP:OD2	47:s:10:ARG:NH1	2.47	0.48
6:A:1361:A:O2'	14:I:31:LEU:HD12	2.13	0.47
15:J:163:LYS:HB2	15:J:166:LYS:HB3	1.96	0.47
30:a:1724:G:H3'	30:a:1725:G:C8	2.49	0.47
30:a:1861:A:H2'	30:a:1862:A:C8	2.48	0.47
30:a:2072:A:H2'	30:a:2073:A:C8	2.49	0.47
30:a:2415:U:H2'	30:a:2416:G:C8	2.49	0.47
33:d:92:ASP:OD2	33:d:92:ASP:N	2.47	0.47
35:f:78:LYS:HB3	35:f:91:GLY:HA2	1.95	0.47
36:g:123:ILE:HD11	36:g:142:VAL:HG11	1.96	0.47
37:i:4:TYR:CG	44:p:100:VAL:HG11	2.48	0.47
11:F:26:TYR:O	11:F:29:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:334:G:H2'	30:a:334:G:N3	2.29	0.47
30:a:433:G:H2'	30:a:435:G:O4'	2.14	0.47
30:a:1437:G:H2'	30:a:1438:C:C6	2.48	0.47
30:a:1984:G:H3'	30:a:1985:A:H5'	1.96	0.47
30:a:2135:A:N3	30:a:2742:C:O2'	2.44	0.47
30:a:2429:A:H2'	30:a:2430:C:H6	1.79	0.47
34:e:159:VAL:HG13	34:e:160:LEU:N	2.30	0.47
42:n:37:ARG:NH2	42:n:54:ASP:OD1	2.45	0.47
42:n:42:ARG:HB2	42:n:113:ILE:HD11	1.96	0.47
42:n:80:LYS:O	42:n:84:VAL:HG23	2.15	0.47
6:A:1288:U:C6	19:N:17:VAL:HG11	2.49	0.47
16:K:77:GLY:O	16:K:81:MET:HG2	2.13	0.47
35:f:59:MET:HE1	35:f:96:CYS:HB3	1.94	0.47
52:x:12:LEU:O	52:x:63:ARG:NH2	2.39	0.47
6:A:906:G:H2'	6:A:907:A:C8	2.49	0.47
6:A:1210:U:O2'	6:A:1308:C:OP1	2.23	0.47
11:F:7:MET:SD	23:R:65:LEU:HD21	2.54	0.47
12:G:141:MET:HE3	12:G:141:MET:O	2.15	0.47
16:K:87:ARG:HD2	16:K:87:ARG:O	2.13	0.47
18:M:11:ARG:HB2	18:M:97:ASP:OD2	2.14	0.47
27:V:20:LYS:NZ	30:a:1069:C:OP1	2.47	0.47
30:a:361:G:N2	30:a:443:G:H22	2.11	0.47
30:a:390:C:H2'	30:a:391:U:C6	2.49	0.47
30:a:1977:U:H2'	30:a:1978:C:H6	1.79	0.47
39:k:88:LYS:HD2	39:k:88:LYS:C	2.40	0.47
30:a:373:G:N2	30:a:437:G:H22	2.12	0.47
30:a:377:G:H2'	30:a:378:A:O4'	2.15	0.47
30:a:407:A:OP2	34:e:173:ASN:HB2	2.14	0.47
30:a:682:U:H2'	30:a:683:G:H8	1.79	0.47
30:a:938:U:H2'	30:a:939:U:C6	2.49	0.47
30:a:1192:C:H2'	30:a:1193:A:O4'	2.14	0.47
30:a:1395:G:H2'	30:a:1396:U:C6	2.49	0.47
30:a:1962:U:OP2	30:a:1967:A:N6	2.35	0.47
30:a:1977:U:H2'	30:a:1978:C:C6	2.48	0.47
30:a:2887:A:O2'	30:a:3032:G:OP1	2.31	0.47
31:b:5:C:OP1	31:b:61:C:O2'	2.32	0.47
6:A:495:A:H2'	6:A:496:C:H6	1.80	0.47
9:D:87:GLN:NE2	9:D:181:PRO:O	2.46	0.47
30:a:361:G:N2	30:a:444:G:N3	2.62	0.47
30:a:431:A:H2'	30:a:432:A:O4'	2.15	0.47
30:a:1151:G:O2'	30:a:1179:A:O2'	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1391:C:H2'	30:a:1392:A:C8	2.49	0.47
30:a:1691:A:O2'	30:a:1692:G:H8	1.97	0.47
32:c:136:ILE:HD13	32:c:142:VAL:HG11	1.96	0.47
48:t:78:VAL:HG22	48:t:85:ASP:OD1	2.15	0.47
49:u:96:ARG:NH1	49:u:96:ARG:HB2	2.29	0.47
5:4:45:TYR:CE1	35:f:185:PRO:HG3	2.49	0.47
6:A:10:G:H4'	6:A:300:A:H4'	1.96	0.47
6:A:920:C:C2	6:A:921:A:C8	3.03	0.47
6:A:1050:U:H4'	6:A:1051:C:O5'	2.13	0.47
12:G:101:ASN:N	12:G:101:ASN:OD1	2.48	0.47
12:G:179:ALA:HB1	12:G:202:TYR:CE1	2.50	0.47
14:I:57:ASP:OD1	14:I:60:GLN:N	2.44	0.47
30:a:361:G:H1	30:a:443:G:H1	1.60	0.47
30:a:436:U:H2'	30:a:437:G:C8	2.50	0.47
30:a:1753:A:H2'	30:a:1754:A:C8	2.50	0.47
30:a:2925:C:O2'	36:g:152:LYS:HE2	2.14	0.47
32:c:147:LEU:HD12	32:c:183:ARG:NH2	2.30	0.47
39:k:79:LEU:HD13	39:k:117:LEU:HB2	1.96	0.47
39:k:80:ASP:OD1	39:k:80:ASP:N	2.48	0.47
39:k:94:VAL:H	39:k:97:LEU:HD23	1.80	0.47
6:A:139:U:H2'	6:A:140:U:C6	2.50	0.47
6:A:339:G:H2'	6:A:340:A:H8	1.80	0.47
6:A:861:C:OP1	13:H:85:LYS:HE3	2.14	0.47
30:a:686:G:O2'	30:a:740:A:N1	2.48	0.47
35:f:117:LEU:HG	35:f:118:PRO:HD3	1.95	0.47
6:A:1237:G:H4'	15:J:56:GLU:OE2	2.15	0.47
6:A:1271:G:H5'	6:A:1272:G:C4	2.50	0.47
6:A:1300:C:H2'	6:A:1301:U:H6	1.80	0.47
9:D:171:ASN:N	9:D:171:ASN:OD1	2.46	0.47
10:E:103:THR:OG1	10:E:145:ASP:O	2.24	0.47
11:F:52:ILE:HG22	11:F:53:GLN:NE2	2.29	0.47
28:X:3:SER:C	28:X:5:ILE:H	2.22	0.47
30:a:51:A:H2'	30:a:52:A:C8	2.50	0.47
30:a:337:G:H2'	30:a:338:U:O4'	2.14	0.47
30:a:418:G:O2'	30:a:419:U:OP1	2.29	0.47
30:a:442:U:H3'	30:a:443:G:H8	1.80	0.47
30:a:2739:G:H2'	30:a:2740:C:C6	2.50	0.47
30:a:3012:U:OP1	33:d:64:LYS:NZ	2.48	0.47
35:f:33:ASN:OD1	35:f:35:MET:HG2	2.15	0.47
35:f:60:ASP:O	35:f:63:ILE:HG13	2.14	0.47
40:l:118:MET:O	40:l:122:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:104:ARG:HB3	43:o:104:ARG:NH1	2.30	0.47
6:A:256:G:OP1	22:Q:77:THR:OG1	2.29	0.47
9:D:28:ARG:HB3	9:D:31:TYR:CZ	2.50	0.47
9:D:141:ARG:HH21	9:D:144:SER:HB2	1.80	0.47
18:M:66:GLU:HB3	24:S:59:SER:HB3	1.97	0.47
30:a:166:A:N3	30:a:2390:C:O2'	2.46	0.47
30:a:344:U:H2'	30:a:345:G:H21	1.79	0.47
30:a:1280:U:O2	39:k:6:HIS:HB3	2.15	0.47
30:a:1361:G:N2	30:a:1404:G:H5''	2.30	0.47
36:g:107:PHE:HB2	36:g:115:VAL:CG1	2.45	0.47
7:B:118:GLU:HA	7:B:142:LYS:HE3	1.97	0.46
18:M:82:LYS:H	18:M:82:LYS:HG3	1.56	0.46
19:N:50:ASP:O	19:N:54:VAL:HG12	2.14	0.46
30:a:568:A:H1'	30:a:569:A:H5''	1.97	0.46
30:a:1717:G:H1'	30:a:1718:G:O4'	2.14	0.46
30:a:2501:G:O2'	30:a:2502:U:O4'	2.28	0.46
30:a:2510:A:H2'	30:a:2511:G:H8	1.74	0.46
30:a:2730:G:N3	38:j:23:ARG:NH2	2.63	0.46
30:a:2807:G:H2'	30:a:2808:C:C6	2.50	0.46
30:a:2830:G:H2'	30:a:2831:U:C6	2.50	0.46
41:m:87:MET:HE1	41:m:116:ILE:HB	1.97	0.46
6:A:362:G:H2'	6:A:363:G:C8	2.50	0.46
6:A:411:G:H2'	6:A:412:G:O4'	2.16	0.46
6:A:1108:U:H4'	18:M:38:GLY:HA3	1.96	0.46
8:C:43:A:H2'	8:C:44:A:C8	2.49	0.46
16:K:52:SER:H	16:K:55:THR:HB	1.79	0.46
30:a:15:U:H5''	54:z:14:ARG:HB3	1.96	0.46
30:a:1906:C:H2'	30:a:1907:A:O4'	2.13	0.46
30:a:2041:G:N7	30:a:2067:A:O2'	2.48	0.46
30:a:2486:G:H22	30:a:2494:U:H3	1.62	0.46
46:r:50:VAL:HG21	46:r:72:MET:HE2	1.97	0.46
6:A:325:U:H2'	6:A:326:G:O4'	2.14	0.46
6:A:467:G:H1'	6:A:468:U:OP2	2.16	0.46
6:A:634:U:O4	6:A:734:G:O2'	2.24	0.46
6:A:929:G:C2	6:A:930:A:C8	3.03	0.46
6:A:994:C:H2'	6:A:995:U:O4'	2.16	0.46
9:D:138:ILE:HB	9:D:175:ILE:HB	1.97	0.46
9:D:157:PHE:CE1	9:D:170:PRO:HG3	2.51	0.46
19:N:33:THR:O	19:N:37:THR:HG22	2.15	0.46
19:N:67:GLU:O	19:N:71:ARG:HG2	2.14	0.46
30:a:637:U:H2'	30:a:638:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1148:U:H3'	30:a:1149:U:H5''	1.96	0.46
30:a:2053:U:H3'	30:a:2054:A:C8	2.50	0.46
30:a:2511:G:H2'	30:a:2512:U:C6	2.50	0.46
33:d:214:LYS:O	33:d:216:ALA:N	2.47	0.46
43:o:13:MET:HE3	43:o:13:MET:HB2	1.75	0.46
49:u:153:TYR:CZ	49:u:155:GLY:HA3	2.51	0.46
6:A:66:U:H2'	6:A:67:C:C6	2.51	0.46
6:A:865:G:OP2	17:L:9:ARG:NH2	2.48	0.46
6:A:1273:A:H2	6:A:1339:G:H1'	1.79	0.46
7:B:14:VAL:O	7:B:204:ASN:HB2	2.15	0.46
30:a:101:G:O6	48:t:111:ARG:NH1	2.49	0.46
30:a:288:G:O2'	30:a:289:U:H5'	2.15	0.46
30:a:1030:A:H2'	30:a:1031:C:C6	2.50	0.46
36:g:119:ALA:HB2	36:g:125:PHE:CE2	2.50	0.46
38:j:120:GLU:HG2	43:o:66:PHE:HE2	1.80	0.46
6:A:38:C:H2'	6:A:39:G:H8	1.81	0.46
7:B:47:LEU:O	7:B:50:ILE:HG22	2.15	0.46
10:E:84:ALA:O	10:E:88:GLU:HG2	2.16	0.46
30:a:57:G:H5'	47:s:79:PRO:HB3	1.97	0.46
30:a:1149:U:O4	30:a:1152:A:H5''	2.16	0.46
30:a:1675:A:H2'	30:a:1676:A:C8	2.51	0.46
30:a:1714:C:H2'	30:a:1715:A:O4'	2.16	0.46
31:b:3:U:H2'	31:b:4:C:C6	2.50	0.46
31:b:13:A:N1	31:b:69:G:O2'	2.48	0.46
31:b:29:A:H2'	31:b:30:C:C6	2.50	0.46
36:g:106:GLU:HA	36:g:106:GLU:OE2	2.15	0.46
9:D:15:LEU:O	9:D:55:LYS:NZ	2.48	0.46
12:G:45:ASN:O	12:G:48:ARG:NH1	2.45	0.46
16:K:86:LYS:HA	16:K:86:LYS:HD2	1.63	0.46
19:N:39:ILE:HD12	19:N:56:LEU:HD11	1.98	0.46
26:U:42:PRO:HA	26:U:45:ILE:HG23	1.97	0.46
30:a:352:G:H2'	30:a:353:A:C4	2.51	0.46
30:a:1912:U:H4'	30:a:1914:C:C6	2.50	0.46
30:a:2706:G:H22	30:a:2721:C:H5	1.62	0.46
34:e:56:THR:O	34:e:60:VAL:HG23	2.16	0.46
35:f:63:ILE:HA	35:f:66:ILE:HG22	1.98	0.46
36:g:23:TYR:HE1	36:g:34:ASN:HB2	1.81	0.46
43:o:111:LYS:HB2	43:o:111:LYS:HE2	1.77	0.46
5:4:25:ARG:O	35:f:111:ARG:NH1	2.49	0.46
6:A:988:G:C6	6:A:1010:C:N4	2.84	0.46
12:G:155:ARG:HG2	12:G:159:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:87:ARG:O	20:O:87:ARG:NH1	2.46	0.46
30:a:1624:A:H2'	30:a:1626:C:H5	1.81	0.46
42:n:34:GLU:OE1	42:n:34:GLU:N	2.30	0.46
46:r:97:ILE:O	46:r:117:SER:OG	2.34	0.46
6:A:733:U:H2'	6:A:734:G:O4'	2.16	0.46
6:A:823:A:H2'	6:A:824:U:C6	2.51	0.46
6:A:1516:G:N7	28:X:7:LYS:HE3	2.31	0.46
14:I:111:ARG:HB2	14:I:119:ARG:HG2	1.97	0.46
21:P:95:GLN:CB	21:P:98:ARG:HH12	2.26	0.46
27:V:21:ARG:HG3	27:V:22:PRO:HD2	1.97	0.46
30:a:720:G:H2'	30:a:721:C:C6	2.51	0.46
30:a:1145:G:H2'	30:a:1146:G:C8	2.50	0.46
6:A:69:A:C2	6:A:220:G:H8	2.34	0.46
6:A:265:G:H2'	6:A:266:U:C6	2.51	0.46
6:A:658:A:H1'	16:K:123:PRO:HB3	1.97	0.46
15:J:46:ALA:HB3	15:J:132:VAL:HG13	1.98	0.46
16:K:29:ILE:HG12	16:K:38:ILE:HG23	1.97	0.46
18:M:6:ILE:HG23	18:M:102:LEU:HA	1.98	0.46
23:R:65:LEU:HD23	23:R:67:LEU:HD21	1.98	0.46
30:a:142:G:N2	30:a:147:G:H22	2.13	0.46
30:a:373:G:N3	30:a:373:G:H2'	2.30	0.46
30:a:826:U:H2'	30:a:827:U:C6	2.51	0.46
30:a:2977:A:H2	30:a:2982:U:H5	1.64	0.46
42:n:88:ILE:HD12	42:n:88:ILE:HA	1.82	0.46
6:A:179:G:C2	6:A:180:A:C8	3.04	0.46
6:A:992:U:O2	6:A:1007:G:O6	2.34	0.46
12:G:23:TYR:CZ	18:M:11:ARG:HB3	2.51	0.46
21:P:23:MET:HG2	21:P:33:ALA:HA	1.98	0.46
26:U:66:MET:HE3	26:U:74:PHE:CE2	2.51	0.46
30:a:653:G:H2'	30:a:2213:A:N7	2.31	0.46
36:g:103:LYS:HB3	36:g:119:ALA:HB3	1.97	0.46
40:l:78:PRO:O	40:l:81:SER:OG	2.33	0.46
41:m:33:ARG:HB3	41:m:114:GLU:HB2	1.97	0.46
52:x:45:ARG:O	52:x:49:VAL:HG23	2.16	0.46
6:A:641:A:H2'	6:A:642:G:H8	1.81	0.45
6:A:729:U:H2'	6:A:730:U:C6	2.51	0.45
6:A:1422:G:H2'	6:A:1423:C:H6	1.81	0.45
8:C:62:C:H2'	8:C:63:G:H8	1.81	0.45
12:G:91:GLU:OE1	12:G:98:ILE:N	2.49	0.45
16:K:99:ARG:NH1	16:K:118:ASP:OD2	2.46	0.45
21:P:44:ALA:O	21:P:45:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2993:U:H2'	30:a:2994:C:H6	1.82	0.45
49:u:33:MET:HG2	49:u:41:ILE:HB	1.98	0.45
53:y:47:MET:O	53:y:51:VAL:HG22	2.15	0.45
6:A:1134:U:H2'	6:A:1135:C:O4'	2.16	0.45
7:B:74:LYS:H	7:B:74:LYS:HD2	1.82	0.45
9:D:174:ARG:C	9:D:175:ILE:HD12	2.41	0.45
30:a:354:U:H2'	30:a:355:U:O4'	2.16	0.45
30:a:1305:G:O3'	30:a:1306:U:H3'	2.15	0.45
30:a:1912:U:H5''	30:a:1913:G:H3'	1.98	0.45
30:a:2818:U:H4'	33:d:87:GLU:OE2	2.16	0.45
6:A:798:A:OP1	6:A:1513:G:O2'	2.32	0.45
6:A:848:A:H2'	6:A:849:A:C8	2.51	0.45
6:A:1202:U:H2'	6:A:1203:C:C6	2.51	0.45
10:E:167:LEU:O	10:E:170:LEU:HB2	2.16	0.45
12:G:87:ARG:O	12:G:91:GLU:HG2	2.16	0.45
12:G:155:ARG:HH21	12:G:192:PHE:HB2	1.82	0.45
13:H:10:MET:SD	13:H:33:LYS:HG2	2.57	0.45
15:J:63:ILE:HG13	15:J:103:TYR:CE1	2.51	0.45
15:J:78:GLU:N	15:J:78:GLU:OE2	2.50	0.45
17:L:87:VAL:HG11	17:L:90:LEU:HD12	1.98	0.45
18:M:78:GLU:O	18:M:80:THR:HG22	2.16	0.45
20:O:23:PRO:HB2	20:O:68:ILE:HD11	1.97	0.45
25:T:59:ASP:OD2	25:T:76:LYS:HD2	2.16	0.45
30:a:548:U:H2'	30:a:549:A:H8	1.81	0.45
30:a:654:A:O2'	45:q:79:LYS:HE3	2.16	0.45
30:a:993:A:H2'	30:a:996:C:H5	1.81	0.45
30:a:1755:A:H2'	30:a:1756:G:H8	1.81	0.45
30:a:1974:A:N6	30:a:2011:G:O2'	2.42	0.45
30:a:2697:C:H2'	30:a:2698:G:H8	1.81	0.45
30:a:2995:C:O2'	54:z:42:HIS:ND1	2.41	0.45
42:n:48:PHE:HD1	42:n:64:SER:HB2	1.81	0.45
6:A:234:A:H2'	6:A:235:C:C6	2.51	0.45
10:E:100:VAL:O	10:E:103:THR:HG22	2.17	0.45
18:M:15:HIS:HA	18:M:18:ILE:HG22	1.97	0.45
18:M:88:MET:N	18:M:88:MET:SD	2.90	0.45
20:O:74:GLU:OE2	20:O:74:GLU:N	2.32	0.45
30:a:1350:G:H3'	30:a:1351:U:H5''	1.96	0.45
30:a:2047:U:OP1	30:a:2592:G:O2'	2.32	0.45
3:2:27:ALA:HB2	39:k:61:PRO:HD3	1.99	0.45
6:A:454:A:H5''	6:A:455:G:N2	2.31	0.45
6:A:683:C:OP1	6:A:684:A:O2'	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1212:C:P	19:N:91:ARG:HH12	2.39	0.45
6:A:1433:A:O2'	6:A:1434:A:H5'	2.17	0.45
12:G:177:LEU:HD23	12:G:177:LEU:H	1.80	0.45
30:a:2:C:H2'	30:a:3:A:H8	1.82	0.45
30:a:814:G:H5'	30:a:815:U:H5''	1.99	0.45
30:a:814:G:O2'	30:a:848:G:H4'	2.16	0.45
30:a:1703:G:OP2	30:a:1704:A:O2'	2.32	0.45
30:a:1866:C:H2'	30:a:1867:C:C6	2.51	0.45
30:a:3077:U:H2'	30:a:3078:U:C6	2.51	0.45
34:e:12:VAL:HG12	34:e:14:GLY:N	2.32	0.45
34:e:155:LYS:NZ	34:e:155:LYS:HB3	2.32	0.45
47:s:3:GLU:HG3	47:s:4:LEU:N	2.31	0.45
6:A:220:G:H2'	6:A:221:C:O4'	2.16	0.45
6:A:386:G:H2'	6:A:387:C:H6	1.82	0.45
6:A:1071:U:H3	6:A:1084:G:H22	1.65	0.45
7:B:87:VAL:HG21	7:B:222:ALA:HB3	1.99	0.45
13:H:39:ILE:HG21	13:H:108:ILE:HD12	1.98	0.45
15:J:148:THR:O	15:J:148:THR:OG1	2.34	0.45
16:K:19:LYS:C	16:K:20:LYS:HD3	2.42	0.45
16:K:20:LYS:HD3	16:K:20:LYS:N	2.30	0.45
23:R:55:VAL:O	23:R:59:ILE:HG12	2.17	0.45
30:a:1724:G:H3'	30:a:1725:G:H8	1.82	0.45
30:a:2978:G:H2'	30:a:2979:U:C4	2.52	0.45
41:m:97:VAL:HG22	41:m:113:ILE:HG13	1.97	0.45
6:A:266:U:H2'	6:A:267:G:O4'	2.17	0.45
6:A:1518:A:H2'	6:A:1519:U:C2	2.52	0.45
12:G:128:ALA:HB3	12:G:131:ARG:HG2	1.98	0.45
16:K:25:GLY:HA2	16:K:43:PRO:HD3	1.99	0.45
16:K:41:THR:HA	16:K:47:VAL:HA	1.98	0.45
18:M:54:SER:HB3	18:M:58:TYR:HB2	1.97	0.45
30:a:235:G:H4'	30:a:236:U:C6	2.52	0.45
30:a:361:G:N2	30:a:443:G:N2	2.65	0.45
30:a:1166:G:O2'	30:a:1168:A:N7	2.45	0.45
30:a:1618:U:H2'	30:a:1619:A:H8	1.82	0.45
35:f:144:GLN:HA	35:f:161:MET:HE1	1.98	0.45
6:A:39:G:H2'	6:A:40:C:C6	2.52	0.45
7:B:102:THR:HG22	7:B:176:GLU:OE1	2.17	0.45
7:B:110:ARG:HD2	7:B:110:ARG:HA	1.73	0.45
30:a:630:U:H2'	30:a:631:G:O4'	2.17	0.45
30:a:869:G:H5'	30:a:870:G:OP1	2.17	0.45
30:a:1052:G:H2'	30:a:1053:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1137:A:H61	30:a:1188:U:H3	1.64	0.45
30:a:1417:G:O6	47:s:25:LEU:HD21	2.16	0.45
30:a:2720:C:O2'	30:a:2721:C:OP2	2.35	0.45
41:m:69:THR:HG22	41:m:70:ILE:N	2.32	0.45
42:n:11:LEU:HD23	42:n:12:SER:H	1.80	0.45
6:A:248:A:C2	6:A:284:A:C5	3.05	0.45
6:A:417:C:C2	6:A:418:G:C8	3.05	0.45
6:A:467:G:H4'	6:A:468:U:O5'	2.16	0.45
6:A:999:A:C2	6:A:1205:A:H1'	2.52	0.45
6:A:1244:G:H2'	6:A:1245:C:C6	2.52	0.45
6:A:1304:A:H1'	26:U:37:ARG:NH1	2.32	0.45
11:F:15:GLU:O	11:F:18:GLN:NE2	2.50	0.45
22:Q:28:ILE:HG21	22:Q:60:ALA:HB3	1.99	0.45
29:Y:14:A:H2'	29:Y:14:A:N3	2.31	0.45
30:a:173:A:H2'	30:a:174:G:O4'	2.16	0.45
30:a:201:G:H2'	30:a:202:A:O4'	2.17	0.45
30:a:373:G:H22	30:a:437:G:H1	1.65	0.45
30:a:1862:A:H2'	30:a:1863:A:H8	1.81	0.45
30:a:1908:C:N4	30:a:1909:C:H41	2.14	0.45
30:a:2496:A:H2'	30:a:2497:G:C8	2.52	0.45
6:A:35:G:C8	6:A:308:A:H1'	2.52	0.45
6:A:301:G:H2'	6:A:302:A:C8	2.51	0.45
7:B:6:THR:HA	7:B:9:LEU:HD12	1.97	0.45
7:B:61:VAL:HA	7:B:65:GLY:HA3	1.99	0.45
9:D:82:GLY:HA3	9:D:192:GLU:HG3	1.98	0.45
9:D:150:ILE:O	9:D:154:ARG:HG3	2.17	0.45
30:a:310:C:H2'	30:a:311:A:C8	2.52	0.45
30:a:1416:U:H2'	47:s:62:MET:HE3	1.99	0.45
30:a:2010:U:H5'	30:a:2154:U:H4'	1.98	0.45
30:a:2263:U:H2'	30:a:2264:A:C8	2.52	0.45
30:a:2913:G:H2'	30:a:2914:G:C8	2.52	0.45
47:s:90:GLU:OE1	47:s:90:GLU:HA	2.16	0.45
6:A:1451:G:H2'	6:A:1452:U:H6	1.82	0.44
7:B:189:ASP:OD2	7:B:189:ASP:N	2.35	0.44
17:L:49:LEU:HD12	17:L:49:LEU:HA	1.83	0.44
20:O:7:LYS:HE2	20:O:7:LYS:HB2	1.85	0.44
21:P:111:GLU:OE2	21:P:114:GLU:HB3	2.17	0.44
30:a:306:G:H4'	30:a:307:U:O5'	2.17	0.44
30:a:372:U:C2	30:a:373:G:C8	3.05	0.44
30:a:1465:G:H2'	30:a:1466:U:C6	2.52	0.44
30:a:1901:U:H2'	30:a:1902:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2220:U:H2'	30:a:2221:C:C6	2.52	0.44
30:a:2819:U:H5''	33:d:89:ARG:NH1	2.31	0.44
36:g:142:VAL:O	36:g:145:GLU:HG3	2.17	0.44
41:m:10:LEU:HB2	41:m:17:GLU:HG3	1.98	0.44
42:n:76:ASP:OD2	42:n:76:ASP:C	2.60	0.44
46:r:56:GLN:HE21	54:z:25:THR:H	1.63	0.44
1:0:29:ASN:C	1:0:31:ARG:H	2.25	0.44
6:A:214:G:H2'	6:A:215:U:H6	1.81	0.44
6:A:1152:G:N1	6:A:1155:A:OP2	2.50	0.44
6:A:1230:U:H2'	6:A:1231:G:H8	1.82	0.44
6:A:1302:G:N1	6:A:1305:A:OP2	2.46	0.44
6:A:1411:U:H2'	6:A:1412:A:C8	2.52	0.44
9:D:105:THR:OG1	9:D:106:ARG:N	2.50	0.44
16:K:22:VAL:HG11	16:K:42:ASP:HB2	1.99	0.44
18:M:32:THR:HG22	18:M:82:LYS:HE2	1.99	0.44
30:a:751:C:H2'	30:a:752:U:C6	2.51	0.44
34:e:133:VAL:HG13	34:e:166:ILE:HG22	1.99	0.44
35:f:111:ARG:NE	35:f:149:GLU:OE1	2.49	0.44
6:A:386:G:H2'	6:A:387:C:C6	2.52	0.44
6:A:641:A:H2'	6:A:642:G:C8	2.51	0.44
30:a:20:U:H2'	30:a:21:C:C6	2.53	0.44
30:a:975:G:C2	30:a:976:G:C5	3.05	0.44
30:a:2248:C:H2'	30:a:2249:C:C6	2.52	0.44
30:a:2490:G:H2'	30:a:2490:G:N3	2.32	0.44
31:b:52:U:H1'	31:b:53:C:H5	1.81	0.44
31:b:66:A:H61	31:b:108:A:H2'	1.81	0.44
39:k:97:LEU:HA	39:k:100:VAL:HG22	1.99	0.44
6:A:428:U:H2'	6:A:429:U:C6	2.53	0.44
6:A:1135:C:H2'	6:A:1136:A:C8	2.53	0.44
15:J:63:ILE:HD12	15:J:104:ASP:O	2.17	0.44
30:a:1902:C:H2'	30:a:1903:G:H8	1.81	0.44
30:a:2753:C:O2'	33:d:157:THR:O	2.28	0.44
30:a:2758:G:O2'	30:a:2761:C:OP2	2.29	0.44
38:j:93:PRO:HG3	38:j:114:ILE:HG13	1.98	0.44
1:0:37:MET:HE2	1:0:37:MET:HB3	1.78	0.44
6:A:959:A:H5'	6:A:959:A:H8	1.81	0.44
6:A:1057:G:H2'	6:A:1058:U:C6	2.52	0.44
6:A:1224:A:H2	6:A:1227:G:N3	2.16	0.44
6:A:1500:A:H2'	6:A:1501:C:H6	1.82	0.44
7:B:73:LYS:O	7:B:77:GLN:HG2	2.18	0.44
16:K:112:GLU:OE2	16:K:112:GLU:N	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:76:C:H2'	30:a:77:C:H6	1.83	0.44
30:a:1002:A:H5''	31:b:98:G:O2'	2.17	0.44
30:a:1176:G:H2'	30:a:1177:U:O4'	2.18	0.44
30:a:2428:G:H2'	30:a:2429:A:H8	1.81	0.44
33:d:44:ARG:NE	33:d:87:GLU:OE1	2.47	0.44
34:e:153:LEU:H	34:e:154:ARG:NH2	2.16	0.44
38:j:64:ARG:HB2	38:j:83:ALA:HB3	2.00	0.44
48:t:46:HIS:N	48:t:46:HIS:ND1	2.65	0.44
54:z:35:CYS:SG	54:z:47:SER:HB2	2.57	0.44
6:A:973:G:O6	6:A:1203:C:N4	2.50	0.44
6:A:1053:G:H8	6:A:1053:G:OP2	2.00	0.44
15:J:172:LYS:O	15:J:173:ARG:HG2	2.18	0.44
30:a:188:A:H2'	30:a:189:A:H8	1.83	0.44
30:a:1771:U:H2'	30:a:1772:G:C8	2.53	0.44
30:a:2289:U:OP1	30:a:2289:U:H6	2.01	0.44
33:d:20:LEU:HD12	33:d:30:VAL:HG11	1.98	0.44
6:A:690:C:H2'	6:A:691:A:H8	1.83	0.44
6:A:1103:U:H1'	6:A:1165:A:C5	2.53	0.44
6:A:1274:A:H2'	6:A:1275:A:H8	1.79	0.44
10:E:160:VAL:O	10:E:163:THR:HG22	2.18	0.44
13:H:43:GLU:HA	13:H:43:GLU:OE2	2.18	0.44
15:J:158:LYS:HB2	15:J:161:LEU:HD12	2.00	0.44
21:P:23:MET:HE3	21:P:32:ARG:O	2.17	0.44
30:a:400:G:H2'	30:a:401:U:O4'	2.17	0.44
30:a:580:A:H2'	30:a:581:G:O4'	2.18	0.44
30:a:935:U:H2'	30:a:936:U:C6	2.53	0.44
30:a:993:A:H2'	30:a:996:C:C5	2.53	0.44
30:a:1615:A:H2'	30:a:1616:G:H8	1.83	0.44
36:g:106:GLU:OE2	36:g:116:ILE:HD13	2.17	0.44
47:s:25:LEU:HD22	47:s:30:THR:HG21	1.98	0.44
6:A:12:A:C6	9:D:201:LYS:HB3	2.53	0.44
6:A:45:G:H2'	6:A:46:G:H8	1.83	0.44
6:A:78:G:H2'	6:A:79:C:H6	1.83	0.44
6:A:512:G:C5	29:Y:22:U:H2'	2.52	0.44
6:A:536:U:H2'	6:A:537:C:C6	2.52	0.44
6:A:717:U:H2'	6:A:718:U:C6	2.52	0.44
6:A:984:A:N1	6:A:1025:G:C6	2.85	0.44
16:K:40:ILE:HG22	16:K:85:MET:HE3	2.00	0.44
30:a:437:G:H2'	30:a:438:G:C8	2.53	0.44
30:a:1195:G:H2'	30:a:1196:U:O4'	2.18	0.44
30:a:1232:U:H2'	30:a:1233:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1912:U:OP2	30:a:1913:G:O2'	2.36	0.44
30:a:2047:U:H2'	30:a:2048:G:O4'	2.18	0.44
30:a:2051:U:H2'	30:a:2052:G:O4'	2.17	0.44
6:A:562:C:H2'	6:A:563:G:O4'	2.17	0.44
6:A:618:U:H2'	6:A:619:U:C6	2.53	0.44
6:A:739:U:OP1	6:A:804:G:O2'	2.35	0.44
9:D:182:THR:O	9:D:185:GLN:N	2.50	0.44
10:E:160:VAL:O	10:E:164:VAL:HG23	2.18	0.44
34:e:125:ARG:HH22	34:e:150:LEU:HD13	1.83	0.44
54:z:45:CYS:CB	54:z:48:CYS:SG	3.05	0.44
6:A:934:U:O4	19:N:105:THR:HG21	2.18	0.43
7:B:50:ILE:HD12	7:B:201:ILE:HG12	2.00	0.43
9:D:57:ARG:HG2	9:D:62:VAL:O	2.18	0.43
21:P:120:ILE:HD12	21:P:123:LYS:HB2	1.99	0.43
30:a:671:U:H2'	30:a:672:U:C6	2.52	0.43
30:a:1429:A:H2'	30:a:1430:A:C8	2.52	0.43
30:a:1904:U:OP2	30:a:1921:G:N2	2.51	0.43
30:a:2214:A:N3	30:a:2637:G:O2'	2.50	0.43
35:f:24:ALA:HA	35:f:27:GLU:HG3	2.00	0.43
39:k:144:THR:O	39:k:145:LYS:HB2	2.17	0.43
5:4:12:THR:N	5:4:24:THR:O	2.42	0.43
6:A:865:G:P	17:L:9:ARG:HH22	2.41	0.43
6:A:989:G:H2'	6:A:990:A:C8	2.53	0.43
17:L:16:ILE:HD12	17:L:16:ILE:N	2.33	0.43
23:R:63:ARG:HD3	23:R:70:TYR:HA	2.00	0.43
30:a:51:A:H2'	30:a:52:A:H8	1.83	0.43
30:a:254:G:H4'	30:a:475:G:C6	2.53	0.43
30:a:817:C:H2'	30:a:818:G:O4'	2.19	0.43
30:a:944:G:O2'	30:a:1000:G:O6	2.35	0.43
30:a:2695:G:H2'	30:a:2696:U:C6	2.53	0.43
38:j:64:ARG:O	38:j:82:ASN:HA	2.18	0.43
1:0:25:ILE:HG12	3:2:34:GLU:HG2	1.99	0.43
5:4:18:CYS:SG	5:4:41:CYS:HB2	2.59	0.43
6:A:1284:C:O2'	14:I:114:LYS:NZ	2.51	0.43
10:E:133:SER:O	10:E:137:VAL:HG23	2.18	0.43
11:F:48:LEU:HD11	11:F:86:MET:HE1	1.99	0.43
30:a:283:U:O2'	30:a:315:G:N2	2.50	0.43
30:a:405:G:H4'	30:a:407:A:N7	2.33	0.43
30:a:608:U:H2'	30:a:609:C:C6	2.53	0.43
30:a:672:U:H2'	30:a:673:A:H8	1.82	0.43
30:a:2933:G:H4'	36:g:4:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2992:G:H2'	30:a:2993:U:H6	1.82	0.43
40:l:134:ARG:CZ	49:u:124:ASN:HD21	2.31	0.43
43:o:106:LYS:HA	43:o:109:LYS:HD2	1.99	0.43
6:A:403:C:O2'	6:A:603:A:N3	2.47	0.43
6:A:428:U:OP1	9:D:28:ARG:NH1	2.49	0.43
6:A:1374:G:H2'	6:A:1375:G:H8	1.83	0.43
9:D:15:LEU:HD12	9:D:51:ARG:HG2	2.00	0.43
18:M:21:SER:OG	18:M:96:VAL:HG11	2.18	0.43
18:M:64:HIS:HB3	24:S:59:SER:OG	2.18	0.43
30:a:339:U:H3'	30:a:340:C:C6	2.53	0.43
30:a:728:G:N2	30:a:731:A:H5''	2.33	0.43
30:a:1481:C:H2'	30:a:1482:G:C8	2.52	0.43
30:a:1866:C:H2'	30:a:1867:C:H6	1.83	0.43
30:a:1980:G:O2'	32:c:257:THR:OG1	2.34	0.43
30:a:2274:U:OP2	51:w:61:ARG:NH2	2.43	0.43
30:a:2288:G:HO2'	30:a:2289:U:P	2.41	0.43
30:a:2496:A:H2'	30:a:2497:G:H8	1.84	0.43
34:e:160:LEU:HD13	34:e:163:SER:O	2.19	0.43
35:f:141:LEU:HD22	35:f:146:MET:HE2	2.01	0.43
41:m:70:ILE:HG22	41:m:72:ASP:H	1.84	0.43
42:n:40:VAL:HG13	42:n:49:VAL:HG22	1.99	0.43
45:q:58:VAL:HG22	45:q:100:ILE:HG23	2.00	0.43
6:A:379:G:OP1	21:P:4:LYS:NZ	2.33	0.43
6:A:849:A:H2'	6:A:850:C:C6	2.53	0.43
6:A:1415:A:H2'	6:A:1416:C:H6	1.83	0.43
7:B:163:TRP:CH2	7:B:187:ILE:HD11	2.54	0.43
19:N:33:THR:HA	19:N:59:HIS:CE1	2.53	0.43
30:a:372:U:C2	30:a:373:G:H8	2.36	0.43
30:a:899:C:H1'	30:a:1301:G:N2	2.33	0.43
30:a:1488:U:H2'	30:a:1489:C:C6	2.53	0.43
46:r:68:ILE:O	46:r:72:MET:HG3	2.19	0.43
6:A:21:U:H2'	6:A:22:C:H6	1.81	0.43
6:A:719:C:H2'	6:A:720:U:H6	1.83	0.43
6:A:719:C:H2'	6:A:720:U:C6	2.54	0.43
6:A:793:U:O2'	6:A:885:A:N1	2.51	0.43
6:A:1055:U:H2'	6:A:1056:C:C6	2.53	0.43
8:C:23:C:H2'	8:C:24:U:C6	2.53	0.43
9:D:116:GLY:O	9:D:117:HIS:ND1	2.51	0.43
15:J:138:ARG:N	15:J:139:PRO:HD2	2.34	0.43
26:U:22:GLN:HG2	26:U:31:ILE:HD11	1.99	0.43
30:a:752:U:H2'	30:a:753:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2980:G:O2'	30:a:2981:U:OP1	2.35	0.43
35:f:31:TYR:HD2	35:f:37:ILE:HG13	1.83	0.43
35:f:179:LEU:HD22	35:f:184:PHE:CE1	2.53	0.43
6:A:113:G:H2'	6:A:114:U:C6	2.54	0.43
6:A:677:A:H2'	6:A:678:A:C8	2.54	0.43
6:A:966:U:H4'	6:A:967:A:O4'	2.18	0.43
6:A:1164:G:N2	6:A:1166:A:H3'	2.34	0.43
7:B:134:GLU:O	7:B:137:MET:HG3	2.18	0.43
11:F:15:GLU:N	11:F:18:GLN:OE1	2.36	0.43
13:H:117:THR:OG1	13:H:120:GLN:HG3	2.19	0.43
16:K:89:ASP:HB2	16:K:115:PRO:HD2	2.00	0.43
30:a:172:U:H2'	30:a:173:A:H8	1.83	0.43
30:a:180:U:H2'	30:a:181:G:C8	2.54	0.43
30:a:440:A:H2'	30:a:441:C:C6	2.53	0.43
30:a:852:U:H2'	30:a:853:G:H8	1.84	0.43
30:a:1192:C:H3'	30:a:1193:A:H8	1.83	0.43
30:a:1364:U:H5	30:a:1402:U:O2	2.01	0.43
30:a:1486:U:H2'	30:a:1487:G:C8	2.54	0.43
30:a:1726:U:H4'	30:a:1727:G:H5'	2.01	0.43
30:a:2972:A:C2	30:a:3073:G:H2'	2.53	0.43
42:n:5:LEU:HD23	42:n:5:LEU:HA	1.81	0.43
46:r:56:GLN:NE2	54:z:25:THR:H	2.17	0.43
48:t:8:LYS:HA	48:t:26:VAL:HG23	2.01	0.43
2:1:24:THR:HG23	2:1:27:GLY:H	1.83	0.43
