



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 11:23 PM EDT

PDB ID : 7UVY / pdb_00007uvy
EMDB ID : EMD-26820
Title : A. baumannii ribosome-Streptothricin-D complex: 70S with P-site tRNA
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2022-05-02
Resolution : 2.39 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:

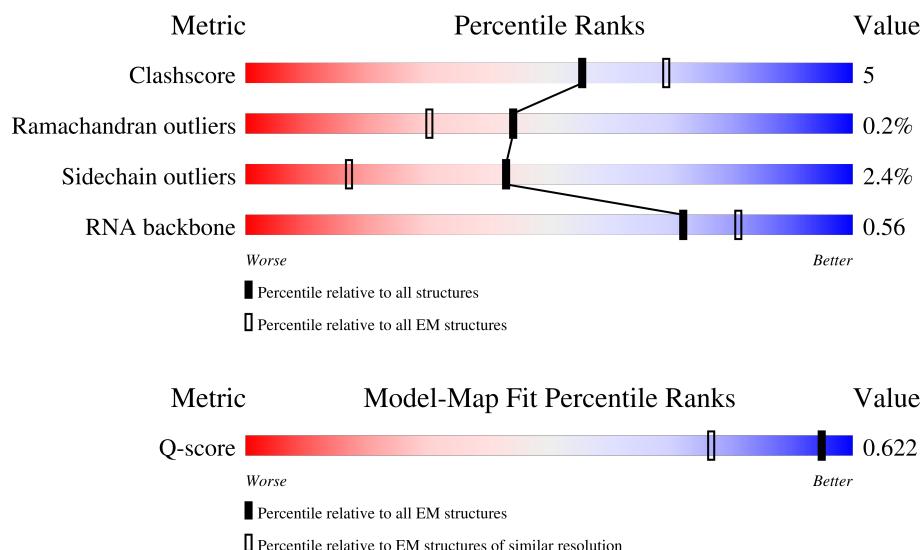
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 2.39 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	4884 (1.90 - 2.89)

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	51	
2	1	44	
3	2	64	

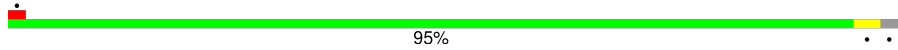
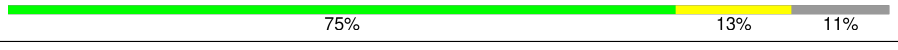
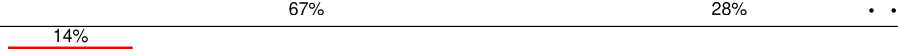
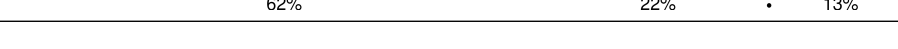
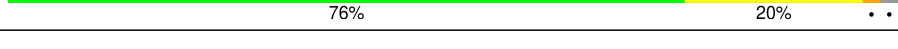
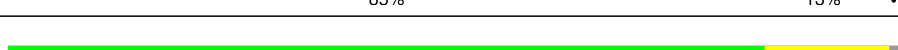
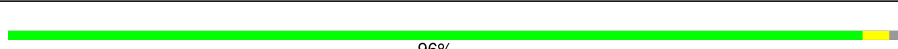
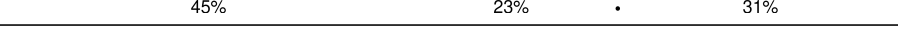
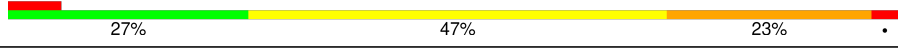
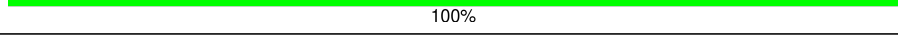
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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	2918	
6	B	115	
7	C	274	
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	

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Mol	Chain	Length	Quality of chain
29	Y	58	
30	Z	61	
31	a	1544	
32	b	250	
33	c	250	
34	d	208	
35	e	165	
36	f	127	
37	g	156	
38	h	131	
39	i	128	
40	j	103	
41	k	128	
42	l	124	
43	m	118	
44	n	101	
45	o	89	
46	p	101	
47	q	85	
48	r	75	
49	s	91	
50	t	88	
51	u	71	
52	v	77	
53	w	3	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 138881 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	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- 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
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2724	Total	C	N	O	P	0	0
			58438	26086	10700	18928	2724		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	144	Total	C	N	O	S	0	0
			1071	663	213	195			

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	116	Total	C	N	O	S	0	0
			873	537	176	158	2		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	117	Total	C	N	O	S	0	0
			919	578	177	164			

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	103	Total	C	N	O		0	0
			766	476	142	148			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	76	Total	C	N	O	S	0	0
			577	358	111	106	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	136	Total	C	N	O	S	0	0
			1073	671	201	194	7		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total	C	N	O	0	0
			426	273	74	79		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	63	Total	C	N	O	S	0	0
			522	327	105	89	1		

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	77	Total	C	N	O	P	S	0	0
			1636	733	291	535	76	1		

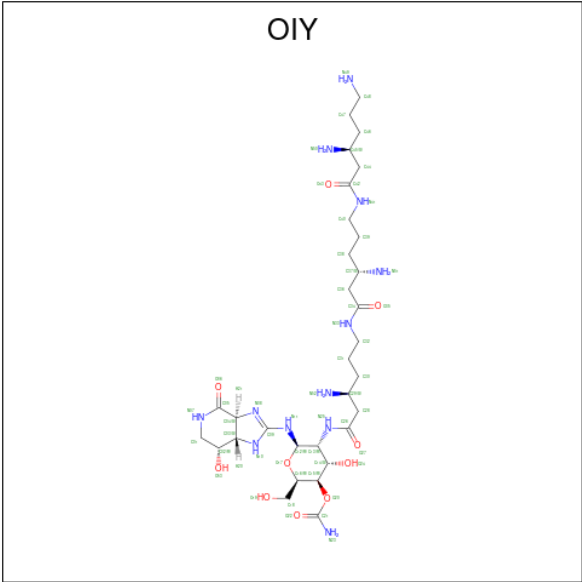
- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	

- Molecule 55 is Streptothricin D (CCD ID: OIY) (formula: C₃₁H₅₈N₁₂O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
55	A	1	Total	C	N	O	0
			40	22	9	9	
55	A	1	Total	C	N	O	0
			47	27	10	10	
55	A	1	Total	C	N	O	0
			53	31	12	10	
55	A	1	Total	C	N	O	0
			53	31	12	10	
55	A	1	Total	C	N	O	0
			35	19	8	8	
55	A	1	Total	C	N	O	0
			44	25	10	9	
55	N	1	Total	C	N	O	0
			35	19	8	8	
55	W	1	Total	C	N	O	0
			53	31	12	10	
55	a	1	Total	C	N	O	0
			35	19	8	8	
55	a	1	Total	C	N	O	0
			53	31	12	10	
55	a	1	Total	C	N	O	0
			53	31	12	10	
55	a	1	Total	C	N	O	0
			35	19	8	8	

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

Mol	Chain	Residues	Atoms		AltConf
56	A	1	Total 1	Mg 1	0

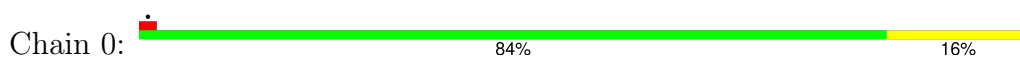
- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	A	4	Total 4	O 4	0
57	R	1	Total 1	O 1	0

3 Residue-property plots

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

- Molecule 1: 50S ribosomal protein L33



- Molecule 2: 50S ribosomal protein L34

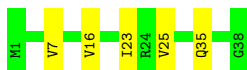


There are no outlier residues recorded for this chain.

- Molecule 3: 50S ribosomal protein L35



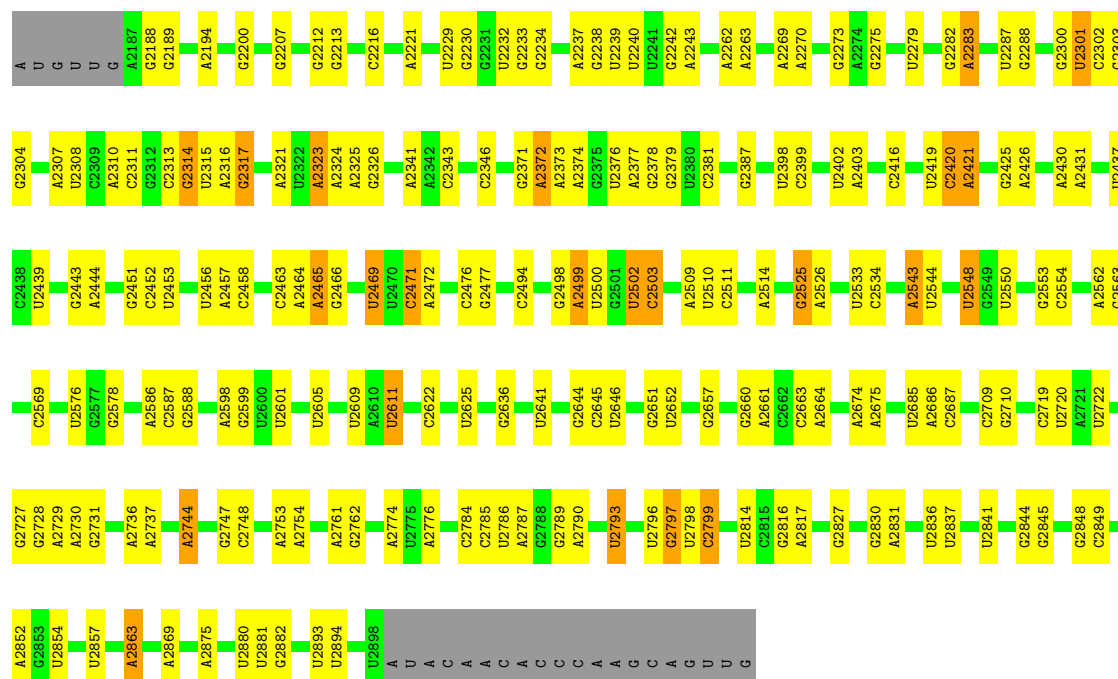
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 23s ribosomal RNA

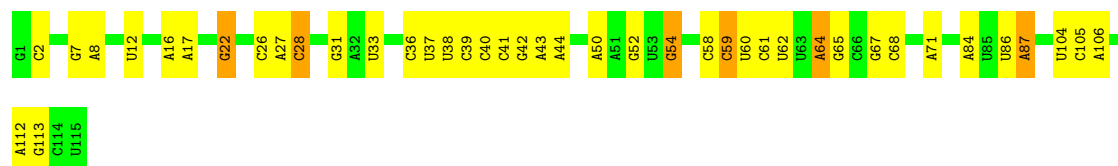


U2035	A1892	G1752	C1575	U1481	A1360	A1166	C	G855	U712	G575	A411	A280
C2039	A1897	G1760	A1577	U1483	G1363	U1170	A	G856	A713	U578	C412	A251
A2048	G1902	A1769	G1579	U1484	G1374	U1171	C	G857	A714	C579	A413	U284
C2051	U1907	A1776	C1580	U1485	U1378	U1172	C	G862	C715	A580	U418	A285
G2052	A1908	A1786	U1581	C1488	A1376	U1173	U	C863	A716	G581	C419	U286
A2056	A1909	U1786	C1582	A1489	A1379	G1179	U	U868	A719	U591	U423	G287
G2057	A1910	A1787	C1583	A1490	A1380	A997	A	U869	A720	U592	G423	U288
A2058	C1910	A1788	U1584	U1491	A1381	A998	A	U870	C721	C593	G424	G289
C2059	3TD1911	C1493	G1585	A1492	A1382	C1004	A	C874	G727	A594	C435	G291
C2060	U1912	C1494	U1586	C1493	U1382	U1009	G	U	A728	U595	U435	U292
C2061	U1913	C1503	A1596	C1494	U1391	C1010	A	A	G740	U596	C455	G297
C2062	A1914	U1504	C1597	C1394	C1394	G1014	A	G	U741	A597	A456	G304
C2063	U1915	A1505	C1598	A1395	A1395	G1014	G	G	U745	A601	G464	G304
A1923	A1923	G1605	G1605	G1406	U1407	G1023	C	G	U745	U605	U308	U308
A1924	A1924	A1606	A1606	U1407	U1407	A1024	C	G	A606	A606	G309	G309
G1925	G1925	A1616	A1616	G1411	G1411	U1025	U	U	A607	A607	U313	U313
G1926	G1926	A1616	A1616	U1412	U1412	A1029	A	A	G773	A612	G331	G331
A1934	A1934	A1630	A1630	G1413	G1413	U1030	C	C	G774	A612	A332	A332
U1942	U1942	G1634	G1634	A1414	A1414	A1036	C	C	A780	G618	U336	U336
C1943	C1943	A1635	A1635	A1422	A1422	A1037	C	C	A781	A625	U345	U345
U1951	U1951	C1812	C1644	C1423	C1423	G1038	A	A	G782	A625	C345	C345
U1952	U1952	A1825	U1645	G1424	G1424	U1039	C	C	G783	G633	G346	G346
C1953	C1953	U1826	U1646	G1425	G1425	C1040	U	U	A635	G633	A347	A347
C1954	C1954	G1647	G1647	A1426	A1426	U1041	U	U	U795	A635	A348	A348
U1959	U1959	C1827	C1654	G1427	G1427	U1042	A	A	G803	G637	C355	C355
U2082	U2082	C1829	U1655	A1428	A1428	A1043	C	C	U811	U637	A356	A356
G2083	G2083	C1833	C1656	A1429	A1429	G1044	C	C	C810	C638	C357	C357
C2089	C2089	C1833	U1657	C1432	C1432	G1048	A	A	C812	U643	U359	U359
C2092	C2092	A1843	G1672	U1433	U1433	C1049	A	A	A817	G649	A361	A361
U2093	U2093	A1844	U1681	A1434	A1434	U1050	G	G	U825	U651	U362	U362
U2094	U2094	G1845	A1682	A1435	A1435	A1051	G	G	U826	U651	G363	G363
C	C	G1845	U1682	A1436	A1436	G	G	G	U826	U655	A364	A364
C	C	A1849	A1682	A1439	A1439	G	G	G	U830	U656	U365	U365
C	C	A1850	A1682	G1441	G1441	G	G	G	U830	U656	G366	G366
C	C	A1854	G1701	C1442	C1442	G	G	G	A831	C669	A367	A367
A	A	A1854	C1724	U1443	U1443	G	G	G	G832	C670	C368	C368
A	A	G1865	U1725	G1447	G1447	G	G	G	U837	A675	G369	G369
A	A	U1866	U1726	U1448	U1448	C	C	C	C838	U684	G371	G371
A	A	A1867	C1726	U1455	U1455	G	G	G	G843	U684	G385	G385
A	A	A1868	G1727	G1462	G1462	G	G	G	A844	A687	A544	A544
A	A	G1869	U1729	A1463	A1463	G	G	G	A845	U688	C391	C391
A	A	A1872	C1731	A1465	A1465	G	G	G	U846	A691	C392	C392
A	A	U1879	U1733	U1477	U1477	A	A	A	A847	A691	G395	G395
A	A	A1881	G1734	G1478	G1478	G	G	G	C848	G698	U571	U571
A	A	G1880	A1735	U1479	U1479	G	G	G	U851	U701	A572	A572
A	A	G1881	G1736	A1480	A1480	G	G	G	G854	G702	A573	A573
A	A	A1885	G1749			C	C	C			U574	U574
A	A	A1886										



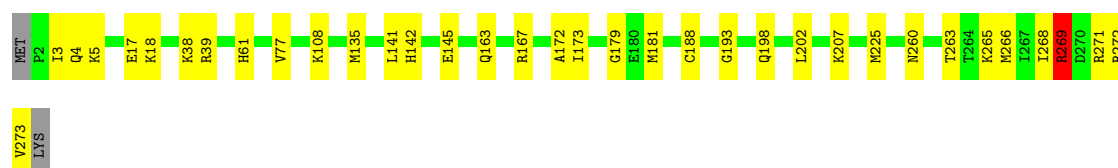
• Molecule 6: 5s ribosomal RNA

Chain B: 63% 31% 5%



• Molecule 7: 50S ribosomal protein L2

Chain C: 86% 12%



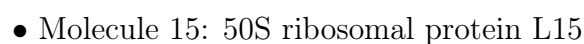
• Molecule 8: 50S ribosomal protein L3

Chain D: 89% 10%



• Molecule 9: 50S ribosomal protein L4

Chain E: 92% 8%

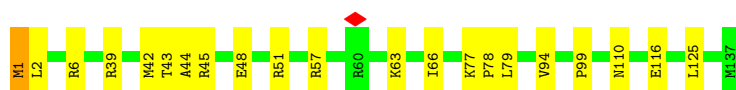


Chain K:  86% 13%



- Molecule 16: 50S ribosomal protein L16

Chain L:  85% 15%



- Molecule 17: 50S ribosomal protein L17

Chain M:  92% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N:  83% 17%



- Molecule 19: 50S ribosomal protein L19

Chain O:  84% 11%



- Molecule 20: 50S ribosomal protein L20

Chain P:  92% 6%



- Molecule 21: 50S ribosomal protein L21

Chain Q:  84% 16%



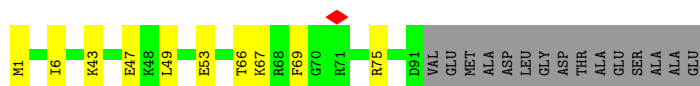
- Molecule 22: 50S ribosomal protein L22

Chain R:  89% 11%



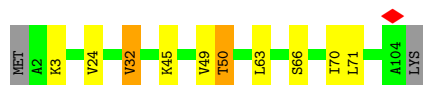
- Molecule 23: 50S ribosomal protein L23

Chain S:  76% 9% 14%



- Molecule 24: 50S ribosomal protein L24

Chain T:  89% 8% . .



- Molecule 25: 50S ribosomal protein L25

Chain U:  92% 7% .



- Molecule 26: 50S ribosomal protein L27

Chain V:  85% 5% 11%



- Molecule 27: 50S ribosomal protein L28

Chain W:  85% 14% .

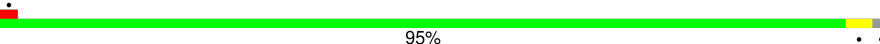


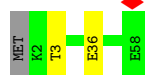
- Molecule 28: 50S ribosomal protein L29

Chain X:  69% 23% 8%



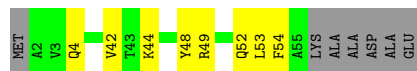
- Molecule 29: 50S ribosomal protein L30

Chain Y:  95%



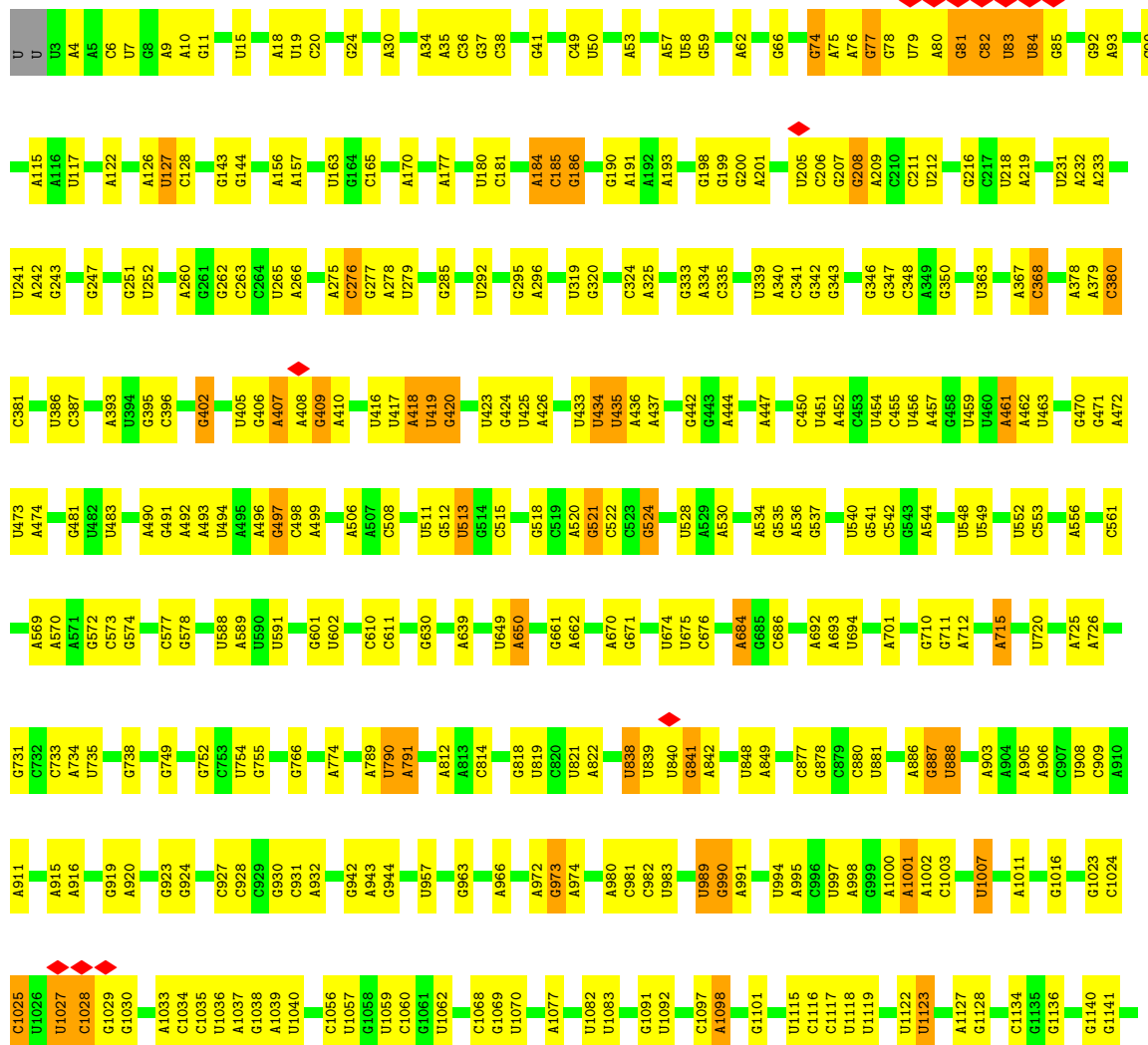
- Molecule 30: 50S ribosomal protein L32