6:A:633:C:H2'	6:A:634:U:C6	2.53	0.43
6:A:717:U:H2'	6:A:718:U:H6	1.82	0.43
6:A:1313:U:H2'	6:A:1314:C:C6	2.53	0.43
6:A:1386:C:O2	6:A:1489:A:N6	2.51	0.43
6:A:1441:U:H2'	6:A:1442:G:H8	1.81	0.43
6:A:1499:U:H2'	6:A:1500:A:C8	2.54	0.43
14:I:21:PRO:O	14:I:25:GLN:HG3	2.19	0.43
30:a:116:G:OP2	30:a:118:A:O2'	2.33	0.43
30:a:145:G:H2'	30:a:146:U:C6	2.53	0.43
30:a:333:U:N3	30:a:334:G:N7	2.67	0.43
30:a:1151:G:H4'	30:a:1153:A:N6	2.34	0.43
30:a:1151:G:H21	30:a:1178:A:H2'	1.83	0.43
30:a:1610:C:H2'	30:a:1611:A:C8	2.54	0.43
30:a:2914:G:H3'	30:a:2915:U:O4'	2.19	0.43
30:a:2922:A:H2'	30:a:2923:A:C8	2.53	0.43
31:b:118:A:H2'	31:b:119:A:O4'	2.19	0.43
32:c:5:LYS:HD2	32:c:17:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:134:ARG:HB3	32:c:134:ARG:NH1	2.34	0.43
6:A:149:G:H2'	6:A:150:A:O4'	2.19	0.43
6:A:806:U:H2'	6:A:807:A:H8	1.83	0.43
6:A:1415:A:H2'	6:A:1416:C:C6	2.53	0.43
21:P:46:PRO:O	21:P:47:SER:C	2.60	0.43
30:a:2:C:H2'	30:a:3:A:C8	2.54	0.43
30:a:405:G:H4'	30:a:407:A:C8	2.53	0.43
30:a:1774:C:N4	30:a:1775:G:O6	2.51	0.43
30:a:2289:U:H2'	30:a:2290:U:O4'	2.18	0.43
34:e:119:ASP:CG	39:k:3:ILE:HG12	2.44	0.43
35:f:127:ASN:ND2	35:f:127:ASN:N	2.66	0.43
40:l:127:MET:HE3	40:l:127:MET:HB3	1.80	0.43
48:t:10:ASP:HB3	48:t:77:LEU:HD21	2.01	0.43
6:A:950:2MG:C2	8:C:34:C:H5'	2.54	0.43
6:A:1375:G:H2'	6:A:1376:C:C6	2.53	0.43
10:E:192:MET:HE3	10:E:192:MET:HB2	1.85	0.43
11:F:81:ILE:HD13	11:F:81:ILE:HA	1.84	0.43
12:G:62:ARG:HA	12:G:97:GLN:HG2	2.00	0.43
13:H:73:ARG:HA	13:H:73:ARG:HD2	1.87	0.43
16:K:42:ASP:OD2	16:K:42:ASP:C	2.62	0.43
20:O:1:MET:HA	20:O:5:GLU:OE2	2.19	0.43
20:O:87:ARG:NH2	30:a:799:U:H3'	2.32	0.43
30:a:620:C:H4'	30:a:621:G:C8	2.53	0.43
30:a:2064:G:H2'	30:a:2065:U:O4'	2.19	0.43
30:a:2374:U:H2'	30:a:2375:U:O4'	2.19	0.43
32:c:172:TYR:CD2	32:c:184:MET:HE3	2.54	0.43
35:f:42:LYS:HG3	35:f:166:VAL:HB	2.01	0.43
46:r:90:GLN:HB2	46:r:123:VAL:HB	2.00	0.43
52:x:41:GLU:OE1	52:x:41:GLU:N	2.41	0.43
6:A:192:G:C6	6:A:202:G:C5	3.07	0.42
6:A:482:G:H2'	6:A:483:C:C6	2.54	0.42
6:A:536:U:H2'	6:A:537:C:H6	1.84	0.42
6:A:969:C:H2'	6:A:970:U:C6	2.54	0.42
12:G:176:THR:HG22	12:G:179:ALA:H	1.84	0.42
30:a:147:G:H1'	30:a:1780:C:O2'	2.18	0.42
30:a:1258:G:H2'	30:a:1259:G:C8	2.54	0.42
30:a:1493:G:H1'	30:a:1769:G:N2	2.33	0.42
30:a:1734:U:H2'	30:a:1735:G:O4'	2.19	0.42
30:a:1902:C:H2'	30:a:1903:G:C8	2.54	0.42
30:a:1918:G:H2'	30:a:1919:U:C6	2.53	0.42
30:a:2425:U:H2'	30:a:2426:U:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1453:C:H2'	6:A:1454:G:O4'	2.19	0.42
9:D:15:LEU:HB3	9:D:55:LYS:HZ3	1.83	0.42
9:D:137:ILE:HG12	9:D:176:LEU:HD13	2.01	0.42
10:E:187:ILE:HG13	10:E:188:ALA:N	2.35	0.42
30:a:270:G:H2'	30:a:271:G:O4'	2.19	0.42
30:a:504:A:H2'	30:a:505:C:C6	2.54	0.42
30:a:905:A:H4'	30:a:921:G:N2	2.34	0.42
30:a:1070:C:H2'	30:a:1071:A:O4'	2.19	0.42
30:a:1649:U:H2'	30:a:1704:A:N6	2.34	0.42
30:a:2025:G:H2'	30:a:2026:C:C6	2.54	0.42
30:a:2050:G:H2'	30:a:2051:U:O4'	2.19	0.42
30:a:2106:U:H2'	30:a:2107:C:H6	1.84	0.42
30:a:2432:G:O2'	30:a:2678:C:OP1	2.29	0.42
30:a:2706:G:N1	30:a:2721:C:H5	2.12	0.42
32:c:24:LEU:HD11	32:c:84:TYR:HB2	2.01	0.42
32:c:124:ASP:OD1	32:c:125:ILE:N	2.52	0.42
33:d:59:GLY:O	33:d:83:ARG:N	2.47	0.42
39:k:123:LEU:HB2	39:k:143:VAL:HG12	2.01	0.42
41:m:82:GLU:O	41:m:86:ARG:HB2	2.20	0.42
6:A:828:A:H2'	6:A:829:C:C6	2.54	0.42
6:A:829:C:H4'	23:R:14:LYS:NZ	2.35	0.42
6:A:990:A:H4'	6:A:1023:C:H4'	2.00	0.42
7:B:58:LYS:HA	7:B:58:LYS:HD3	1.72	0.42
17:L:72:HIS:HE2	17:L:74:LEU:HD12	1.84	0.42
19:N:37:THR:HG23	19:N:39:ILE:HG13	2.01	0.42
30:a:305:U:H2'	30:a:306:G:N2	2.34	0.42
30:a:532:A:C2	34:e:48:ARG:HG3	2.54	0.42
30:a:947:G:H2'	30:a:948:A:O4'	2.18	0.42
30:a:1084:A:H2'	30:a:1085:G:O4'	2.19	0.42
30:a:1881:G:OP2	30:a:1882:A:O2'	2.33	0.42
30:a:2234:A:OP2	30:a:2234:A:H8	2.02	0.42
30:a:2248:C:H2'	30:a:2249:C:H6	1.84	0.42
30:a:2546:C:H2'	30:a:2547:G:O4'	2.19	0.42
34:e:63:GLY:HA3	34:e:82:ARG:HG2	2.00	0.42
34:e:157:LEU:HD12	34:e:182:ALA:HA	2.01	0.42
34:e:210:ARG:CZ	34:e:210:ARG:HB3	2.49	0.42
44:p:109:LEU:HD23	44:p:109:LEU:HA	1.82	0.42
47:s:26:LEU:HD21	47:s:31:TYR:CE2	2.55	0.42
6:A:187:C:O2'	25:T:84:ASN:OD1	2.31	0.42
6:A:474:G:H2'	6:A:475:U:C6	2.53	0.42
6:A:576:C:H2'	6:A:577:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1240:A:OP1	18:M:47:ASN:ND2	2.49	0.42
6:A:1511:C:H2'	6:A:1512:G:C8	2.55	0.42
7:B:107:ILE:O	7:B:111:ILE:HG12	2.18	0.42
7:B:155:MET:HE2	7:B:155:MET:HB3	1.86	0.42
13:H:3:MET:HE2	13:H:3:MET:HA	2.01	0.42
30:a:568:A:N3	30:a:570:G:H5''	2.34	0.42
30:a:718:A:H2'	30:a:719:A:C8	2.55	0.42
30:a:948:A:H2'	30:a:949:G:C8	2.54	0.42
30:a:1199:U:H2'	30:a:1200:U:H6	1.83	0.42
30:a:1251:C:H2'	30:a:1252:C:C6	2.54	0.42
30:a:1260:U:H2'	30:a:1261:U:O4'	2.20	0.42
30:a:1631:G:H2'	30:a:1632:U:C6	2.54	0.42
30:a:2694:C:H2'	30:a:2695:G:O4'	2.19	0.42
34:e:157:LEU:HD13	34:e:157:LEU:HA	1.95	0.42
37:i:104:ALA:O	37:i:108:MET:HG3	2.20	0.42
49:u:29:VAL:HG21	49:u:50:THR:HG21	2.01	0.42
6:A:449:G:O6	6:A:467:G:O2'	2.34	0.42
6:A:575:U:H2'	6:A:576:C:C6	2.55	0.42
6:A:652:A:H2'	6:A:653:A:C8	2.54	0.42
6:A:1040:A:O2'	12:G:155:ARG:NH1	2.51	0.42
6:A:1267:U:O4	18:M:9:ARG:NH2	2.52	0.42
7:B:187:ILE:HD12	7:B:214:LEU:HD13	2.01	0.42
10:E:104:ILE:O	10:E:121:PRO:HB3	2.20	0.42
13:H:22:HIS:O	13:H:69:TYR:OH	2.30	0.42
19:N:91:ARG:HB2	19:N:98:VAL:HG12	2.01	0.42
30:a:172:U:H2'	30:a:173:A:C8	2.54	0.42
30:a:587:U:H2'	30:a:588:G:O4'	2.19	0.42
30:a:948:A:H2'	30:a:949:G:H8	1.85	0.42
30:a:1160:A:N6	30:a:1171:A:N1	2.67	0.42
30:a:2287:G:H1'	30:a:2288:G:H5'	2.01	0.42
30:a:2934:C:H2'	30:a:2935:A:O4'	2.20	0.42
31:b:28:C:H2'	31:b:29:A:O4'	2.19	0.42
33:d:57:GLY:O	33:d:58:TYR:HB3	2.19	0.42
34:e:160:LEU:C	34:e:162:ARG:N	2.75	0.42
41:m:38:VAL:HG22	41:m:111:ALA:HB2	2.01	0.42
6:A:270:U:H2'	6:A:271:U:C6	2.54	0.42
6:A:1268:C:H2'	6:A:1269:U:C6	2.54	0.42
6:A:1505:MA6:H8	6:A:1505:MA6:O5'	2.19	0.42
7:B:81:VAL:O	7:B:85:THR:OG1	2.28	0.42
11:F:43:TRP:HB2	11:F:60:TYR:HB2	2.01	0.42
14:I:79:ARG:HE	14:I:79:ARG:HB3	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:135:G:OP1	30:a:1767:G:H5''	2.20	0.42
30:a:979:U:H2'	30:a:981:C:H41	1.84	0.42
30:a:1014:G:H3'	30:a:1015:U:C6	2.55	0.42
30:a:2919:G:H2'	30:a:2920:A:C8	2.55	0.42
32:c:5:LYS:HE2	32:c:5:LYS:HB3	1.86	0.42
35:f:86:PHE:HB2	35:f:88:LEU:HD22	2.02	0.42
35:f:146:MET:HB3	35:f:146:MET:HE3	1.77	0.42
36:g:20:ASP:OD1	36:g:20:ASP:N	2.52	0.42
52:x:48:GLU:OE1	52:x:48:GLU:HA	2.19	0.42
6:A:214:G:H2'	6:A:215:U:C6	2.55	0.42
6:A:561:U:H2'	6:A:562:C:H6	1.83	0.42
6:A:1167:G:H1'	6:A:1168:G:C5	2.55	0.42
21:P:95:GLN:HB2	21:P:98:ARG:NH1	2.28	0.42
30:a:658:A:OP2	30:a:2681:C:O2'	2.38	0.42
30:a:764:G:H2'	30:a:765:G:H8	1.85	0.42
47:s:20:GLU:OE1	47:s:20:GLU:N	2.41	0.42
5:4:60:ARG:HA	5:4:63:ARG:CZ	2.50	0.42
6:A:449:G:N1	6:A:468:U:OP2	2.51	0.42
6:A:584:A:H2'	6:A:585:A:H8	1.84	0.42
6:A:1301:U:H2'	6:A:1302:G:O4'	2.20	0.42
7:B:166:ASP:OD2	7:B:169:LYS:HB2	2.20	0.42
15:J:156:ARG:O	15:J:158:LYS:HE3	2.20	0.42
17:L:72:HIS:NE2	17:L:74:LEU:HD12	2.35	0.42
30:a:629:C:H2'	30:a:630:U:O4'	2.20	0.42
30:a:1183:C:H2'	30:a:1184:U:O4'	2.19	0.42
30:a:2001:U:H2'	32:c:157:ARG:HB2	2.02	0.42
31:b:66:A:N6	31:b:108:A:H2'	2.35	0.42
54:z:48:CYS:SG	54:z:57:ARG:NH2	2.93	0.42
6:A:161:A:H2'	6:A:162:A:O4'	2.20	0.42
6:A:478:A:O2'	6:A:479:G:C8	2.73	0.42
6:A:1497:C:H2'	6:A:1498:G:H8	1.85	0.42
9:D:165:TRP:CD1	9:D:181:PRO:HB3	2.55	0.42
11:F:56:SER:OG	11:F:56:SER:O	2.32	0.42
30:a:406:G:OP2	34:e:138:PRO:HA	2.20	0.42
35:f:31:TYR:CD2	35:f:37:ILE:HG13	2.54	0.42
43:o:14:ARG:H	43:o:77:HIS:CD2	2.38	0.42
46:r:62:GLU:O	46:r:66:LYS:HG3	2.20	0.42
48:t:116:LEU:HD23	48:t:116:LEU:H	1.84	0.42
6:A:229:G:H2'	6:A:230:A:C8	2.55	0.42
6:A:1033:G:H5''	24:S:3:LYS:HG2	2.01	0.42
14:I:69:ILE:HD11	14:I:127:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:93:PRO:O	14:I:96:GLN:HG2	2.20	0.42
21:P:9:ARG:C	21:P:10:LEU:HD12	2.44	0.42
30:a:26:G:H22	30:a:600:G:H1'	1.85	0.42
30:a:238:U:H2'	30:a:239:G:O4'	2.20	0.42
30:a:271:G:O2'	30:a:272:A:OP1	2.36	0.42
30:a:2066:G:C2	30:a:2067:A:H1'	2.55	0.42
30:a:2180:C:H5'	33:d:128:MET:CE	2.49	0.42
30:a:2560:A:C5	30:a:2561:G:H1'	2.55	0.42
36:g:47:ASP:O	36:g:47:ASP:CG	2.62	0.42
4:3:26:ILE:HD12	4:3:26:ILE:C	2.45	0.41
5:4:8:ASP:OD2	5:4:8:ASP:C	2.62	0.41
6:A:90:U:H1'	6:A:91:G:O5'	2.20	0.41
6:A:177:C:H2'	6:A:178:G:H5''	2.02	0.41
6:A:520:U:H2'	6:A:521:A:H8	1.85	0.41
7:B:137:MET:HA	7:B:140:ARG:HG2	2.01	0.41
9:D:197:GLU:HA	9:D:197:GLU:OE2	2.20	0.41
10:E:104:ILE:HD12	10:E:170:LEU:HD11	2.01	0.41
12:G:133:MET:HE3	12:G:150:ILE:HG22	2.02	0.41
15:J:61:VAL:HG21	15:J:125:ILE:HD12	2.02	0.41
15:J:93:PRO:HA	15:J:96:THR:HG22	2.02	0.41
18:M:26:VAL:HG22	18:M:36:VAL:HG21	2.01	0.41
19:N:87:TYR:O	19:N:91:ARG:HG2	2.20	0.41
19:N:91:ARG:HA	19:N:91:ARG:HD2	1.92	0.41
20:O:87:ARG:N	20:O:87:ARG:HD3	2.35	0.41
30:a:18:G:H2'	30:a:19:A:C8	2.55	0.41
30:a:145:G:H2'	30:a:146:U:H6	1.85	0.41
30:a:422:U:H2'	30:a:423:G:O4'	2.20	0.41
30:a:1607:A:H4'	30:a:1608:C:O4'	2.20	0.41
31:b:5:C:OP1	31:b:62:U:H5'	2.19	0.41
38:j:34:TYR:N	38:j:37:ASP:OD2	2.42	0.41
46:r:128:GLU:CD	46:r:128:GLU:H	2.28	0.41
6:A:97:C:H2'	6:A:98:U:H5'	2.02	0.41
6:A:352:G:H2'	6:A:353:G:C8	2.55	0.41
6:A:373:A:H2'	6:A:374:C:O4'	2.19	0.41
6:A:934:U:OP2	19:N:102:ARG:HD2	2.20	0.41
6:A:970:U:H2'	6:A:971:G:O4'	2.20	0.41
6:A:1236:A:H2'	6:A:1237:G:C8	2.55	0.41
6:A:1299:U:P	26:U:5:LEU:HB2	2.60	0.41
11:F:91:MET:HE2	11:F:91:MET:HB3	1.84	0.41
15:J:54:ARG:NH1	15:J:150:ASP:OD1	2.53	0.41
30:a:3:A:N6	30:a:3079:C:H42	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:975:G:H2'	30:a:976:G:C8	2.55	0.41
30:a:1984:G:C6	30:a:2385:U:H5''	2.55	0.41
30:a:2014:U:H2'	30:a:2015:C:C6	2.56	0.41
30:a:2113:G:O2'	30:a:2151:G:O6	2.34	0.41
30:a:2871:U:H5''	30:a:2872:G:C8	2.54	0.41
30:a:2961:U:P	30:a:2961:U:H3'	2.60	0.41
34:e:160:LEU:CB	34:e:164:ASP:HB2	2.48	0.41
41:m:65:PHE:O	41:m:68:ARG:HB2	2.21	0.41
6:A:45:G:H2'	6:A:46:G:C8	2.55	0.41
11:F:75:LEU:O	11:F:79:LEU:HG	2.20	0.41
23:R:33:ILE:HD12	23:R:68:LEU:HD22	2.02	0.41
30:a:2468:A:H4'	30:a:2469:A:O4'	2.21	0.41
43:o:10:LYS:HE2	43:o:10:LYS:HB2	1.90	0.41
45:q:27:ASP:OD2	45:q:27:ASP:N	2.52	0.41
6:A:1314:C:H5''	19:N:28:THR:HG21	2.03	0.41
6:A:1497:C:H2'	6:A:1498:G:C8	2.55	0.41
8:C:9:G:O2'	8:C:10:G:N7	2.45	0.41
15:J:133:ASP:OD2	15:J:136:ALA:HB3	2.20	0.41
21:P:45:ASP:CB	21:P:46:PRO:HD3	2.49	0.41
30:a:670:G:H22	39:k:34:ARG:NH1	2.18	0.41
30:a:936:U:H2'	30:a:937:G:H8	1.85	0.41
30:a:1156:A:O2'	30:a:2656:U:O3'	2.35	0.41
30:a:1982:G:N7	32:c:179:SER:OG	2.47	0.41
30:a:2194:U:H2'	30:a:2195:G:O4'	2.21	0.41
33:d:20:LEU:O	33:d:27:LEU:HD12	2.20	0.41
33:d:21:TRP:CE2	33:d:27:LEU:HD13	2.56	0.41
45:q:56:VAL:HA	45:q:102:GLY:HA2	2.02	0.41
48:t:26:VAL:HG12	48:t:38:VAL:HG22	2.01	0.41
6:A:26:G:H2'	6:A:27:C:C6	2.55	0.41
6:A:36:A:OP2	6:A:400:C:O2'	2.33	0.41
6:A:401:G:H2'	6:A:402:C:C6	2.56	0.41
6:A:624:A:C5	13:H:112:SER:HA	2.56	0.41
6:A:852:C:H2'	6:A:853:U:O4'	2.20	0.41
9:D:118:PHE:O	9:D:119:LEU:HD23	2.20	0.41
10:E:201:GLU:OE1	10:E:201:GLU:HA	2.19	0.41
14:I:13:MET:HE3	14:I:14:VAL:H	1.84	0.41
30:a:279:A:H62	30:a:319:G:N2	2.18	0.41
30:a:742:U:H2'	30:a:743:C:C6	2.55	0.41
30:a:1010:A:H2'	30:a:1011:A:C8	2.55	0.41
30:a:1912:U:H5''	30:a:1914:C:H5'	2.02	0.41
31:b:90:A:C2	31:b:91:U:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:38:ARG:HA	36:g:38:ARG:HD3	1.81	0.41
38:j:112:MET:HE2	38:j:112:MET:HA	2.02	0.41
6:A:23:C:H2'	6:A:24:U:C6	2.56	0.41
6:A:201:U:H4'	22:Q:4:ASN:HD22	1.85	0.41
6:A:831:G:H5'	6:A:832:G:OP2	2.21	0.41
6:A:938:G:H2'	6:A:939:A:H8	1.85	0.41
6:A:989:G:H3'	6:A:1009:G:N2	2.36	0.41
6:A:1312:C:H2'	6:A:1313:U:C6	2.55	0.41
7:B:16:PHE:O	7:B:204:ASN:ND2	2.53	0.41
9:D:52:GLU:CD	9:D:191:ASN:HB2	2.45	0.41
30:a:141:A:H2'	30:a:142:G:C8	2.56	0.41
30:a:432:A:H2'	30:a:433:G:O4'	2.21	0.41
30:a:672:U:H2'	30:a:673:A:C8	2.55	0.41
30:a:824:A:H1'	30:a:825:C:H5	1.86	0.41
30:a:1402:U:O2'	30:a:2193:G:O2'	2.38	0.41
30:a:2098:3TD:H2'	30:a:2099:A:O4'	2.21	0.41
30:a:2288:G:H1'	30:a:2289:U:OP2	2.21	0.41
30:a:2584:G:H1'	30:a:2585:G:N7	2.36	0.41
30:a:2649:C:H2'	30:a:2650:G:O4'	2.20	0.41
30:a:2956:C:H2'	30:a:2957:A:O4'	2.21	0.41
30:a:3026:G:H2'	30:a:3027:U:C6	2.56	0.41
35:f:105:MET:HE2	35:f:105:MET:HB3	1.94	0.41
36:g:72:LEU:HD12	36:g:72:LEU:HA	1.87	0.41
6:A:886:G:H2'	6:A:887:G:H8	1.85	0.41
6:A:1002:U:H2'	6:A:1003:G:O4'	2.21	0.41
6:A:1164:G:N7	15:J:142:LYS:NZ	2.38	0.41
6:A:1217:A:H2'	6:A:1218:U:C6	2.55	0.41
6:A:1266:A:H5'	18:M:42:LEU:HD12	2.03	0.41
7:B:54:TYR:CE1	7:B:58:LYS:HE2	2.56	0.41
12:G:17:ASP:N	12:G:17:ASP:OD2	2.54	0.41
14:I:26:LEU:HG	14:I:101:MET:HE2	2.02	0.41
30:a:353:A:H2'	30:a:354:U:H5	1.86	0.41
30:a:445:U:H2'	30:a:446:G:H8	1.84	0.41
30:a:459:G:OP2	30:a:512:A:N6	2.54	0.41
30:a:488:U:H2'	30:a:489:G:O4'	2.21	0.41
30:a:1661:C:H2'	30:a:1662:U:C6	2.56	0.41
30:a:2831:U:H2'	30:a:2832:C:C6	2.56	0.41
34:e:15:LYS:HE2	34:e:15:LYS:N	2.36	0.41
36:g:53:VAL:HG11	36:g:69:THR:HG23	2.03	0.41
52:x:34:GLN:HB3	52:x:40:LEU:HB2	2.02	0.41
1:0:18:GLU:OE1	1:0:18:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:48:LYS:HB3	5:4:48:LYS:HE3	1.95	0.41
6:A:569:G:N1	6:A:736:C:OP2	2.54	0.41
6:A:1159:C:H2'	6:A:1160:G:H8	1.86	0.41
6:A:1184:G:H2'	6:A:1185:U:C6	2.56	0.41
6:A:1333:G:H5''	15:J:152:ARG:HB2	2.02	0.41
7:B:45:GLN:H	7:B:45:GLN:HG2	1.66	0.41
12:G:7:PRO:HA	12:G:11:ARG:HH21	1.85	0.41
12:G:165:GLU:OE2	12:G:166:GLY:N	2.54	0.41
20:O:27:VAL:HG12	20:O:83:LEU:HD13	2.03	0.41
28:X:21:LEU:O	28:X:28:ARG:NH2	2.53	0.41
30:a:31:C:N4	30:a:536:A:OP2	2.54	0.41
30:a:331:C:O2'	30:a:332:U:O5'	2.36	0.41
30:a:622:U:O2'	44:p:49:ASP:OD1	2.32	0.41
30:a:1836:U:C4	41:m:8:PRO:HG2	2.55	0.41
30:a:2036:A:N1	30:a:2269:G:H1'	2.36	0.41
30:a:2704:U:O2'	30:a:2829:U:OP1	2.24	0.41
30:a:2871:U:H5''	30:a:2872:G:H8	1.85	0.41
30:a:3071:A:H2'	30:a:3072:G:O4'	2.20	0.41
34:e:153:LEU:C	34:e:154:ARG:HE	2.29	0.41
49:u:81:ASP:N	49:u:81:ASP:OD1	2.51	0.41
5:4:65:TYR:CE2	26:U:5:LEU:HD12	2.55	0.41
6:A:79:C:H2'	6:A:80:C:H6	1.85	0.41
6:A:300:A:H2'	6:A:301:G:C8	2.56	0.41
6:A:409:C:OP1	9:D:107:ARG:NH1	2.54	0.41
6:A:678:A:H2'	6:A:679:U:C6	2.55	0.41
6:A:1357:G:C2	6:A:1358:G:C8	3.09	0.41
6:A:1388:G:H2'	6:A:1389:4OC:O4'	2.20	0.41
11:F:87:ARG:HG2	11:F:88:THR:H	1.86	0.41
12:G:115:VAL:O	12:G:119:ILE:HG13	2.20	0.41
15:J:41:ARG:HA	15:J:42:PRO:HD3	1.88	0.41
15:J:149:ARG:NH1	15:J:150:ASP:O	2.54	0.41
21:P:52:ASP:O	21:P:56:VAL:HG12	2.20	0.41
21:P:100:ASN:OD1	21:P:103:ASP:HB2	2.21	0.41
30:a:330:C:N4	30:a:331:C:H41	2.19	0.41
30:a:377:G:O6	30:a:432:A:N6	2.54	0.41
30:a:649:U:H2'	30:a:650:U:O4'	2.21	0.41
30:a:838:U:H2'	30:a:839:G:C8	2.51	0.41
30:a:911:U:O2'	39:k:52:GLY:HA3	2.21	0.41
30:a:913:U:H4'	30:a:916:G:N1	2.36	0.41
30:a:1138:G:N2	30:a:1168:A:H1'	2.30	0.41
30:a:1142:G:N2	30:a:1163:C:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1486:U:H2'	30:a:1487:G:H8	1.86	0.41
30:a:1664:U:H2'	30:a:1665:C:C6	2.55	0.41
30:a:1709:G:N2	30:a:1729:G:O6	2.54	0.41
30:a:2025:G:H2'	30:a:2026:C:H6	1.86	0.41
30:a:2500:G:H5''	30:a:2501:G:OP2	2.21	0.41
30:a:2555:A:H2'	30:a:2556:C:C6	2.56	0.41
30:a:2929:G:O6	30:a:2937:C:H5''	2.21	0.41
30:a:2978:G:H21	30:a:2981:U:C5'	2.33	0.41
32:c:267:LEU:HD13	32:c:267:LEU:HA	1.80	0.41
33:d:20:LEU:HD11	33:d:194:LEU:HD13	2.02	0.41
35:f:59:MET:O	35:f:63:ILE:HG23	2.21	0.41
39:k:96:ASP:O	39:k:100:VAL:HG13	2.20	0.41
42:n:98:THR:O	42:n:98:THR:OG1	2.38	0.41
48:t:45:LYS:HG3	48:t:63:ILE:O	2.21	0.41
49:u:159:LEU:H	49:u:159:LEU:HD12	1.85	0.41
6:A:26:G:H2'	6:A:27:C:H6	1.85	0.41
6:A:638:G:O2'	20:O:26:GLN:OE1	2.38	0.41
6:A:1109:G:N2	6:A:1110:U:O4	2.54	0.41
16:K:54:GLY:HA2	16:K:58:PHE:O	2.21	0.41
18:M:19:ASP:OD1	18:M:23:ARG:NH1	2.54	0.41
19:N:14:ARG:HE	19:N:42:ASP:HA	1.85	0.41
20:O:74:GLU:H	20:O:74:GLU:CD	2.18	0.41
30:a:442:U:H3'	30:a:443:G:C8	2.55	0.41
30:a:1358:U:H2'	30:a:1359:G:O4'	2.21	0.41
30:a:1462:C:H2'	30:a:1463:C:C6	2.55	0.41
30:a:1919:U:H2'	30:a:1920:G:O4'	2.21	0.41
35:f:102:GLY:N	35:f:105:MET:HE2	2.36	0.41
47:s:10:ARG:HG2	52:x:29:PHE:CD2	2.56	0.41
50:v:38:VAL:CG1	50:v:59:LEU:HB2	2.50	0.41
53:y:11:LYS:HB2	53:y:54:LEU:HD22	2.03	0.41
6:A:745:G:H2'	6:A:746:C:C6	2.55	0.40
6:A:1010:C:H2'	6:A:1011:C:O4'	2.21	0.40
6:A:1134:U:O4'	15:J:60:ARG:HD3	2.21	0.40
6:A:1400:A:H2	6:A:1474:G:H22	1.69	0.40
8:C:58:A:O2'	8:C:60:U:OP2	2.31	0.40
12:G:11:ARG:NH1	12:G:177:LEU:HA	2.36	0.40
12:G:72:PRO:HA	12:G:75:VAL:HG12	2.03	0.40
12:G:195:ILE:O	12:G:195:ILE:HG13	2.18	0.40
13:H:40:LEU:HB3	13:H:46:ILE:HG12	2.03	0.40
16:K:132:ARG:CZ	16:K:132:ARG:HB3	2.51	0.40
19:N:12:ASP:OD2	19:N:12:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:16:HIS:CD2	20:O:19:ASP:HB2	2.56	0.40
30:a:54:G:H2'	30:a:55:A:C8	2.55	0.40
30:a:1142:G:C8	30:a:1143:U:H2'	2.56	0.40
30:a:1189:G:H2'	30:a:1190:G:C8	2.55	0.40
30:a:1685:G:H2'	30:a:1686:C:O4'	2.21	0.40
30:a:2008:A:H2'	30:a:2009:C:C6	2.56	0.40
30:a:2176:U:H4'	33:d:139:THR:OG1	2.21	0.40
30:a:2247:C:H2'	30:a:2248:C:H6	1.85	0.40
30:a:2832:C:H2'	30:a:2833:U:H6	1.86	0.40
36:g:105:LEU:HD12	36:g:105:LEU:HA	1.82	0.40
37:i:36:LEU:O	37:i:51:GLY:HA3	2.21	0.40
47:s:14:LEU:O	52:x:32:ARG:NH1	2.54	0.40
6:A:408:G:H5'	9:D:5:THR:OG1	2.21	0.40
6:A:439:U:H2'	6:A:440:U:C6	2.56	0.40
6:A:499:G:H1	6:A:515:A:P	2.44	0.40
6:A:933:A:H2'	6:A:934:U:C6	2.56	0.40
6:A:968:C:H2'	6:A:969:C:H6	1.86	0.40
6:A:1020:G:C2	6:A:1021:G:H1'	2.57	0.40
6:A:1027:U:H2'	6:A:1028:C:O4'	2.21	0.40
6:A:1056:C:H2'	6:A:1057:G:C8	2.54	0.40
6:A:1202:U:OP1	24:S:3:LYS:HE3	2.21	0.40
6:A:1396:A:H5''	30:a:2098:3TD:H10	2.03	0.40
13:H:50:LYS:HD3	13:H:51:VAL:H	1.86	0.40
14:I:57:ASP:O	14:I:61:THR:HG22	2.21	0.40
14:I:78:ARG:HH11	14:I:78:ARG:HG2	1.86	0.40
16:K:73:ALA:HB1	16:K:106:LEU:HD13	2.02	0.40
16:K:125:ASN:HB3	16:K:126:GLY:H	1.70	0.40
26:U:3:ARG:HH12	26:U:10:PHE:HD1	1.70	0.40
30:a:659:U:H2'	30:a:660:G:C8	2.56	0.40
30:a:898:U:H2'	30:a:899:C:H6	1.86	0.40
30:a:2927:C:H2'	30:a:2928:U:C6	2.56	0.40
32:c:134:ARG:HA	32:c:168:ARG:HD3	2.03	0.40
49:u:107:LEU:HD23	49:u:139:ILE:HG23	2.02	0.40
6:A:1088:C:H4'	7:B:97:LEU:HD13	2.04	0.40
6:A:1092:C:C4	6:A:1093:G:C8	3.10	0.40
6:A:1277:C:H2'	6:A:1278:C:C6	2.57	0.40
7:B:112:ALA:HA	7:B:115:LYS:HG2	2.03	0.40
7:B:172:LEU:O	7:B:176:GLU:HG3	2.22	0.40
9:D:3:ARG:HG3	9:D:110:ARG:HH21	1.86	0.40
20:O:42:LYS:HE2	20:O:42:LYS:HB3	1.68	0.40
22:Q:45:MET:HE3	22:Q:45:MET:HB3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1709:G:O6	30:a:1726:U:O2'	2.34	0.40
34:e:13:LYS:HD2	34:e:13:LYS:HA	1.72	0.40
34:e:29:VAL:HG12	34:e:30:ASN:H	1.87	0.40
35:f:11:PRO:HB3	35:f:107:GLU:OE1	2.21	0.40
39:k:99:SER:HA	39:k:103:VAL:HG12	2.03	0.40
53:y:37:ILE:N	53:y:37:ILE:HD12	2.37	0.40
6:A:37:A:H2'	6:A:38:C:C6	2.56	0.40
6:A:392:U:H2'	6:A:393:G:H8	1.86	0.40
6:A:614:U:H5'	6:A:615:G:C8	2.57	0.40
6:A:892:A:H2'	6:A:893:A:C8	2.56	0.40
6:A:976:U:H4'	6:A:977:G:H5''	2.03	0.40
10:E:170:LEU:HD23	10:E:170:LEU:HA	1.90	0.40
14:I:42:ILE:HG21	14:I:116:MET:HB3	2.04	0.40
15:J:173:ARG:HG2	15:J:173:ARG:NH1	2.37	0.40
16:K:70:GLN:O	16:K:74:GLU:HG2	2.21	0.40
21:P:40:TYR:CZ	21:P:42:PRO:HB3	2.56	0.40
30:a:381:G:H2'	30:a:382:U:C6	2.57	0.40
30:a:2141:C:H2'	30:a:2142:G:H8	1.87	0.40
30:a:2398:G:H2'	30:a:2399:G:H8	1.86	0.40
30:a:2749:G:H2'	30:a:2750:C:C6	2.56	0.40
30:a:3027:U:H2'	30:a:3028:G:O4'	2.21	0.40
41:m:77:HIS:O	41:m:78:ILE:C	2.65	0.40
6:A:1161:G:H2'	6:A:1162:A:H8	1.86	0.40
6:A:1236:A:H2	6:A:1357:G:H1'	1.86	0.40
14:I:60:GLN:OE1	14:I:60:GLN:C	2.64	0.40
16:K:89:ASP:OD2	16:K:89:ASP:C	2.64	0.40
30:a:384:A:N1	30:a:407:A:O2'	2.51	0.40
30:a:1315:G:H2'	30:a:1316:U:O4'	2.21	0.40
30:a:1754:A:H2'	30:a:1755:A:H8	1.85	0.40
30:a:1984:G:N1	30:a:2384:G:OP1	2.44	0.40
30:a:2185:U:H2'	30:a:2186:G:C8	2.56	0.40
30:a:2245:A:O2'	30:a:2246:C:H5'	2.20	0.40
30:a:2817:C:H5''	33:d:85:LEU:O	2.21	0.40
35:f:17:TYR:HA	35:f:21:ILE:HG12	2.04	0.40
36:g:35:PHE:HB2	36:g:76:MET:HE3	2.04	0.40
39:k:134:GLU:HA	39:k:137:GLU:OE2	2.21	0.40
42:n:44:SER:O	42:n:77:LYS:NZ	2.48	0.40
46:r:82:ARG:HB3	46:r:82:ARG:NH1	2.36	0.40
47:s:27:ASP:OD1	47:s:27:ASP:C	2.64	0.40
47:s:27:ASP:OD1	47:s:28:GLN:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	65/68 (96%)	65 (100%)	0	0	100	100
4	3	35/37 (95%)	35 (100%)	0	0	100	100
5	4	64/69 (93%)	57 (89%)	7 (11%)	0	100	100
7	B	231/283 (82%)	214 (93%)	15 (6%)	2 (1%)	14	27
9	D	198/201 (98%)	184 (93%)	14 (7%)	0	100	100
10	E	177/215 (82%)	174 (98%)	3 (2%)	0	100	100
11	F	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
12	G	204/269 (76%)	198 (97%)	6 (3%)	0	100	100
13	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
14	I	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
15	J	132/173 (76%)	120 (91%)	11 (8%)	1 (1%)	16	31
16	K	115/135 (85%)	105 (91%)	9 (8%)	1 (1%)	14	27
17	L	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
18	M	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	24
19	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
20	O	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
21	P	126/147 (86%)	112 (89%)	13 (10%)	1 (1%)	16	31
22	Q	88/90 (98%)	78 (89%)	9 (10%)	1 (1%)	11	22
23	R	65/79 (82%)	60 (92%)	4 (6%)	1 (2%)	8	16
24	S	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	13
25	T	85/88 (97%)	85 (100%)	0	0	100	100
26	U	82/93 (88%)	75 (92%)	6 (7%)	1 (1%)	10	20
27	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	X	30/33 (91%)	29 (97%)	0	1 (3%)	3	4
32	c	272/278 (98%)	260 (96%)	11 (4%)	1 (0%)	30	49
33	d	212/223 (95%)	204 (96%)	8 (4%)	0	100	100
34	e	208/301 (69%)	178 (86%)	26 (12%)	4 (2%)	6	11
35	f	182/210 (87%)	169 (93%)	13 (7%)	0	100	100
36	g	175/180 (97%)	168 (96%)	7 (4%)	0	100	100
37	i	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
38	j	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
39	k	142/146 (97%)	124 (87%)	17 (12%)	1 (1%)	18	34
40	l	134/139 (96%)	125 (93%)	9 (7%)	0	100	100
41	m	118/187 (63%)	110 (93%)	7 (6%)	1 (1%)	16	31
42	n	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
43	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
44	p	117/123 (95%)	116 (99%)	1 (1%)	0	100	100
45	q	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
46	r	130/153 (85%)	125 (96%)	5 (4%)	0	100	100
47	s	93/102 (91%)	85 (91%)	7 (8%)	1 (1%)	11	22
48	t	103/122 (84%)	94 (91%)	8 (8%)	1 (1%)	12	24
49	u	177/205 (86%)	168 (95%)	9 (5%)	0	100	100
50	v	76/89 (85%)	74 (97%)	1 (1%)	1 (1%)	9	18
51	w	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	13
52	x	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
53	y	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
54	z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
All	All	5646/6322 (89%)	5320 (94%)	304 (5%)	22 (0%)	31	49