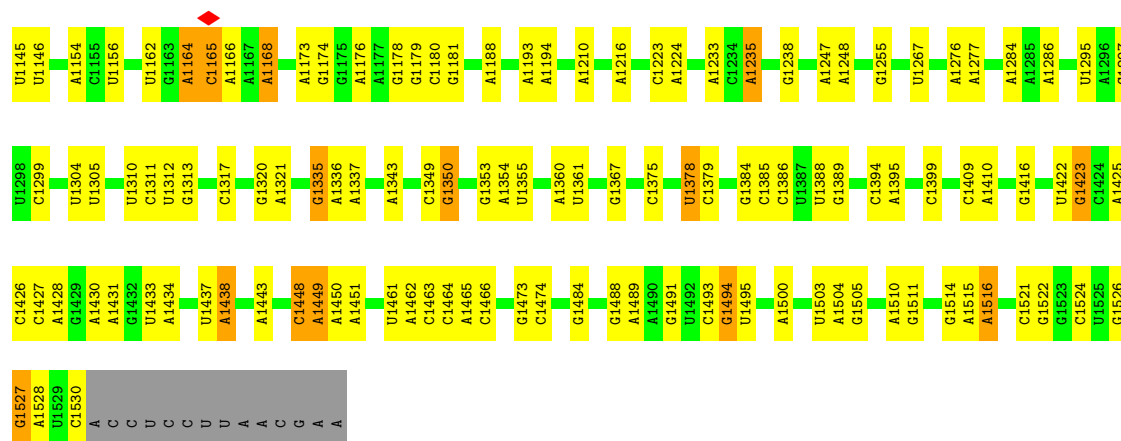
Chain Z:  75% 13% 11%



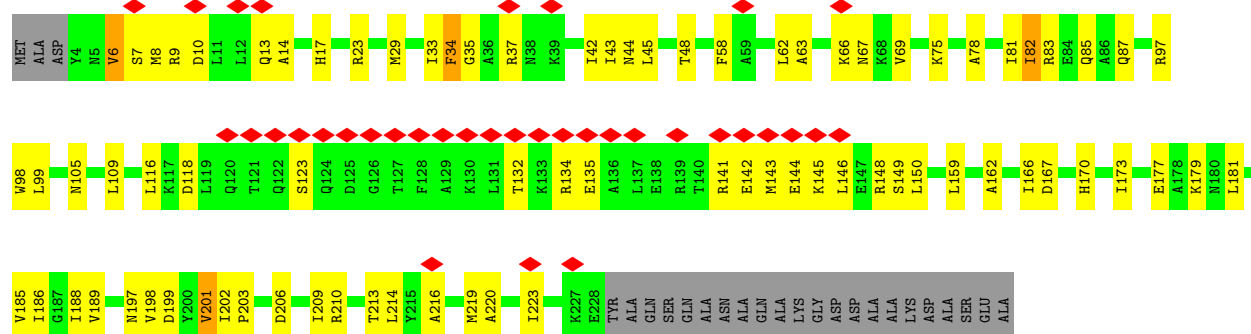
- Molecule 31: 16s Ribosomal RNA

Chain a:  67% 28%

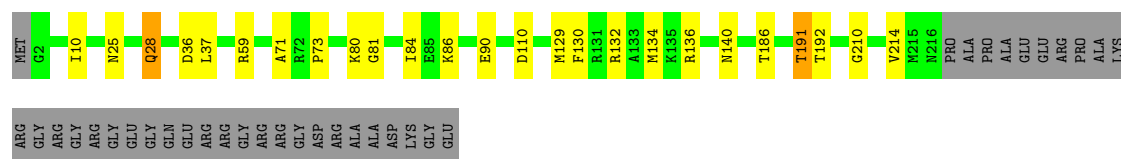




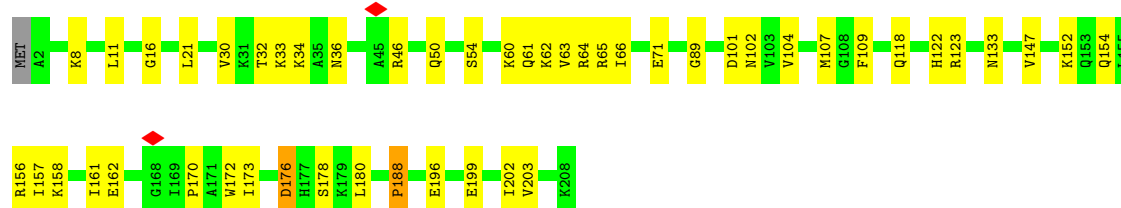
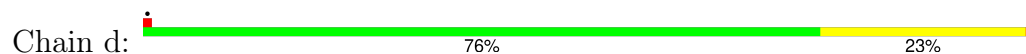
• Molecule 32: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S3

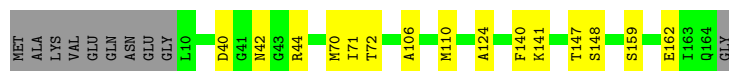


• Molecule 34: 30S ribosomal protein S4



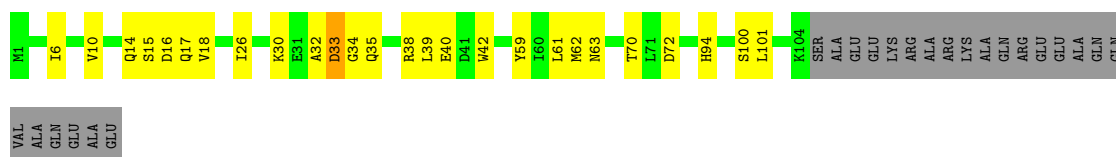
• Molecule 35: 30S ribosomal protein S5

Chain e: 



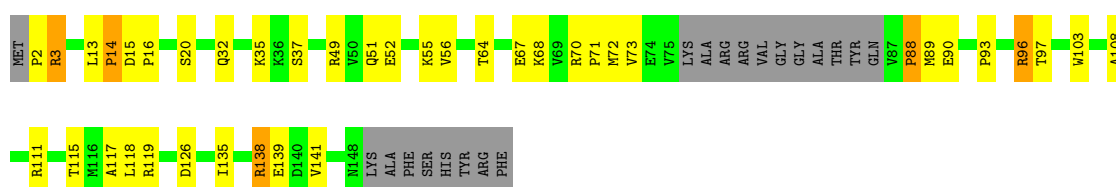
- Molecule 36: 30S ribosomal protein S6

Chain f: 



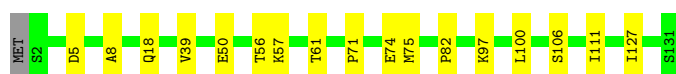
- Molecule 37: 30S ribosomal protein S7

Chain g: 



- Molecule 38: 30S ribosomal protein S8

Chain h: 



- Molecule 39: 30S ribosomal protein S9

Chain i: 



- Molecule 40: 30S ribosomal protein S10

Chain j: 



- Molecule 41: 30S ribosomal protein S11

Chain k: 



- Molecule 42: 30S ribosomal protein S12

Chain l: 76% 20% ..



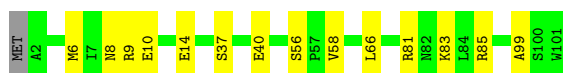
- Molecule 43: 30S ribosomal protein S13

Chain m: 85% 13% .



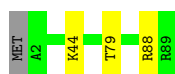
- Molecule 44: 30S ribosomal protein S14

Chain n: 85% 14% .



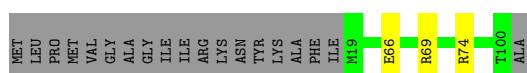
- Molecule 45: 30S ribosomal protein S15

Chain o: 96% ..



- Molecule 46: 30S ribosomal protein S16

Chain p: 78% 19% .



- Molecule 47: 30S ribosomal protein S17

Chain q: 75% 16% 7% .

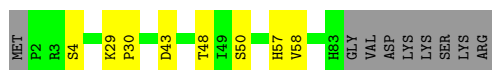
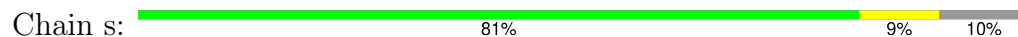


- Molecule 48: 30S ribosomal protein S18

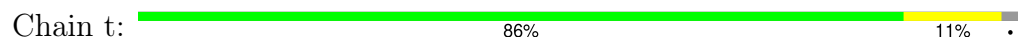
Chain r: 45% 23% 31% .



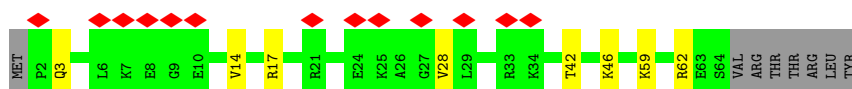
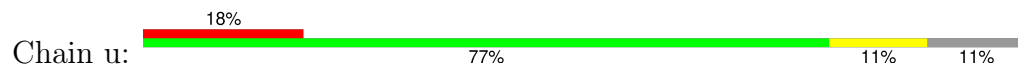
- Molecule 49: 30S ribosomal protein S19



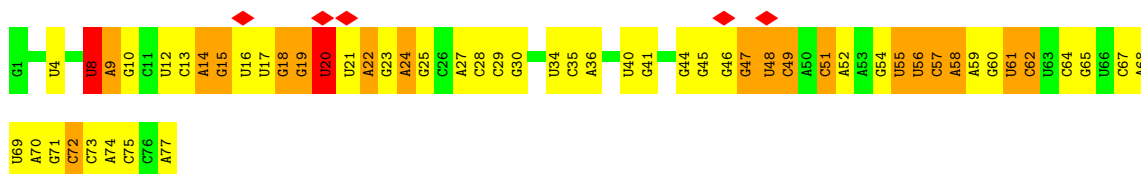
- Molecule 50: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S21



- Molecule 52: tRNA-met



- Molecule 53: mRNA



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.869	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.72, 0.72, 0.72	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, 3TD, OIY, OMG, H2U, MA6, 2MG, 4OC, 6MZ, PSU, OMU, 5MU, 2MA, UR3, ZN, 7MG, MG, 5MC

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	0.16	0/434	0.34	0/573
2	1	0.15	0/367	0.34	0/481
3	2	0.16	0/515	0.40	0/678
4	3	0.17	0/296	0.39	0/389
5	A	0.19	0/65086	0.33	0/101513
6	B	0.15	0/2739	0.29	0/4266
7	C	0.23	0/2152	0.46	0/2891
8	D	0.18	0/1590	0.38	0/2142
9	E	0.18	0/1537	0.40	0/2073
10	F	0.19	0/1390	0.52	0/1863
11	G	0.18	0/1337	0.44	0/1807
12	H	0.18	0/461	0.51	0/616
13	I	0.17	0/1151	0.40	0/1551
14	J	0.17	0/956	0.39	0/1286
15	K	0.16	0/1079	0.34	0/1439
16	L	0.17	0/1104	0.40	0/1475
17	M	0.17	0/956	0.39	0/1282
18	N	0.15	0/881	0.44	0/1177
19	O	0.17	0/931	0.39	0/1249
20	P	0.19	0/947	0.36	0/1262
21	Q	0.17	0/818	0.36	0/1094
22	R	0.17	0/831	0.34	0/1113
23	S	0.15	0/716	0.36	0/957
24	T	0.14	0/770	0.34	0/1034
25	U	0.16	0/770	0.38	0/1036
26	V	0.17	0/585	0.39	0/783
27	W	0.16	0/642	0.36	0/856
28	X	0.16	0/487	0.38	0/646
29	Y	0.17	0/460	0.32	0/614
30	Z	0.15	0/453	0.32	0/604
31	a	0.17	0/36476	0.31	0/56895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.18	0/1799	0.41	0/2429
33	c	0.17	0/1714	0.40	0/2304
34	d	0.19	0/1653	0.48	1/2213 (0.0%)
35	e	0.17	0/1141	0.38	0/1537
36	f	0.17	0/882	0.43	0/1189
37	g	0.23	0/1087	0.59	1/1456 (0.1%)
38	h	0.16	0/993	0.36	0/1331
39	i	0.18	0/1002	0.42	0/1339
40	j	0.19	0/811	0.50	0/1096
41	k	0.18	0/878	0.44	0/1189
42	l	0.18	0/958	0.42	0/1284
43	m	0.18	0/913	0.48	2/1226 (0.2%)
44	n	0.19	0/803	0.36	0/1071
45	o	0.17	0/715	0.33	0/958
46	p	0.15	0/655	0.37	0/879
47	q	0.16	0/628	0.40	0/847
48	r	0.18	0/432	0.44	0/583
49	s	0.17	0/664	0.35	0/897
50	t	0.18	0/669	0.32	0/892
51	u	0.13	0/528	0.33	0/697
52	v	0.17	0/1739	0.31	0/2709
53	w	0.10	0/72	0.16	0/110
All	All	0.18	0/149653	0.34	4/223881 (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
7	C	0	1
21	Q	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	14	PRO	CA-N-CD	-6.40	103.04	112.00
43	m	64	PRO	CA-C-N	-6.04	115.25	122.44
43	m	64	PRO	C-N-CA	-6.04	115.25	122.44
34	d	188	PRO	CA-N-CD	-5.21	104.71	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	269	ARG	Sidechain
21	Q	51	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	8	0
2	1	363	0	401	0	0
3	2	509	0	566	3	0
4	3	295	0	326	3	0
5	A	58438	0	29389	332	0
6	B	2450	0	1241	16	0
7	C	2111	0	2176	37	0
8	D	1572	0	1610	13	0
9	E	1516	0	1569	8	0
10	F	1370	0	1420	55	0
11	G	1318	0	1373	28	0
12	H	458	0	480	9	0
13	I	1125	0	1148	5	0
14	J	946	0	1007	3	0
15	K	1071	0	1141	10	0
16	L	1087	0	1162	15	0
17	M	942	0	987	1	0
18	N	873	0	917	11	0
19	O	919	0	973	12	0
20	P	934	0	997	5	0
21	Q	807	0	842	8	0
22	R	826	0	894	9	0
23	S	710	0	768	7	0
24	T	766	0	816	4	0
25	U	760	0	783	3	0
26	V	577	0	580	3	0
27	W	632	0	667	7	0
28	X	486	0	528	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Y	455	0	476	0	0
30	Z	447	0	435	6	0
31	a	32782	0	16508	256	0
32	b	1769	0	1787	54	0
33	c	1690	0	1774	13	0
34	d	1631	0	1691	34	0
35	e	1129	0	1174	10	0
36	f	867	0	868	15	0
37	g	1073	0	1118	28	0
38	h	985	0	1047	11	0
39	i	991	0	1048	8	0
40	j	801	0	832	12	0
41	k	862	0	877	19	0
42	l	945	0	998	22	0
43	m	903	0	962	8	0
44	n	792	0	833	13	0
45	o	705	0	712	2	0
46	p	644	0	655	2	0
47	q	621	0	665	8	0
48	r	426	0	447	9	0
49	s	646	0	663	4	0
50	t	663	0	715	8	0
51	u	522	0	565	5	0
52	v	1636	0	835	44	0
53	w	65	0	33	0	0
54	3	1	0	0	0	0
55	A	272	0	0	4	0
55	N	35	0	0	1	0
55	W	53	0	0	2	0
55	a	176	0	0	1	0
56	A	1	0	0	0	0
57	A	4	0	0	0	0
57	R	1	0	0	0	0
All	All	138881	0	92941	1135	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 5.