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	100	MET
22	Q	9	THR
24	S	27	CYS
26	U	84	VAL
28	X	4	VAL

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Mol	Chain	Res	Type
34	e	133	VAL
34	e	151	ALA
47	s	93	ARG
16	K	23	VAL
18	M	6	ILE
34	e	159	VAL
21	P	112	ALA
32	c	262	LYS
15	J	43	ALA
23	R	73	THR
34	e	186	ASN
41	m	37	THR
48	t	64	ILE
51	w	41	ASN
50	v	73	ARG
7	B	4	VAL
39	k	124	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/51 (92%)	47 (100%)	0	100	100
2	1	36/36 (100%)	35 (97%)	1 (3%)	38	66
3	2	54/55 (98%)	53 (98%)	1 (2%)	50	76
4	3	35/35 (100%)	35 (100%)	0	100	100
5	4	56/59 (95%)	52 (93%)	4 (7%)	13	29
7	B	197/234 (84%)	189 (96%)	8 (4%)	27	53
9	D	175/176 (99%)	169 (97%)	6 (3%)	32	60
10	E	130/155 (84%)	125 (96%)	5 (4%)	29	56
11	F	89/89 (100%)	87 (98%)	2 (2%)	45	73
12	G	160/200 (80%)	155 (97%)	5 (3%)	35	62
13	H	108/109 (99%)	104 (96%)	4 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	I	132/133 (99%)	125 (95%)	7 (5%)	20	42
15	J	97/131 (74%)	94 (97%)	3 (3%)	35	62
16	K	88/101 (87%)	83 (94%)	5 (6%)	18	39
17	L	103/104 (99%)	99 (96%)	4 (4%)	28	55
18	M	89/93 (96%)	87 (98%)	2 (2%)	45	73
19	N	99/100 (99%)	97 (98%)	2 (2%)	48	75
20	O	74/74 (100%)	73 (99%)	1 (1%)	59	81
21	P	103/115 (90%)	99 (96%)	4 (4%)	28	55
22	Q	81/81 (100%)	78 (96%)	3 (4%)	30	57
23	R	55/65 (85%)	53 (96%)	2 (4%)	31	58
24	S	48/49 (98%)	47 (98%)	1 (2%)	47	74
25	T	68/69 (99%)	64 (94%)	4 (6%)	18	37
26	U	72/80 (90%)	69 (96%)	3 (4%)	26	52
27	V	16/17 (94%)	16 (100%)	0	100	100
28	X	28/29 (97%)	27 (96%)	1 (4%)	31	58
32	c	216/220 (98%)	209 (97%)	7 (3%)	34	62
33	d	166/172 (96%)	165 (99%)	1 (1%)	78	91
34	e	165/237 (70%)	157 (95%)	8 (5%)	23	46
35	f	154/175 (88%)	146 (95%)	8 (5%)	21	42
36	g	150/152 (99%)	144 (96%)	6 (4%)	28	54
37	i	118/120 (98%)	114 (97%)	4 (3%)	32	60
38	j	101/101 (100%)	98 (97%)	3 (3%)	36	64
39	k	111/113 (98%)	107 (96%)	4 (4%)	31	58
40	l	108/110 (98%)	105 (97%)	3 (3%)	38	66
41	m	100/142 (70%)	96 (96%)	4 (4%)	28	54
42	n	95/96 (99%)	92 (97%)	3 (3%)	34	62
43	o	97/99 (98%)	96 (99%)	1 (1%)	68	86
44	p	98/99 (99%)	96 (98%)	2 (2%)	48	75
45	q	84/84 (100%)	74 (88%)	10 (12%)	5	11
46	r	105/118 (89%)	100 (95%)	5 (5%)	23	46
47	s	84/89 (94%)	83 (99%)	1 (1%)	63	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	t	91/103 (88%)	87 (96%)	4 (4%)	25	50
49	u	149/168 (89%)	143 (96%)	6 (4%)	28	54
50	v	60/67 (90%)	57 (95%)	3 (5%)	22	44
51	w	52/53 (98%)	50 (96%)	2 (4%)	29	56
52	x	61/68 (90%)	59 (97%)	2 (3%)	33	61
53	y	53/55 (96%)	51 (96%)	2 (4%)	29	56
54	z	51/52 (98%)	49 (96%)	2 (4%)	28	55
All	All	4709/5133 (92%)	4540 (96%)	169 (4%)	32	58

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	24	THR
3	2	38	SER
5	4	10	ARG
5	4	23	THR
5	4	28	SER
5	4	62	GLU
7	B	1	MET
7	B	20	THR
7	B	155	MET
7	B	164	VAL
7	B	182	ILE
7	B	189	ASP
7	B	193	ASP
7	B	208	ILE
9	D	41	THR
9	D	47	SER
9	D	112	MET
9	D	134	THR
9	D	146	ASP
9	D	190	VAL
10	E	108	VAL
10	E	111	GLU
10	E	146	VAL
10	E	151	LEU
10	E	192	MET
11	F	19	VAL
11	F	88	THR
12	G	93	LEU

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Mol	Chain	Res	Type
12	G	97	GLN
12	G	103	LEU
12	G	161	MET
12	G	197	VAL
13	H	10	MET
13	H	40	LEU
13	H	76	SER
13	H	123	GLU
14	I	12	VAL
14	I	31	LEU
14	I	33	ASP
14	I	40	GLN
14	I	55	ASN
14	I	68	ASN
14	I	146	GLU
15	J	86	HIS
15	J	105	VAL
15	J	148	THR
16	K	22	VAL
16	K	47	VAL
16	K	83	HIS
16	K	111	LEU
16	K	125	ASN
17	L	41	THR
17	L	73	ASN
17	L	101	SER
17	L	104	THR
18	M	76	ILE
18	M	99	GLU
19	N	4	LEU
19	N	103	THR
20	O	9	ILE
21	P	3	THR
21	P	53	SER
21	P	62	VAL
21	P	124	SER
22	Q	24	MET
22	Q	34	ASP
22	Q	62	MET
23	R	44	VAL
23	R	67	LEU
24	S	44	LEU

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Mol	Chain	Res	Type
25	T	17	SER
25	T	22	LYS
25	T	33	ARG
25	T	37	ARG
26	U	62	VAL
26	U	71	LEU
26	U	79	THR
28	X	30	ARG
32	c	23	GLU
32	c	34	LEU
32	c	44	ASN
32	c	95	LEU
32	c	119	SER
32	c	169	GLU
32	c	267	LEU
33	d	94	SER
34	e	7	ILE
34	e	71	LYS
34	e	134	ASP
34	e	150	LEU
34	e	158	VAL
34	e	179	VAL
34	e	185	LEU
34	e	210	ARG
35	f	41	GLU
35	f	73	LYS
35	f	77	THR
35	f	81	LYS
35	f	121	ARG
35	f	127	ASN
35	f	141	LEU
35	f	146	MET
36	g	60	ARG
36	g	72	LEU
36	g	81	THR
36	g	118	ASP
36	g	124	THR
36	g	135	VAL
37	i	30	THR
37	i	91	GLU
37	i	98	ARG
37	i	102	GLU

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Mol	Chain	Res	Type
38	j	28	SER
38	j	65	THR
38	j	73	ASP
39	k	103	VAL
39	k	114	THR
39	k	117	LEU
39	k	143	VAL
40	l	18	THR
40	l	52	ILE
40	l	94	ILE
41	m	23	ASN
41	m	57	THR
41	m	113	ILE
41	m	114	GLU
42	n	11	LEU
42	n	47	VAL
42	n	72	GLU
43	o	30	VAL
44	p	93	LYS
44	p	108	SER
45	q	6	ARG
45	q	14	VAL
45	q	21	GLU
45	q	23	ASP
45	q	36	THR
45	q	49	ASP
45	q	51	ASP
45	q	59	THR
45	q	83	LYS
45	q	95	VAL
46	r	1	MET
46	r	3	LYS
46	r	5	GLU
46	r	41	VAL
46	r	102	ILE
47	s	6	ILE
48	t	33	ARG
48	t	37	VAL
48	t	42	ASN
48	t	46	HIS
49	u	8	LYS
49	u	61	LEU

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Mol	Chain	Res	Type
49	u	81	ASP
49	u	102	ASP
49	u	124	ASN
49	u	150	THR
50	v	49	ASP
50	v	75	ARG
50	v	83	VAL
51	w	25	THR
51	w	47	MET
52	x	8	GLU
52	x	39	GLN
53	y	22	GLU
53	y	58	GLU
54	z	11	SER
54	z	56	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	32	HIS
5	4	34	ASN
7	B	15	HIS
7	B	160	GLN
7	B	204	ASN
9	D	54	GLN
10	E	155	ASN
12	G	6	ASN
12	G	45	ASN
12	G	113	GLN
13	H	18	ASN
13	H	22	HIS
15	J	88	GLN
19	N	52	GLN
25	T	7	GLN
32	c	44	ASN
32	c	96	HIS
32	c	135	ASN
33	d	143	HIS
34	e	93	HIS
34	e	102	GLN
35	f	75	GLN
35	f	127	ASN

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Mol	Chain	Res	Type
35	f	130	GLN
37	i	130	HIS
39	k	106	ASN
39	k	133	GLN
41	m	31	HIS
41	m	62	ASN
49	u	134	ASN
51	w	48	ASN
54	z	12	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	9/22 (40%)	4 (44%)	0
30	a	2891/3086 (93%)	518 (17%)	0
31	b	117/120 (97%)	11 (9%)	0
6	A	1503/1537 (97%)	253 (16%)	17 (1%)
8	C	75/77 (97%)	13 (17%)	1 (1%)
All	All	4595/4842 (94%)	799 (17%)	18 (0%)

All (799) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A
6	A	9	U
6	A	10	G
6	A	13	G
6	A	36	A
6	A	43	G
6	A	51	C
6	A	52	U
6	A	55	A
6	A	58	C
6	A	74	A
6	A	82	U
6	A	91	G
6	A	92	G
6	A	93	G
6	A	96	G
6	A	98	U
6	A	119	A

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Mol	Chain	Res	Type
6	A	120	A
6	A	121	C
6	A	130	A
6	A	143	C
6	A	164	C
6	A	173	A
6	A	174	U
6	A	178	G
6	A	183	G
6	A	184	G
6	A	185	A
6	A	192	G
6	A	204	G
6	A	205	G
6	A	213	A
6	A	214	G
6	A	218	C
6	A	222	G
6	A	226	G
6	A	233	G
6	A	242	C
6	A	247	C
6	A	249	G
6	A	253	G
6	A	268	G
6	A	269	C
6	A	291	G
6	A	308	A
6	A	323	A
6	A	331	A
6	A	332	C
6	A	349	G
6	A	354	C
6	A	356	G
6	A	358	A
6	A	369	U
6	A	374	C
6	A	390	G
6	A	399	A
6	A	408	G
6	A	414	U
6	A	415	G

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Mol	Chain	Res	Type
6	A	416	A
6	A	417	C
6	A	420	C
6	A	423	U
6	A	424	C
6	A	425	G
6	A	426	G
6	A	431	U
6	A	441	U
6	A	453	A
6	A	455	G
6	A	461	G
6	A	463	G
6	A	466	G
6	A	467	G
6	A	468	U
6	A	474	G
6	A	476	A
6	A	477	A
6	A	478	A
6	A	491	A
6	A	492	A
6	A	493	C
6	A	499	G
6	A	500	C
6	A	503	G
6	A	509	G7M
6	A	513	U
6	A	514	G
6	A	515	A
6	A	529	A
6	A	546	U
6	A	554	A
6	A	555	A
6	A	558	G
6	A	559	G
6	A	578	C
6	A	600	C
6	A	614	U
6	A	615	G
6	A	635	U
6	A	647	G

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Mol	Chain	Res	Type
6	A	703	A
6	A	704	G
6	A	716	G
6	A	729	U
6	A	730	U
6	A	737	G
6	A	759	A
6	A	774	A
6	A	775	U
6	A	776	A
6	A	791	G
6	A	797	A
6	A	799	C
6	A	803	G
6	A	825	U
6	A	826	C
6	A	827	C
6	A	828	A
6	A	831	G
6	A	832	G
6	A	837	G
6	A	874	G
6	A	898	A
6	A	900	G
6	A	910	G
6	A	911	G
6	A	918	C
6	A	919	A
6	A	944	U
6	A	945	U
6	A	950	2MG
6	A	952	A
6	A	953	A
6	A	955	G
6	A	956	C
6	A	959	A
6	A	960	G
6	A	961	A
6	A	975	U
6	A	976	U
6	A	977	G
6	A	978	A

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Mol	Chain	Res	Type
6	A	984	A
6	A	987	G
6	A	988	G
6	A	989	G
6	A	990	A
6	A	992	U
6	A	993	G
6	A	994	C
6	A	1003	G
6	A	1004	G
6	A	1009	G
6	A	1010	C
6	A	1012	U
6	A	1015	U
6	A	1021	G
6	A	1025	G
6	A	1026	U
6	A	1027	U
6	A	1029	A
6	A	1030	C
6	A	1031	A
6	A	1038	G
6	A	1040	A
6	A	1041	U
6	A	1050	U
6	A	1051	C
6	A	1053	G
6	A	1055	U
6	A	1066	G
6	A	1070	U
6	A	1079	G
6	A	1080	U
6	A	1086	A
6	A	1088	C
6	A	1110	U
6	A	1111	U
6	A	1121	U
6	A	1122	U
6	A	1125	G
6	A	1126	G
6	A	1131	G
6	A	1132	A

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Mol	Chain	Res	Type
6	A	1138	U
6	A	1140	G
6	A	1145	C
6	A	1146	G
6	A	1153	U
6	A	1162	A
6	A	1168	G
6	A	1170	G
6	A	1182	A
6	A	1183	A
6	A	1188	U
6	A	1192	G
6	A	1198	U
6	A	1199	A
6	A	1200	U
6	A	1210	U
6	A	1213	A
6	A	1224	A
6	A	1227	G
6	A	1237	G
6	A	1242	U
6	A	1244	G
6	A	1246	G
6	A	1256	G
6	A	1261	A
6	A	1266	A
6	A	1272	G
6	A	1273	A
6	A	1274	A
6	A	1278	C
6	A	1285	A
6	A	1286	G
6	A	1291	G
6	A	1298	G
6	A	1303	C
6	A	1306	C
6	A	1326	G
6	A	1332	A
6	A	1333	G
6	A	1339	G
6	A	1351	C
6	A	1368	U