All (1135) 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)
5:A:1036:A:N6	5:A:1113:G:H1	1.44	1.14
7:C:269:ARG:HH11	7:C:269:ARG:HB3	1.09	1.08
52:v:27:A:N6	52:v:45:G:H1	1.51	1.08
31:a:75:A:N6	31:a:92:G:H1	1.59	0.97
31:a:74:G:H1	31:a:93:A:H61	0.99	0.97
7:C:269:ARG:HB3	7:C:269:ARG:NH1	1.83	0.91
31:a:75:A:H61	31:a:92:G:H1	0.94	0.90
31:a:74:G:H1	31:a:93:A:N6	1.69	0.90
31:a:1007:U:H3	31:a:1016:G:H1	0.88	0.88
31:a:454:U:H3	31:a:470:G:H1	1.23	0.83
5:A:1050:U:H3	5:A:1103:A:H61	1.29	0.81
5:A:279:U:H3	5:A:366:G:H1	0.85	0.81
34:d:32:THR:HG23	34:d:34:LYS:H	1.47	0.79
10:F:58:GLN:HG2	10:F:65:PRO:HD3	1.65	0.79
27:W:17:ASN:OD1	55:W:101:OIY:N49	2.16	0.78
31:a:1162:U:H3	31:a:1168:A:H61	1.32	0.78
52:v:19:G:H3'	52:v:20:H2U:H2'	1.65	0.76
48:r:41:PRO:HG2	48:r:44:ILE:HD12	1.68	0.75
5:A:279:U:O2	5:A:366:G:N2	2.20	0.75
5:A:347:A:H1'	5:A:348:A:H2	1.52	0.75
18:N:35:HIS:ND1	18:N:54:THR:OG1	2.20	0.74
5:A:1521:G:H1	5:A:1544:G:H22	1.32	0.74
16:L:1:MET:HE1	16:L:45:ARG:HG2	1.68	0.74
52:v:27:A:N1	52:v:45:G:N2	2.32	0.74
5:A:2469:U:OP1	5:A:2471:C:N4	2.21	0.73
5:A:1036:A:N1	5:A:1113:G:N2	2.30	0.73
11:G:47:GLU:CD	11:G:48:GLY:H	1.97	0.73
7:C:108:LYS:HA	7:C:108:LYS:HE2	1.70	0.72
5:A:2315:U:O2'	5:A:2317:G:N7	2.21	0.72
5:A:1297:A:OP2	5:A:1605:G:O2'	2.08	0.71
31:a:1098:A:OP2	32:b:97:ARG:NH1	2.24	0.71
10:F:34:ILE:HG13	10:F:96:MET:HE3	1.72	0.70
31:a:74:G:N2	31:a:93:A:N1	2.33	0.70
31:a:520:A:N6	42:l:89:ASP:OD2	2.17	0.70
5:A:1854:A:H61	5:A:1880:G:H1'	1.54	0.70
5:A:2844:G:O2'	5:A:2863:A:N1	2.24	0.70
37:g:72:MET:HG2	37:g:73:VAL:HG23	1.72	0.70
5:A:2287:U:H2'	5:A:2288:G:C8	2.26	0.70
52:v:52:A:H61	52:v:64:C:H42	1.37	0.70
5:A:1595:A:H5''	5:A:1596:A:H5'	1.74	0.70
55:W:101:OIY:O24	55:W:101:OIY:N23	2.25	0.70
32:b:33:ILE:O	32:b:34:PHE:HD1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:4:ARG:HB2	15:K:7:GLU:HG3	1.73	0.69
50:t:42:GLY:HA2	50:t:86:LEU:HD11	1.75	0.69
14:J:97:ARG:NH1	31:a:335:C:OP2	2.24	0.69
31:a:522:C:OP1	42:l:86:ARG:NH2	2.25	0.69
31:a:670:A:H2'	31:a:671:G:C8	2.27	0.69
48:r:22:ASP:OD1	48:r:23:TYR:N	2.26	0.69
5:A:1854:A:N6	5:A:1880:G:H1'	2.07	0.68
5:A:1580:C:O2'	5:A:1583:C:N3	2.23	0.68
31:a:471:G:H2'	31:a:472:A:C8	2.29	0.68
33:c:129:MET:SD	33:c:132:ARG:NH2	2.67	0.68
19:O:30:VAL:HG22	19:O:47:GLU:HG3	1.75	0.68
46:p:66:GLU:OE2	46:p:69:ARG:NH2	2.25	0.68
5:A:854:G:H2'	5:A:855:G:C8	2.28	0.68
31:a:1223:C:H2'	43:m:102:THR:HG22	1.74	0.68
14:J:47:ILE:HG13	14:J:48:PRO:HD2	1.75	0.67
7:C:269:ARG:HH11	7:C:269:ARG:CB	1.99	0.67
6:B:41:C:O2	10:F:92:ARG:NH1	2.27	0.67
7:C:181:MET:HE2	7:C:269:ARG:NH1	2.09	0.67
10:F:56:ASP:OD2	10:F:150:ARG:NH1	2.27	0.67
34:d:11:LEU:HD22	34:d:65:ARG:HE	1.60	0.67
52:v:21:U:H1'	52:v:22:A:H2'	1.77	0.67
16:L:57:ARG:NH2	16:L:116:GLU:OE1	2.28	0.66
9:E:7:SER:OG	9:E:121:GLU:OE2	2.13	0.66
5:A:2324:A:H2'	5:A:2325:A:C8	2.30	0.66
5:A:52:G:H5''	5:A:53:G:H5'	1.76	0.66
5:A:1412:C:O2'	5:A:1585:G:O2'	2.14	0.66
31:a:943:A:H2'	31:a:944:G:C8	2.31	0.66
32:b:142:GLU:O	32:b:146:LEU:HD12	1.95	0.66
5:A:2744:A:H1'	11:G:67:THR:HG22	1.78	0.65
22:R:95:ARG:HB3	22:R:95:ARG:NH1	2.11	0.65
1:O:6:ARG:NH1	1:O:49:LYS:O	2.30	0.65
7:C:181:MET:HB2	7:C:269:ARG:HH12	1.60	0.65
5:A:2048:A:H4'	8:D:151:GLN:O	1.97	0.65
7:C:271:ARG:NE	7:C:273:VAL:HG12	2.10	0.65
31:a:1068:C:H2'	31:a:1069:G:H8	1.61	0.65
41:k:67:GLU:HG2	41:k:98:ALA:HB1	1.79	0.65
52:v:27:A:H61	52:v:45:G:H1	0.75	0.64
31:a:1353:G:H2'	31:a:1354:A:C8	2.32	0.64
42:l:110:ARG:NH2	42:l:112:GLN:O	2.30	0.64
23:S:66:THR:HG22	23:S:75:ARG:HG3	1.77	0.64
31:a:470:G:H2'	31:a:471:G:C8	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:994:U:H2'	31:a:995:A:H8	1.61	0.64
5:A:1798:A:H2'	5:A:1799:A:C8	2.32	0.64
5:A:482:A:OP1	24:T:45:LYS:NZ	2.31	0.64
5:A:2753:A:N1	11:G:67:THR:HG21	2.13	0.64
34:d:147:VAL:O	34:d:152:LYS:NZ	2.31	0.64
5:A:2188:G:H2'	5:A:2189:G:C8	2.33	0.64
31:a:1127:A:H2'	31:a:1128:G:H8	1.62	0.64
32:b:123:SER:HB2	32:b:143:MET:HE1	1.79	0.64
44:n:10:GLU:O	44:n:14:GLU:HG3	1.99	0.63
31:a:498:C:H2'	31:a:499:A:H8	1.62	0.63
31:a:423:U:OP2	31:a:424:G:O2'	2.14	0.63
31:a:1313:G:H4'	44:n:58:VAL:HG11	1.81	0.63
31:a:1320:G:H2'	31:a:1321:A:C8	2.34	0.63
37:g:93:PRO:HA	37:g:96:ARG:HG3	1.79	0.63
5:A:1843:A:H2	5:A:1844:A:H62	1.46	0.62
10:F:11:GLU:HG3	10:F:12:LEU:HD12	1.81	0.62
41:k:80:ASN:HB3	41:k:105:LYS:NZ	2.15	0.62
5:A:1185:G:H5'	15:K:34:GLY:HA2	1.81	0.62
1:0:13:THR:HB	1:0:38:LYS:HE3	1.82	0.62
19:O:40:ARG:NH1	31:a:341:C:OP1	2.32	0.62
5:A:1104:G:N2	5:A:1105:U:O4	2.33	0.62
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.81	0.62
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.82	0.62
5:A:2323:A:H2'	5:A:2324:A:C8	2.35	0.62
10:F:29:PRO:HB3	10:F:160:ALA:HB2	1.81	0.62
15:K:93:SER:OG	15:K:95:GLU:OE1	2.17	0.62
7:C:135:MET:O	7:C:167:ARG:NH2	2.33	0.62
10:F:162:THR:OG1	10:F:163:ASP:N	2.27	0.62
31:a:78:G:H2'	31:a:79:U:C6	2.35	0.62
5:A:1792:U:H2'	5:A:1793:C:C6	2.35	0.62
6:B:26:C:H5''	18:N:32:THR:HG21	1.82	0.61
31:a:498:C:H2'	31:a:499:A:C8	2.34	0.61
31:a:710:G:H2'	31:a:711:G:C8	2.35	0.61
39:i:37:PHE:O	39:i:43:ARG:NH1	2.33	0.61
5:A:579:C:H2'	5:A:580:A:C8	2.35	0.61
10:F:36:LEU:HB2	10:F:89:VAL:HG23	1.82	0.61
8:D:20:GLY:HA3	19:O:83:VAL:HG23	1.80	0.61
36:f:26:ILE:HD11	36:f:39:LEU:HD13	1.82	0.61
24:T:49:VAL:HG23	24:T:50:THR:HG23	1.83	0.61
41:k:80:ASN:HB3	41:k:105:LYS:HZ2	1.66	0.61
5:A:286:U:H2'	5:A:287:G:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2587:C:H2'	5:A:2588:G:H8	1.65	0.61
32:b:33:ILE:HG22	32:b:35:GLY:H	1.66	0.61
5:A:1464:A:H2'	5:A:1465:A:C8	2.36	0.61
5:A:2543:A:H2'	5:A:2544:U:C6	2.36	0.60
31:a:725:A:H2'	31:a:726:A:C8	2.36	0.60
25:U:80:ALA:HB3	25:U:94:ASP:HB2	1.84	0.60
41:k:36:ARG:HG3	41:k:36:ARG:HH11	1.66	0.60
13:I:19:ASP:O	13:I:23:LYS:NZ	2.34	0.60
52:v:18:G:N1	52:v:56:PSU:O2'	2.32	0.60
48:r:42:SER:OG	48:r:47:THR:O	2.19	0.60
7:C:4:GLN:NE2	7:C:18:LYS:HB2	2.16	0.60
5:A:2587:C:H2'	5:A:2588:G:C8	2.36	0.60
32:b:82:ILE:HD11	32:b:166:ILE:HG13	1.83	0.60
42:l:35:THR:N	42:l:54:ARG:O	2.33	0.60
5:A:847:A:H2'	5:A:848:C:C6	2.37	0.60
34:d:101:ASP:OD1	34:d:102:ASN:N	2.34	0.60
9:E:4:LYS:HE2	9:E:4:LYS:HA	1.83	0.60
5:A:579:C:H2'	5:A:580:A:H8	1.68	0.59
11:G:17:VAL:HG11	11:G:50:LEU:HD21	1.85	0.59
31:a:75:A:N1	31:a:92:G:N2	2.45	0.59
5:A:1885:A:H2'	5:A:1886:A:C8	2.38	0.59
10:F:164:ASP:OD1	10:F:164:ASP:N	2.35	0.59
31:a:1527:G:O6	51:u:46:LYS:NZ	2.36	0.59
31:a:198:G:H21	31:a:462:A:H61	1.50	0.59
31:a:207:G:O2'	31:a:208:G:O4'	2.16	0.59
39:i:128:ARG:NH2	52:v:34:U:OP2	2.35	0.59
5:A:2082:U:H2'	5:A:2083:G:C8	2.38	0.59
32:b:62:LEU:HD12	32:b:67:ASN:HB2	1.83	0.59
40:j:80:THR:O	40:j:83:THR:OG1	2.17	0.59
5:A:1792:U:H2'	5:A:1793:C:H6	1.67	0.59
32:b:69:VAL:HG22	32:b:162:ALA:HB3	1.85	0.59
43:m:66:GLU:O	43:m:70:ARG:HG2	2.01	0.59
5:A:1036:A:H61	5:A:1113:G:H1	0.69	0.59
10:F:170:MET:HE1	10:F:177:PHE:O	2.03	0.59
18:N:2:ASN:OD1	18:N:2:ASN:N	2.36	0.59
31:a:711:G:H2'	31:a:712:A:C8	2.38	0.59
52:v:15:G:N1	52:v:49:C:N3	2.50	0.59
1:O:26:MET:HE1	1:O:30:MET:HE2	1.85	0.58
19:O:91:ARG:NH2	19:O:113:ILE:O	2.35	0.58
31:a:339:U:O2'	31:a:342:G:O6	2.18	0.58
5:A:1428:A:H2'	5:A:1429:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:167:ARG:HA	7:C:172:ALA:HA	1.85	0.58
8:D:6:VAL:HG11	8:D:79:LEU:HD11	1.85	0.58
40:j:52:LEU:HD23	40:j:62:ARG:HG2	1.85	0.58
52:v:15:G:N1	52:v:49:C:C2	2.71	0.58
37:g:111:ARG:NH2	37:g:126:ASP:OD2	2.30	0.58
5:A:1647:G:O2'	17:M:106:ASP:OD2	2.18	0.58
5:A:2067:A:H2'	5:A:2068:C:C6	2.39	0.58
34:d:154:GLN:O	34:d:157:ILE:HG22	2.04	0.58
5:A:1050:U:H3	5:A:1103:A:N6	1.99	0.58
5:A:2463:C:H2'	5:A:2464:A:O4'	2.03	0.58
10:F:4:LEU:HD23	10:F:7:ARG:HD3	1.86	0.58
10:F:38:MET:HG3	10:F:152:MET:HB2	1.85	0.58
11:G:120:GLY:O	11:G:135:SER:OG	2.18	0.57
31:a:143:G:H2'	31:a:144:G:C8	2.39	0.57
7:C:3:ILE:HD11	7:C:202:LEU:HD13	1.86	0.57
30:Z:52:GLN:OE1	30:Z:53:LEU:N	2.37	0.57
32:b:85:GLN:HG3	32:b:220:ALA:HB2	1.84	0.57
48:r:34:THR:OG1	48:r:36:ASN:OD1	2.19	0.57
5:A:2282:G:H4'	5:A:2283:A:O4'	2.04	0.57
13:I:77:HIS:ND1	13:I:78:THR:O	2.37	0.57
5:A:591:U:H2'	5:A:592:U:C6	2.39	0.57
5:A:606:A:H2'	5:A:607:A:C8	2.40	0.57
34:d:152:LYS:HG2	34:d:180:LEU:HD12	1.85	0.57
5:A:741:U:O2'	5:A:1657:U:OP1	2.23	0.57
5:A:1523:A:H2'	5:A:1524:A:H8	1.68	0.57
6:B:87:A:OP2	16:L:39:ARG:NE	2.33	0.57
40:j:66:GLU:HB3	44:n:99:ALA:HB2	1.87	0.57
10:F:31:ILE:HD11	10:F:156:ILE:HB	1.85	0.57
19:O:40:ARG:HH22	31:a:341:C:H5''	1.69	0.57
5:A:2325:A:H2'	5:A:2326:G:C8	2.40	0.57
10:F:54:VAL:HG13	10:F:65:PRO:HG2	1.86	0.57
37:g:108:ALA:O	37:g:119:ARG:HD2	2.05	0.57
6:B:52:G:N2	10:F:26:MET:SD	2.76	0.56
31:a:433:U:O2'	34:d:156:ARG:NH2	2.38	0.56
31:a:451:U:C2	31:a:452:A:C8	2.93	0.56
31:a:1422:U:O2'	31:a:1423:G:H5'	2.03	0.56
5:A:413:C:H2'	5:A:414:A:C8	2.41	0.56
5:A:1531:C:O2'	5:A:1533:U:O4	2.16	0.56
5:A:2063:G:H1	5:A:2439:U:H3	1.53	0.56
5:A:2188:G:H2'	5:A:2189:G:H8	1.71	0.56
5:A:2465:A:N6	5:A:2477:G:O2'	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:37:ARG:HD3	32:b:42:ILE:HD13	1.88	0.56
38:h:18:GLN:HG2	38:h:71:PRO:HB3	1.86	0.56
5:A:2736:A:H2'	5:A:2737:A:C8	2.40	0.56
12:H:54:LEU:O	12:H:57:GLN:NE2	2.38	0.56
31:a:417:U:H4'	31:a:418:A:OP2	2.05	0.56
5:A:740:G:H2'	5:A:741:U:C6	2.39	0.56
5:A:1530:A:H3'	5:A:1531:C:H4'	1.88	0.56
31:a:265:U:H2'	31:a:266:A:C8	2.41	0.56
31:a:1038:G:H2'	31:a:1039:A:C8	2.40	0.56
34:d:158:LYS:O	34:d:162:GLU:HG2	2.06	0.56
41:k:110:THR:HG22	51:u:3:GLN:HA	1.86	0.56
44:n:37:SER:OG	44:n:40:GLU:OE2	2.20	0.56
5:A:12:A:H2'	5:A:13:A:C8	2.40	0.56
5:A:817:A:OP2	5:A:1182:G:N2	2.32	0.56
31:a:156:A:H2'	31:a:157:A:O4'	2.05	0.56
40:j:6:ILE:HB	40:j:76:ILE:HB	1.87	0.56
5:A:2510:U:H2'	5:A:2511:C:H6	1.71	0.56
22:R:65:ASP:N	22:R:65:ASP:OD1	2.39	0.56
31:a:1059:U:H2'	31:a:1060:C:C6	2.41	0.56
5:A:2060:C:H2'	5:A:2061:C:C6	2.41	0.56
10:F:65:PRO:HA	10:F:89:VAL:HG13	1.88	0.56
11:G:15:VAL:HA	11:G:27:LYS:O	2.05	0.56
33:c:130:PHE:O	33:c:134:MET:HG3	2.06	0.56
5:A:71:G:H2'	5:A:72:C:H6	1.70	0.55
5:A:596:U:H2'	5:A:597:A:H8	1.72	0.55
31:a:1461:U:H2'	31:a:1462:A:H8	1.71	0.55
5:A:1583:C:H3'	5:A:1584:A:H8	1.70	0.55
19:O:5:HIS:O	19:O:9:GLN:HG3	2.07	0.55
31:a:473:U:H2'	31:a:474:A:C8	2.41	0.55
31:a:733:C:H2'	31:a:734:A:C8	2.41	0.55
5:A:1790:A:H2'	5:A:1791:C:C6	2.42	0.55
10:F:110:ARG:HB3	10:F:137:VAL:HG13	1.88	0.55
5:A:347:A:H1'	5:A:348:A:C2	2.38	0.55
5:A:1037:A:H2	5:A:1112:G:H22	1.54	0.55
5:A:2300:G:H22	5:A:2308:U:H3	1.55	0.55
30:Z:42:VAL:HG22	30:Z:48:TYR:HB2	1.88	0.55
5:A:637:U:H2'	5:A:638:C:C6	2.42	0.55
5:A:2242:G:H2'	5:A:2243:A:H8	1.72	0.55
10:F:36:LEU:HD22	10:F:154:ILE:HG13	1.89	0.55
19:O:103:LEU:HD11	19:O:113:ILE:HD11	1.89	0.55
22:R:95:ARG:HB3	22:R:95:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:107:MET:HE2	34:d:173:ILE:HD11	1.88	0.55
34:d:157:ILE:HG23	34:d:158:LYS:HD3	1.88	0.55
42:l:88:LYS:HG3	42:l:88:LYS:O	2.05	0.55
5:A:19:U:O2	5:A:2622:C:H4'	2.07	0.55
5:A:976:A:H2'	5:A:979:C:H42	1.72	0.55
5:A:1287:G:N7	55:A:3004:OIY:N52	2.54	0.55
5:A:1634:G:H2'	5:A:1635:A:C8	2.42	0.55
6:B:64:A:H61	6:B:104:U:H2'	1.72	0.55
32:b:63:ALA:HB2	32:b:223:ILE:HD12	1.88	0.55
34:d:8:LYS:HD3	34:d:21:LEU:HB3	1.89	0.55
52:v:69:U:H2'	52:v:70:A:H8	1.71	0.55
5:A:199:G:O2'	5:A:675:A:N1	2.37	0.55
19:O:30:VAL:HB	19:O:88:GLU:HG2	1.89	0.55
28:X:4:LYS:HE3	28:X:4:LYS:HA	1.89	0.55
37:g:15:ASP:HB3	37:g:20:SER:H	1.71	0.55
12:H:8:ARG:HA	12:H:14:LYS:HA	1.88	0.55
38:h:39:VAL:HG21	38:h:111:ILE:HG22	1.88	0.55
5:A:1827:G:OP1	55:A:3006:OIY:N11	2.40	0.54
31:a:199:G:H1'	31:a:461:A:H61	1.71	0.54
31:a:419:U:O2'	31:a:420:G:O5'	2.25	0.54
5:A:1680:G:H2'	5:A:1681:U:C6	2.42	0.54
31:a:512:G:H2'	31:a:513:PSU:H6	1.73	0.54
5:A:418:U:H2'	5:A:419:C:C6	2.42	0.54
5:A:2510:U:H2'	5:A:2511:C:C6	2.42	0.54
5:A:2798:U:H2'	5:A:2799:C:C6	2.42	0.54
5:A:280:A:H2'	5:A:281:A:C8	2.42	0.54
34:d:63:VAL:HG21	34:d:202:ILE:HD11	1.89	0.54
5:A:1790:A:H2'	5:A:1791:C:H6	1.71	0.54
31:a:1123:U:O4	40:j:9:ARG:NH1	2.41	0.54
5:A:413:C:H2'	5:A:414:A:H8	1.72	0.54
32:b:189:VAL:HG21	32:b:201:VAL:HG23	1.90	0.54
5:A:1523:A:H2'	5:A:1524:A:C8	2.43	0.54
5:A:2242:G:H2'	5:A:2243:A:C8	2.43	0.54
11:G:124:GLU:HG3	11:G:132:ILE:HB	1.90	0.54
31:a:19:U:H2'	31:a:20:C:C6	2.43	0.54
31:a:588:U:H2'	31:a:589:A:H8	1.73	0.54
31:a:754:U:OP1	31:a:819:U:O2'	2.23	0.53
5:A:830:U:H2'	5:A:831:A:C8	2.43	0.53
5:A:365:U:H4'	5:A:366:G:O5'	2.08	0.53
5:A:1172:U:H2'	5:A:1173:G:C4	2.43	0.53
32:b:75:LYS:NZ	32:b:206:ASP:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:72:HIS:CE1	42:l:74:LEU:HB2	2.43	0.53
5:A:830:U:H2'	5:A:831:A:H8	1.73	0.53
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.90	0.53
50:t:39:ILE:HD11	50:t:83:VAL:HG23	1.89	0.53
31:a:1524:C:OP2	51:u:42:THR:HG22	2.09	0.53
32:b:179:LYS:HD2	32:b:197:ASN:HD21	1.73	0.53
11:G:16:THR:HG23	11:G:27:LYS:HB2	1.89	0.53
31:a:435:U:C2	31:a:436:A:C8	2.96	0.53
5:A:533:U:O2'	20:P:49:ASP:OD2	2.18	0.53
5:A:1182:G:H5'	21:Q:83:TYR:CE1	2.44	0.53
5:A:1749:G:N2	5:A:1752:G:OP2	2.36	0.53
31:a:451:U:H2'	31:a:452:A:H8	1.73	0.53
31:a:1388:U:H2'	31:a:1389:G:C8	2.44	0.53
31:a:79:U:H2'	31:a:80:A:H8	1.74	0.53
37:g:2:PRO:O	37:g:3:ARG:HB2	2.09	0.53
39:i:110:GLU:OE1	39:i:113:LYS:NZ	2.37	0.53
31:a:1068:C:H2'	31:a:1069:G:C8	2.43	0.53
48:r:26:ILE:HD12	48:r:27:ASP:N	2.24	0.53
10:F:134:GLU:HA	10:F:149:ILE:HG22	1.92	0.52
31:a:37:G:H2'	31:a:38:C:C6	2.44	0.52
31:a:473:U:H2'	31:a:474:A:H8	1.74	0.52
31:a:1409:C:H2'	31:a:1410:A:C8	2.44	0.52
36:f:10:VAL:HG11	36:f:18:VAL:HG12	1.91	0.52
37:g:71:PRO:HG3	37:g:103:TRP:CZ3	2.44	0.52
49:s:50:SER:HB3	49:s:57:HIS:HB3	1.91	0.52
37:g:90:GLU:OE1	37:g:90:GLU:N	2.42	0.52
5:A:71:G:H2'	5:A:72:C:C6	2.44	0.52
8:D:182:SER:HB3	8:D:191:VAL:HB	1.92	0.52
31:a:588:U:H2'	31:a:589:A:C8	2.43	0.52
31:a:1437:U:H3'	31:a:1438:A:C8	2.44	0.52
43:m:37:VAL:HG12	43:m:39:ILE:HG13	1.92	0.52
52:v:69:U:H2'	52:v:70:A:C8	2.43	0.52
5:A:596:U:H2'	5:A:597:A:C8	2.45	0.52
7:C:179:GLY:O	7:C:269:ARG:NH2	2.43	0.52
5:A:1733:U:H3'	5:A:1734:G:C8	2.45	0.52
10:F:115:ARG:CZ	10:F:177:PHE:HE2	2.22	0.52
11:G:127:THR:OG1	11:G:128:ALA:N	2.43	0.52
32:b:135:GLU:N	32:b:135:GLU:OE1	2.43	0.52
38:h:18:GLN:CG	38:h:71:PRO:HB3	2.39	0.52
5:A:691:A:OP2	7:C:39:ARG:NH1	2.42	0.52
5:A:2533:U:H2'	5:A:2534:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:67:LYS:NZ	23:S:69:PHE:HB2	2.24	0.52
31:a:456:U:H2'	31:a:457:A:H8	1.74	0.52
31:a:534:A:H2'	31:a:535:G:H8	1.75	0.52
39:i:5:TYR:OH	39:i:7:THR:OG1	2.28	0.52
5:A:1111:C:H2'	5:A:1112:G:C8	2.45	0.52
5:A:1529:U:H3'	5:A:1530:A:H8	1.75	0.52
5:A:2674:A:H2'	5:A:2675:A:C8	2.45	0.52
10:F:74:ILE:HB	10:F:79:ILE:HD11	1.91	0.52
31:a:989:U:H4'	31:a:990:G:O5'	2.08	0.52
52:v:8:4SU:OP2	52:v:8:4SU:H6	2.10	0.52
31:a:534:A:H2'	31:a:535:G:C8	2.45	0.52
41:k:49:GLN:HB2	41:k:51:PHE:HE1	1.75	0.52
52:v:74:A:H5'	52:v:75:C:H5'	1.92	0.52
31:a:127:U:H2'	31:a:128:C:C6	2.46	0.51
48:r:21:ILE:HD13	48:r:55:LEU:HD12	1.92	0.51
5:A:2310:A:H2'	5:A:2311:C:C6	2.46	0.51
6:B:16:A:H2'	6:B:17:A:H8	1.75	0.51
31:a:1173:A:H2'	31:a:1174:G:C8	2.45	0.51
38:h:5:ASP:OD2	38:h:8:ALA:HB3	2.11	0.51
5:A:2237:A:H2'	5:A:2238:G:C8	2.46	0.51
5:A:2371:G:H5'	5:A:2372:A:OP2	2.10	0.51
31:a:232:A:H2'	31:a:233:A:C8	2.45	0.51
31:a:674:U:H3	31:a:710:G:H22	1.58	0.51
5:A:1348:A:H2'	5:A:1349:A:C8	2.46	0.51
33:c:80:LYS:NZ	33:c:80:LYS:HB3	2.25	0.51
41:k:80:ASN:OD1	41:k:80:ASN:N	2.42	0.51
5:A:357:C:H2'	5:A:358:A:C8	2.46	0.51
5:A:997:A:H2'	5:A:998:A:C8	2.45	0.51
31:a:184:A:O4'	50:t:84:LYS:NZ	2.41	0.51
31:a:506:A:N3	31:a:540:U:O2'	2.40	0.51
5:A:811:U:H2'	5:A:812:C:H6	1.76	0.51
26:V:32:THR:H	26:V:35:ASN:ND2	2.08	0.51
31:a:686:C:OP1	41:k:45:THR:OG1	2.24	0.51
32:b:33:ILE:O	32:b:34:PHE:CD1	2.61	0.51
32:b:179:LYS:HD2	32:b:197:ASN:ND2	2.25	0.51
5:A:2239:U:H2'	5:A:2240:U:C6	2.45	0.51
55:A:3002:OIY:O43	27:W:2:SER:N	2.44	0.51
10:F:8:TYR:HA	10:F:12:LEU:HD13	1.92	0.51
11:G:84:GLU:HA	11:G:133:LEU:O	2.11	0.51
31:a:1311:C:H2'	31:a:1312:U:C6	2.45	0.51
52:v:12:U:H2'	52:v:13:C:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2798:U:H2'	5:A:2799:C:H6	1.76	0.51
7:C:142:HIS:ND1	7:C:193:GLY:O	2.33	0.51
7:C:181:MET:HE2	7:C:269:ARG:CZ	2.40	0.51
31:a:821:U:H2'	31:a:822:A:C8	2.45	0.51
31:a:386:U:H2'	31:a:387:C:C6	2.45	0.51
34:d:50:GLN:HB3	34:d:54:SER:HB3	1.91	0.51
40:j:10:LEU:HD22	40:j:98:VAL:HG22	1.92	0.51
5:A:593:C:H2'	5:A:594:A:H5''	1.92	0.51
5:A:2070:U:H2'	5:A:2071:U:C6	2.46	0.51
31:a:35:A:H2'	31:a:36:C:H6	1.76	0.51
31:a:1127:A:H2'	31:a:1128:G:C8	2.45	0.51
37:g:32:GLN:O	37:g:35:LYS:HG3	2.11	0.51
5:A:308:U:H2'	5:A:309:G:O4'	2.10	0.50
5:A:637:U:H2'	5:A:638:C:H6	1.75	0.50
31:a:1011:A:C2	31:a:1216:A:H1'	2.46	0.50
36:f:42:TRP:CZ2	36:f:61:LEU:HD12	2.46	0.50
10:F:135:GLN:NE2	10:F:148:ARG:O	2.44	0.50
31:a:190:G:H4'	50:t:59:ASP:HB3	1.93	0.50
31:a:915:A:H2'	31:a:916:A:C8	2.46	0.50
33:c:191:THR:HG22	33:c:192:THR:H	1.77	0.50
5:A:578:U:H2'	5:A:579:C:C6	2.46	0.50
5:A:592:U:H2'	5:A:593:C:C6	2.47	0.50
5:A:2789:G:H2'	5:A:2790:A:C8	2.46	0.50
31:a:649:U:O4	31:a:749:G:O2'	2.27	0.50
34:d:176:ASP:OD1	34:d:178:SER:OG	2.29	0.50
37:g:16:PRO:HA	39:i:44:MET:HE2	1.92	0.50
1:O:26:MET:HE1	1:O:30:MET:HB2	1.91	0.50
7:C:4:GLN:HE22	7:C:18:LYS:HB2	1.77	0.50
18:N:56:ASP:OD1	18:N:57:ALA:N	2.44	0.50
22:R:83:LYS:HB3	22:R:95:ARG:HH12	1.76	0.50
31:a:610:C:H2'	31:a:611:C:C6	2.46	0.50
38:h:74:GLU:OE2	38:h:97:LYS:NZ	2.40	0.50
51:u:14:VAL:HG12	51:u:17:ARG:HH21	1.76	0.50
23:S:43:LYS:O	23:S:47:GLU:HG3	2.12	0.50
31:a:1488:G:H2'	31:a:1489:A:C8	2.46	0.50
5:A:2586:A:H2'	5:A:2587:C:H6	1.76	0.50
23:S:67:LYS:HZ2	23:S:69:PHE:HB2	1.76	0.50
31:a:333:G:H2'	31:a:334:A:C8	2.46	0.50
36:f:40:GLU:OE2	36:f:100:SER:HB3	2.12	0.50
37:g:64:THR:HG22	37:g:68:LYS:NZ	2.26	0.50
47:q:76:LEU:HD12	47:q:77:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2789:G:H2'	5:A:2790:A:H8	1.77	0.50
31:a:218:U:H2'	31:a:219:A:C8	2.47	0.50
31:a:733:C:H2'	31:a:734:A:H8	1.76	0.50
31:a:1461:U:H2'	31:a:1462:A:C8	2.47	0.50
32:b:219:MET:O	32:b:223:ILE:HG22	2.12	0.50
37:g:67:GLU:OE2	37:g:70:ARG:NH1	2.40	0.50
41:k:34:THR:HG23	41:k:35:ASP:O	2.11	0.50
5:A:1568:A:H2'	5:A:1569:A:C8	2.47	0.50
31:a:454:U:H2'	31:a:455:C:C6	2.46	0.50
31:a:1027:U:H5'	31:a:1028:C:O4'	2.12	0.50
35:e:147:THR:OG1	35:e:148:SER:N	2.44	0.50
42:l:33:VAL:HG22	42:l:79:VAL:HG22	1.93	0.50
52:v:44:G:H2'	52:v:45:G:C8	2.47	0.50
5:A:701:U:H2'	5:A:702:G:O4'	2.11	0.50
31:a:218:U:H2'	31:a:219:A:H8	1.76	0.50
32:b:6:VAL:HG11	32:b:214:LEU:HD21	1.93	0.50
34:d:104:VAL:HG13	34:d:109:PHE:HB2	1.93	0.50
31:a:79:U:H2'	31:a:80:A:C8	2.46	0.49
31:a:490:A:H2'	31:a:491:G:C8	2.46	0.49
31:a:821:U:H2'	31:a:822:A:H8	1.77	0.49
32:b:144:GLU:O	32:b:148:ARG:HG2	2.12	0.49
37:g:55:LYS:HE2	37:g:55:LYS:H	1.76	0.49
5:A:478:A:N3	5:A:480:G:H5''	2.27	0.49
5:A:605:U:C5	5:A:618:G:C5	3.00	0.49
10:F:56:ASP:O	10:F:60:ILE:HG13	2.12	0.49
31:a:818:G:H2'	31:a:819:U:C6	2.48	0.49
41:k:63:GLN:O	41:k:67:GLU:HG3	2.12	0.49
5:A:869:U:H2'	5:A:870:U:C6	2.47	0.49
31:a:536:A:H2'	31:a:537:G:C8	2.46	0.49
31:a:1449:A:H2'	31:a:1450:A:C8	2.47	0.49
5:A:944:A:H2'	5:A:945:C:C6	2.46	0.49
5:A:1535:U:H2'	5:A:1536:G:C8	2.47	0.49
5:A:1849:A:H2'	5:A:1850:A:C8	2.48	0.49
31:a:650:A:C6	38:h:57:LYS:HG3	2.47	0.49
33:c:25:ASN:HB2	33:c:28:GLN:OE1	2.11	0.49
52:v:15:G:C6	52:v:49:C:O2	2.66	0.49
5:A:1193:U:H2'	5:A:1194:U:C6	2.48	0.49
8:D:42:GLU:OE2	8:D:42:GLU:N	2.46	0.49
37:g:70:ARG:HH21	37:g:97:THR:HG23	1.78	0.49
5:A:1464:A:H2'	5:A:1465:A:H8	1.77	0.49
5:A:2525:G:H5''	5:A:2526:A:H5''	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2644:G:N7	55:A:3005:OIY:N52	2.60	0.49
31:a:661:G:H22	31:a:738:G:H1	1.58	0.49
31:a:839:U:H1'	31:a:841:G:H1	1.78	0.49
31:a:973:G:OP2	31:a:1355:U:O2'	2.29	0.49
35:e:71:ILE:HG12	35:e:140:PHE:CZ	2.47	0.49
5:A:2651:G:O2'	5:A:2660:G:O6	2.25	0.49
8:D:85:VAL:HG21	8:D:90:LEU:HD13	1.94	0.49
16:L:1:MET:O	16:L:2:LEU:HB2	2.12	0.49
31:a:82:C:H2'	31:a:84:U:H3	1.78	0.49
33:c:36:ASP:OD1	33:c:59:ARG:NH2	2.45	0.49
5:A:1794:U:OP2	7:C:273:VAL:HB	2.13	0.49
8:D:13:THR:OG1	8:D:14:ARG:N	2.45	0.49
31:a:1378:U:H2'	31:a:1379:C:C6	2.48	0.49
31:a:1427:C:H2'	31:a:1428:A:C8	2.47	0.49
34:d:16:GLY:O	34:d:46:ARG:NH2	2.39	0.49
35:e:44:ARG:HH11	35:e:72:THR:HG22	1.78	0.49
5:A:844:A:H4'	5:A:845:A:O5'	2.13	0.49
5:A:2324:A:H2'	5:A:2325:A:H8	1.76	0.49
31:a:692:A:H2'	31:a:693:A:C8	2.48	0.49
31:a:1488:G:H2'	31:a:1489:A:H8	1.78	0.49
52:v:20:H2U:OP2	52:v:20:H2U:H3'	2.12	0.49
31:a:36:C:H2'	31:a:37:G:H8	1.78	0.49
32:b:17:HIS:HB3	32:b:45:LEU:HD21	1.94	0.49
33:c:210:GLY:O	33:c:214:VAL:HG23	2.13	0.49
37:g:49:ARG:O	37:g:52:GLU:HG3	2.13	0.49
40:j:15:HIS:HA	40:j:18:ILE:HG22	1.95	0.49
5:A:698:G:O2'	5:A:1630:A:N3	2.44	0.48
31:a:242:A:C2	31:a:278:A:C5	3.00	0.48
31:a:251:G:H2'	31:a:252:U:C6	2.48	0.48
31:a:942:G:C2	31:a:943:A:C8	3.01	0.48
3:2:33:THR:OG1	5:A:2416:C:OP1	2.25	0.48
5:A:1411:G:H2'	5:A:1412:C:C6	2.48	0.48
5:A:1844:A:H2'	5:A:1845:G:H8	1.78	0.48
5:A:2797:G:H2'	5:A:2798:U:C6	2.48	0.48
31:a:231:U:H2'	31:a:232:A:C8	2.48	0.48
31:a:436:A:C4	31:a:437:A:C8	3.01	0.48
44:n:6:MET:SD	44:n:9:ARG:NH2	2.86	0.48
52:v:9:A:O2'	52:v:10:G:N7	2.43	0.48
1:0:6:ARG:HG2	1:0:50:ILE:HD12	1.95	0.48
5:A:101:U:H2'	5:A:102:A:C8	2.48	0.48
5:A:157:U:H2'	5:A:158:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1481:U:H2'	5:A:1482:C:C6	2.48	0.48
5:A:1491:A:H2'	5:A:1493:C:C5	2.49	0.48
5:A:2034:G:H2'	5:A:2035:U:O4'	2.14	0.48
41:k:81:LEU:HD22	41:k:104:TYR:HB3	1.95	0.48
52:v:15:G:N2	52:v:60:G:C5	2.82	0.48
52:v:24:A:H2'	52:v:25:G:C8	2.48	0.48
5:A:1243:G:C4	9:E:82:LYS:HE2	2.48	0.48
11:G:51:GLN:OE1	11:G:51:GLN:HA	2.12	0.48
55:N:201:OIY:O20	55:N:201:OIY:O19	2.31	0.48
31:a:58:U:H2'	31:a:59:G:C8	2.48	0.48
32:b:9:ARG:NH2	32:b:13:GLN:HG2	2.27	0.48
34:d:199:GLU:HA	34:d:202:ILE:HD12	1.96	0.48
36:f:14:GLN:O	36:f:18:VAL:HG13	2.12	0.48
31:a:1002:A:C5	31:a:1003:C:H1'	2.48	0.48
32:b:58:PHE:HD2	32:b:186:ILE:HD11	1.78	0.48
5:A:1843:A:H2'	5:A:1844:A:C8	2.49	0.48
12:H:54:LEU:HA	12:H:57:GLN:OE1	2.14	0.48
27:W:39:TRP:HE1	27:W:41:GLU:HG2	1.78	0.48
34:d:36:ASN:HA	34:d:46:ARG:HD2	1.95	0.48
34:d:158:LYS:O	34:d:161:ILE:HG13	2.13	0.48
11:G:43:LEU:O	11:G:44:LYS:HD2	2.14	0.48
18:N:63:THR:OG1	18:N:66:ASN:ND2	2.47	0.48
31:a:58:U:H2'	31:a:59:G:H8	1.78	0.48
31:a:450:C:H2'	31:a:451:U:H6	1.79	0.48
31:a:943:A:H2'	31:a:944:G:H8	1.78	0.48
5:A:1681:U:H2'	5:A:1682:A:C8	2.49	0.48
5:A:2548:OMU:H6	5:A:2548:OMU:O5'	2.13	0.48
10:F:57:MET:SD	10:F:87:CYS:HB3	2.53	0.48
36:f:42:TRP:HB2	36:f:59:TYR:HB2	1.96	0.48
41:k:60:PHE:O	41:k:64:VAL:HG23	2.14	0.48
10:F:4:LEU:HA	10:F:7:ARG:HB3	1.95	0.48
15:K:2:THR:OG1	15:K:3:LEU:N	2.43	0.48
16:L:51:ARG:HD3	16:L:66:ILE:HD11	1.95	0.48
31:a:499:A:OP1	42:l:115:SER:OG	2.22	0.48
32:b:14:ALA:HA	32:b:210:ARG:NH1	2.29	0.48
37:g:70:ARG:HG2	37:g:96:ARG:HB3	1.95	0.48
42:l:42:PRO:HB3	42:l:89:ASP:OD1	2.13	0.48
5:A:782:G:H5'	5:A:783:G:OP1	2.14	0.47
5:A:2880:U:H1'	30:Z:49:ARG:HD3	1.95	0.47
11:G:23:GLN:NE2	11:G:34:SER:OG	2.44	0.47
31:a:734:A:H2'	31:a:735:U:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:28:C:H2'	52:v:29:C:H6	1.79	0.47
5:A:1482:C:H2'	5:A:1483:U:O4'	2.15	0.47
7:C:4:GLN:HE21	7:C:18:LYS:NZ	2.12	0.47
31:a:577:C:H2'	31:a:578:G:O4'	2.14	0.47
52:v:18:G:H1	52:v:56:PSU:HO2'	1.57	0.47
52:v:35:C:H2'	52:v:36:A:C8	2.49	0.47
1:0:26:MET:CE	1:0:30:MET:HB2	2.44	0.47
5:A:521:G:H2'	5:A:522:C:C6	2.49	0.47
5:A:831:A:H2'	5:A:832:G:C8	2.50	0.47
5:A:1605:G:N3	5:A:1605:G:H2'	2.30	0.47
6:B:112:A:H2'	6:B:113:G:C8	2.50	0.47
11:G:47:GLU:CD	11:G:48:GLY:N	2.70	0.47
31:a:208:G:H2'	31:a:209:A:H8	1.79	0.47
42:l:87:VAL:HG21	42:l:90:LEU:HB2	1.95	0.47
5:A:1025:A:N6	5:A:1122:G:H2'	2.30	0.47
5:A:1311:A:H2'	5:A:1312:G:H8	1.79	0.47
8:D:196:ILE:HD12	8:D:204:VAL:HG11	1.97	0.47
31:a:395:G:H2'	31:a:396:C:C6	2.49	0.47
5:A:811:U:H2'	5:A:812:C:C6	2.49	0.47
5:A:862:G:H2'	5:A:863:C:C6	2.49	0.47
5:A:2457:A:H2'	5:A:2458:C:C6	2.48	0.47
31:a:542:C:H5'	34:d:71:GLU:HB2	1.96	0.47
33:c:86:LYS:O	33:c:90:GLU:HG2	2.14	0.47
37:g:49:ARG:NH1	37:g:118:LEU:HD12	2.30	0.47
38:h:50:GLU:HG2	38:h:61:THR:HB	1.95	0.47
1:0:6:ARG:HG3	1:0:6:ARG:HH11	1.78	0.47
5:A:568:G:H2'	5:A:2026:6MZ:N7	2.30	0.47
5:A:1311:A:H2'	5:A:1312:G:C8	2.50	0.47
5:A:1356:G:H2'	5:A:1357:C:C6	2.49	0.47
9:E:1:MET:HE1	9:E:18:PHE:C	2.40	0.47
10:F:11:GLU:HB2	10:F:15:LYS:HE3	1.96	0.47
31:a:30:A:O2'	31:a:292:U:OP1	2.29	0.47
31:a:1311:C:H2'	31:a:1312:U:H6	1.78	0.47
38:h:106:SER:HB2	38:h:127:ILE:HD11	1.97	0.47
47:q:58:ASP:OD2	47:q:83:ALA:N	2.48	0.47
5:A:655:U:H2'	5:A:656:U:C6	2.49	0.47
5:A:740:G:H2'	5:A:741:U:H6	1.78	0.47
5:A:2021:C:H2'	5:A:2022:U:C6	2.49	0.47
5:A:2341:A:N3	5:A:2377:A:H2'	2.30	0.47
10:F:50:LEU:O	10:F:54:VAL:HG23	2.15	0.47
16:L:43:THR:HG22	16:L:94:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:36:GLY:HA3	25:U:97:ARG:HB2	1.96	0.47
31:a:409:G:N2	31:a:424:G:H1'	2.30	0.47
31:a:693:A:H2'	31:a:694:U:H6	1.79	0.47
5:A:34:G:N2	5:A:511:G:H1'	2.30	0.47
5:A:846:U:H2'	5:A:847:A:C8	2.49	0.47
5:A:868:U:OP1	16:L:6:ARG:NH2	2.47	0.47
5:A:2553:G:H2'	5:A:2554:C:C6	2.50	0.47
15:K:82:SER:HB3	15:K:116:GLY:HA3	1.97	0.47
22:R:73:THR:HB	22:R:106:LYS:HB2	1.96	0.47
52:v:60:G:H2'	52:v:61:U:O4'	2.14	0.47
5:A:1503:C:O2'	5:A:1505:A:N7	2.48	0.47
5:A:2730:A:H2'	5:A:2731:G:O4'	2.15	0.47
19:O:91:ARG:NH1	19:O:115:GLU:HB2	2.30	0.47