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Mol	Chain	Res	Type
6	A	1382	C
6	A	1385	A
6	A	1401	U
6	A	1406	G
6	A	1415	A
6	A	1429	G
6	A	1433	A
6	A	1437	G
6	A	1438	U
6	A	1439	U
6	A	1440	G
6	A	1474	G
6	A	1479	A
6	A	1480	A
6	A	1481	G
6	A	1484	G
6	A	1493	U
6	A	1504	G
6	A	1506	MA6
6	A	1516	G
6	A	1517	G
6	A	1518	A
6	A	1519	U
6	A	1520	C
6	A	1521	A
8	C	6	G
8	C	9	G
8	C	16	C
8	C	17	C
8	C	17(A)	U
8	C	18	G
8	C	19	G
8	C	20	U
8	C	21	A
8	C	47	U
8	C	48	C
8	C	69	C
8	C	76	A
29	Y	19	U
29	Y	20	U
29	Y	21	U
29	Y	22	U

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Mol	Chain	Res	Type
30	a	11	G
30	a	12	U
30	a	32	U
30	a	34	G
30	a	42	G
30	a	44	G
30	a	50	G
30	a	62	G
30	a	70	A
30	a	73	A
30	a	74	G
30	a	82	G
30	a	91	A
30	a	92	G
30	a	93	C
30	a	99	G
30	a	101	G
30	a	117	A
30	a	118	A
30	a	119	U
30	a	132	A
30	a	133	A
30	a	135	G
30	a	136	U
30	a	147	G
30	a	166	A
30	a	169	G
30	a	171	A
30	a	180	U
30	a	185	G
30	a	188	A
30	a	203	A
30	a	206	A
30	a	222	G
30	a	223	A
30	a	229	A
30	a	230	A
30	a	235	G
30	a	236	U
30	a	237	G
30	a	240	A
30	a	255	G

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Mol	Chain	Res	Type
30	a	272	A
30	a	273	G
30	a	275	C
30	a	276	U
30	a	279	A
30	a	283	U
30	a	284	G
30	a	285	U
30	a	286	G
30	a	287	U
30	a	288	G
30	a	290	G
30	a	307	U
30	a	308	U
30	a	309	G
30	a	310	C
30	a	312	U
30	a	313	G
30	a	314	U
30	a	318	G
30	a	322	U
30	a	324	U
30	a	325	G
30	a	332	U
30	a	337	G
30	a	338	U
30	a	339	U
30	a	345	G
30	a	346	C
30	a	347	C
30	a	348	G
30	a	353	A
30	a	354	U
30	a	356	G
30	a	357	G
30	a	358	C
30	a	359	C
30	a	360	A
30	a	362	U
30	a	366	A
30	a	367	A
30	a	369	U

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Mol	Chain	Res	Type
30	a	370	G
30	a	373	G
30	a	375	G
30	a	377	G
30	a	378	A
30	a	379	A
30	a	380	G
30	a	387	C
30	a	389	U
30	a	393	G
30	a	396	A
30	a	402	A
30	a	408	G
30	a	415	A
30	a	419	U
30	a	423	G
30	a	431	A
30	a	433	G
30	a	434	C
30	a	435	G
30	a	445	U
30	a	447	U
30	a	451	G
30	a	454	G
30	a	455	C
30	a	460	A
30	a	475	G
30	a	476	U
30	a	477	G
30	a	478	G
30	a	480	A
30	a	494	U
30	a	500	G
30	a	501	A
30	a	516	U
30	a	532	A
30	a	533	C
30	a	535	G
30	a	536	A
30	a	537	U
30	a	540	U
30	a	544	U

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Mol	Chain	Res	Type
30	a	545	G
30	a	546	A
30	a	569	A
30	a	570	G
30	a	589	A
30	a	592	G
30	a	593	A
30	a	596	U
30	a	618	G
30	a	619	C
30	a	620	C
30	a	621	G
30	a	631	G
30	a	632	U
30	a	633	G
30	a	634	U
30	a	635	G
30	a	646	G
30	a	656	G
30	a	657	A
30	a	658	A
30	a	674	G
30	a	675	U
30	a	676	G
30	a	687	A
30	a	698	U
30	a	699	G
30	a	700	G
30	a	701	U
30	a	704	G
30	a	713	A
30	a	720	G
30	a	723	A
30	a	731	A
30	a	734	G
30	a	739	G
30	a	740	A
30	a	741	G
30	a	770	A
30	a	771	U
30	a	794	G
30	a	797	G

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Mol	Chain	Res	Type
30	a	802	G
30	a	815	U
30	a	832	U
30	a	849	A
30	a	860	G
30	a	861	G
30	a	867	A
30	a	869	G
30	a	870	G
30	a	875	U
30	a	877	A
30	a	890	G
30	a	897	C
30	a	912	U
30	a	930	G
30	a	931	G
30	a	944	G
30	a	951	A
30	a	966	G
30	a	968	G
30	a	969	C
30	a	970	U
30	a	971	U
30	a	973	U
30	a	974	C
30	a	979	U
30	a	981	C
30	a	994	A
30	a	1014	G
30	a	1015	U
30	a	1028	A
30	a	1029	G
30	a	1042	A
30	a	1044	G
30	a	1057	G
30	a	1063	A
30	a	1066	A
30	a	1079	A
30	a	1096	G
30	a	1105	G
30	a	1109	G
30	a	1116	U

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Mol	Chain	Res	Type
30	a	1120	G
30	a	1124	U
30	a	1128	U
30	a	1129	A
30	a	1130	G
30	a	1135	C
30	a	1137	A
30	a	1140	A
30	a	1141	G
30	a	1144	U
30	a	1145	G
30	a	1149	U
30	a	1150	G
30	a	1153	A
30	a	1154	G
30	a	1156	A
30	a	1157	G
30	a	1159	C
30	a	1161	U
30	a	1162	C
30	a	1163	C
30	a	1164	U
30	a	1165	U
30	a	1171	A
30	a	1178	A
30	a	1179	A
30	a	1181	A
30	a	1183	C
30	a	1188	U
30	a	1191	U
30	a	1194	A
30	a	1195	G
30	a	1196	U
30	a	1211	A
30	a	1215	U
30	a	1216	A
30	a	1218	C
30	a	1225	U
30	a	1227	A
30	a	1254	G
30	a	1255	U
30	a	1256	G

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Mol	Chain	Res	Type
30	a	1257	U
30	a	1283	G
30	a	1297	G
30	a	1306	U
30	a	1307	G
30	a	1327	G
30	a	1333	G
30	a	1348	G
30	a	1351	U
30	a	1376	A
30	a	1377	U
30	a	1388	U
30	a	1397	C
30	a	1405	U
30	a	1417	G
30	a	1420	U
30	a	1426	C
30	a	1428	U
30	a	1441	A
30	a	1455	U
30	a	1460	A
30	a	1471	A
30	a	1472	U
30	a	1493	G
30	a	1601	G
30	a	1607	A
30	a	1608	C
30	a	1625	U
30	a	1626	C
30	a	1630	G
30	a	1633	G
30	a	1639	U
30	a	1641	U
30	a	1642	C
30	a	1663	G
30	a	1667	G
30	a	1673	U
30	a	1674	A
30	a	1685	G
30	a	1688	U
30	a	1690	A
30	a	1691	A

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Mol	Chain	Res	Type
30	a	1692	G
30	a	1695	U
30	a	1697	A
30	a	1706	G
30	a	1710	A
30	a	1713	C
30	a	1714	C
30	a	1717	G
30	a	1718	G
30	a	1719	U
30	a	1720	U
30	a	1721	G
30	a	1724	G
30	a	1725	G
30	a	1726	U
30	a	1727	G
30	a	1737	U
30	a	1743	A
30	a	1749	G
30	a	1752	A
30	a	1761	G
30	a	1763	G
30	a	1769	G
30	a	1791	U
30	a	1792	A
30	a	1794	A
30	a	1818	U
30	a	1830	A
30	a	1832	C
30	a	1837	G
30	a	1838	A
30	a	1858	G
30	a	1897	G
30	a	1904	U
30	a	1905	G
30	a	1906	C
30	a	1908	C
30	a	1911	G
30	a	1912	U
30	a	1913	G
30	a	1914	C
30	a	1915	G

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Mol	Chain	Res	Type
30	a	1916	G
30	a	1919	U
30	a	1929	G
30	a	1939	G
30	a	1947	G
30	a	1956	A
30	a	1965	C
30	a	1974	A
30	a	1983	C
30	a	1984	G
30	a	1985	A
30	a	1999	U
30	a	2012	A
30	a	2031	A
30	a	2041	G
30	a	2042	A
30	a	2052	G
30	a	2053	U
30	a	2054	A
30	a	2055	U
30	a	2066	G
30	a	2067	A
30	a	2068	A
30	a	2069	C
30	a	2089	G
30	a	2096	A
30	a	2097	C
30	a	2098	3TD
30	a	2101	A
30	a	2103	C
30	a	2112	G
30	a	2113	G
30	a	2120	A
30	a	2121	A
30	a	2124	C
30	a	2138	U
30	a	2150	C
30	a	2153	A
30	a	2154	U
30	a	2155	G
30	a	2174	U
30	a	2176	U

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Mol	Chain	Res	Type
30	a	2203	A
30	a	2204	U
30	a	2206	A
30	a	2210	G
30	a	2214	A
30	a	2215	G
30	a	2216	A
30	a	2222	G
30	a	2226	C
30	a	2233	C
30	a	2235	G
30	a	2238	C
30	a	2239	G
30	a	2243	A
30	a	2245	A
30	a	2246	C
30	a	2275	G
30	a	2278	G
30	a	2280	U
30	a	2282	G
30	a	2283	G
30	a	2284	G
30	a	2287	G
30	a	2288	G
30	a	2289	U
30	a	2291	U
30	a	2361	C
30	a	2364	A
30	a	2366	U
30	a	2367	G
30	a	2369	U
30	a	2381	A
30	a	2384	G
30	a	2385	U
30	a	2386	G
30	a	2393	G
30	a	2394	A
30	a	2395	U
30	a	2407	A
30	a	2420	G
30	a	2421	G
30	a	2460	A

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Mol	Chain	Res	Type
30	a	2461	G
30	a	2464	G
30	a	2465	C
30	a	2469	A
30	a	2470	A
30	a	2487	U
30	a	2489	G
30	a	2490	G
30	a	2493	A
30	a	2501	G
30	a	2502	U
30	a	2503	G
30	a	2509	A
30	a	2517	A
30	a	2518	A
30	a	2529	C
30	a	2532	U
30	a	2536	A
30	a	2543	G
30	a	2565	G
30	a	2567	A
30	a	2585	G
30	a	2588	U
30	a	2607	A
30	a	2608	A
30	a	2611	G
30	a	2612	A
30	a	2617	A
30	a	2623	C
30	a	2627	2MG
30	a	2630	A
30	a	2655	C
30	a	2657	C
30	a	2658	A
30	a	2673	U
30	a	2676	G
30	a	2680	OMC
30	a	2684	G
30	a	2687	G
30	a	2688	U
30	a	2700	A
30	a	2702	C

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Mol	Chain	Res	Type
30	a	2712	G
30	a	2717	G
30	a	2721	C
30	a	2722	C
30	a	2748	A
30	a	2749	G
30	a	2763	G
30	a	2764	G
30	a	2767	U
30	a	2784	A
30	a	2791	U
30	a	2792	C
30	a	2795	U
30	a	2796	A
30	a	2811	A
30	a	2828	C
30	a	2836	A
30	a	2845	G
30	a	2852	G
30	a	2870	G
30	a	2872	G
30	a	2873	C
30	a	2896	G
30	a	2908	C
30	a	2914	G
30	a	2915	U
30	a	2926	G
30	a	2930	A
30	a	2939	A
30	a	2948	G
30	a	2960	A
30	a	2962	A
30	a	2963	A
30	a	2971	C
30	a	2972	A
30	a	2973	C
30	a	2978	G
30	a	2979	U
30	a	2981	U
30	a	2982	U
30	a	2983	C
30	a	2988	U

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Mol	Chain	Res	Type
30	a	3013	U
30	a	3014	G
30	a	3015	A
30	a	3041	G
30	a	3047	G
30	a	3052	G
30	a	3053	A
30	a	3063	A
30	a	3064	U
30	a	3066	G
30	a	3071	A
30	a	3073	G
30	a	3074	A
30	a	3075	C
31	b	34	G
31	b	35	U
31	b	45	A
31	b	52	U
31	b	56	U
31	b	84	C
31	b	91	U
31	b	100	A
31	b	109	C
31	b	110	G
31	b	119	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	9	U
6	A	90	U
6	A	418	G
6	A	467	G
6	A	869	G
6	A	1009	G
6	A	1050	U
6	A	1052	A
6	A	1130	G
6	A	1131	G
6	A	1187	A
6	A	1271	G
6	A	1350	A

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Mol	Chain	Res	Type
6	A	1384	C
6	A	1479	A
6	A	1480	A
6	A	1520	C
8	C	17(A)	U

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

34 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
6	5MC	A	951	6	19,22,23	4.50	8 (42%)	26,32,35	0.99	1 (3%)
30	5MC	a	2145	30	19,22,23	4.36	8 (42%)	26,32,35	1.08	2 (7%)
30	PSU	a	2786	30	18,21,22	0.91	1 (5%)	21,30,33	0.77	0
30	5MU	a	2122	30	19,22,23	0.30	0	27,32,35	0.41	0
6	5MC	A	1387	6	19,22,23	4.48	8 (42%)	26,32,35	1.07	1 (3%)
30	PSU	a	2094	30	18,21,22	0.92	1 (5%)	21,30,33	0.67	0
30	PSU	a	2762	30	18,21,22	0.95	1 (5%)	21,30,33	0.90	1 (4%)
8	5MU	C	54	8	19,22,23	0.25	0	27,32,35	0.42	0
6	G7M	A	509	6	23,26,27	2.61	9 (39%)	34,39,42	1.72	7 (20%)
6	4OC	A	1389	6	20,23,24	3.10	8 (40%)	25,32,35	0.92	1 (4%)
6	2MG	A	950	6	23,26,27	3.12	8 (34%)	33,38,41	2.51	12 (36%)
30	3TD	a	2098	30	19,22,23	4.13	7 (36%)	23,32,35	1.86	5 (21%)
30	PSU	a	2686	30	18,21,22	0.92	1 (5%)	21,30,33	0.74	0
30	2MA	a	2685	30,56	22,25,26	0.85	1 (4%)	32,37,40	1.20	5 (15%)
6	PSU	A	498	56,6	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
8	PSU	C	55	8	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
6	5MC	A	1394	6	19,22,23	4.37	8 (42%)	26,32,35	1.03	2 (7%)
30	PSU	a	2787	30	18,21,22	0.94	1 (5%)	21,30,33	0.77	0
6	UR3	A	1485	6	19,22,23	2.70	8 (42%)	26,32,35	1.63	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	2MG	A	1503	6	23,26,27	3.05	8 (34%)	33,38,41	2.62	12 (36%)
30	PSU	a	2639	30	18,21,22	0.92	1 (5%)	21,30,33	0.74	0
30	2MG	a	2627	30	23,26,27	3.03	8 (34%)	33,38,41	2.46	12 (36%)
6	5MC	A	1391	6	19,22,23	4.40	8 (42%)	26,32,35	0.96	2 (7%)
30	2MG	a	2018	30	23,26,27	3.04	8 (34%)	33,38,41	2.62	12 (36%)
8	4SU	C	8	8	18,21,22	3.75	7 (38%)	25,30,33	2.31	4 (16%)
30	OMU	a	2734	30	19,22,23	2.90	6 (31%)	25,31,34	1.89	5 (20%)
30	PSU	a	2100	30	18,21,22	0.90	1 (5%)	21,30,33	0.66	0
30	PSU	a	1038	30	18,21,22	0.91	1 (5%)	21,30,33	0.88	0
30	OMC	a	2680	30,56	19,22,23	3.16	8 (42%)	25,31,34	0.89	0
30	H2U	a	2631	30	18,21,22	3.06	5 (27%)	19,30,33	1.49	4 (21%)
6	MA6	A	1506	6	23,26,27	1.41	4 (17%)	33,38,41	3.15	13 (39%)
30	OMG	a	2433	30,8	23,26,27	2.53	9 (39%)	32,38,41	2.41	11 (34%)
8	5MC	C	32	8	19,22,23	4.42	8 (42%)	26,32,35	1.01	1 (3%)
6	MA6	A	1505	6	23,26,27	1.38	4 (17%)	33,38,41	3.02	12 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MC	A	951	6	-	0/7/25/26	0/2/2/2
30	5MC	a	2145	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2786	30	-	0/7/25/26	0/2/2/2
30	5MU	a	2122	30	-	0/7/25/26	0/2/2/2
6	5MC	A	1387	6	-	2/7/25/26	0/2/2/2
30	PSU	a	2094	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2762	30	-	0/7/25/26	0/2/2/2
8	5MU	C	54	8	-	0/7/25/26	0/2/2/2
6	G7M	A	509	6	-	3/7/25/26	0/3/3/3
6	4OC	A	1389	6	-	1/9/29/30	0/2/2/2
6	2MG	A	950	6	-	0/9/27/28	0/3/3/3
30	3TD	a	2098	30	-	2/7/25/26	0/2/2/2
30	PSU	a	2686	30	-	1/7/25/26	0/2/2/2
30	2MA	a	2685	30,56	-	1/7/25/26	0/3/3/3
6	PSU	A	498	56,6	-	0/7/25/26	0/2/2/2
8	PSU	C	55	8	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5MC	A	1394	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2787	30	-	0/7/25/26	0/2/2/2
6	UR3	A	1485	6	-	0/7/25/26	0/2/2/2
6	2MG	A	1503	6	-	0/9/27/28	0/3/3/3
30	PSU	a	2639	30	-	0/7/25/26	0/2/2/2
30	2MG	a	2627	30	-	2/9/27/28	0/3/3/3
6	5MC	A	1391	6	-	0/7/25/26	0/2/2/2
30	2MG	a	2018	30	-	2/9/27/28	0/3/3/3
8	4SU	C	8	8	-	0/7/25/26	0/2/2/2
30	OMU	a	2734	30	-	0/9/27/28	0/2/2/2
30	PSU	a	2100	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1038	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2680	30,56	-	0/9/27/28	0/2/2/2
30	H2U	a	2631	30	-	0/7/38/39	0/2/2/2
6	MA6	A	1506	6	-	2/11/29/30	0/3/3/3
30	OMG	a	2433	30,8	-	1/9/27/28	0/3/3/3
8	5MC	C	32	8	-	0/7/25/26	0/2/2/2
6	MA6	A	1505	6	-	0/11/29/30	0/3/3/3