4:3:25:VAL:HB	4:3:35:GLN:HB2	1.96	0.46
12:H:54:LEU:HD12	12:H:57:GLN:HE22	1.80	0.46
32:b:149:SER:HB2	32:b:150:LEU:HD12	1.98	0.46
5:A:2273:G:OP2	26:V:10:THR:HG21	2.15	0.46
31:a:206:C:H4'	31:a:207:G:H5'	1.97	0.46
31:a:1521:C:H2'	31:a:1522:G:C8	2.50	0.46
32:b:123:SER:CB	32:b:143:MET:HE1	2.45	0.46
5:A:2229:U:H2'	5:A:2230:G:C8	2.50	0.46
18:N:1:MET:HB3	18:N:1:MET:HE2	1.82	0.46
21:Q:40:MET:HE3	21:Q:49:ILE:HG12	1.96	0.46
31:a:35:A:H2'	31:a:36:C:C6	2.50	0.46
31:a:930:G:O6	37:g:3:ARG:NH2	2.49	0.46
32:b:10:ASP:O	32:b:13:GLN:HG3	2.15	0.46
38:h:5:ASP:HB2	38:h:82:PRO:HG2	1.98	0.46
5:A:418:U:H2'	5:A:419:C:H6	1.80	0.46
5:A:574:U:H2'	5:A:575:G:C8	2.51	0.46
5:A:1509:U:H2'	5:A:1510:G:H5'	1.97	0.46
5:A:1529:U:H3'	5:A:1530:A:C8	2.51	0.46
5:A:2827:G:O2'	5:A:2880:U:OP1	2.26	0.46
10:F:93:GLY:O	10:F:96:MET:HG2	2.15	0.46
31:a:18:A:H8	31:a:1077:A:O2'	1.98	0.46
31:a:1433:U:H2'	31:a:1434:A:C8	2.51	0.46
32:b:48:THR:OG1	32:b:203:PRO:O	2.33	0.46
34:d:8:LYS:HB2	34:d:21:LEU:HG	1.97	0.46
36:f:32:ALA:O	36:f:33:ASP:HB2	2.15	0.46
52:v:13:C:H2'	52:v:14:A:H5''	1.97	0.46
5:A:1381:A:H2'	5:A:1382:U:C6	2.51	0.46
5:A:1843:A:H2'	5:A:1844:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:38:HIS:HB3	11:G:41:VAL:HG23	1.98	0.46
20:P:78:ARG:HA	20:P:78:ARG:HD3	1.66	0.46
31:a:818:G:H2'	31:a:819:U:H6	1.80	0.46
39:i:79:HIS:O	39:i:83:ARG:HG3	2.14	0.46
5:A:177:G:H2'	5:A:178:U:C6	2.50	0.46
5:A:580:A:H2'	5:A:581:G:C8	2.51	0.46
5:A:1681:U:H2'	5:A:1682:A:H8	1.80	0.46
5:A:2509:A:H2'	5:A:2510:U:C6	2.51	0.46
10:F:119:ALA:HB2	10:F:177:PHE:CE1	2.50	0.46
16:L:6:ARG:HB2	16:L:6:ARG:NH1	2.31	0.46
15:K:131:LYS:HB2	15:K:131:LYS:HE2	1.76	0.46
31:a:434:U:H5''	34:d:122:HIS:HB3	1.97	0.46
31:a:1036:U:H2'	31:a:1037:A:C8	2.51	0.46
37:g:72:MET:SD	37:g:72:MET:N	2.84	0.46
42:l:36:ARG:HG2	42:l:38:TYR:HD1	1.79	0.46
42:l:59:SER:HB2	42:l:61:PHE:HD2	1.81	0.46
52:v:71:G:O2'	52:v:72:C:H5'	2.15	0.46
5:A:1380:A:O2'	5:A:1391:U:O2	2.33	0.46
5:A:2451:G:H2'	5:A:2452:C:C6	2.51	0.46
5:A:2586:A:H2'	5:A:2587:C:C6	2.49	0.46
7:C:198:GLN:N	7:C:198:GLN:OE1	2.48	0.46
11:G:98:VAL:HG12	11:G:125:THR:HG23	1.98	0.46
31:a:1057:U:P	44:n:85:ARG:HH22	2.39	0.46
7:C:5:LYS:HB2	7:C:17:GLU:CD	2.40	0.46
28:X:6:LEU:HA	28:X:9:LYS:HD2	1.98	0.46
31:a:454:U:H2'	31:a:455:C:H6	1.81	0.46
31:a:908:U:H2'	31:a:909:C:C6	2.50	0.46
31:a:997:U:H2'	31:a:998:A:H8	1.81	0.46
32:b:145:LYS:HA	32:b:145:LYS:HD3	1.82	0.46
32:b:188:ILE:HD13	32:b:202:ILE:HB	1.98	0.46
36:f:16:ASP:OD1	36:f:17:GLN:N	2.49	0.46
4:3:23:ILE:HD13	5:A:1029:A:H1'	1.98	0.46
5:A:2645:C:H2'	5:A:2646:U:H6	1.80	0.46
19:O:88:GLU:N	19:O:88:GLU:OE2	2.48	0.46
31:a:472:A:H2'	31:a:473:U:C6	2.51	0.46
32:b:173:ILE:O	32:b:177:GLU:HG2	2.15	0.46
43:m:34:LEU:HD22	43:m:39:ILE:HB	1.98	0.46
5:A:363:G:OP2	5:A:364:A:O2'	2.33	0.45
5:A:2747:G:H4'	11:G:4:VAL:HG23	1.98	0.45
6:B:16:A:H2'	6:B:17:A:C8	2.50	0.45
31:a:877:C:OP1	42:l:5:ASN:ND2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:919:G:H2'	31:a:920:A:C8	2.51	0.45
34:d:62:LYS:O	34:d:66:ILE:HG13	2.17	0.45
42:l:34:CYS:HA	42:l:55:VAL:HA	1.98	0.45
5:A:1171:U:H3'	5:A:1172:U:H6	1.81	0.45
5:A:1193:U:C2	5:A:1194:U:C5	3.04	0.45
5:A:2301:U:H2'	5:A:2302:C:C6	2.50	0.45
5:A:2469:U:H2'	5:A:2469:U:O2	2.15	0.45
11:G:2:SER:O	11:G:6:LYS:HG2	2.15	0.45
18:N:69:ALA:O	18:N:73:VAL:HG23	2.16	0.45
28:X:10:SER:H	28:X:13:GLU:CD	2.25	0.45
49:s:30:PRO:HA	49:s:48:THR:HG23	1.98	0.45
5:A:284:U:H2'	5:A:285:A:C8	2.51	0.45
5:A:1172:U:H3'	5:A:1173:G:C8	2.52	0.45
6:B:43:A:C4	6:B:44:A:C8	3.05	0.45
7:C:173:ILE:HG23	7:C:268:ILE:HD13	1.97	0.45
7:C:260:ASN:HD21	7:C:263:THR:HG23	1.82	0.45
13:I:98:GLU:CD	13:I:98:GLU:H	2.24	0.45
16:L:63:LYS:HB3	16:L:63:LYS:HE2	1.68	0.45
20:P:58:ARG:HA	20:P:61:TRP:CE3	2.51	0.45
32:b:6:VAL:HG12	32:b:10:ASP:HB2	1.99	0.45
37:g:51:GLN:O	37:g:55:LYS:HA	2.16	0.45
47:q:24:VAL:HG11	47:q:62:ILE:HD13	1.97	0.45
5:A:1344:C:C2	5:A:1345:C:C5	3.05	0.45
10:F:132:LEU:HD23	10:F:152:MET:HE3	1.99	0.45
31:a:380:C:H2'	31:a:381:C:H6	1.80	0.45
33:c:81:GLY:O	33:c:84:ILE:HG13	2.17	0.45
47:q:80:VAL:HG12	47:q:81:GLU:HG3	1.98	0.45
52:v:51:C:H2'	52:v:52:A:H8	1.81	0.45
5:A:837:U:H2'	5:A:838:C:C6	2.52	0.45
5:A:2502:U:O2'	5:A:2503:C:OP1	2.26	0.45
12:H:5:LEU:HD12	12:H:17:ASP:HB2	1.99	0.45
31:a:887:G:H4'	31:a:888:U:O5'	2.17	0.45
32:b:185:VAL:N	32:b:199:ASP:OD1	2.41	0.45
5:A:1406:G:H2'	5:A:1407:U:C6	2.52	0.45
6:B:22:G:N7	6:B:54:G:H2'	2.32	0.45
31:a:1001:A:C8	31:a:1023:G:C8	3.05	0.45
32:b:83:ARG:O	32:b:87:GLN:HG2	2.17	0.45
34:d:89:GLY:HA3	34:d:199:GLU:HG3	1.99	0.45
35:e:110:MET:HE3	35:e:110:MET:HB2	1.64	0.45
49:s:29:LYS:NZ	49:s:29:LYS:HB3	2.30	0.45
5:A:687:A:H2'	5:A:688:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1194:U:H2'	5:A:1195:C:H6	1.82	0.45
5:A:1597:U:H2'	5:A:1598:C:H6	1.82	0.45
21:Q:28:GLU:CD	21:Q:29:SER:H	2.25	0.45
27:W:36:HIS:HD2	27:W:56:MET:SD	2.39	0.45
30:Z:52:GLN:OE1	30:Z:54:PHE:N	2.50	0.45
31:a:1038:G:H2'	31:a:1039:A:H8	1.81	0.45
31:a:1118:U:H2'	31:a:1119:U:C6	2.52	0.45
31:a:1425:A:H2'	31:a:1426:C:C6	2.52	0.45
32:b:141:ARG:O	32:b:145:LYS:HG2	2.17	0.45
5:A:86:C:HO2'	5:A:348:A:H8	1.61	0.45
5:A:234:A:C2	5:A:2403:A:H1'	2.52	0.45
5:A:2262:A:H4'	5:A:2263:A:N3	2.32	0.45
31:a:231:U:H2'	31:a:232:A:H8	1.82	0.45
31:a:552:U:H2'	31:a:553:C:C6	2.51	0.45
36:f:15:SER:O	36:f:18:VAL:HG22	2.16	0.45
43:m:12:ASN:OD1	43:m:46:ARG:NH1	2.50	0.45
5:A:1867:A:H2'	5:A:1868:A:C8	2.52	0.45
5:A:2533:U:H2'	5:A:2534:C:H6	1.81	0.45
27:W:17:ASN:OD1	27:W:27:ARG:HD2	2.17	0.45
31:a:380:C:H2'	31:a:381:C:C6	2.52	0.45
31:a:521:G:H2'	31:a:522:C:C6	2.52	0.45
43:m:27:ARG:O	43:m:31:LYS:HG3	2.16	0.45
5:A:46:G:H2'	5:A:47:U:C6	2.52	0.45
5:A:189:A:H2'	5:A:190:C:C6	2.52	0.45
5:A:1567:A:OP1	7:C:61:HIS:NE2	2.38	0.45
5:A:2784:C:H2'	5:A:2785:C:C6	2.51	0.45
9:E:122:GLU:OE1	9:E:123:PHE:N	2.48	0.45
52:v:19:G:H3'	52:v:20:H2U:C2'	2.41	0.45
5:A:1680:G:H2'	5:A:1681:U:H6	1.82	0.44
31:a:367:A:H2'	31:a:368:C:O4'	2.17	0.44
31:a:536:A:H2'	31:a:537:G:H8	1.83	0.44
52:v:14:A:C6	52:v:15:G:H1'	2.52	0.44
52:v:15:G:O6	52:v:49:C:O2	2.35	0.44
31:a:887:G:H1'	31:a:903:A:N6	2.32	0.44
32:b:37:ARG:H	32:b:42:ILE:HG12	1.82	0.44
24:T:32:VAL:HG13	24:T:63:LEU:HD12	1.99	0.44
28:X:41:HIS:HA	28:X:44:GLN:HG3	1.97	0.44
31:a:200:G:H2'	31:a:201:A:O4'	2.16	0.44
31:a:470:G:H2'	31:a:471:G:H8	1.77	0.44
35:e:40:ASP:OD1	35:e:42:ASN:N	2.34	0.44
5:A:189:A:H2'	5:A:190:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:669:C:H2'	5:A:670:C:C6	2.53	0.44
11:G:4:VAL:O	11:G:69:ARG:HD2	2.16	0.44
21:Q:37:ASP:OD1	21:Q:37:ASP:N	2.37	0.44
31:a:37:G:O2'	42:l:115:SER:O	2.32	0.44
31:a:378:A:H2'	31:a:379:A:C8	2.52	0.44
31:a:734:A:H2'	31:a:735:U:C6	2.51	0.44
37:g:115:THR:HG22	37:g:117:ALA:N	2.31	0.44
40:j:23:GLN:OE1	40:j:23:GLN:HA	2.18	0.44
1:O:6:ARG:HG3	1:O:50:ILE:HA	1.99	0.44
10:F:31:ILE:HG13	10:F:96:MET:HE1	1.99	0.44
11:G:71:VAL:O	11:G:75:LEU:HG	2.17	0.44
31:a:78:G:H2'	31:a:79:U:H6	1.79	0.44
31:a:402:G:H21	34:d:118:GLN:HE22	1.64	0.44
31:a:766:G:H4'	31:a:1510:A:H4'	1.99	0.44
31:a:886:A:H5'	31:a:888:U:H1'	2.00	0.44
31:a:1070:U:O2	32:b:105:ASN:ND2	2.49	0.44
34:d:170:PRO:HB2	34:d:172:TRP:CZ3	2.52	0.44
41:k:20:ALA:HB3	41:k:83:VAL:HG22	1.99	0.44
5:A:715:C:H2'	5:A:716:A:O4'	2.16	0.44
7:C:181:MET:CB	7:C:269:ARG:HH12	2.30	0.44
31:a:1056:C:O2'	44:n:85:ARG:NH1	2.51	0.44
32:b:75:LYS:H	32:b:75:LYS:HG3	1.63	0.44
32:b:167:ASP:OD1	32:b:170:HIS:N	2.40	0.44
47:q:76:LEU:HD12	47:q:77:VAL:H	1.83	0.44
5:A:1844:A:H2'	5:A:1845:G:C8	2.53	0.44
8:D:26:THR:HG21	8:D:196:ILE:HG12	1.98	0.44
11:G:43:LEU:HD11	11:G:50:LEU:HD23	1.99	0.44
21:Q:21:LYS:HG2	21:Q:93:PHE:CD1	2.53	0.44
32:b:81:ILE:HG21	32:b:213:THR:HA	1.98	0.44
37:g:13:LEU:HD23	37:g:14:PRO:O	2.18	0.44
37:g:135:ILE:HD12	37:g:138:ARG:HG2	1.99	0.44
52:v:15:G:H22	52:v:49:C:N4	2.16	0.44
5:A:908:A:H2'	5:A:909:A:C8	2.53	0.44
5:A:1537:C:H3'	5:A:1538:A:H8	1.83	0.44
5:A:2727:G:H2'	5:A:2728:G:C8	2.52	0.44
10:F:5:LYS:HD3	10:F:97:TYR:CE2	2.53	0.44
10:F:120:LYS:O	10:F:122:PHE:N	2.51	0.44
12:H:1:MET:HG2	12:H:23:ALA:HA	2.00	0.44
31:a:83:U:OP2	31:a:84:U:N3	2.50	0.44
31:a:1140:G:H2'	31:a:1141:G:H8	1.83	0.44
40:j:85:ASP:OD1	40:j:85:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:51:PHE:HB3	41:k:55:ARG:HB3	1.99	0.44
44:n:56:SER:OG	44:n:58:VAL:HG22	2.17	0.44
47:q:26:ILE:HB	47:q:43:THR:HG23	1.99	0.44
5:A:727:G:C8	7:C:207:LYS:HD2	2.53	0.44
5:A:780:A:C2	7:C:225:MET:HG2	2.53	0.44
5:A:1427:G:H2'	5:A:1428:A:C8	2.53	0.44
5:A:1844:A:H2'	5:A:1845:G:O4'	2.18	0.44
31:a:905:A:H2'	31:a:906:A:H8	1.82	0.44
31:a:1493:C:H2'	31:a:1494:G:O4'	2.18	0.44
36:f:38:ARG:HB3	36:f:63:ASN:HB2	1.99	0.44
43:m:39:ILE:HD12	43:m:56:ILE:HD11	1.99	0.44
44:n:83:LYS:HD3	44:n:83:LYS:HA	1.77	0.44
48:r:50:ARG:HG3	48:r:53:ARG:NH2	2.33	0.44
5:A:215:C:H2'	5:A:216:C:H6	1.82	0.43
5:A:358:A:H2'	5:A:359:U:C6	2.53	0.43
5:A:1314:C:O2'	5:A:1315:C:H5'	2.18	0.43
5:A:2269:A:H2'	5:A:2270:A:C8	2.53	0.43
5:A:2287:U:H2'	5:A:2288:G:H8	1.81	0.43
8:D:58:GLU:CD	8:D:58:GLU:H	2.26	0.43
10:F:141:ILE:HD13	10:F:145:LYS:HB2	2.00	0.43
31:a:177:A:C6	31:a:191:A:C8	3.06	0.43
31:a:211:C:H2'	31:a:212:U:C6	2.53	0.43
31:a:1335:G:H2'	31:a:1336:A:C8	2.53	0.43
31:a:1510:A:H2'	31:a:1511:G:C8	2.53	0.43
32:b:159:LEU:HD13	32:b:181:LEU:HD13	2.00	0.43
52:v:54:G:H3'	52:v:55:5MU:H73	2.00	0.43
5:A:1577:A:H2'	5:A:1578:A:C8	2.53	0.43
5:A:1597:U:H2'	5:A:1598:C:C6	2.53	0.43
5:A:1732:C:H2'	5:A:1733:U:C6	2.52	0.43
5:A:2456:U:C2	5:A:2457:A:C8	3.06	0.43
31:a:572:G:O2'	31:a:818:G:OP2	2.32	0.43
31:a:905:A:H2'	31:a:906:A:C8	2.52	0.43
5:A:9:G:H2'	5:A:10:U:C6	2.53	0.43
5:A:712:U:OP2	45:o:88:ARG:NH1	2.50	0.43
5:A:1193:U:H2'	5:A:1194:U:H6	1.83	0.43
5:A:1316:A:C4	5:A:1317:A:C8	3.07	0.43
5:A:1786:U:H2'	5:A:1787:A:C5	2.52	0.43
5:A:2611:U:C2	30:Z:4:GLN:HA	2.54	0.43
10:F:115:ARG:HG2	10:F:115:ARG:HH11	1.83	0.43
16:L:48:GLU:OE1	16:L:51:ARG:NH2	2.39	0.43
18:N:98:TYR:OH	18:N:110:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:295:G:H2'	31:a:296:A:C8	2.53	0.43
31:a:1117:C:H2'	31:a:1118:U:H6	1.82	0.43
31:a:1117:C:H2'	31:a:1118:U:C6	2.53	0.43
5:A:12:A:H2'	5:A:13:A:H8	1.80	0.43
5:A:1489:A:H2'	5:A:1490:A:C8	2.54	0.43
6:B:58:C:H2'	6:B:59:C:C6	2.54	0.43
10:F:136:ILE:O	10:F:137:VAL:HB	2.17	0.43
10:F:137:VAL:HG12	10:F:137:VAL:O	2.18	0.43
31:a:1448:C:H5	31:a:1449:A:C4	2.37	0.43
5:A:86:C:O2'	5:A:348:A:H8	2.01	0.43
5:A:1880:G:O2'	5:A:1881:A:H8	2.01	0.43
7:C:265:LYS:HE2	7:C:266:MET:HE2	1.99	0.43
28:X:48:LYS:O	28:X:52:ARG:HG3	2.18	0.43
31:a:81:G:H3'	31:a:82:C:H6	1.84	0.43
31:a:260:A:H4'	47:q:66:ARG:HD2	1.99	0.43
31:a:346:G:H2'	31:a:347:G:C8	2.53	0.43
35:e:70:MET:HE3	35:e:70:MET:HB3	1.79	0.43
5:A:148:A:OP2	5:A:148:A:H8	2.01	0.43
5:A:1583:C:H3'	5:A:1584:A:C8	2.53	0.43
5:A:2451:G:H2'	5:A:2452:C:H6	1.83	0.43
5:A:2893:U:H2'	5:A:2894:U:C6	2.54	0.43
31:a:184:A:C8	50:t:84:LYS:HD2	2.53	0.43
31:a:886:A:H4'	31:a:887:G:OP1	2.18	0.43
31:a:1116:C:H2'	31:a:1117:C:H6	1.83	0.43
33:c:37:LEU:HD13	44:n:66:LEU:HD11	1.99	0.43
34:d:60:LYS:O	34:d:64:ARG:HG2	2.18	0.43
5:A:68:A:O3'	28:X:32:LYS:NZ	2.43	0.43
5:A:478:A:H4'	5:A:479:A:OP1	2.18	0.43
5:A:1885:A:H2'	5:A:1886:A:H8	1.83	0.43
5:A:2420:C:OP2	5:A:2421:A:H2'	2.19	0.43
6:B:37:U:H2'	6:B:38:U:C2	2.54	0.43
20:P:86:ALA:HB2	20:P:116:ALA:HB2	1.99	0.43
21:Q:75:ILE:HG13	21:Q:86:GLN:HG2	2.00	0.43
31:a:838:U:H3'	31:a:839:U:O2	2.19	0.43
32:b:66:LYS:O	32:b:66:LYS:HG3	2.19	0.43
5:A:2060:C:H2'	5:A:2061:C:H6	1.83	0.43
5:A:2313:C:H2'	5:A:2314:G:C8	2.54	0.43
6:B:60:U:H2'	6:B:61:C:C6	2.54	0.43
11:G:42:GLU:OE2	11:G:55:ALA:N	2.52	0.43
31:a:180:U:C2	31:a:181:C:C5	3.06	0.43
37:g:115:THR:HG22	37:g:117:ALA:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:102:A:H2'	5:A:103:U:C6	2.54	0.43
5:A:1394:C:H2'	5:A:1395:A:H8	1.84	0.43
31:a:122:A:OP1	31:a:602:U:O2'	2.25	0.43
31:a:409:G:O6	34:d:33:LYS:HB2	2.18	0.43
32:b:85:GLN:HG2	32:b:216:ALA:C	2.43	0.43
5:A:1442:C:H2'	5:A:1443:U:C6	2.54	0.43
5:A:1513:A:C2'	5:A:1514:U:H5'	2.49	0.43
7:C:108:LYS:HD2	7:C:198:GLN:NE2	2.33	0.43
31:a:37:G:H2'	31:a:38:C:H6	1.84	0.43
31:a:1023:G:N3	31:a:1023:G:H2'	2.34	0.43
32:b:43:ILE:H	32:b:43:ILE:HG13	1.68	0.43
34:d:172:TRP:CD1	34:d:188:PRO:HD3	2.54	0.43
34:d:196:GLU:OE2	34:d:196:GLU:N	2.38	0.43
52:v:40:U:H2'	52:v:41:G:H8	1.83	0.43
5:A:161:A:H2'	5:A:162:A:C8	2.54	0.42
5:A:279:U:H2'	5:A:364:A:N6	2.34	0.42
5:A:1004:C:OP1	13:I:37:ARG:NH1	2.48	0.42
5:A:1048:G:H2'	5:A:1049:C:O4'	2.19	0.42
5:A:1164:G:H2'	5:A:1165:U:C6	2.54	0.42
24:T:3:LYS:HD2	24:T:3:LYS:HA	1.86	0.42
33:c:110:ASP:OD2	33:c:140:ASN:HB3	2.18	0.42
50:t:78:ARG:O	50:t:82:GLN:HG3	2.19	0.42
5:A:2212:G:H2'	5:A:2213:G:C8	2.54	0.42
5:A:2663:C:H2'	5:A:2664:A:O4'	2.19	0.42
6:B:12:U:OP2	6:B:68:C:O2'	2.37	0.42
31:a:407:A:O2'	34:d:33:LYS:NZ	2.51	0.42
31:a:880:C:O2'	31:a:881:U:H5'	2.19	0.42
31:a:1145:U:H2'	31:a:1146:U:O4'	2.19	0.42
32:b:219:MET:HA	32:b:219:MET:HE2	2.01	0.42
36:f:72:ASP:OD1	36:f:72:ASP:N	2.52	0.42
42:l:57:LEU:HD11	42:l:82:ILE:HD11	2.01	0.42
5:A:138:A:H2'	5:A:139:C:H6	1.85	0.42
5:A:288:U:H2'	5:A:289:G:C8	2.54	0.42
5:A:2232:U:H2'	5:A:2233:G:O4'	2.19	0.42
18:N:44:ASP:OD1	18:N:46:GLY:N	2.52	0.42
27:W:67:VAL:O	27:W:71:LEU:HG	2.20	0.42
31:a:511:U:N3	31:a:512:G:N7	2.67	0.42
31:a:675:U:H2'	31:a:676:C:H6	1.84	0.42
31:a:789:A:H1'	31:a:790:U:OP2	2.19	0.42
31:a:1024:C:H2'	31:a:1025:C:C6	2.54	0.42
5:A:669:C:H2'	5:A:670:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:57:MET:HE2	10:F:89:VAL:HG22	2.01	0.42
11:G:33:LEU:HD13	11:G:75:LEU:HD22	2.01	0.42
18:N:98:TYR:CE2	18:N:103:LYS:HG3	2.55	0.42
22:R:38:PHE:CE1	30:Z:44:LYS:HE2	2.55	0.42
31:a:275:A:H4'	31:a:276:C:O5'	2.18	0.42
31:a:319:U:H2'	31:a:320:G:O4'	2.19	0.42
31:a:1349:C:H2'	31:a:1350:G:C8	2.54	0.42
31:a:1430:A:H2'	31:a:1431:A:C8	2.54	0.42
32:b:132:THR:HG21	32:b:134:ARG:NH2	2.34	0.42
47:q:12:LYS:HE2	47:q:12:LYS:HB3	1.68	0.42
48:r:47:THR:HG22	48:r:48:LYS:O	2.19	0.42
52:v:67:C:H2'	52:v:68:A:C8	2.54	0.42
5:A:1103:A:N3	5:A:1103:A:H2'	2.34	0.42
31:a:1247:A:H2'	31:a:1248:A:C8	2.54	0.42
31:a:1464:C:H2'	31:a:1465:A:H8	1.85	0.42
39:i:39:ARG:HE	39:i:39:ARG:HB3	1.80	0.42
41:k:36:ARG:HG3	41:k:36:ARG:NH1	2.34	0.42
52:v:29:C:H2'	52:v:30:G:H8	1.85	0.42
52:v:61:U:H5'	52:v:62:C:C5	2.54	0.42
5:A:291:G:H2'	5:A:292:U:C6	2.55	0.42
5:A:1424:G:H2'	5:A:1425:G:H8	1.84	0.42
5:A:1654:C:H2'	5:A:1655:U:H6	1.84	0.42
5:A:1924:A:H2'	5:A:1925:G:O4'	2.19	0.42
5:A:1942:U:H2'	5:A:1943:C:H6	1.85	0.42
5:A:2287:U:OP1	5:A:2376:U:O2'	2.36	0.42
11:G:85:ARG:HD2	11:G:85:ARG:HA	1.64	0.42
20:P:84:LYS:HE2	20:P:84:LYS:HB2	1.88	0.42
31:a:848:U:H2'	31:a:849:A:C8	2.54	0.42
31:a:1304:U:H2'	31:a:1305:U:C6	2.54	0.42
55:a:1602:OIY:O53	35:e:141:LYS:HE2	2.19	0.42
36:f:61:LEU:HD23	36:f:62:MET:N	2.34	0.42
41:k:17:GLU:HB3	41:k:36:ARG:HD3	2.01	0.42
49:s:43:ASP:OD1	49:s:43:ASP:N	2.51	0.42
5:A:1481:U:H2'	5:A:1482:C:H6	1.83	0.42
8:D:33:ASN:N	8:D:33:ASN:HD22	2.17	0.42
12:H:50:ARG:HA	12:H:50:ARG:HD2	1.79	0.42
14:J:63:VAL:HG12	14:J:106:LEU:HD11	2.01	0.42
31:a:200:G:C4	31:a:201:A:C8	3.08	0.42
31:a:497:G:H2'	31:a:498:C:H6	1.84	0.42
31:a:1007:U:O4	31:a:1016:G:O6	2.37	0.42
31:a:1473:G:H2'	31:a:1474:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:34:ALA:HB2	40:j:83:THR:HG21	2.02	0.42
52:v:28:C:H2'	52:v:29:C:C6	2.55	0.42
5:A:37:G:H2'	5:A:38:C:C6	2.54	0.42
5:A:355:C:H2'	5:A:356:A:C8	2.55	0.42
5:A:575:G:O2'	5:A:1249:A:OP1	2.38	0.42
5:A:1953:C:H2'	5:A:1954:C:H6	1.84	0.42
5:A:2641:U:H4'	5:A:2728:G:O2'	2.19	0.42
5:A:2793:U:O4	5:A:2797:G:N2	2.41	0.42
31:a:185:C:H4'	31:a:186:G:O5'	2.19	0.42
31:a:548:U:H2'	31:a:549:U:H6	1.83	0.42
5:A:2836:U:H2'	5:A:2837:U:C6	2.55	0.42
10:F:108:ILE:HD12	10:F:176:PRO:HG3	2.01	0.42
16:L:6:ARG:HB2	16:L:6:ARG:HH11	1.85	0.42
31:a:715:A:H5'	41:k:118:ASN:OD1	2.19	0.42
31:a:789:A:H1'	31:a:791:A:N7	2.35	0.42
31:a:1527:G:H2'	31:a:1528:A:C8	2.55	0.42
45:o:44:LYS:HA	45:o:44:LYS:HD3	1.83	0.42
5:A:794:C:H2'	5:A:795:U:C6	2.55	0.42
7:C:181:MET:HB2	7:C:269:ARG:NH1	2.29	0.42
10:F:23:LYS:HB2	10:F:23:LYS:HE2	1.81	0.42
13:I:73:LYS:HA	13:I:73:LYS:HD3	1.92	0.42
15:K:89:GLY:O	15:K:120:ARG:NH2	2.53	0.42
31:a:99:C:OP1	50:t:12:ARG:NH1	2.49	0.42
31:a:455:C:H2'	31:a:456:U:H6	1.85	0.42
31:a:1034:C:H2'	31:a:1035:C:C6	2.54	0.42
31:a:1164:A:H4'	31:a:1165:C:C5	2.54	0.42
43:m:44:LYS:HB2	43:m:47:GLU:OE2	2.20	0.42
52:v:18:G:H3'	52:v:57:C:N3	2.35	0.42
5:A:719:A:H2'	5:A:720:A:C8	2.54	0.41
5:A:720:A:H2'	5:A:721:C:C6	2.55	0.41
5:A:1039:G:H2'	5:A:1040:C:C6	2.54	0.41
5:A:1732:C:H2'	5:A:1733:U:H6	1.84	0.41
7:C:272:ARG:HD2	7:C:272:ARG:N	2.35	0.41
31:a:184:A:N7	50:t:84:LYS:HD2	2.35	0.41
31:a:275:A:H5''	31:a:277:G:O4'	2.20	0.41
31:a:878:G:P	42:l:9:ARG:HH22	2.43	0.41
31:a:982:C:H2'	31:a:983:U:C6	2.55	0.41
31:a:1310:U:H2'	31:a:1311:C:C6	2.55	0.41
32:b:34:PHE:CD1	32:b:44:ASN:HB3	2.55	0.41
32:b:99:LEU:HD23	32:b:99:LEU:HA	1.89	0.41
36:f:30:LYS:HA	36:f:33:ASP:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:88:PRO:O	37:g:89:MET:HB2	2.19	0.41
5:A:712:U:H5'	5:A:713:A:OP2	2.20	0.41
5:A:1479:U:H2'	5:A:1480:A:C8	2.55	0.41
31:a:980:A:H2	31:a:981:C:C6	2.39	0.41
34:d:123:ARG:HD2	34:d:133:ASN:HB3	2.02	0.41
34:d:199:GLU:O	34:d:203:VAL:HG23	2.20	0.41
52:v:51:C:H2'	52:v:52:A:C8	2.55	0.41
5:A:34:G:H22	5:A:511:G:H1'	1.85	0.41
5:A:1105:U:H2'	5:A:1106:C:C6	2.55	0.41
5:A:1729:U:H2'	5:A:1730:U:C6	2.55	0.41
19:O:37:GLU:O	19:O:40:ARG:N	2.50	0.41
28:X:5:ASP:OD1	28:X:5:ASP:N	2.52	0.41
31:a:1115:U:H1'	31:a:1176:A:C5	2.55	0.41
31:a:1154:A:C2	31:a:1178:G:C4	3.09	0.41
31:a:1462:A:H2'	31:a:1463:C:H6	1.85	0.41
32:b:75:LYS:HD2	32:b:167:ASP:HB2	2.01	0.41
42:l:50:ARG:HD2	42:l:90:LEU:HD11	2.02	0.41
3:2:24:LYS:HB3	15:K:64:PRO:HG2	2.03	0.41
5:A:34:G:O2'	5:A:35:A:OP2	2.32	0.41
5:A:2719:C:H2'	5:A:2720:U:O4'	2.20	0.41
6:B:27:A:H2'	6:B:28:C:C6	2.55	0.41
8:D:36:THR:HG22	8:D:74:VAL:HG21	2.02	0.41
10:F:75:ALA:HB2	52:v:58:A:H5'	2.03	0.41
10:F:110:ARG:CB	10:F:137:VAL:HG13	2.50	0.41
10:F:162:THR:HG23	10:F:165:GLU:OE1	2.20	0.41
28:X:28:LEU:HB3	28:X:43:VAL:HG12	2.01	0.41
31:a:601:G:H2'	31:a:602:U:O4'	2.20	0.41
31:a:675:U:H2'	31:a:676:C:C6	2.55	0.41
36:f:34:GLY:C	36:f:35:GLN:HG3	2.46	0.41
41:k:97:ARG:HG3	41:k:97:ARG:HH11	1.85	0.41
5:A:26:A:H2'	5:A:27:U:C6	2.56	0.41
5:A:580:A:H2'	5:A:581:G:H8	1.85	0.41
7:C:181:MET:H	7:C:269:ARG:HH12	1.68	0.41
35:e:40:ASP:OD1	35:e:40:ASP:C	2.64	0.41
42:l:72:HIS:ND1	42:l:74:LEU:HB2	2.34	0.41
42:l:87:VAL:O	42:l:88:LYS:HB3	2.19	0.41
10:F:32:THR:OG1	10:F:157:THR:O	2.32	0.41
10:F:60:ILE:HG22	10:F:99:PHE:HE1	1.85	0.41
12:H:52:ALA:HB1	12:H:56:LYS:NZ	2.35	0.41
27:W:43:GLU:OE1	27:W:45:ARG:NE	2.50	0.41
31:a:1039:A:O2'	31:a:1040:U:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:136:ARG:CZ	33:c:136:ARG:HB2	2.50	0.41
37:g:138:ARG:HG3	37:g:139:GLU:N	2.34	0.41
5:A:1654:C:C2	5:A:1655:U:C5	3.09	0.41
5:A:2061:C:H2'	5:A:2062:C:H6	1.86	0.41
5:A:2373:A:H2'	5:A:2374:A:C8	2.56	0.41
7:C:135:MET:HE3	7:C:141:LEU:HD22	2.03	0.41
7:C:145:GLU:HB3	7:C:188:CYS:HB3	2.02	0.41
7:C:271:ARG:CZ	7:C:273:VAL:HG12	2.51	0.41
25:U:35:TYR:O	25:U:96:LYS:HA	2.21	0.41
31:a:1057:U:OP1	44:n:85:ARG:NH2	2.54	0.41
31:a:1384:G:H2'	31:a:1385:C:H6	1.85	0.41
31:a:1428:A:H2	31:a:1466:C:H42	1.66	0.41
31:a:1504:A:H2'	31:a:1505:G:C8	2.56	0.41
36:f:101:LEU:HD23	36:f:101:LEU:HA	1.86	0.41
38:h:75:MET:HE3	38:h:75:MET:HB3	1.88	0.41
52:v:71:G:C2'	52:v:72:C:H5'	2.51	0.41
5:A:1439:A:C4	5:A:1440:G:C8	3.08	0.41
16:L:77:LYS:HA	16:L:78:PRO:HD3	1.84	0.41
5:A:494:G:H21	22:R:61:ASN:HD21	1.69	0.41
5:A:1040:C:H2'	5:A:1041:A:C8	2.55	0.41
5:A:1317:A:C5	5:A:1318:C:C5	3.09	0.41
5:A:1833:C:O2'	5:A:1923:A:N3	2.42	0.41
5:A:1942:U:H2'	5:A:1943:C:C6	2.55	0.41
5:A:2061:C:C2	5:A:2062:C:C5	3.09	0.41
5:A:2066:A:H2'	5:A:2067:A:C8	2.56	0.41
5:A:2212:G:H2'	5:A:2213:G:H8	1.85	0.41
5:A:2830:G:H2'	5:A:2875:A:H61	1.86	0.41
10:F:130:MET:HE2	10:F:154:ILE:HD13	2.02	0.41
10:F:133:LYS:O	10:F:134:GLU:HB2	2.20	0.41
10:F:167:ARG:O	10:F:170:MET:HG3	2.20	0.41
11:G:30:LYS:HE3	11:G:81:GLU:O	2.21	0.41
21:Q:71:LYS:HB2	21:Q:71:LYS:HE3	1.86	0.41
31:a:81:G:H3'	31:a:82:C:C6	2.55	0.41
31:a:208:G:C2	31:a:209:A:C8	3.09	0.41
31:a:405:U:H2'	31:a:406:G:O4'	2.21	0.41
31:a:610:C:H2'	31:a:611:C:H6	1.85	0.41
31:a:1235:A:H2	31:a:1238:G:N3	2.19	0.41
32:b:14:ALA:HA	32:b:210:ARG:HH11	1.86	0.41
32:b:78:ALA:HB1	32:b:82:ILE:HD13	2.02	0.41
32:b:98:TRP:NE1	32:b:177:GLU:OE2	2.51	0.41
40:j:51:VAL:HG13	44:n:81:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:74:LEU:HD23	41:k:74:LEU:HA	1.95	0.41
42:l:5:ASN:O	42:l:9:ARG:HG3	2.21	0.41
52:v:47:G:H8	52:v:48:U:C4	2.38	0.41
3:2:28:LYS:HA	3:2:28:LYS:HD2	1.90	0.41
5:A:2841:U:H5''	19:O:55:ASN:O	2.21	0.41
10:F:123:ASP:OD1	10:F:123:ASP:N	2.53	0.41
23:S:47:GLU:OE2	23:S:53:GLU:HA	2.21	0.41
31:a:684:A:C2	31:a:701:A:C5	3.09	0.41
31:a:754:U:H2'	31:a:755:G:O4'	2.21	0.41
32:b:109:LEU:HA	32:b:109:LEU:HD12	1.86	0.41
40:j:47:GLU:O	40:j:66:GLU:HA	2.21	0.41
46:p:74:ARG:HA	46:p:74:ARG:HD2	1.94	0.41
5:A:31:G:O2'	22:R:78:GLU:O	2.39	0.40
5:A:492:G:H2'	5:A:493:G:O4'	2.21	0.40
5:A:845:A:OP2	5:A:846:U:H5	2.05	0.40
5:A:2308:U:O3'	10:F:68:THR:HG21	2.21	0.40
7:C:163:GLN:OE1	7:C:163:GLN:HA	2.21	0.40
9:E:110:GLU:HB3	15:K:3:LEU:HD22	2.03	0.40
11:G:43:LEU:HD21	11:G:50:LEU:HD23	2.03	0.40
18:N:30:ASN:OD1	18:N:31:ARG:N	2.54	0.40
31:a:77:G:C2	31:a:78:G:C5	3.09	0.40
5:A:2645:C:H2'	5:A:2646:U:C6	2.55	0.40
7:C:181:MET:CE	7:C:269:ARG:NH1	2.79	0.40
10:F:11:GLU:HB2	10:F:15:LYS:NZ	2.36	0.40
21:Q:2:TYR:CE1	21:Q:13:ARG:HD2	2.56	0.40
31:a:548:U:H2'	31:a:549:U:C6	2.55	0.40
33:c:71:ALA:C	33:c:73:PRO:HD3	2.46	0.40
37:g:13:LEU:HA	37:g:14:PRO:HD2	1.89	0.40
37:g:135:ILE:O	37:g:139:GLU:HG3	2.22	0.40
42:l:86:ARG:HE	42:l:86:ARG:HB3	1.76	0.40
5:A:578:U:H2'	5:A:579:C:H6	1.85	0.40
5:A:633:C:O2'	5:A:637:U:OP1	2.37	0.40
5:A:1786:U:H2'	5:A:1787:A:N7	2.36	0.40
9:E:4:LYS:NZ	9:E:8:GLY:O	2.47	0.40
10:F:135:GLN:H	10:F:135:GLN:HG2	1.68	0.40
31:a:541:G:OP1	34:d:61:GLN:NE2	2.54	0.40
31:a:991:A:N3	44:n:8:ASN:ND2	2.68	0.40
48:r:25:ASP:O	48:r:29:LEU:HG	2.21	0.40
4:3:16:VAL:HG22	4:3:25:VAL:HG22	2.03	0.40
5:A:391:C:H2'	5:A:392:C:H6	1.86	0.40
5:A:1549:U:H2'	5:A:1550:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:7:G:C2	6:B:8:A:C8	3.10	0.40
8:D:111:ASP:OD1	8:D:176:GLN:HA	2.22	0.40
10:F:77:PHE:HB2	10:F:79:ILE:HG13	2.03	0.40
12:H:37:VAL:HG22	12:H:38:ALA:H	1.86	0.40
16:L:39:ARG:HB3	16:L:99:PRO:HD3	2.04	0.40
23:S:49:LEU:HD13	28:X:26:PHE:CZ	2.56	0.40
31:a:650:A:C5	38:h:57:LYS:HG3	2.56	0.40
31:a:1464:C:H2'	31:a:1465:A:C8	2.56	0.40
32:b:29:MET:O	32:b:33:ILE:HG13	2.20	0.40
35:e:159:SER:HB2	35:e:162:GLU:OE2	2.21	0.40
39:i:57:GLU:N	39:i:57:GLU:CD	2.79	0.40
5:A:288:U:H2'	5:A:289:G:H8	1.86	0.40
5:A:464:G:H2'	5:A:465:A:C8	2.56	0.40
5:A:1805:A:H2'	5:A:1806:A:C8	2.56	0.40
5:A:2848:G:H2'	5:A:2849:C:O4'	2.21	0.40
7:C:38:LYS:HE2	7:C:38:LYS:HB2	1.89	0.40
9:E:56:LYS:NZ	9:E:56:LYS:HB3	2.37	0.40
10:F:108:ILE:HG21	10:F:176:PRO:HB3	2.04	0.40
11:G:72:LEU:HD23	11:G:72:LEU:HA	1.91	0.40
16:L:1:MET:O	16:L:44:ALA:HB1	2.21	0.40
16:L:42:MET:HE3	16:L:125:LEU:HD22	2.03	0.40
23:S:1:MET:HB3	23:S:1:MET:HE2	1.76	0.40
26:V:74:GLN:H	26:V:74:GLN:HG3	1.65	0.40
31:a:207:G:O2'	31:a:208:G:O5'	2.39	0.40
35:e:106:ALA:HB2	35:e:124:ALA:HB3	2.03	0.40
51:u:59:LYS:HA	51:u:62:ARG:NE	2.36	0.40
52:v:28:C:C2	52:v:29:C:C5	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	C	270/274 (98%)	262 (97%)	8 (3%)	0	100	100
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	157 (91%)	12 (7%)	3 (2%)	7	10
11	G	172/177 (97%)	166 (96%)	5 (3%)	1 (1%)	21	32
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	J	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	18	28
17	M	117/125 (94%)	113 (97%)	4 (3%)	0	100	100
18	N	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
19	O	115/122 (94%)	114 (99%)	1 (1%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	12	20
22	R	107/109 (98%)	107 (100%)	0	0	100	100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100	100
24	T	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
25	U	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
26	V	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	213 (96%)	8 (4%)	2 (1%)	14	22
33	c	213/250 (85%)	206 (97%)	7 (3%)	0	100	100
34	d	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
35	e	153/165 (93%)	151 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	f	102/127 (80%)	99 (97%)	2 (2%)	1 (1%)	12	20
37	g	132/156 (85%)	123 (93%)	7 (5%)	2 (2%)	8	12
38	h	128/131 (98%)	126 (98%)	2 (2%)	0	100	100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100	100
40	j	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
41	k	115/128 (90%)	111 (96%)	4 (4%)	0	100	100
42	l	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100
47	q	77/85 (91%)	75 (97%)	2 (3%)	0	100	100
48	r	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
49	s	80/91 (88%)	79 (99%)	1 (1%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
All	All	5414/5872 (92%)	5265 (97%)	138 (2%)	11 (0%)	44	58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	137	VAL
32	b	8	MET
36	f	33	ASP
37	g	88	PRO
37	g	3	ARG
11	G	13	ASN
10	F	5	LYS
32	b	7	SER
10	F	121	SER
16	L	79	LEU
21	Q	52	PRO

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	47/47 (100%)	46 (98%)	1 (2%)	47	69
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	51 (98%)	1 (2%)	50	71
4	3	33/33 (100%)	32 (97%)	1 (3%)	36	58
7	C	218/220 (99%)	216 (99%)	2 (1%)	70	85
8	D	166/167 (99%)	164 (99%)	2 (1%)	63	81
9	E	155/155 (100%)	150 (97%)	5 (3%)	34	56
10	F	144/147 (98%)	137 (95%)	7 (5%)	22	39
11	G	139/142 (98%)	131 (94%)	8 (6%)	18	32
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	115 (98%)	3 (2%)	42	64
14	J	103/103 (100%)	101 (98%)	2 (2%)	50	71
15	K	106/108 (98%)	102 (96%)	4 (4%)	29	49
16	L	113/113 (100%)	111 (98%)	2 (2%)	51	73
17	M	96/101 (95%)	93 (97%)	3 (3%)	35	57
18	N	85/85 (100%)	83 (98%)	2 (2%)	43	65
19	O	99/102 (97%)	98 (99%)	1 (1%)	68	84
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	83 (99%)	1 (1%)	63	81
22	R	88/88 (100%)	86 (98%)	2 (2%)	44	66
23	S	77/87 (88%)	76 (99%)	1 (1%)	61	80
24	T	83/85 (98%)	77 (93%)	6 (7%)	13	23
25	U	79/80 (99%)	78 (99%)	1 (1%)	61	80
26	V	59/64 (92%)	59 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	52 (98%)	1 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	Y	53/54 (98%)	51 (96%)	2 (4%)	29	49
30	Z	46/50 (92%)	46 (100%)	0	100	100
32	b	185/200 (92%)	176 (95%)	9 (5%)	22	39
33	c	175/198 (88%)	171 (98%)	4 (2%)	44	66
34	d	170/171 (99%)	168 (99%)	2 (1%)	63	81
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	91 (97%)	3 (3%)	34	56
37	g	113/128 (88%)	108 (96%)	5 (4%)	25	43
38	h	108/109 (99%)	106 (98%)	2 (2%)	50	71
39	i	99/100 (99%)	97 (98%)	2 (2%)	48	70
40	j	89/91 (98%)	86 (97%)	3 (3%)	32	54
41	k	88/98 (90%)	85 (97%)	3 (3%)	32	54
42	l	104/106 (98%)	99 (95%)	5 (5%)	23	40
43	m	95/98 (97%)	94 (99%)	1 (1%)	65	82
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	70 (99%)	1 (1%)	59	79
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	71/76 (93%)	67 (94%)	4 (6%)	19	33
48	r	46/66 (70%)	44 (96%)	2 (4%)	26	44
49	s	70/78 (90%)	68 (97%)	2 (3%)	37	60
50	t	65/67 (97%)	64 (98%)	1 (2%)	57	77
51	u	54/62 (87%)	53 (98%)	1 (2%)	50	71
All	All	4485/4756 (94%)	4377 (98%)	108 (2%)	43	65