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2098	3TD	C6-C5	12.83	1.49	1.35
6	A	951	5MC	C6-C5	9.70	1.50	1.34
6	A	1387	5MC	C6-C5	9.61	1.50	1.34
6	A	1394	5MC	C6-C5	9.53	1.50	1.34
8	C	32	5MC	C6-C5	9.53	1.50	1.34
6	A	951	5MC	C5-C4	9.43	1.51	1.44
6	A	1391	5MC	C6-C5	9.39	1.49	1.34
30	a	2631	H2U	C2-N1	9.37	1.48	1.35
30	a	2145	5MC	C6-C5	9.36	1.49	1.34
6	A	1387	5MC	C5-C4	9.26	1.51	1.44
30	a	2098	3TD	C2-N1	9.09	1.48	1.37
6	A	1391	5MC	C5-C4	9.01	1.50	1.44
8	C	32	5MC	C5-C4	8.96	1.50	1.44
30	a	2145	5MC	C5-C4	8.96	1.50	1.44
6	A	1394	5MC	C5-C4	8.80	1.50	1.44
6	A	950	2MG	C2-N3	8.12	1.47	1.32
30	a	2627	2MG	C2-N3	7.89	1.47	1.32
6	A	1503	2MG	C2-N3	7.86	1.47	1.32
30	a	2018	2MG	C2-N3	7.82	1.46	1.32
6	A	951	5MC	C4-N3	7.61	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1387	5MC	C4-N3	7.54	1.46	1.34
8	C	32	5MC	C4-N3	7.54	1.46	1.34
30	a	2145	5MC	C4-N3	7.43	1.46	1.34
6	A	1391	5MC	C4-N3	7.41	1.46	1.34
6	A	1394	5MC	C4-N3	7.35	1.45	1.34
8	C	8	4SU	C2-N3	7.26	1.50	1.38
8	C	8	4SU	C2-N1	7.23	1.49	1.38
6	A	950	2MG	C4-N3	7.12	1.50	1.34
8	C	32	5MC	C2-N3	7.11	1.50	1.36
30	a	2018	2MG	C4-N3	7.08	1.50	1.34
6	A	1389	4OC	C4-N3	7.07	1.44	1.32
6	A	1485	UR3	C2-N1	7.05	1.48	1.38
6	A	1387	5MC	C2-N3	7.02	1.50	1.36
6	A	951	5MC	C2-N3	7.01	1.50	1.36
6	A	1391	5MC	C2-N3	7.00	1.50	1.36
30	a	2145	5MC	C2-N3	6.95	1.50	1.36
30	a	2627	2MG	C4-N3	6.95	1.50	1.34
30	a	2734	OMU	C2-N1	6.91	1.49	1.38
6	A	1503	2MG	C4-N3	6.90	1.50	1.34
6	A	1394	5MC	C2-N3	6.89	1.50	1.36
30	a	2680	OMC	C2-N3	6.81	1.49	1.36
6	A	950	2MG	C2-N2	6.79	1.47	1.33
8	C	8	4SU	C4-N3	6.78	1.44	1.37
30	a	2433	OMG	C4-N3	6.62	1.49	1.34
30	a	2018	2MG	C2-N2	6.59	1.47	1.33
30	a	2734	OMU	C2-N3	6.57	1.49	1.38
6	A	1503	2MG	C2-N2	6.51	1.47	1.33
6	A	509	G7M	C4-N3	6.48	1.49	1.34
30	a	2631	H2U	C2-N3	6.38	1.49	1.38
30	a	2627	2MG	C2-N2	6.37	1.46	1.33
6	A	1389	4OC	C6-C5	6.15	1.49	1.35
6	A	1389	4OC	C2-N3	6.04	1.48	1.36
6	A	1485	UR3	C6-C5	6.02	1.49	1.35
8	C	8	4SU	C5-C4	6.01	1.49	1.42
30	a	2680	OMC	C6-C5	5.82	1.48	1.35
30	a	2098	3TD	C6-N1	5.80	1.45	1.36
6	A	951	5MC	C4-N4	5.79	1.48	1.34
6	A	1387	5MC	C4-N4	5.78	1.48	1.34
6	A	951	5MC	C6-N1	5.76	1.47	1.38
6	A	1387	5MC	C6-N1	5.76	1.47	1.38
8	C	32	5MC	C4-N4	5.76	1.48	1.34
6	A	1394	5MC	C4-N4	5.75	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1391	5MC	C6-N1	5.74	1.47	1.38
6	A	1391	5MC	C4-N4	5.72	1.48	1.34
30	a	2145	5MC	C4-N4	5.71	1.48	1.34
30	a	2734	OMU	C6-C5	5.67	1.48	1.35
6	A	1394	5MC	C6-N1	5.62	1.47	1.38
8	C	32	5MC	C6-N1	5.59	1.47	1.38
8	C	8	4SU	C6-C5	5.56	1.48	1.35
30	a	2433	OMG	C2-N3	5.52	1.46	1.33
30	a	2145	5MC	C6-N1	5.43	1.47	1.38
6	A	509	G7M	C2-N3	5.33	1.46	1.33
30	a	2433	OMG	C2-N2	5.32	1.46	1.34
30	a	2680	OMC	C4-N3	5.27	1.44	1.34
6	A	950	2MG	C2-N1	5.21	1.45	1.36
6	A	1503	2MG	C2-N1	5.16	1.44	1.36
30	a	2018	2MG	C2-N1	4.98	1.44	1.36
8	C	8	4SU	C4-S4	-4.86	1.60	1.68
30	a	2627	2MG	C2-N1	4.85	1.44	1.36
30	a	2680	OMC	C4-N4	4.84	1.45	1.33
6	A	509	G7M	C2-N2	4.75	1.45	1.34
6	A	1387	5MC	C2-N1	4.73	1.50	1.40
30	a	2631	H2U	C4-N3	4.69	1.45	1.37
6	A	1485	UR3	C2-N3	4.69	1.48	1.39
6	A	509	G7M	C5-N7	-4.64	1.33	1.39
30	a	2098	3TD	C2-N3	4.64	1.48	1.38
6	A	1394	5MC	C2-N1	4.60	1.49	1.40
6	A	1391	5MC	C2-N1	4.52	1.49	1.40
6	A	951	5MC	C2-N1	4.51	1.49	1.40
8	C	32	5MC	C2-N1	4.49	1.49	1.40
30	a	2145	5MC	C2-N1	4.45	1.49	1.40
30	a	2680	OMC	C2-N1	4.40	1.49	1.40
30	a	2680	OMC	O2-C2	-4.34	1.15	1.23
6	A	1389	4OC	C4-N4	4.34	1.45	1.36
6	A	1389	4OC	C2-N1	4.04	1.48	1.40
6	A	509	G7M	C5-C6	3.74	1.53	1.43
6	A	1389	4OC	C5-C4	3.65	1.49	1.41
8	C	55	PSU	C6-C5	3.59	1.39	1.35
30	a	2094	PSU	C6-C5	3.57	1.39	1.35
30	a	2686	PSU	C6-C5	3.57	1.39	1.35
30	a	2787	PSU	C6-C5	3.55	1.39	1.35
6	A	1506	MA6	C6-N6	3.55	1.46	1.36
30	a	2762	PSU	C6-C5	3.53	1.39	1.35
30	a	1038	PSU	C6-C5	3.53	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2639	PSU	C6-C5	3.51	1.39	1.35
6	A	498	PSU	C6-C5	3.51	1.39	1.35
30	a	2680	OMC	C6-N1	3.49	1.46	1.38
30	a	2786	PSU	C6-C5	3.49	1.39	1.35
6	A	1505	MA6	C6-N6	3.48	1.46	1.36
30	a	2100	PSU	C6-C5	3.46	1.39	1.35
30	a	2734	OMU	C4-N3	3.41	1.44	1.38
6	A	1506	MA6	C5-C4	-3.16	1.33	1.39
6	A	1389	4OC	C6-N1	3.12	1.45	1.38
30	a	2627	2MG	C5-N7	-3.08	1.32	1.39
6	A	1505	MA6	C5-C4	-3.01	1.33	1.39
30	a	2734	OMU	O2-C2	-2.99	1.17	1.23
30	a	2433	OMG	O6-C6	-2.97	1.17	1.23
6	A	1389	4OC	O2-C2	-2.95	1.18	1.23
6	A	1485	UR3	C6-N1	2.88	1.45	1.38
30	a	2018	2MG	C5-N7	-2.88	1.33	1.39
6	A	1503	2MG	C5-C6	2.82	1.54	1.44
6	A	950	2MG	C5-C6	2.79	1.54	1.44
30	a	2734	OMU	O4-C4	-2.79	1.19	1.24
30	a	2433	OMG	C2-N1	2.78	1.44	1.37
30	a	2018	2MG	C5-C6	2.77	1.54	1.44
6	A	1503	2MG	C5-N7	-2.73	1.33	1.39
6	A	950	2MG	C5-N7	-2.73	1.33	1.39
6	A	1506	MA6	C5-N7	-2.71	1.34	1.39
6	A	509	G7M	C2-N1	2.70	1.44	1.37
30	a	2627	2MG	C5-C6	2.69	1.54	1.44
8	C	8	4SU	C6-N1	2.68	1.44	1.38
30	a	2433	OMG	C5-C6	2.67	1.54	1.44
6	A	509	G7M	O6-C6	-2.64	1.18	1.23
30	a	2631	H2U	O2-C2	-2.63	1.18	1.23
30	a	2627	2MG	O6-C6	-2.63	1.18	1.23
6	A	1505	MA6	C5-N7	-2.60	1.34	1.39
30	a	2098	3TD	C4-N3	2.59	1.45	1.40
6	A	1391	5MC	O2-C2	-2.55	1.19	1.23
6	A	950	2MG	C6-N1	2.55	1.43	1.38
6	A	1394	5MC	O2-C2	-2.51	1.19	1.23
30	a	2018	2MG	O6-C6	-2.51	1.18	1.23
8	C	32	5MC	O2-C2	-2.49	1.19	1.23
30	a	2145	5MC	O2-C2	-2.49	1.19	1.23
6	A	1503	2MG	O6-C6	-2.48	1.18	1.23
6	A	1387	5MC	O2-C2	-2.46	1.19	1.23
6	A	1503	2MG	C6-N1	2.46	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2018	2MG	C6-N1	2.45	1.43	1.38
30	a	2680	OMC	C5-C4	2.45	1.48	1.42
6	A	951	5MC	O2-C2	-2.43	1.19	1.23
30	a	2685	2MA	C6-N6	-2.42	1.28	1.34
30	a	2433	OMG	C5-N7	-2.41	1.34	1.39
6	A	950	2MG	O6-C6	-2.41	1.19	1.23
30	a	2433	OMG	C6-N1	2.37	1.43	1.38
6	A	1485	UR3	O4-C4	-2.34	1.18	1.23
30	a	2631	H2U	O4-C4	-2.33	1.18	1.23
6	A	509	G7M	C6-N1	2.29	1.43	1.38
6	A	1485	UR3	C4-N3	2.28	1.45	1.40
6	A	1505	MA6	C8-N9	-2.27	1.33	1.37
6	A	1485	UR3	O2-C2	-2.25	1.18	1.22
6	A	1506	MA6	C8-N9	-2.24	1.33	1.37
6	A	1485	UR3	C5-C4	2.19	1.49	1.43
30	a	2098	3TD	O4-C4	-2.18	1.18	1.23
6	A	509	G7M	C4-N9	-2.17	1.32	1.38
30	a	2627	2MG	C6-N1	2.15	1.42	1.38
30	a	2098	3TD	O2-C2	-2.06	1.19	1.23
30	a	2433	OMG	C4-N9	-2.03	1.32	1.38

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1506	MA6	N1-C6-N6	-11.15	103.27	116.86
6	A	1505	MA6	N1-C6-N6	-10.56	103.99	116.86
8	C	8	4SU	C4-N3-C2	-7.90	119.74	127.31
30	a	2018	2MG	C2-N3-C4	7.36	121.21	112.00
6	A	1506	MA6	C5-C6-N6	7.19	136.72	125.33
30	a	2433	OMG	C1'-N9-C8	-6.79	107.45	126.73
6	A	1505	MA6	C5-C6-N6	6.61	135.79	125.33
6	A	1503	2MG	C2-N3-C4	6.44	120.06	112.00
6	A	950	2MG	C2-N3-C4	6.29	119.87	112.00
30	a	2627	2MG	C2-N3-C4	6.21	119.77	112.00
30	a	2018	2MG	C5-C4-N3	-6.19	118.53	128.39
30	a	2734	OMU	C4-N3-C2	-5.91	119.28	126.61
30	a	2098	3TD	N1-C2-N3	5.85	120.39	116.13
6	A	1485	UR3	C4-N3-C2	-5.83	119.89	124.58
6	A	1505	MA6	N1-C2-N3	-5.79	119.82	128.58
6	A	950	2MG	C1'-N9-C4	-5.79	109.39	126.49
6	A	1506	MA6	N1-C2-N3	-5.68	119.98	128.58
6	A	1503	2MG	C1'-N9-C4	-5.67	109.73	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2627	2MG	C5-C4-N3	-5.56	119.54	128.39
6	A	1503	2MG	C1'-N9-C8	5.52	142.41	126.73
6	A	950	2MG	C1'-N9-C8	5.50	142.36	126.73
30	a	2433	OMG	C1'-N9-C4	5.47	142.64	126.49
8	C	8	4SU	C5-C4-N3	5.39	119.77	114.75
6	A	1503	2MG	C5-C4-N3	-5.27	120.00	128.39
6	A	950	2MG	C5-C4-N3	-5.11	120.27	128.39
30	a	2627	2MG	C1'-N9-C4	-5.00	111.72	126.49
6	A	1506	MA6	C5-C4-N3	-4.92	119.95	126.72
6	A	1505	MA6	C5-C4-N3	-4.91	119.96	126.72
30	a	2018	2MG	C2-N1-C6	-4.87	118.66	124.55
30	a	2627	2MG	C1'-N9-C8	4.85	140.51	126.73
30	a	2627	2MG	C2-N1-C6	-4.67	118.90	124.55
6	A	1503	2MG	C2-N1-C6	-4.64	118.94	124.55
30	a	2433	OMG	C5-C4-N3	-4.59	121.09	128.39
6	A	509	G7M	C2-N3-C4	4.37	119.83	112.30
30	a	2433	OMG	C2-N3-C4	4.28	119.67	112.30
6	A	1506	MA6	N9-C8-N7	-4.26	107.90	113.94
30	a	2018	2MG	C1'-N9-C4	-4.23	114.00	126.49
30	a	2018	2MG	C1'-N9-C8	4.21	138.69	126.73
6	A	950	2MG	C2-N1-C6	-4.15	119.53	124.55
30	a	2734	OMU	N3-C2-N1	4.06	120.18	114.89
6	A	1505	MA6	N9-C8-N7	-4.02	108.23	113.94
30	a	2018	2MG	N1-C2-N2	4.00	120.64	116.56
6	A	509	G7M	C5-C6-N1	3.98	120.08	111.84
6	A	1503	2MG	N1-C2-N2	3.96	120.61	116.56
8	C	8	4SU	C5-C4-S4	-3.93	119.81	124.31
30	a	2098	3TD	C4-N3-C2	-3.93	120.45	124.61
30	a	2018	2MG	N9-C4-N3	3.91	133.78	125.95
6	A	1506	MA6	C4-C5-C6	3.90	119.94	115.91
8	C	8	4SU	N3-C2-N1	3.88	119.94	114.89
6	A	509	G7M	C5-C4-N3	-3.85	120.88	128.15
6	A	1505	MA6	C4-C5-C6	3.75	119.79	115.91
6	A	1485	UR3	C5-C4-N3	3.75	119.97	115.04
30	a	2734	OMU	C5-C4-N3	3.69	119.97	114.80
30	a	2433	OMG	N9-C8-N7	-3.69	106.55	113.40
30	a	2631	H2U	N3-C2-N1	3.61	120.28	116.65
6	A	1387	5MC	C5-C6-N1	-3.56	119.45	123.31
30	a	2145	5MC	C5-C6-N1	-3.53	119.48	123.31
30	a	2627	2MG	N9-C4-N3	3.42	132.78	125.95
6	A	1505	MA6	C2-N3-C4	3.42	120.17	111.83
6	A	1506	MA6	C2-N3-C4	3.40	120.12	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1505	MA6	C2-N1-C6	3.36	120.05	111.83
6	A	951	5MC	C5-C6-N1	-3.35	119.67	123.31
6	A	1506	MA6	C2-N1-C6	3.34	120.00	111.83
6	A	509	G7M	O6-C6-C5	-3.32	120.60	128.01
30	a	2685	2MA	C5-C4-N3	-3.32	123.68	127.18
6	A	509	G7M	N9-C4-N3	3.23	132.42	125.95
8	C	32	5MC	C5-C6-N1	-3.17	119.87	123.31
30	a	2734	OMU	O4-C4-C5	-3.11	119.80	125.16
30	a	2433	OMG	C2-N1-C6	-3.10	119.49	125.11
6	A	1394	5MC	C5-C6-N1	-3.07	119.98	123.31
30	a	2098	3TD	C1'-C5-C4	3.07	122.26	117.61
6	A	950	2MG	N1-C2-N2	3.05	119.67	116.56
6	A	1505	MA6	N3-C4-N9	3.05	132.35	127.17
6	A	950	2MG	N9-C4-N3	3.02	132.00	125.95
6	A	1506	MA6	C5-N7-C8	3.02	108.19	103.45
6	A	950	2MG	N9-C8-N7	-2.94	107.95	113.40
30	a	2433	OMG	N9-C4-N3	2.93	131.81	125.95
30	a	2631	H2U	C5-C6-N1	2.93	120.38	111.52
6	A	1503	2MG	N9-C4-N3	2.91	131.78	125.95
30	a	2018	2MG	C5-C6-N1	2.91	120.67	113.25
6	A	509	G7M	C2-N1-C6	-2.91	119.83	125.11
6	A	1503	2MG	N9-C8-N7	-2.89	108.03	113.40
30	a	2631	H2U	C5-C4-N3	2.81	119.68	116.69
6	A	1506	MA6	N3-C4-N9	2.80	131.93	127.17
6	A	1503	2MG	C5-C6-N1	2.78	120.32	113.25
6	A	1391	5MC	C5-C6-N1	-2.77	120.30	123.31
6	A	1503	2MG	CM2-N2-C2	-2.77	117.70	123.65
30	a	2433	OMG	C5-C6-N1	2.75	120.26	113.25
6	A	1505	MA6	C5-N7-C8	2.72	107.73	103.45
30	a	2627	2MG	N9-C8-N7	-2.71	108.37	113.40
30	a	2627	2MG	C5-C6-N1	2.71	120.15	113.25
6	A	950	2MG	C5-C6-N1	2.71	120.14	113.25
30	a	2018	2MG	O6-C6-C5	-2.69	119.42	126.53
30	a	2631	H2U	O2-C2-N1	-2.66	119.91	123.10
30	a	2685	2MA	N3-C2-N1	-2.59	121.19	125.77
30	a	2433	OMG	O6-C6-C5	-2.58	119.72	126.53
6	A	509	G7M	N9-C8-N7	-2.55	106.29	112.48
30	a	2627	2MG	N1-C2-N2	2.55	119.16	116.56
6	A	950	2MG	O6-C6-C5	-2.52	119.89	126.53
30	a	2627	2MG	O6-C6-C5	-2.47	120.01	126.53
6	A	1503	2MG	O6-C6-C5	-2.47	120.02	126.53
30	a	2685	2MA	CM2-C2-N1	2.45	120.80	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2627	2MG	CM2-N2-C2	-2.43	118.42	123.65
30	a	2018	2MG	N9-C8-N7	-2.42	108.90	113.40
6	A	1506	MA6	C4-C5-N7	-2.39	107.84	110.58
30	a	2018	2MG	CM2-N2-C2	-2.37	118.55	123.65
30	a	2762	PSU	C3'-C2'-C1'	2.37	104.48	101.69
30	a	2098	3TD	C6-C5-C4	2.35	119.77	118.19
30	a	2145	5MC	CM5-C5-C6	-2.35	119.67	122.85
30	a	2433	OMG	C8-N7-C5	2.29	108.35	104.26
30	a	2685	2MA	C2-N1-C6	2.29	121.61	118.10
30	a	2734	OMU	O2-C2-N1	-2.25	119.86	122.80
6	A	1389	4OC	C6-C5-C4	2.25	119.71	117.00
6	A	1505	MA6	C4-N9-C8	2.23	108.08	105.74
6	A	1503	2MG	C8-N7-C5	2.12	108.04	104.26
6	A	1506	MA6	C5-C4-N9	2.12	108.12	105.81
6	A	1506	MA6	C4-N9-C8	2.10	107.94	105.74
6	A	950	2MG	N1-C2-N3	-2.10	120.14	123.68
30	a	2098	3TD	O4'-C1'-C2'	2.09	108.04	105.15
30	a	2433	OMG	C8-N9-C4	2.07	109.90	106.03
6	A	950	2MG	C8-N7-C5	2.06	107.93	104.26
30	a	2018	2MG	N1-C2-N3	-2.06	120.21	123.68
6	A	1394	5MC	C5-C4-N3	-2.06	119.65	121.75
30	a	2685	2MA	N3-C4-N9	2.03	129.57	126.99
6	A	1391	5MC	CM5-C5-C6	-2.02	120.11	122.85
6	A	1505	MA6	C4-C5-N7	-2.02	108.27	110.58
30	a	2627	2MG	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1506	MA6	O4'-C4'-C5'-O5'
30	a	2098	3TD	O4'-C4'-C5'-O5'
6	A	509	G7M	C3'-C4'-C5'-O5'
30	a	2098	3TD	C3'-C4'-C5'-O5'
30	a	2627	2MG	C3'-C4'-C5'-O5'
6	A	1387	5MC	O4'-C4'-C5'-O5'
30	a	2627	2MG	O4'-C4'-C5'-O5'
6	A	509	G7M	O4'-C4'-C5'-O5'
6	A	1506	MA6	C3'-C4'-C5'-O5'
30	a	2018	2MG	O4'-C4'-C5'-O5'
30	a	2018	2MG	C3'-C4'-C5'-O5'
6	A	1387	5MC	C3'-C4'-C5'-O5'

Continued on next page...

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Mol	Chain	Res	Type	Atoms
30	a	2433	OMG	C1'-C2'-O2'-CM2
6	A	509	G7M	C4'-C5'-O5'-P
6	A	1389	4OC	O4'-C4'-C5'-O5'
30	a	2686	PSU	O4'-C4'-C5'-O5'
30	a	2685	2MA	C4'-C5'-O5'-P

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1389	4OC	1	0
6	A	950	2MG	1	0
30	a	2098	3TD	2	0
6	A	1503	2MG	2	0
30	a	2631	H2U	1	0
6	A	1506	MA6	2	0
6	A	1505	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 309 ligands modelled in this entry, 307 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	V7A	a	3145	56	37,38,38	1.09	2 (5%)	43,60,60	0.92	1 (2%)
57	V7A	A	1602	56	37,38,38	1.11	2 (5%)	43,60,60	1.02	3 (6%)

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	V7A	a	3145	56	-	8/13/72/72	0/4/4/4
57	V7A	A	1602	56	-	5/13/72/72	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A	1602	V7A	CBC-NBD	5.10	1.48	1.33
57	a	3145	V7A	CBC-NBD	5.01	1.47	1.33
57	a	3145	V7A	OAY-CAH	2.23	1.27	1.23
57	A	1602	V7A	OAY-CAH	2.12	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	1602	V7A	CAH-CAI-CAL	2.93	121.12	118.80
57	A	1602	V7A	OBA-CAM-CAL	-2.41	106.29	110.14
57	a	3145	V7A	CAM-CAP-CAQ	2.39	119.55	115.75
57	A	1602	V7A	OAZ-CAL-CAM	2.28	116.67	113.37

There are no chirality outliers.

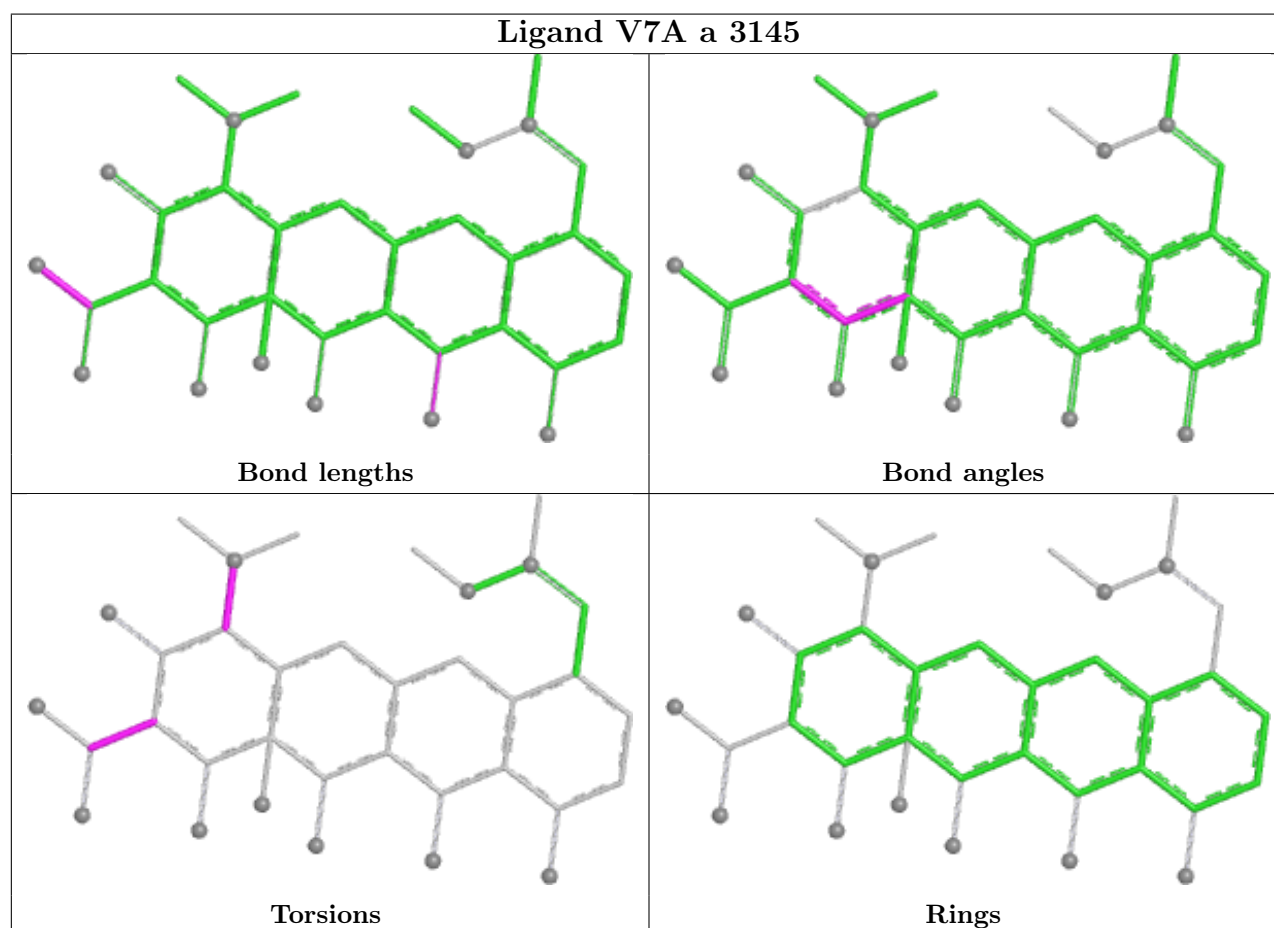
All (13) torsion outliers are listed below:

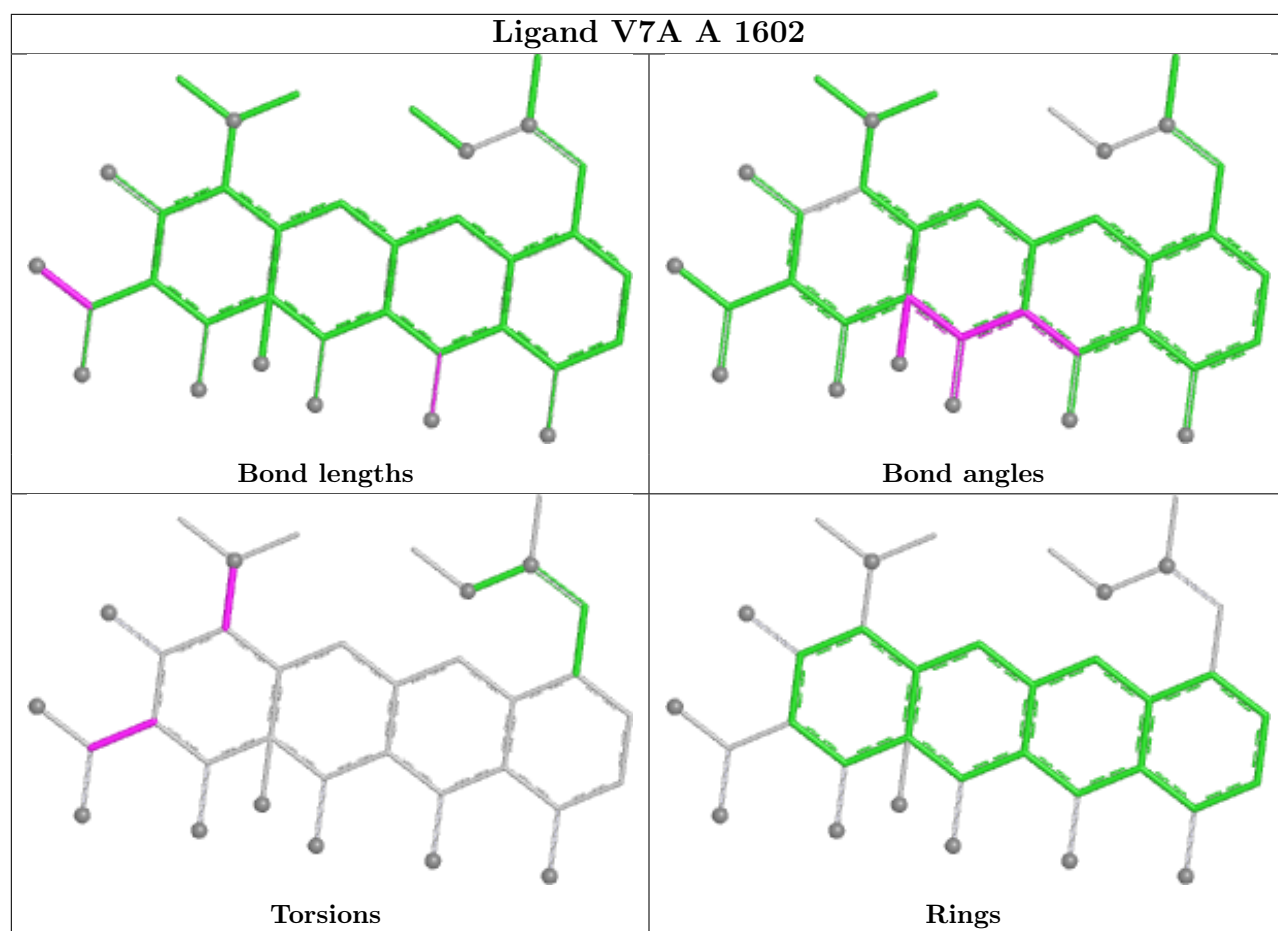
Mol	Chain	Res	Type	Atoms
57	A	1602	V7A	CAN-CAO-NBF-CBG
57	A	1602	V7A	CAP-CAQ-CBC-NBD
57	A	1602	V7A	CAP-CAQ-CBC-OBE
57	a	3145	V7A	CAR-CAO-NBF-CBG
57	a	3145	V7A	CAR-CAO-NBF-CBH
57	a	3145	V7A	CAP-CAQ-CBC-OBE
57	a	3145	V7A	CAR-CAQ-CBC-NBD
57	a	3145	V7A	CAR-CAQ-CBC-OBE
57	A	1602	V7A	CAR-CAQ-CBC-NBD
57	A	1602	V7A	CAR-CAQ-CBC-OBE
57	a	3145	V7A	CAP-CAQ-CBC-NBD
57	a	3145	V7A	CAN-CAO-NBF-CBG
57	a	3145	V7A	CAN-CAO-NBF-CBH

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

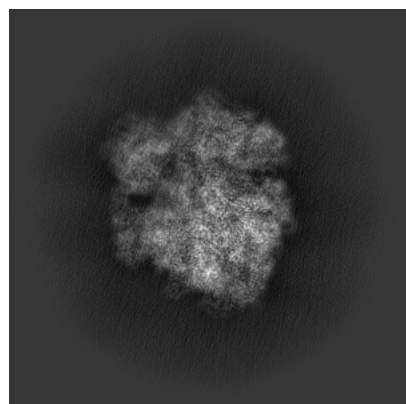
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71683. These allow visual inspection of the internal detail of the map and identification of artifacts.