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	25	THR
3	2	64	ILE
4	3	7	VAL
7	C	77	VAL
7	C	269	ARG
8	D	3	ILE
8	D	98	THR

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Mol	Chain	Res	Type
9	E	6	VAL
9	E	119	LEU
9	E	125	VAL
9	E	154	GLU
9	E	199	LEU
10	F	50	LEU
10	F	59	LEU
10	F	89	VAL
10	F	90	THR
10	F	106	ILE
10	F	152	MET
10	F	164	ASP
11	G	11	VAL
11	G	16	THR
11	G	41	VAL
11	G	67	THR
11	G	76	VAL
11	G	81	GLU
11	G	105	LEU
11	G	170	LEU
13	I	1	MET
13	I	17	VAL
13	I	70	LEU
14	J	116	SER
14	J	122	LEU
15	K	12	GLU
15	K	17	GLU
15	K	88	GLU
15	K	137	ILE
16	L	1	MET
16	L	110	ASN
17	M	6	SER
17	M	98	LEU
17	M	116	VAL
18	N	10	ARG
18	N	58	SER
19	O	68	SER
21	Q	53	VAL
22	R	67	ASP
22	R	109	VAL
23	S	6	ILE
24	T	24	VAL

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Mol	Chain	Res	Type
24	T	32	VAL
24	T	50	THR
24	T	66	SER
24	T	70	ILE
24	T	71	LEU
25	U	28	SER
28	X	56	LEU
29	Y	3	THR
29	Y	36	GLU
32	b	6	VAL
32	b	23	ARG
32	b	34	PHE
32	b	82	ILE
32	b	116	LEU
32	b	118	ASP
32	b	198	VAL
32	b	201	VAL
32	b	209	ILE
33	c	10	ILE
33	c	28	GLN
33	c	186	THR
33	c	191	THR
34	d	30	VAL
34	d	176	ASP
36	f	6	ILE
36	f	70	THR
36	f	94	HIS
37	g	37	SER
37	g	56	VAL
37	g	96	ARG
37	g	138	ARG
37	g	141	VAL
38	h	56	THR
38	h	100	LEU
39	i	35	GLN
39	i	70	ILE
40	j	6	ILE
40	j	81	ASP
40	j	92	LEU
41	k	17	GLU
41	k	37	GLN
41	k	80	ASN

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Mol	Chain	Res	Type
42	l	55	VAL
42	l	59	SER
42	l	67	ILE
42	l	74	LEU
42	l	107	VAL
43	m	63	VAL
45	o	79	THR
47	q	24	VAL
47	q	30	VAL
47	q	38	SER
47	q	59	VAL
48	r	35	GLU
48	r	36	ASN
49	s	4	SER
49	s	58	VAL
50	t	77	SER
51	u	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	53	HIS
8	D	63	ASN
8	D	133	GLN
10	F	24	ASN
11	G	88	GLN
12	H	28	ASN
13	I	12	GLN
13	I	47	HIS
16	L	22	HIS
17	M	72	ASN
18	N	66	ASN
20	P	44	GLN
24	T	38	ASN
25	U	58	ASN
26	V	35	ASN
27	W	20	HIS
27	W	35	HIS
29	Y	24	GLN
32	b	20	HIS
33	c	54	ASN
33	c	140	ASN

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Mol	Chain	Res	Type
34	d	198	ASN
35	e	164	GLN
38	h	42	GLN
38	h	98	GLN
39	i	48	GLN
40	j	58	ASN
41	k	117	HIS
42	l	96	HIS
45	o	48	HIS
45	o	50	HIS
50	t	80	ASN
51	u	43	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	207 (13%)	0
5	A	2720/2918 (93%)	379 (13%)	19 (0%)
52	v	76/77 (98%)	28 (36%)	0
53	w	2/3 (66%)	0	0
6	B	114/115 (99%)	21 (18%)	1 (0%)
All	All	4439/4657 (95%)	635 (14%)	20 (0%)

All (635) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	22	G
5	A	50	G
5	A	53	G
5	A	67	G
5	A	78	A
5	A	81	A
5	A	82	G
5	A	91	A
5	A	92	G
5	A	104	C
5	A	109	G
5	A	110	A
5	A	125	A
5	A	126	A
5	A	127	U

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Mol	Chain	Res	Type
5	A	138	A
5	A	139	C
5	A	147	A
5	A	148	A
5	A	149	G
5	A	170	A
5	A	203	A
5	A	206	A
5	A	222	G
5	A	223	A
5	A	228	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	237	G
5	A	240	A
5	A	246	U
5	A	252	G
5	A	255	G
5	A	257	G
5	A	262	A
5	A	279	U
5	A	285	A
5	A	297	G
5	A	304	G
5	A	313	A
5	A	331	G
5	A	332	A
5	A	336	U
5	A	345	C
5	A	347	A
5	A	348	A
5	A	360	A
5	A	361	A
5	A	365	U
5	A	366	G
5	A	367	A
5	A	369	G
5	A	370	A
5	A	371	G
5	A	385	G
5	A	395	G

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Mol	Chain	Res	Type
5	A	403	A
5	A	410	G
5	A	411	A
5	A	423	G
5	A	435	C
5	A	455	C
5	A	456	A
5	A	479	A
5	A	480	G
5	A	493	G
5	A	504	A
5	A	529	G
5	A	531	A
5	A	544	U
5	A	545	C
5	A	546	G
5	A	548	G
5	A	554	A
5	A	561	A
5	A	571	U
5	A	573	A
5	A	594	A
5	A	595	G
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	635	A
5	A	643	U
5	A	649	G
5	A	651	U
5	A	684	U
5	A	712	U
5	A	713	A
5	A	714	A
5	A	728	A
5	A	745	U
5	A	762	A
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G

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Mol	Chain	Res	Type
5	A	783	G
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	843	G
5	A	845	A
5	A	851	U
5	A	857	G
5	A	900	C
5	A	905	G
5	A	908	A
5	A	929	C
5	A	930	U
5	A	931	A
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1030	U
5	A	1036	A
5	A	1043	A
5	A	1044	G
5	A	1051	A
5	A	1104	G
5	A	1105	U
5	A	1106	C
5	A	1107	G
5	A	1108	A
5	A	1109	G
5	A	1125	G
5	A	1128	G
5	A	1129	U
5	A	1130	A

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Mol	Chain	Res	Type
5	A	1131	A
5	A	1132	C
5	A	1140	A
5	A	1148	U
5	A	1149	G
5	A	1166	A
5	A	1170	U
5	A	1173	G
5	A	1174	U
5	A	1245	G
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1316	A
5	A	1320	U
5	A	1324	U
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1374	U
5	A	1378	A
5	A	1411	G
5	A	1412	C
5	A	1414	A
5	A	1422	A
5	A	1423	C
5	A	1428	A
5	A	1432	C
5	A	1433	U
5	A	1435	A
5	A	1447	G
5	A	1448	U
5	A	1455	U
5	A	1462	G
5	A	1477	U
5	A	1478	G
5	A	1483	U
5	A	1484	U
5	A	1485	A

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Mol	Chain	Res	Type
5	A	1488	C
5	A	1494	C
5	A	1503	C
5	A	1504	U
5	A	1505	A
5	A	1511	A
5	A	1514	U
5	A	1519	U
5	A	1520	A
5	A	1523	A
5	A	1527	U
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1535	U
5	A	1536	G
5	A	1537	C
5	A	1538	A
5	A	1539	G
5	A	1542	A
5	A	1543	A
5	A	1564	A
5	A	1567	A
5	A	1574	U
5	A	1576	U
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1605	G
5	A	1606	A
5	A	1616	A
5	A	1644	C
5	A	1645	U
5	A	1646	U
5	A	1647	G
5	A	1672	G
5	A	1701	G
5	A	1724	C

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Mol	Chain	Res	Type
5	A	1726	C
5	A	1727	G
5	A	1729	U
5	A	1733	U
5	A	1734	G
5	A	1736	G
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1807	G
5	A	1812	C
5	A	1825	A
5	A	1829	C
5	A	1844	A
5	A	1854	A
5	A	1865	G
5	A	1869	G
5	A	1872	A
5	A	1879	U
5	A	1881	A
5	A	1892	A
5	A	1897	A
5	A	1902	G
5	A	1908	A
5	A	1909	A
5	A	1910	C
5	A	1915	A
5	A	1923	A
5	A	1925	G
5	A	1926	G
5	A	1934	A
5	A	1951	U
5	A	1959	U
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1983	G
5	A	1987	U

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Mol	Chain	Res	Type
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG
5	A	2089	G
5	A	2092	C
5	A	2093	U
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2216	C
5	A	2221	A
5	A	2234	G
5	A	2275	G
5	A	2279	U
5	A	2283	A
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2307	A
5	A	2314	G
5	A	2316	A
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2343	C
5	A	2346	C
5	A	2372	A
5	A	2378	G
5	A	2379	G
5	A	2381	C
5	A	2387	G
5	A	2398	U
5	A	2399	C

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Mol	Chain	Res	Type
5	A	2402	U
5	A	2420	C
5	A	2421	A
5	A	2425	G
5	A	2426	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2465	A
5	A	2466	G
5	A	2469	U
5	A	2471	C
5	A	2472	A
5	A	2476	C
5	A	2494	C
5	A	2498	G
5	A	2499	2MA
5	A	2502	U
5	A	2503	C
5	A	2514	A
5	A	2525	G
5	A	2543	A
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2569	C
5	A	2578	G
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2609	U
5	A	2611	U
5	A	2625	U
5	A	2636	G
5	A	2652	U
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2709	C

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Mol	Chain	Res	Type
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2744	A
5	A	2748	C
5	A	2754	A
5	A	2761	A
5	A	2762	G
5	A	2774	A
5	A	2776	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2799	C
5	A	2814	U
5	A	2816	G
5	A	2817	A
5	A	2831	A
5	A	2845	G
5	A	2852	A
5	A	2854	U
5	A	2857	U
5	A	2863	A
5	A	2869	A
5	A	2881	U
5	A	2882	G
6	B	2	C
6	B	22	G
6	B	28	C
6	B	31	G
6	B	33	U
6	B	36	C
6	B	39	C
6	B	40	C
6	B	42	G
6	B	50	A
6	B	54	G
6	B	59	C
6	B	62	U
6	B	64	A

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Mol	Chain	Res	Type
6	B	65	G
6	B	67	G
6	B	71	A
6	B	84	A
6	B	87	A
6	B	105	C
6	B	106	A
31	a	4	A
31	a	6	C
31	a	7	U
31	a	9	A
31	a	10	A
31	a	11	G
31	a	15	U
31	a	24	G
31	a	34	A
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A
31	a	57	A
31	a	62	A
31	a	66	G
31	a	74	G
31	a	76	A
31	a	77	G
31	a	81	G
31	a	82	C
31	a	83	U
31	a	84	U
31	a	85	G
31	a	115	A
31	a	117	U
31	a	126	A
31	a	127	U
31	a	163	U
31	a	165	C
31	a	170	A
31	a	184	A
31	a	185	C
31	a	186	G
31	a	193	A

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Mol	Chain	Res	Type
31	a	205	U
31	a	208	G
31	a	216	G
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	279	U
31	a	285	G
31	a	324	C
31	a	325	A
31	a	340	A
31	a	343	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	380	C
31	a	393	A
31	a	402	G
31	a	407	A
31	a	408	A
31	a	409	G
31	a	410	A
31	a	416	U
31	a	418	A
31	a	419	U
31	a	420	G
31	a	425	U
31	a	426	A
31	a	434	U
31	a	435	U
31	a	442	G
31	a	444	A
31	a	447	A
31	a	459	U
31	a	461	A
31	a	463	U
31	a	481	G
31	a	483	U

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Mol	Chain	Res	Type
31	a	492	A
31	a	493	A
31	a	494	U
31	a	496	A
31	a	497	G
31	a	508	C
31	a	515	C
31	a	518	G
31	a	521	G
31	a	524	7MG
31	a	528	U
31	a	530	A
31	a	544	A
31	a	556	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	574	G
31	a	591	U
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	684	A
31	a	715	A
31	a	720	U
31	a	731	G
31	a	752	G
31	a	774	A
31	a	790	U
31	a	791	A
31	a	812	A
31	a	814	C
31	a	838	U
31	a	840	U
31	a	841	G
31	a	842	A
31	a	887	G
31	a	888	U
31	a	911	A
31	a	923	G

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Mol	Chain	Res	Type
31	a	924	G
31	a	927	C
31	a	928	C
31	a	931	C
31	a	932	A
31	a	957	U
31	a	963	2MG
31	a	966	A
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	1000	A
31	a	1001	A
31	a	1007	U
31	a	1025	C
31	a	1027	U
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1033	A
31	a	1062	U
31	a	1082	U
31	a	1083	U
31	a	1091	G
31	a	1092	U
31	a	1097	C
31	a	1098	A
31	a	1101	G
31	a	1122	U
31	a	1123	U
31	a	1134	C
31	a	1136	G
31	a	1156	U
31	a	1164	A
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1181	G

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Mol	Chain	Res	Type
31	a	1188	A
31	a	1193	A
31	a	1194	A
31	a	1210	A
31	a	1224	A
31	a	1233	A
31	a	1235	A
31	a	1255	G
31	a	1267	U
31	a	1276	A
31	a	1277	A
31	a	1284	A
31	a	1286	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1317	C
31	a	1335	G
31	a	1337	A
31	a	1343	A
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1375	C
31	a	1378	U
31	a	1386	C
31	a	1394	C
31	a	1395	A
31	a	1416	G
31	a	1423	G
31	a	1438	A
31	a	1443	A
31	a	1448	C
31	a	1449	A
31	a	1451	A
31	a	1484	G
31	a	1491	G
31	a	1494	G
31	a	1500	A
31	a	1503	U
31	a	1514	G

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Mol	Chain	Res	Type
31	a	1516	MA6
31	a	1526	G
31	a	1527	G
31	a	1530	C
52	v	4	U
52	v	8	4SU
52	v	9	A
52	v	14	A
52	v	15	G
52	v	16	U
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U
52	v	22	A
52	v	23	G
52	v	24	A
52	v	46	G
52	v	47	G
52	v	48	U
52	v	49	C
52	v	51	C
52	v	55	5MU
52	v	57	C
52	v	58	A
52	v	59	A
52	v	61	U
52	v	62	C
52	v	65	G
52	v	72	C
52	v	73	C
52	v	77	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	91	A
5	A	109	G
5	A	256	C
5	A	364	A
5	A	365	U
5	A	368	C

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Mol	Chain	Res	Type
5	A	424	G
5	A	478	A
5	A	496	A
5	A	782	G
5	A	844	A
5	A	1127	U
5	A	1173	G
5	A	1179	G
5	A	1187	G
5	A	1880	G
5	A	2419	U
5	A	2443	G
5	A	2502	U
6	B	86	U

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

28 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
31	7MG	a	524	31	23,26,27	1.09	1 (4%)	27,39,42	0.89	2 (7%)
31	PSU	a	513	31	18,21,22	1.10	1 (5%)	21,30,33	1.85	5 (23%)
31	4OC	a	1399	31	20,23,24	3.13	8 (40%)	25,32,35	0.99	1 (4%)
5	PSU	A	1913	5	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
52	5MU	v	55	52	19,22,23	0.41	0	27,32,35	0.61	0
5	PSU	A	2576	5	18,21,22	1.10	2 (11%)	21,30,33	1.98	5 (23%)
31	2MG	a	1204	31	23,26,27	0.45	0	33,38,41	0.53	0
52	4SU	v	8	52	18,21,22	4.40	8 (44%)	25,30,33	2.23	4 (16%)
5	OMG	A	2247	5,52	23,26,27	0.50	0	32,38,41	0.45	0
5	PSU	A	2500	5	18,21,22	1.07	1 (5%)	21,30,33	1.85	4 (19%)
5	PSU	A	2601	5	18,21,22	1.05	1 (5%)	21,30,33	1.84	3 (14%)
5	3TD	A	1911	5	19,22,23	4.39	6 (31%)	23,32,35	1.73	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	v	56	52	18,21,22	1.16	1 (5%)	21,30,33	1.88	5 (23%)
5	6MZ	A	2026	5	22,25,26	2.54	4 (18%)	29,36,39	3.27	10 (34%)
31	UR3	a	1495	31	19,22,23	2.86	7 (36%)	26,32,35	1.61	3 (11%)
52	H2U	v	20	52	18,21,22	0.52	0	19,30,33	0.98	1 (5%)
5	7MG	A	2065	5	23,26,27	1.07	1 (4%)	27,39,42	0.94	2 (7%)
5	PSU	A	1907	5	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
31	MA6	a	1516	31	23,26,27	1.42	4 (17%)	33,38,41	3.28	13 (39%)
5	PSU	A	2453	5	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
5	5MU	A	1935	5	19,22,23	0.45	0	27,32,35	0.52	0
5	OMU	A	2548	5	19,22,23	3.03	8 (42%)	25,31,34	1.83	5 (20%)
5	2MA	A	2499	5	22,25,26	3.89	9 (40%)	32,37,40	2.62	10 (31%)
31	2MG	a	963	31	23,26,27	0.47	0	33,38,41	0.55	0
31	5MC	a	964	31	19,22,23	0.55	0	26,32,35	0.60	0
5	2MG	A	2441	5	23,26,27	0.50	0	33,38,41	0.46	0
5	PSU	A	952	5	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
31	MA6	a	1515	31	23,26,27	1.43	4 (17%)	33,38,41	3.20	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
31	7MG	a	524	31	-	2/7/37/38	0/3/3/3
31	PSU	a	513	31	-	0/7/25/26	0/2/2/2
31	4OC	a	1399	31	-	1/9/29/30	0/2/2/2
5	PSU	A	1913	5	-	0/7/25/26	0/2/2/2
52	5MU	v	55	52	-	3/7/25/26	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
52	4SU	v	8	52	-	2/7/25/26	0/2/2/2
5	OMG	A	2247	5,52	-	0/9/27/28	0/3/3/3
5	PSU	A	2500	5	-	1/7/25/26	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
52	PSU	v	56	52	-	4/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	2/9/27/28	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	H2U	v	20	52	-	3/7/38/39	0/2/2/2
5	7MG	A	2065	5	-	0/7/37/38	0/3/3/3
5	PSU	A	1907	5	-	0/7/25/26	0/2/2/2
31	MA6	a	1516	31	-	0/11/29/30	0/3/3/3
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	0/9/27/28	0/2/2/2
5	2MA	A	2499	5	-	2/7/25/26	0/3/3/3
31	2MG	a	963	31	-	0/9/27/28	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.15	1.49	1.35
5	A	2499	2MA	C4-N3	11.85	1.49	1.34
5	A	1911	3TD	C2-N1	10.57	1.50	1.37
5	A	2026	6MZ	C6-N6	10.16	1.45	1.34
52	v	8	4SU	C2-N1	9.42	1.53	1.38
52	v	8	4SU	C4-N3	8.89	1.46	1.37
52	v	8	4SU	C5-C4	7.20	1.51	1.42
5	A	2499	2MA	C2-N3	7.19	1.46	1.34
52	v	8	4SU	C2-N3	7.15	1.50	1.38
5	A	2548	OMU	C2-N1	7.04	1.49	1.38
31	a	1495	UR3	C2-N1	6.95	1.48	1.38
31	a	1399	4OC	C4-N3	6.86	1.44	1.32
5	A	2499	2MA	C6-N1	6.81	1.44	1.35
5	A	2548	OMU	C2-N3	6.80	1.49	1.38
31	a	1495	UR3	C6-C5	6.69	1.50	1.35
52	v	8	4SU	C6-C5	6.42	1.49	1.35
31	a	1399	4OC	C6-C5	6.28	1.49	1.35
31	a	1399	4OC	C2-N3	6.14	1.48	1.36
5	A	2499	2MA	C2-N1	5.84	1.44	1.34
5	A	1911	3TD	C6-N1	5.73	1.45	1.36
5	A	2548	OMU	C6-C5	5.58	1.48	1.35
31	a	1495	UR3	C2-N3	5.48	1.49	1.39
5	A	1911	3TD	C2-N3	4.91	1.48	1.38
52	v	8	4SU	C4-S4	-4.83	1.60	1.68
31	a	1399	4OC	C4-N4	4.76	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C5-C6	4.63	1.53	1.41
31	a	524	7MG	C5-N7	4.52	1.41	1.35
5	A	2065	7MG	C5-N7	4.45	1.41	1.35
5	A	2548	OMU	C4-N3	4.23	1.45	1.38
31	a	1399	4OC	C2-N1	4.15	1.48	1.40
31	a	1515	MA6	C6-N6	3.91	1.47	1.36
31	a	1516	MA6	C6-N6	3.90	1.47	1.36
52	v	56	PSU	C6-C5	3.80	1.39	1.35
5	A	1913	PSU	C6-C5	3.77	1.39	1.35
5	A	1907	PSU	C6-C5	3.65	1.39	1.35
5	A	2499	2MA	C6-N6	-3.63	1.24	1.34
31	a	1399	4OC	C5-C4	3.55	1.48	1.41
31	a	513	PSU	C6-C5	3.53	1.39	1.35
5	A	2500	PSU	C6-C5	3.46	1.39	1.35
5	A	2601	PSU	C6-C5	3.44	1.39	1.35
5	A	952	PSU	C6-C5	3.38	1.39	1.35
5	A	2453	PSU	C6-C5	3.35	1.39	1.35
5	A	2576	PSU	C6-C5	3.29	1.38	1.35
31	a	1495	UR3	C6-N1	3.28	1.45	1.38
5	A	2026	6MZ	C5-N7	-3.20	1.33	1.39
31	a	1399	4OC	C6-N1	3.17	1.45	1.38
5	A	2548	OMU	O4-C4	-3.10	1.18	1.24
31	a	1515	MA6	C5-C4	-3.09	1.33	1.39
5	A	2026	6MZ	C5-C4	-3.07	1.33	1.39
5	A	1911	3TD	C4-N3	3.05	1.46	1.40
31	a	1516	MA6	C5-C4	-2.99	1.33	1.39
31	a	1399	4OC	O2-C2	-2.92	1.18	1.23
5	A	2548	OMU	C6-N1	2.71	1.44	1.38
5	A	2026	6MZ	C8-N9	-2.71	1.32	1.37
5	A	2548	OMU	O2-C2	-2.63	1.18	1.23
52	v	8	4SU	O2-C2	-2.60	1.18	1.23
31	a	1516	MA6	C5-N7	-2.54	1.34	1.39
31	a	1515	MA6	C5-N7	-2.54	1.34	1.39
52	v	8	4SU	C6-N1	2.48	1.44	1.38
31	a	1495	UR3	C4-N3	2.43	1.45	1.40
5	A	2499	2MA	C5-N7	-2.43	1.34	1.39
5	A	2499	2MA	C4-N9	-2.41	1.32	1.37
31	a	1515	MA6	C8-N9	-2.33	1.33	1.37
5	A	1911	3TD	O2-C2	-2.32	1.19	1.23
5	A	2548	OMU	C5-C4	2.25	1.48	1.43
31	a	1516	MA6	C8-N9	-2.25	1.33	1.37
5	A	2499	2MA	C8-N7	2.22	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1495	UR3	C5-C4	2.21	1.49	1.43
31	a	1495	UR3	O2-C2	-2.13	1.18	1.22
5	A	2576	PSU	O4'-C1'	-2.09	1.41	1.43

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1516	MA6	N1-C6-N6	-11.95	102.29	116.86
31	a	1515	MA6	N1-C6-N6	-11.40	102.97	116.86
5	A	2026	6MZ	C4-N9-C1'	-8.87	105.88	126.63
5	A	2026	6MZ	C1'-N9-C8	8.86	146.76	127.09
31	a	1516	MA6	C5-C6-N6	8.01	138.01	125.33
31	a	1515	MA6	C5-C6-N6	7.65	137.44	125.33
52	v	8	4SU	C4-N3-C2	-7.57	120.06	127.31
5	A	2499	2MA	C1'-N9-C8	-6.82	111.97	127.09
5	A	2499	2MA	N9-C8-N7	-5.98	105.45	113.94
5	A	2026	6MZ	C5-C4-N3	-5.90	118.60	126.72
31	a	1495	UR3	C4-N3-C2	-5.68	120.00	124.58
5	A	2548	OMU	C4-N3-C2	-5.61	119.65	126.61
31	a	1516	MA6	N1-C2-N3	-5.45	120.33	128.58
31	a	1515	MA6	N1-C2-N3	-5.40	120.41	128.58
5	A	2499	2MA	C5-C4-N3	-5.32	121.58	127.18
5	A	1911	3TD	N1-C2-N3	5.29	119.98	116.13
52	v	8	4SU	C5-C4-N3	5.14	119.53	114.75
5	A	2026	6MZ	C4-C5-C6	5.12	121.03	116.78
5	A	2499	2MA	C4-N9-C8	5.10	111.10	105.74
5	A	952	PSU	C4-N3-C2	-4.99	119.50	126.37
31	a	1516	MA6	C5-C4-N3	-4.98	119.86	126.72
31	a	1515	MA6	C5-C4-N3	-4.94	119.92	126.72
5	A	2026	6MZ	N1-C2-N3	-4.92	121.13	128.58
5	A	2453	PSU	C4-N3-C2	-4.91	119.60	126.37
5	A	2500	PSU	C4-N3-C2	-4.83	119.72	126.37
5	A	2576	PSU	N1-C2-N3	4.82	120.25	115.17
5	A	2601	PSU	C4-N3-C2	-4.81	119.74	126.37
5	A	1913	PSU	C4-N3-C2	-4.80	119.76	126.37
5	A	2576	PSU	C4-N3-C2	-4.80	119.76	126.37
5	A	952	PSU	N1-C2-N3	4.75	120.18	115.17
5	A	2453	PSU	N1-C2-N3	4.71	120.13	115.17
5	A	2500	PSU	N1-C2-N3	4.69	120.12	115.17
5	A	1907	PSU	C4-N3-C2	-4.69	119.91	126.37
52	v	56	PSU	N1-C2-N3	4.66	120.08	115.17
52	v	56	PSU	C4-N3-C2	-4.64	119.99	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1913	PSU	N1-C2-N3	4.62	120.05	115.17
5	A	1907	PSU	N1-C2-N3	4.61	120.03	115.17
31	a	513	PSU	N1-C2-N3	4.59	120.00	115.17
5	A	2601	PSU	N1-C2-N3	4.57	119.99	115.17
31	a	513	PSU	C4-N3-C2	-4.53	120.13	126.37
5	A	2499	2MA	C4-N9-C1'	4.40	136.93	126.63
31	a	1515	MA6	C4-C5-C6	4.38	120.44	115.91
31	a	1515	MA6	N9-C8-N7	-4.32	107.80	113.94
31	a	1516	MA6	C4-C5-C6	4.21	120.26	115.91
31	a	1516	MA6	N9-C8-N7	-4.18	108.01	113.94
5	A	1911	3TD	C4-N3-C2	-4.02	120.35	124.61
5	A	2548	OMU	N3-C2-N1	4.00	120.10	114.89
52	v	8	4SU	C5-C4-S4	-3.95	119.80	124.31
5	A	2026	6MZ	N3-C4-N9	3.89	133.78	127.17
5	A	2499	2MA	N3-C4-N9	3.77	131.78	126.99
52	v	8	4SU	N3-C2-N1	3.68	119.68	114.89
31	a	1495	UR3	C5-C4-N3	3.60	119.78	115.04
5	A	2548	OMU	C5-C4-N3	3.51	119.72	114.80
5	A	2026	6MZ	N9-C8-N7	-3.51	108.96	113.94
5	A	2499	2MA	C5-N7-C8	3.41	108.81	103.45
5	A	2026	6MZ	C2-N3-C4	3.39	120.11	111.83
5	A	2499	2MA	N3-C2-N1	-3.37	119.83	125.77
31	a	1516	MA6	C2-N1-C6	3.32	119.94	111.83
31	a	1516	MA6	C2-N3-C4	3.31	119.91	111.83
31	a	1515	MA6	C2-N1-C6	3.29	119.87	111.83
31	a	1515	MA6	C2-N3-C4	3.25	119.77	111.83
52	v	20	H2U	C5-C4-N3	-3.23	113.25	116.69
31	a	1515	MA6	N3-C4-N9	3.05	132.36	127.17
5	A	2548	OMU	O4-C4-C5	-3.02	119.95	125.16
5	A	2576	PSU	O2-C2-N1	-3.00	119.70	122.79
31	a	1515	MA6	C5-N7-C8	2.97	108.11	103.45
5	A	2453	PSU	O2-C2-N1	-2.94	119.76	122.79
31	a	1516	MA6	C5-N7-C8	2.94	108.06	103.45
31	a	1516	MA6	N3-C4-N9	2.91	132.12	127.17
5	A	952	PSU	O2-C2-N1	-2.85	119.85	122.79
31	a	513	PSU	O2-C2-N1	-2.75	119.95	122.79
5	A	1911	3TD	C1'-C5-C4	2.74	121.76	117.61
52	v	56	PSU	O2-C2-N1	-2.72	119.98	122.79
5	A	1907	PSU	O2-C2-N1	-2.71	120.00	122.79
31	a	513	PSU	C6-N1-C2	-2.68	120.20	122.69
5	A	2026	6MZ	C5-N7-C8	2.67	107.64	103.45
31	a	1399	4OC	C6-C5-C4	2.63	120.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2500	PSU	O2-C2-N1	-2.59	120.12	122.79
5	A	1913	PSU	O2-C2-N1	-2.57	120.14	122.79
5	A	2576	PSU	O4'-C1'-C2'	2.54	108.67	105.15
52	v	56	PSU	C6-N1-C2	-2.53	120.34	122.69
5	A	2576	PSU	C6-N1-C2	-2.52	120.36	122.69
5	A	2601	PSU	O2-C2-N1	-2.51	120.20	122.79
31	a	1515	MA6	C4-N9-C8	2.44	108.30	105.74
5	A	2065	7MG	C5-C4-N9	2.41	109.42	106.33
31	a	524	7MG	C4-C5-N7	2.38	108.19	105.38
52	v	56	PSU	O4'-C1'-C2'	2.38	108.45	105.15
5	A	1907	PSU	C6-N1-C2	-2.38	120.48	122.69
31	a	513	PSU	O4'-C1'-C2'	2.34	108.38	105.15
31	a	1516	MA6	C4-C5-N7	-2.34	107.91	110.58
31	a	524	7MG	C5-C4-N9	2.30	109.28	106.33
5	A	2548	OMU	O2-C2-N1	-2.28	119.83	122.80
5	A	2065	7MG	C4-C5-N7	2.27	108.06	105.38
5	A	2499	2MA	C4-C5-N7	-2.26	108.00	110.58
31	a	1495	UR3	C6-N1-C2	-2.25	119.96	121.80
5	A	2453	PSU	C6-N1-C2	-2.24	120.61	122.69
31	a	1515	MA6	C4-C5-N7	-2.20	108.06	110.58
5	A	2499	2MA	CM2-C2-N1	2.20	120.42	117.13
5	A	2026	6MZ	C5-C6-N1	2.17	120.48	118.15
31	a	1516	MA6	C4-N9-C8	2.16	108.00	105.74
5	A	2500	PSU	C6-N1-C2	-2.15	120.70	122.69
5	A	2453	PSU	O4'-C1'-C2'	2.13	108.10	105.15
5	A	1913	PSU	C6-N1-C2	-2.11	120.74	122.69
5	A	952	PSU	C6-N1-C2	-2.06	120.78	122.69
31	a	1516	MA6	C5-C4-N9	2.02	108.02	105.81