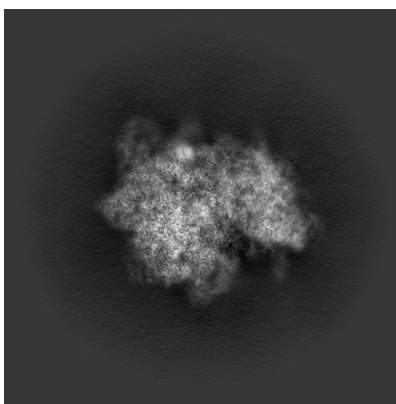
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

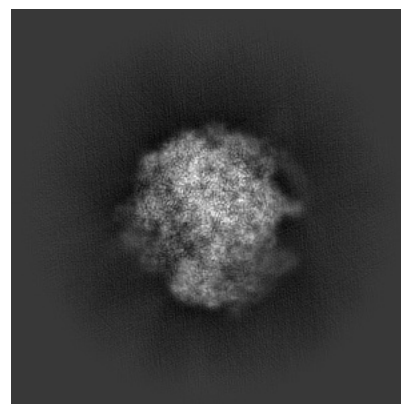
6.1.1 Primary map



X

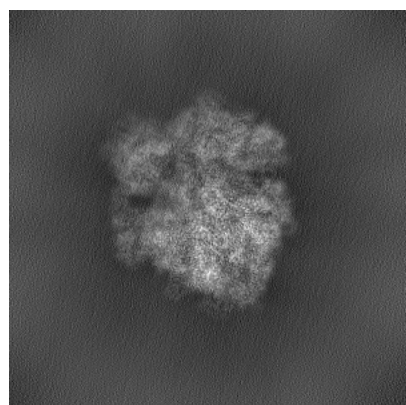


Y

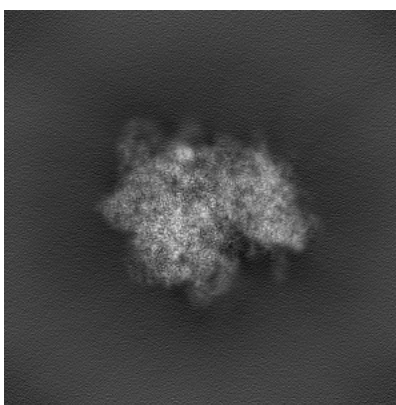


Z

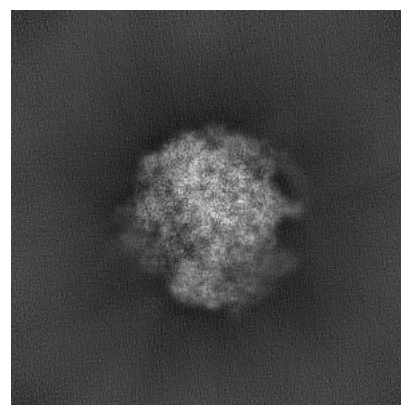
6.1.2 Raw map



X



Y

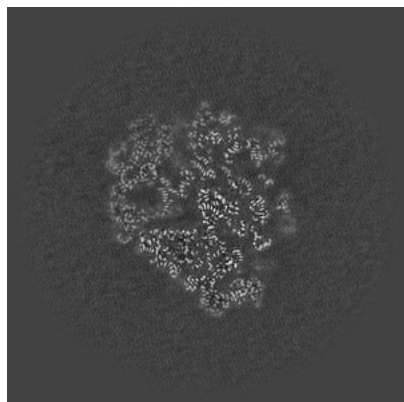


Z

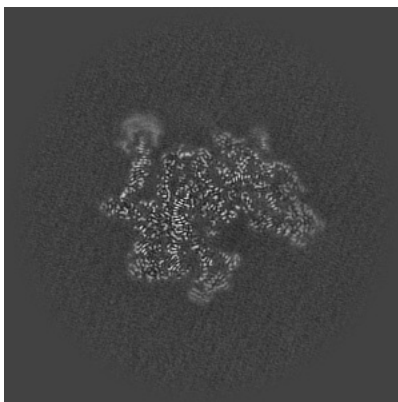
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

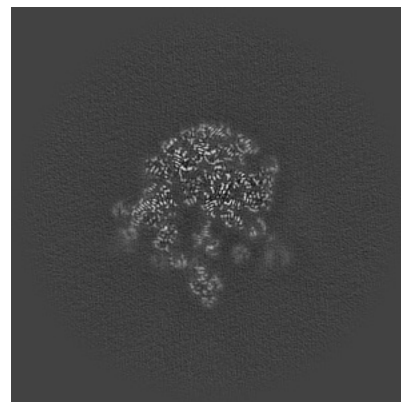
6.2.1 Primary map



X Index: 220

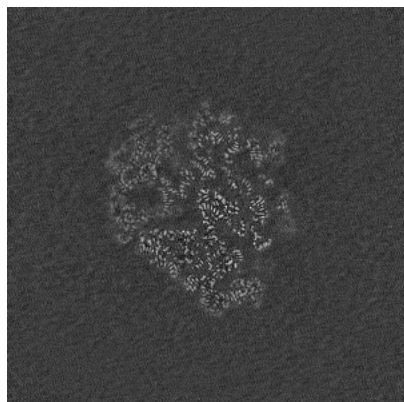


Y Index: 220

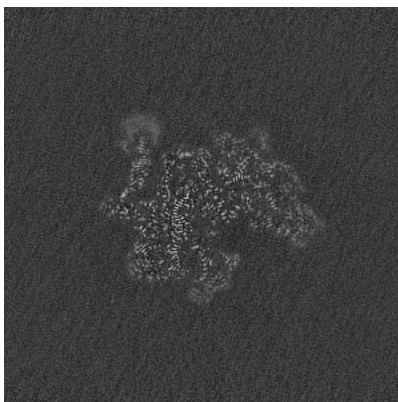


Z Index: 220

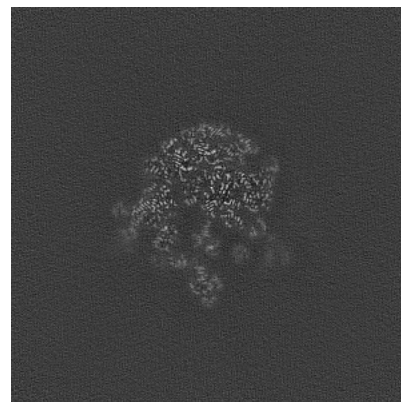
6.2.2 Raw map



X Index: 220



Y Index: 220

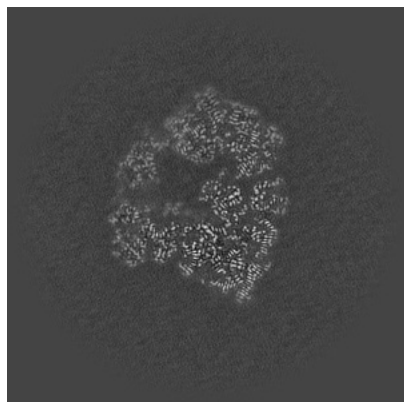


Z Index: 220

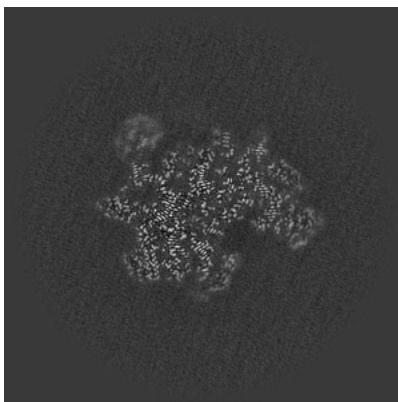
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

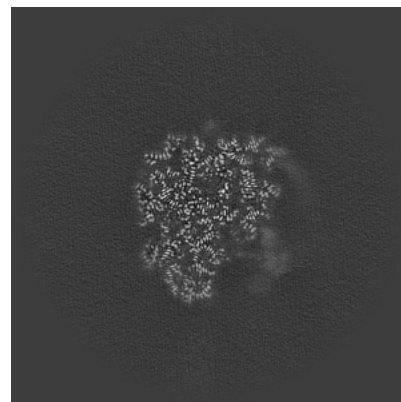
6.3.1 Primary map



X Index: 203

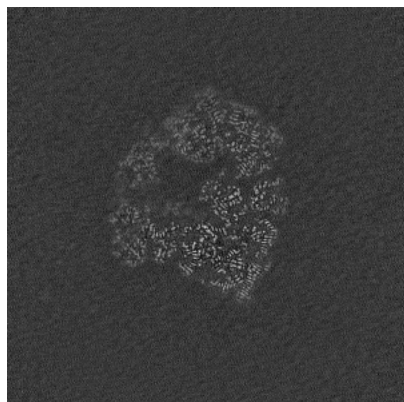


Y Index: 225

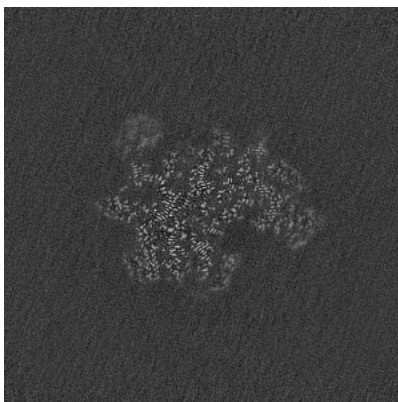


Z Index: 190

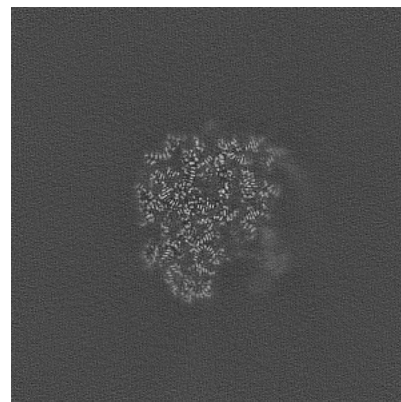
6.3.2 Raw map



X Index: 203



Y Index: 225

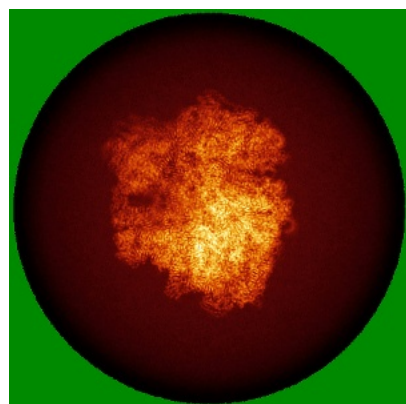


Z Index: 190

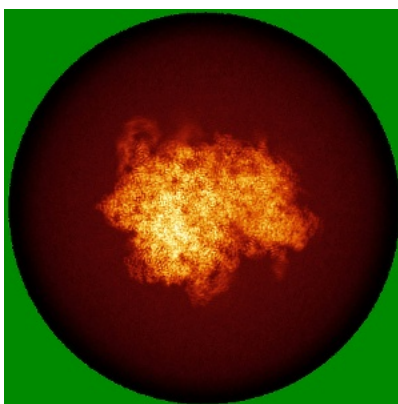
The images above show the largest variance slices of the map in three orthogonal directions.

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

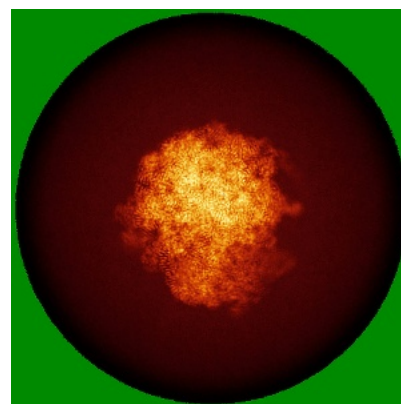
6.4.1 Primary map



X

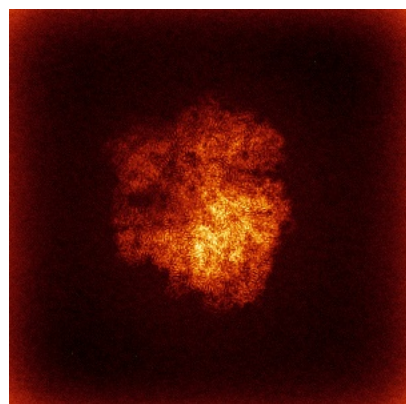


Y

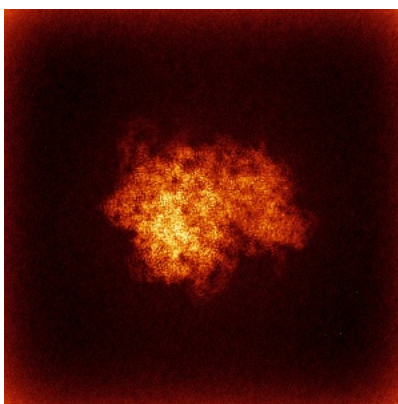


Z

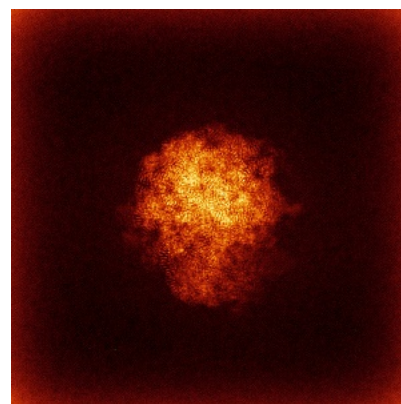
6.4.2 Raw map



X



Y

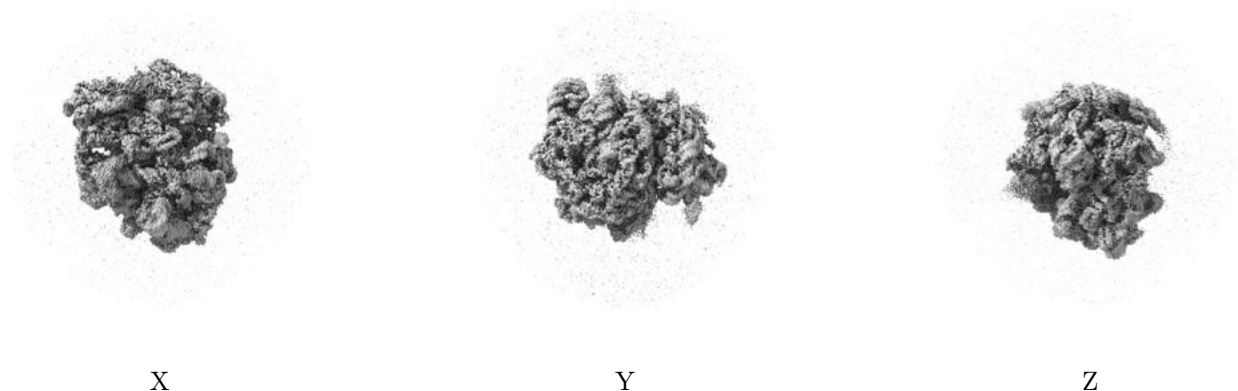


Z

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

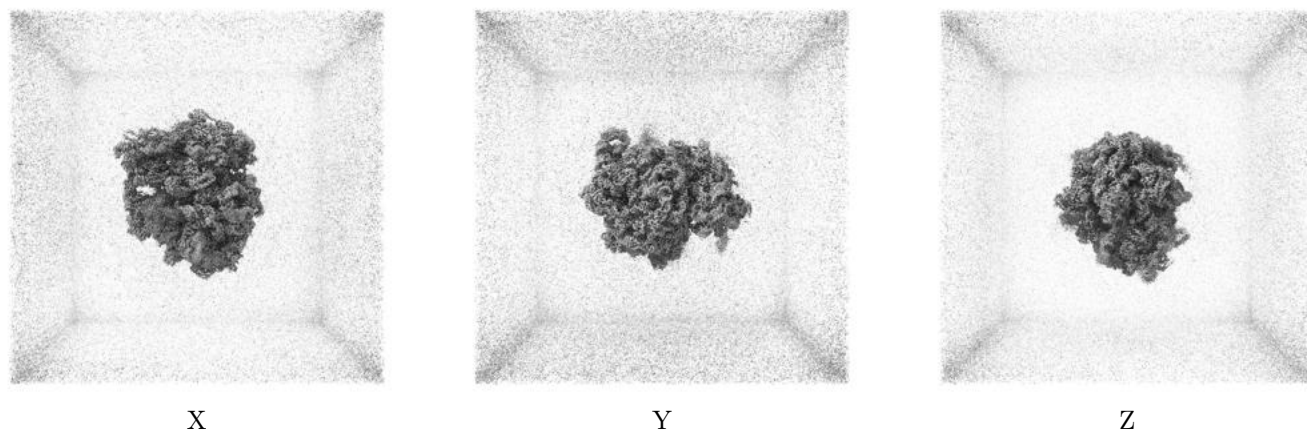
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



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

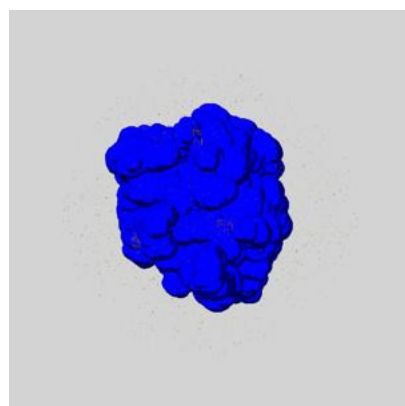
6.6 Mask visualisation [i](#)

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

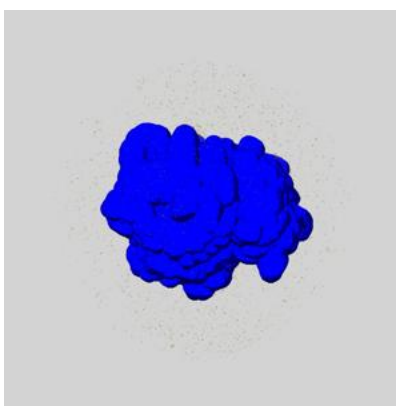
A mask typically either:

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

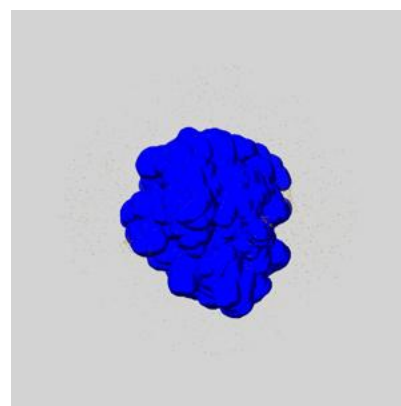
6.6.1 emd_71683_msk_1.map [i](#)



X



Y

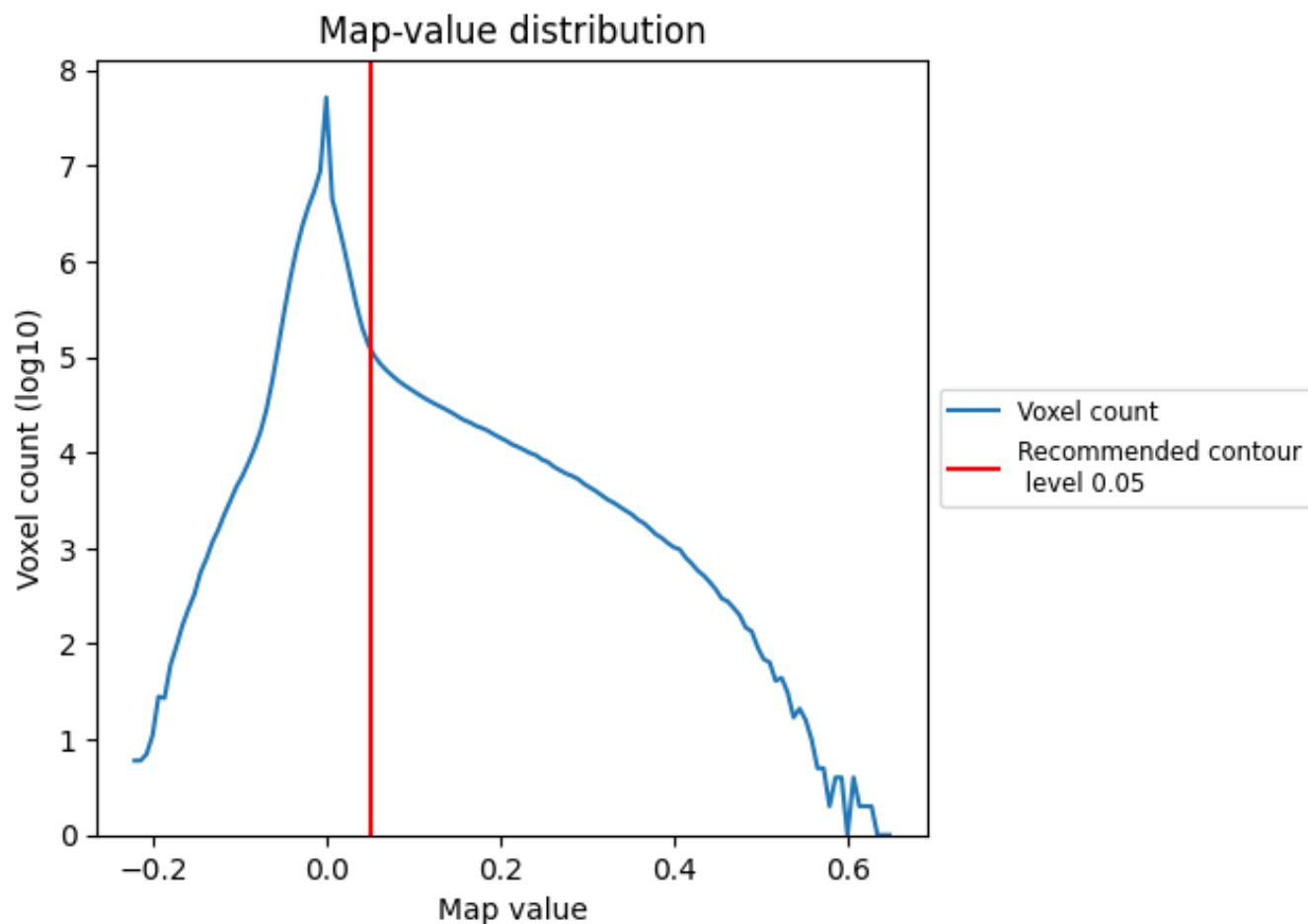


Z

7 Map analysis [i](#)

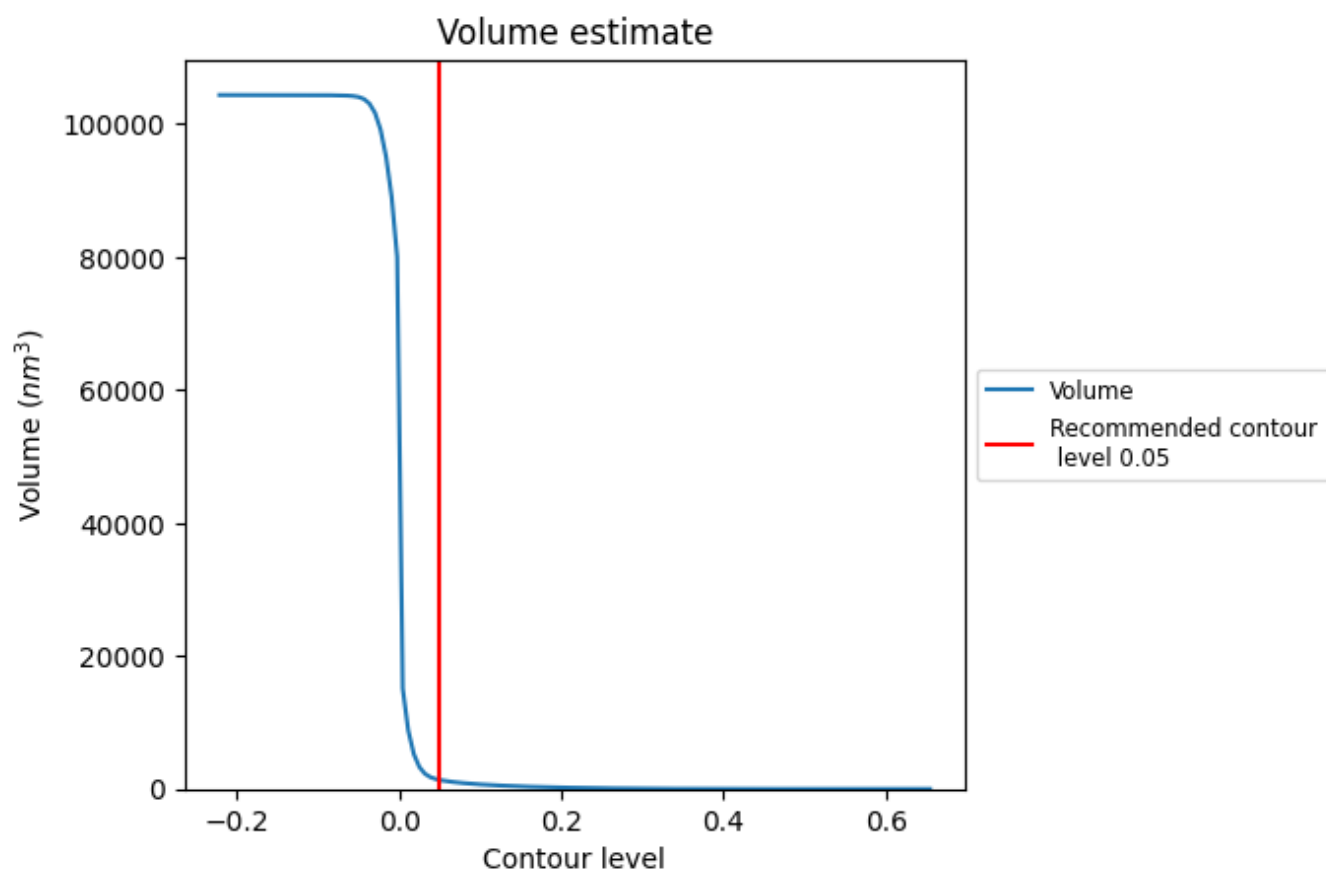
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

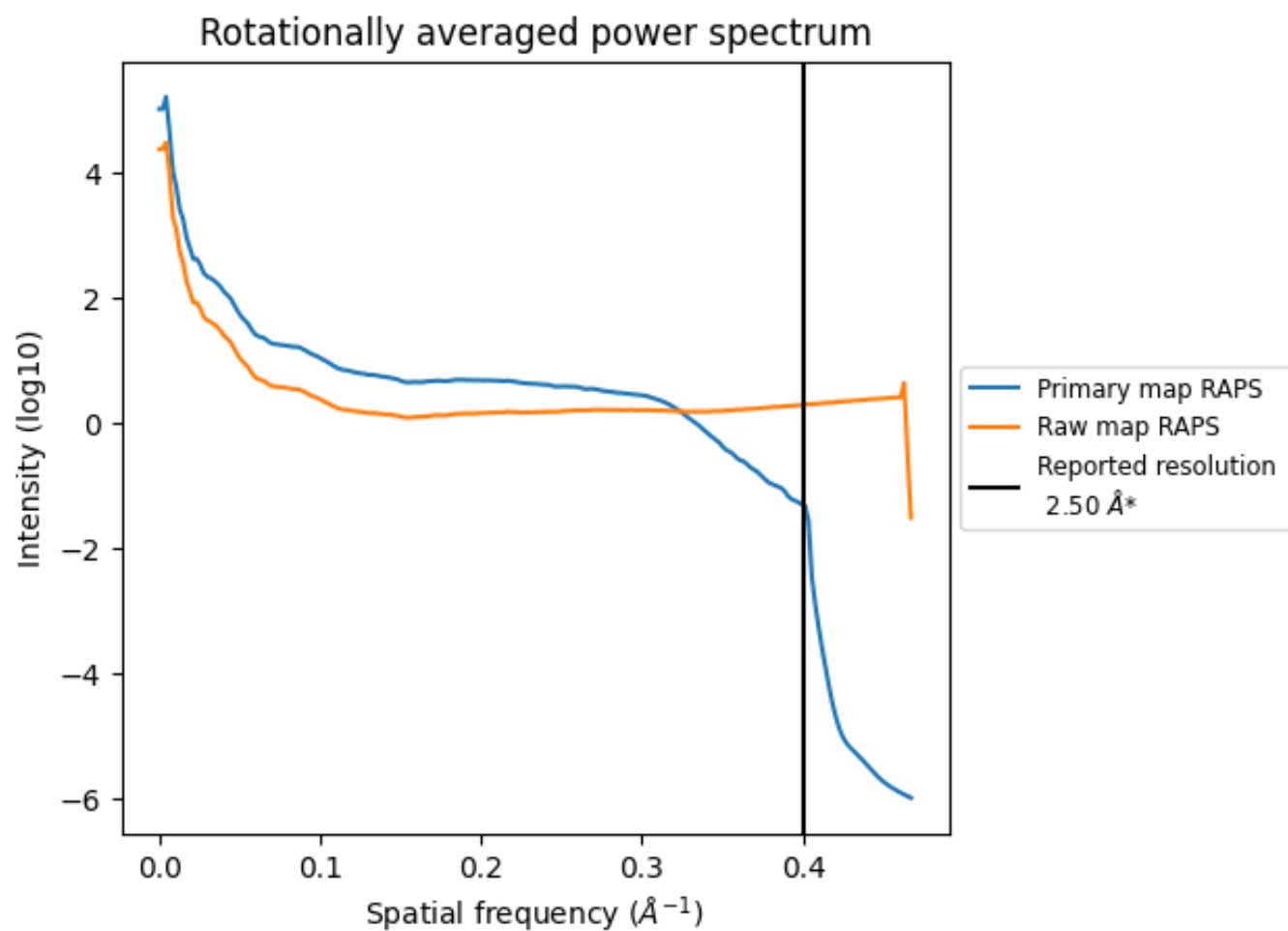
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1360 nm^3 ; this corresponds to an approximate mass of 1229 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

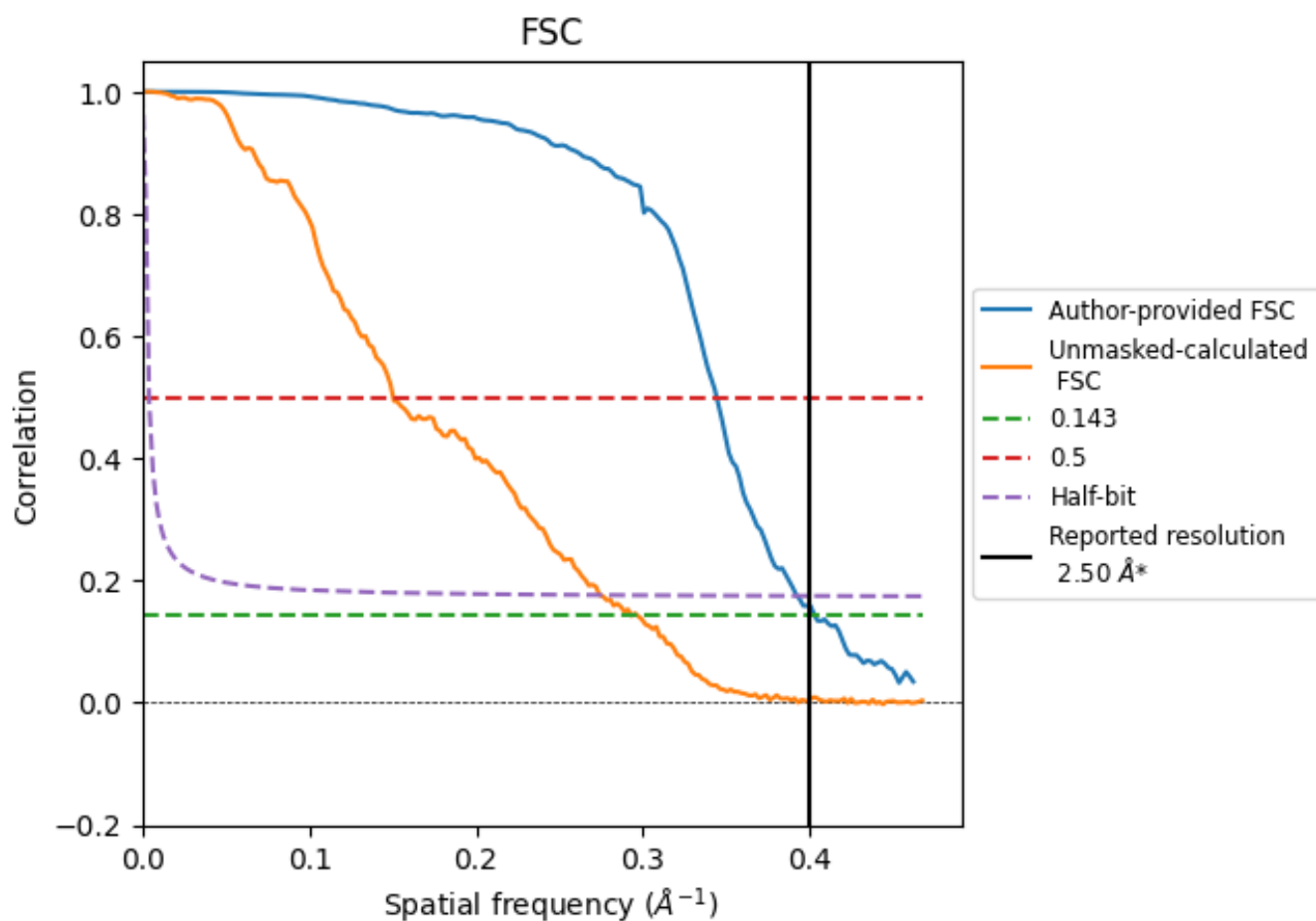


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

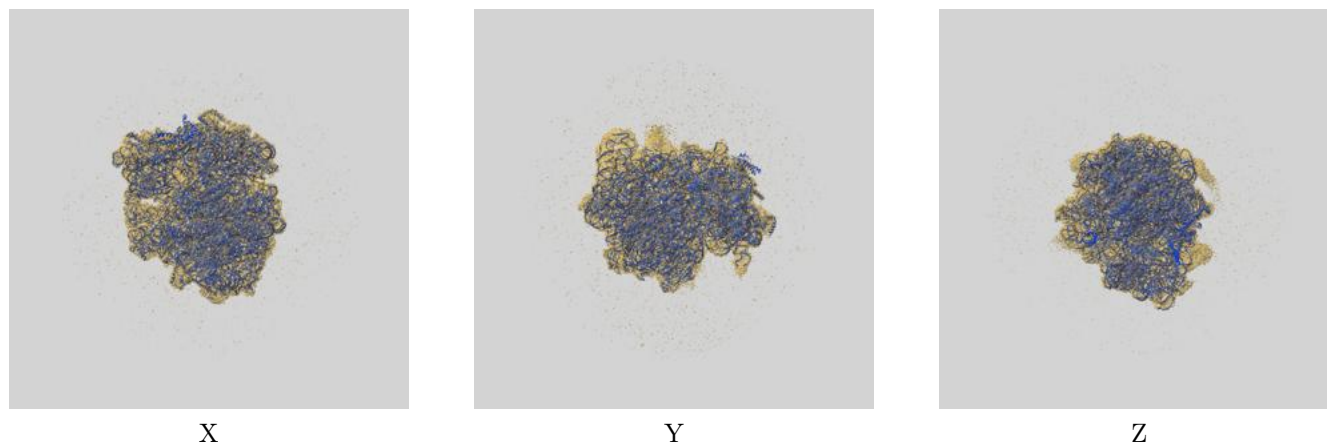
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.91	2.55
Unmasked-calculated*	3.41	6.65	3.65

*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 3.41 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

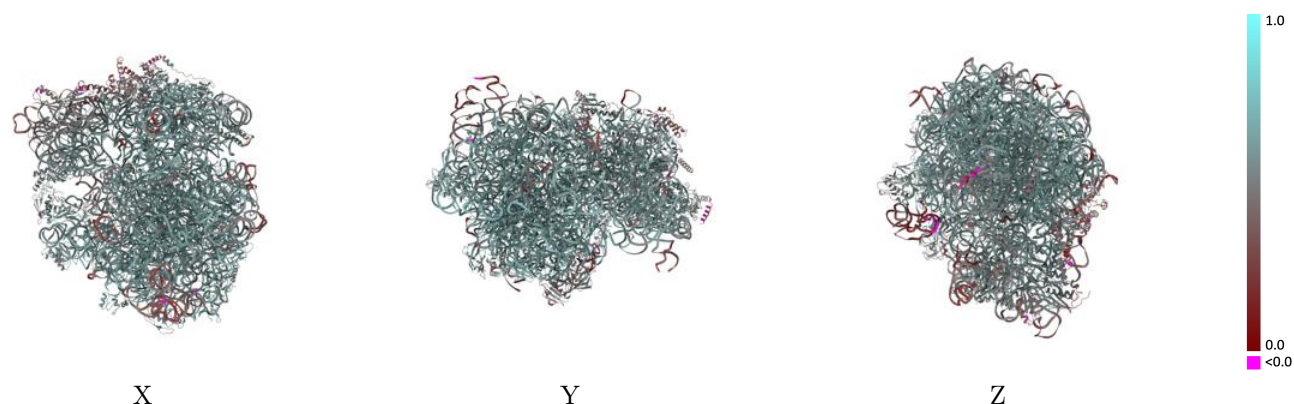
This section contains information regarding the fit between EMDB map EMD-71683 and PDB model 9PJ8. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



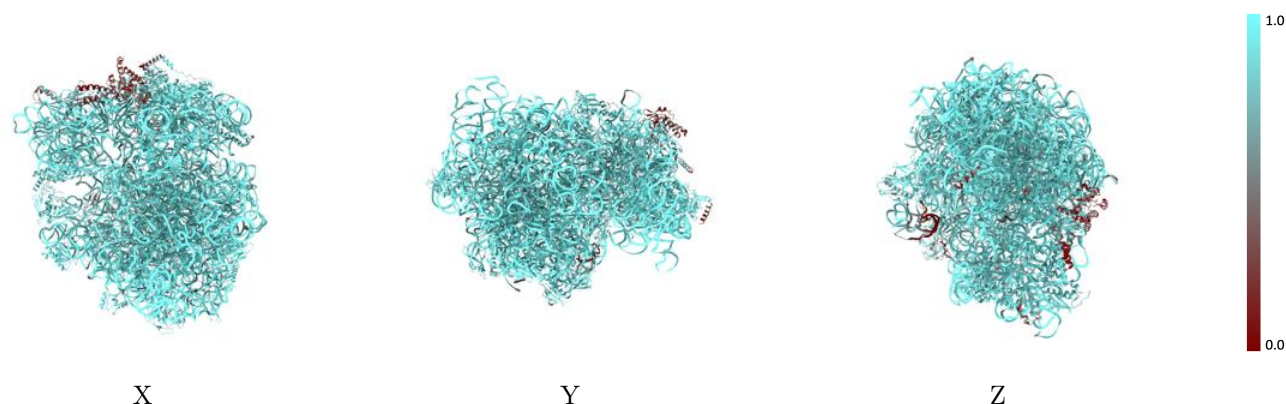
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



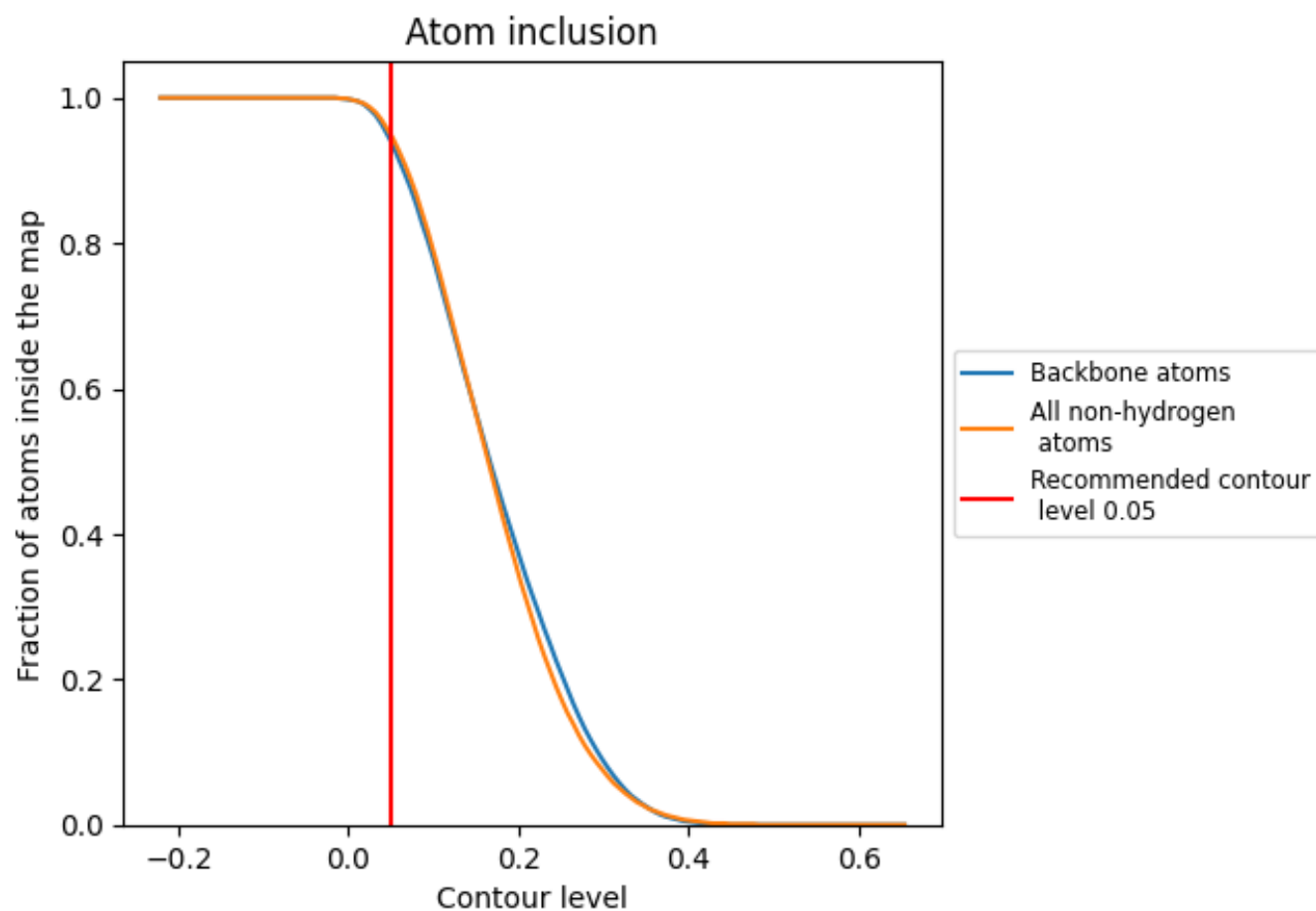
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5680
0	 0.9580	 0.6020
1	 0.9940	 0.6400
2	 0.9680	 0.6250
3	 0.9490	 0.6080
4	 0.8960	 0.5030
A	 0.9830	 0.5610
B	 0.2570	 0.3670
C	 0.9610	 0.5600
D	 0.9060	 0.5040
E	 0.8750	 0.5530
F	 0.8960	 0.5240
G	 0.7980	 0.5000
H	 0.9390	 0.5740
I	 0.9020	 0.5240
J	 0.8970	 0.4760
K	 0.9510	 0.5540
L	 0.9390	 0.5870
M	 0.7200	 0.4460
N	 0.8750	 0.5200
O	 0.9460	 0.5570
P	 0.8710	 0.4960
Q	 0.8920	 0.5490
R	 0.8510	 0.5230
S	 0.8900	 0.5480
T	 0.9310	 0.5590
U	 0.9260	 0.5000
V	 0.9770	 0.6370
X	 0.9110	 0.5860
Y	 0.7390	 0.4520
a	 0.9710	 0.5830
b	 0.9960	 0.5910
c	 0.9670	 0.6220
d	 0.9750	 0.6070
e	 0.9510	 0.5800



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.9440	 0.5440
g	 0.9040	 0.4950
i	 0.9730	 0.6160
j	 0.9390	 0.5990
k	 0.9490	 0.5950
l	 0.9640	 0.6060
m	 0.9690	 0.6070
n	 0.9590	 0.5610
o	 0.9460	 0.6060
p	 0.9620	 0.6130
q	 0.9530	 0.5900
r	 0.9460	 0.6060
s	 0.9590	 0.5900
t	 0.9420	 0.5670
u	 0.7270	 0.4660
v	 0.9630	 0.6220
w	 0.9800	 0.6260
x	 0.9360	 0.5610
y	 0.9510	 0.6100
z	 0.9610	 0.6170