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	55	5MU	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C4'-C5'-O5'
52	v	56	PSU	O4'-C1'-C5-C4
52	v	56	PSU	O4'-C1'-C5-C6
31	a	524	7MG	C3'-C4'-C5'-O5'
52	v	8	4SU	C3'-C4'-C5'-O5'
52	v	56	PSU	C3'-C4'-C5'-O5'
52	v	56	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	A	1911	3TD	O4'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	2026	6MZ	O4'-C4'-C5'-O5'
31	a	524	7MG	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
5	A	2026	6MZ	C3'-C4'-C5'-O5'
52	v	20	H2U	C3'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
52	v	20	H2U	C4'-C5'-O5'-P
52	v	55	5MU	C4'-C5'-O5'-P
5	A	2500	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	513	PSU	1	0
52	v	55	5MU	1	0
52	v	8	4SU	1	0
52	v	56	PSU	2	0
5	A	2026	6MZ	1	0
52	v	20	H2U	3	0
5	A	2548	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
55	OIY	a	1603	-	54,55,55	1.80	11 (20%)	55,74,74	1.61	8 (14%)
55	OIY	a	1601	-	36,37,55	1.34	6 (16%)	37,52,74	1.69	4 (10%)
55	OIY	A	3005	-	36,37,55	1.34	6 (16%)	37,52,74	1.98	6 (16%)
55	OIY	W	101	-	54,55,55	1.80	11 (20%)	55,74,74	1.61	8 (14%)
55	OIY	a	1604	-	36,37,55	1.30	6 (16%)	37,52,74	1.79	5 (13%)
55	OIY	A	3006	-	45,46,55	1.67	9 (20%)	46,63,74	1.57	6 (13%)
55	OIY	A	3003	-	54,55,55	1.80	11 (20%)	55,74,74	1.51	7 (12%)
55	OIY	A	3001	-	41,42,55	1.66	9 (21%)	43,58,74	1.64	6 (13%)
55	OIY	N	201	-	36,37,55	1.36	6 (16%)	37,52,74	1.66	5 (13%)
55	OIY	A	3002	-	48,49,55	1.84	12 (25%)	50,67,74	1.91	9 (18%)
55	OIY	a	1602	-	54,55,55	1.79	10 (18%)	55,74,74	1.53	8 (14%)
55	OIY	A	3004	-	54,55,55	1.77	10 (18%)	55,74,74	1.56	6 (10%)

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
55	OIY	a	1603	-	-	7/44/89/89	0/3/3/3
55	OIY	a	1601	-	-	3/22/67/89	0/3/3/3
55	OIY	A	3005	-	-	7/22/67/89	0/3/3/3
55	OIY	W	101	-	-	11/44/89/89	0/3/3/3
55	OIY	a	1604	-	-	3/22/67/89	0/3/3/3
55	OIY	A	3006	-	-	14/33/78/89	0/3/3/3
55	OIY	A	3003	-	-	17/44/89/89	0/3/3/3
55	OIY	A	3001	-	-	5/28/73/89	0/3/3/3
55	OIY	N	201	-	-	4/22/67/89	0/3/3/3
55	OIY	A	3002	-	-	15/36/81/89	0/3/3/3
55	OIY	a	1602	-	-	13/44/89/89	0/3/3/3
55	OIY	A	3004	-	-	12/44/89/89	0/3/3/3

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3002	OIY	C34-N33	6.90	1.49	1.33
55	a	1602	OIY	C34-N33	6.77	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3006	OIY	C34-N33	6.71	1.49	1.33
55	a	1603	OIY	C34-N33	6.70	1.49	1.33
55	W	101	OIY	C34-N33	6.70	1.49	1.33
55	A	3004	OIY	C34-N33	6.68	1.49	1.33
55	A	3003	OIY	C34-N33	6.67	1.49	1.33
55	A	3001	OIY	C34-N33	6.65	1.49	1.33
55	A	3003	OIY	C42-N41	6.20	1.48	1.33
55	a	1602	OIY	C42-N41	6.13	1.47	1.33
55	W	101	OIY	C42-N41	6.12	1.47	1.33
55	A	3004	OIY	C42-N41	6.12	1.47	1.33
55	a	1603	OIY	C42-N41	6.08	1.47	1.33
55	A	3002	OIY	C42-N41	5.10	1.47	1.34
55	a	1603	OIY	C05-N07	3.93	1.40	1.33
55	A	3006	OIY	C05-N07	3.91	1.40	1.33
55	a	1602	OIY	C05-N07	3.89	1.40	1.33
55	N	201	OIY	C05-N07	3.85	1.40	1.33
55	W	101	OIY	C05-N07	3.85	1.40	1.33
55	A	3003	OIY	C05-N07	3.83	1.40	1.33
55	a	1601	OIY	C05-N07	3.82	1.40	1.33
55	A	3002	OIY	C05-N07	3.77	1.40	1.33
55	A	3005	OIY	C05-N07	3.70	1.40	1.33
55	A	3004	OIY	C05-N07	3.70	1.40	1.33
55	A	3001	OIY	C05-N07	3.68	1.40	1.33
55	a	1604	OIY	C05-N07	3.56	1.39	1.33
55	A	3005	OIY	C01-C02	3.34	1.55	1.52
55	A	3002	OIY	C01-C02	3.29	1.55	1.52
55	W	101	OIY	C01-C02	3.28	1.55	1.52
55	A	3004	OIY	C01-C02	3.25	1.55	1.52
55	A	3006	OIY	C01-C02	3.24	1.55	1.52
55	a	1604	OIY	C01-C02	3.21	1.55	1.52
55	a	1601	OIY	C01-C02	3.20	1.55	1.52
55	A	3003	OIY	C01-C02	3.13	1.55	1.52
55	a	1603	OIY	C01-C02	3.10	1.55	1.52
55	N	201	OIY	C01-C02	3.10	1.55	1.52
55	A	3001	OIY	C01-C02	3.06	1.55	1.52
55	a	1603	OIY	C02-C03	-2.99	1.50	1.53
55	a	1601	OIY	C02-C03	-2.97	1.50	1.53
55	a	1602	OIY	C01-C02	2.92	1.55	1.52
55	N	201	OIY	C02-C03	-2.87	1.50	1.53
55	A	3003	OIY	C02-C03	-2.87	1.50	1.53
55	a	1602	OIY	C02-C03	-2.86	1.50	1.53
55	W	101	OIY	C02-C03	-2.85	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3006	OIY	C02-C03	-2.84	1.50	1.53
55	A	3004	OIY	C02-C03	-2.74	1.50	1.53
55	A	3005	OIY	C02-C03	-2.72	1.50	1.53
55	N	201	OIY	C01-N07	2.69	1.49	1.46
55	A	3002	OIY	C02-C03	-2.67	1.50	1.53
55	a	1603	OIY	C01-N07	2.66	1.49	1.46
55	a	1604	OIY	C02-C03	-2.65	1.50	1.53
55	A	3003	OIY	C01-N07	2.64	1.49	1.46
55	a	1601	OIY	C01-N07	2.62	1.49	1.46
55	W	101	OIY	C01-N07	2.61	1.49	1.46
55	A	3001	OIY	C02-C03	-2.60	1.50	1.53
55	a	1602	OIY	C01-N07	2.60	1.49	1.46
55	A	3005	OIY	C01-N07	2.58	1.49	1.46
55	A	3006	OIY	C01-N07	2.58	1.49	1.46
55	A	3004	OIY	C01-N07	2.56	1.49	1.46
55	A	3002	OIY	C01-N07	2.55	1.49	1.46
55	A	3002	OIY	C26-N25	2.46	1.39	1.34
55	A	3005	OIY	C26-N25	2.43	1.39	1.34
55	a	1604	OIY	C01-N07	2.41	1.48	1.46
55	a	1603	OIY	C26-N25	2.40	1.39	1.34
55	A	3004	OIY	C26-N25	2.40	1.39	1.34
55	A	3001	OIY	C36-C34	2.39	1.56	1.51
55	N	201	OIY	C26-N25	2.39	1.39	1.34
55	A	3003	OIY	C26-N25	2.38	1.39	1.34
55	A	3001	OIY	C26-N25	2.38	1.39	1.34
55	A	3002	OIY	C44-C42	2.37	1.55	1.50
55	A	3006	OIY	C26-N25	2.37	1.39	1.34
55	W	101	OIY	C26-N25	2.35	1.39	1.34
55	a	1602	OIY	C26-N25	2.35	1.39	1.34
55	a	1604	OIY	C26-N25	2.35	1.39	1.34
55	a	1601	OIY	C26-N25	2.33	1.38	1.34
55	A	3005	OIY	C21-N23	2.32	1.37	1.33
55	A	3001	OIY	C01-N07	2.30	1.48	1.46
55	A	3001	OIY	C21-N23	2.30	1.37	1.33
55	W	101	OIY	C21-N23	2.29	1.37	1.33
55	a	1604	OIY	C21-N23	2.29	1.37	1.33
55	a	1603	OIY	C21-N23	2.28	1.37	1.33
55	N	201	OIY	C21-N23	2.26	1.37	1.33
55	a	1602	OIY	C21-N23	2.26	1.37	1.33
55	A	3006	OIY	C21-N23	2.25	1.37	1.33
55	A	3004	OIY	C21-N23	2.24	1.37	1.33
55	A	3003	OIY	C21-N23	2.24	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1601	OIY	C21-N23	2.22	1.37	1.33
55	A	3002	OIY	C36-C34	2.21	1.56	1.51
55	A	3002	OIY	C21-N23	2.18	1.37	1.33
55	a	1602	OIY	O43-C42	-2.16	1.19	1.23
55	W	101	OIY	O43-C42	-2.15	1.19	1.23
55	A	3004	OIY	O43-C42	-2.13	1.19	1.23
55	a	1603	OIY	O43-C42	-2.13	1.19	1.23
55	A	3002	OIY	O35-C34	-2.12	1.19	1.23
55	W	101	OIY	O35-C34	-2.11	1.19	1.23
55	A	3003	OIY	C36-C34	2.11	1.56	1.51
55	A	3003	OIY	O43-C42	-2.10	1.19	1.23
55	A	3003	OIY	O35-C34	-2.09	1.19	1.23
55	a	1602	OIY	O35-C34	-2.09	1.19	1.23
55	a	1603	OIY	O35-C34	-2.06	1.19	1.23
55	A	3006	OIY	C36-C34	2.06	1.56	1.51
55	A	3004	OIY	O35-C34	-2.06	1.19	1.23
55	A	3006	OIY	O35-C34	-2.05	1.19	1.23
55	A	3001	OIY	O35-C34	-2.04	1.19	1.23
55	W	101	OIY	C36-C34	2.03	1.56	1.51
55	a	1603	OIY	C36-C34	2.02	1.56	1.51
55	A	3002	OIY	O43-C42	-2.00	1.18	1.23

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1604	OIY	C02-C01-N07	8.06	118.04	109.83
55	A	3002	OIY	C02-C01-N07	7.72	117.69	109.83
55	W	101	OIY	C02-C01-N07	7.65	117.63	109.83
55	a	1601	OIY	C02-C01-N07	7.48	117.45	109.83
55	A	3001	OIY	C02-C01-N07	7.39	117.36	109.83
55	A	3004	OIY	C02-C01-N07	7.28	117.25	109.83
55	A	3006	OIY	C02-C01-N07	7.25	117.22	109.83
55	A	3005	OIY	C02-C01-N07	7.20	117.17	109.83
55	A	3003	OIY	C02-C01-N07	7.10	117.06	109.83
55	N	201	OIY	C02-C01-N07	7.04	117.00	109.83
55	a	1602	OIY	C02-C01-N07	7.00	116.96	109.83
55	a	1603	OIY	C02-C01-N07	6.88	116.84	109.83
55	A	3002	OIY	O17-C12-C13	5.51	112.73	108.97
55	A	3005	OIY	C12-C13-N25	5.13	117.38	111.12
55	A	3004	OIY	O06-C05-N07	3.72	127.45	122.41
55	A	3002	OIY	C36-C34-N33	3.69	121.67	115.97
55	A	3005	OIY	O06-C05-N07	3.69	127.41	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1603	OIY	C36-C34-N33	3.67	121.64	115.97
55	A	3002	OIY	C28-C26-N25	-3.61	111.33	116.25
55	A	3004	OIY	C28-C26-N25	-3.53	111.44	116.25
55	A	3005	OIY	C28-C26-N25	-3.50	111.47	116.25
55	a	1604	OIY	C28-C26-N25	-3.46	111.53	116.25
55	W	101	OIY	C28-C26-N25	-3.45	111.54	116.25
55	a	1603	OIY	C28-C26-N25	-3.42	111.58	116.25
55	A	3003	OIY	C28-C26-N25	-3.39	111.63	116.25
55	a	1604	OIY	O06-C05-N07	3.38	126.99	122.41
55	A	3001	OIY	C28-C26-N25	-3.37	111.66	116.25
55	N	201	OIY	C28-C26-N25	-3.35	111.68	116.25
55	a	1602	OIY	C28-C26-N25	-3.34	111.70	116.25
55	A	3006	OIY	C28-C26-N25	-3.33	111.70	116.25
55	a	1601	OIY	C28-C26-N25	-3.28	111.77	116.25
55	N	201	OIY	O06-C05-N07	3.26	126.83	122.41
55	a	1602	OIY	C03-N10-C09	-3.24	106.75	112.17
55	a	1601	OIY	O06-C05-N07	3.23	126.78	122.41
55	A	3006	OIY	O06-C05-N07	3.23	126.78	122.41
55	A	3003	OIY	O06-C05-N07	3.17	126.71	122.41
55	A	3002	OIY	O06-C05-N07	3.12	126.64	122.41
55	A	3005	OIY	C13-N25-C26	3.00	127.32	122.90
55	a	1603	OIY	O17-C12-C13	3.00	111.02	108.97
55	a	1602	OIY	O17-C12-N11	2.99	113.60	108.12
55	A	3002	OIY	C16-O17-C12	2.95	116.57	112.47
55	a	1603	OIY	O06-C05-N07	2.93	126.38	122.41
55	a	1603	OIY	C44-C42-N41	2.87	120.41	115.97
55	A	3004	OIY	C36-C34-N33	2.86	120.38	115.97
55	a	1604	OIY	O17-C12-C13	2.83	110.90	108.97
55	a	1603	OIY	C03-N10-C09	-2.79	107.50	112.17
55	W	101	OIY	O06-C05-N07	2.77	126.16	122.41
55	A	3003	OIY	C03-N10-C09	-2.77	107.55	112.17
55	A	3005	OIY	C03-N10-C09	-2.73	107.61	112.17
55	A	3006	OIY	C03-N10-C09	-2.72	107.62	112.17
55	N	201	OIY	C03-N10-C09	-2.69	107.67	112.17
55	a	1602	OIY	O06-C05-N07	2.68	126.05	122.41
55	A	3004	OIY	C03-N10-C09	-2.65	107.74	112.17
55	A	3003	OIY	C44-C42-N41	2.64	120.05	115.97
55	W	101	OIY	C36-C34-N33	2.62	120.02	115.97
55	a	1601	OIY	C03-N10-C09	-2.61	107.81	112.17
55	A	3001	OIY	O17-C12-N11	2.59	112.87	108.12
55	A	3006	OIY	C36-C34-N33	2.57	119.94	115.97
55	W	101	OIY	C03-N10-C09	-2.53	107.95	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	3002	OIY	C03-N10-C09	-2.50	107.99	112.17
55	W	101	OIY	C44-C42-N41	2.48	119.81	115.97
55	A	3002	OIY	C44-C42-N41	2.41	120.24	116.12
55	a	1602	OIY	C36-C34-N33	2.33	119.57	115.97
55	a	1602	OIY	C44-C42-N41	2.30	119.53	115.97
55	N	201	OIY	O17-C12-C13	2.27	110.52	108.97
55	a	1604	OIY	C03-N10-C09	-2.26	108.39	112.17
55	A	3004	OIY	C44-C42-N41	2.24	119.43	115.97
55	W	101	OIY	N11-C09-N10	-2.23	114.80	122.00
55	A	3003	OIY	C36-C34-N33	2.21	119.39	115.97
55	A	3001	OIY	O06-C05-N07	2.17	125.36	122.41
55	A	3003	OIY	N11-C09-N10	-2.10	115.20	122.00
55	a	1603	OIY	N11-C09-N10	-2.06	115.33	122.00
55	A	3001	OIY	C36-C34-N33	2.04	120.07	116.34
55	A	3001	OIY	C12-C13-N25	2.03	113.60	111.12
55	a	1602	OIY	C40-N41-C42	-2.03	119.05	122.82
55	W	101	OIY	O17-C12-N11	2.02	111.83	108.12
55	A	3002	OIY	O35-C34-N33	-2.01	119.09	123.03
55	A	3006	OIY	O17-C12-C13	2.01	110.34	108.97

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	3002	OIY	C28-C29-C30-C31
55	A	3002	OIY	N52-C29-C30-C31
55	A	3002	OIY	C36-C37-C38-C39
55	A	3002	OIY	N51-C37-C38-C39
55	A	3003	OIY	C12-C13-N25-C26
55	A	3003	OIY	C28-C29-C30-C31
55	A	3003	OIY	C34-C36-C37-N51
55	A	3004	OIY	C26-C28-C29-N52
55	A	3004	OIY	C36-C37-C38-C39
55	A	3004	OIY	C42-C44-C45-N50
55	A	3005	OIY	C12-C13-N25-C26
55	A	3005	OIY	C14-C15-O20-C21
55	A	3005	OIY	C16-C15-O20-C21
55	A	3005	OIY	C26-C28-C29-C30
55	A	3005	OIY	C26-C28-C29-N52
55	A	3006	OIY	N23-C21-O20-C15
55	A	3006	OIY	O22-C21-O20-C15
55	A	3006	OIY	C26-C28-C29-N52

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Mol	Chain	Res	Type	Atoms
55	A	3006	OIY	C28-C29-C30-C31
55	W	101	OIY	N23-C21-O20-C15
55	W	101	OIY	O22-C21-O20-C15
55	W	101	OIY	C28-C29-C30-C31
55	a	1602	OIY	C26-C28-C29-N52
55	a	1602	OIY	C34-C36-C37-C38
55	a	1602	OIY	C34-C36-C37-N51
55	a	1602	OIY	C44-C45-C46-C47
55	a	1602	OIY	N50-C45-C46-C47
55	a	1603	OIY	C28-C29-C30-C31
55	a	1603	OIY	N52-C29-C30-C31
55	a	1603	OIY	C44-C45-C46-C47
55	A	3001	OIY	O17-C16-C18-O19
55	A	3002	OIY	C36-C34-N33-C32
55	a	1602	OIY	C44-C42-N41-C40
55	a	1603	OIY	C36-C34-N33-C32
55	A	3001	OIY	C15-C16-C18-O19
55	A	3002	OIY	O17-C16-C18-O19
55	A	3002	OIY	O35-C34-N33-C32
55	a	1602	OIY	O43-C42-N41-C40
55	a	1603	OIY	O35-C34-N33-C32
55	a	1601	OIY	O17-C16-C18-O19
55	A	3001	OIY	C30-C31-C32-N33
55	A	3004	OIY	C30-C31-C32-N33
55	a	1603	OIY	C38-C39-C40-N41
55	A	3003	OIY	C15-C16-C18-O19
55	A	3006	OIY	C15-C16-C18-O19
55	a	1604	OIY	C15-C16-C18-O19
55	A	3006	OIY	O17-C16-C18-O19
55	A	3004	OIY	C15-C16-C18-O19
55	W	101	OIY	C38-C39-C40-N41
55	A	3003	OIY	O17-C16-C18-O19
55	a	1601	OIY	C15-C16-C18-O19
55	a	1604	OIY	O17-C16-C18-O19
55	A	3004	OIY	O17-C16-C18-O19
55	W	101	OIY	O17-C16-C18-O19
55	W	101	OIY	C45-C46-C47-C48
55	A	3002	OIY	C29-C30-C31-C32
55	A	3003	OIY	C37-C38-C39-C40
55	A	3002	OIY	C26-C28-C29-C30
55	A	3003	OIY	C34-C36-C37-C38
55	A	3004	OIY	C26-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
55	a	1602	OIY	O17-C16-C18-O19
55	A	3006	OIY	C29-C30-C31-C32
55	N	201	OIY	C15-C16-C18-O19
55	A	3002	OIY	C15-C16-C18-O19
55	A	3003	OIY	C38-C39-C40-N41
55	W	101	OIY	C42-C44-C45-C46
55	N	201	OIY	O17-C16-C18-O19
55	A	3004	OIY	O35-C34-C36-C37
55	N	201	OIY	C26-C28-C29-N52
55	a	1602	OIY	C14-C15-O20-C21
55	A	3006	OIY	C36-C37-C38-C39
55	A	3006	OIY	N51-C37-C38-C39
55	W	101	OIY	N52-C29-C30-C31
55	W	101	OIY	C36-C37-C38-C39
55	W	101	OIY	N51-C37-C38-C39
55	A	3004	OIY	N33-C34-C36-C37
55	A	3006	OIY	C12-C13-N25-C26
55	a	1603	OIY	C29-C30-C31-C32
55	A	3003	OIY	C14-C13-N25-C26
55	A	3003	OIY	C42-C44-C45-C46
55	a	1602	OIY	C26-C28-C29-C30
55	A	3006	OIY	C14-C13-N25-C26
55	A	3003	OIY	C30-C31-C32-N33
55	a	1602	OIY	C31-C32-N33-C34
55	A	3004	OIY	C37-C38-C39-C40
55	A	3002	OIY	O35-C34-C36-C37
55	A	3002	OIY	N25-C26-C28-C29
55	A	3006	OIY	C34-C36-C37-C38
55	A	3001	OIY	C26-C28-C29-N52
55	A	3006	OIY	C34-C36-C37-N51
55	W	101	OIY	C26-C28-C29-N52
55	A	3003	OIY	C29-C30-C31-C32
55	A	3003	OIY	N33-C34-C36-C37
55	a	1602	OIY	N25-C26-C28-C29
55	A	3003	OIY	O17-C12-N11-C09
55	A	3002	OIY	O27-C26-C28-C29
55	A	3003	OIY	O35-C34-C36-C37
55	a	1602	OIY	O27-C26-C28-C29
55	A	3001	OIY	N08-C09-N11-C12
55	A	3002	OIY	N08-C09-N11-C12
55	A	3003	OIY	N52-C29-C30-C31
55	A	3003	OIY	N08-C09-N11-C12

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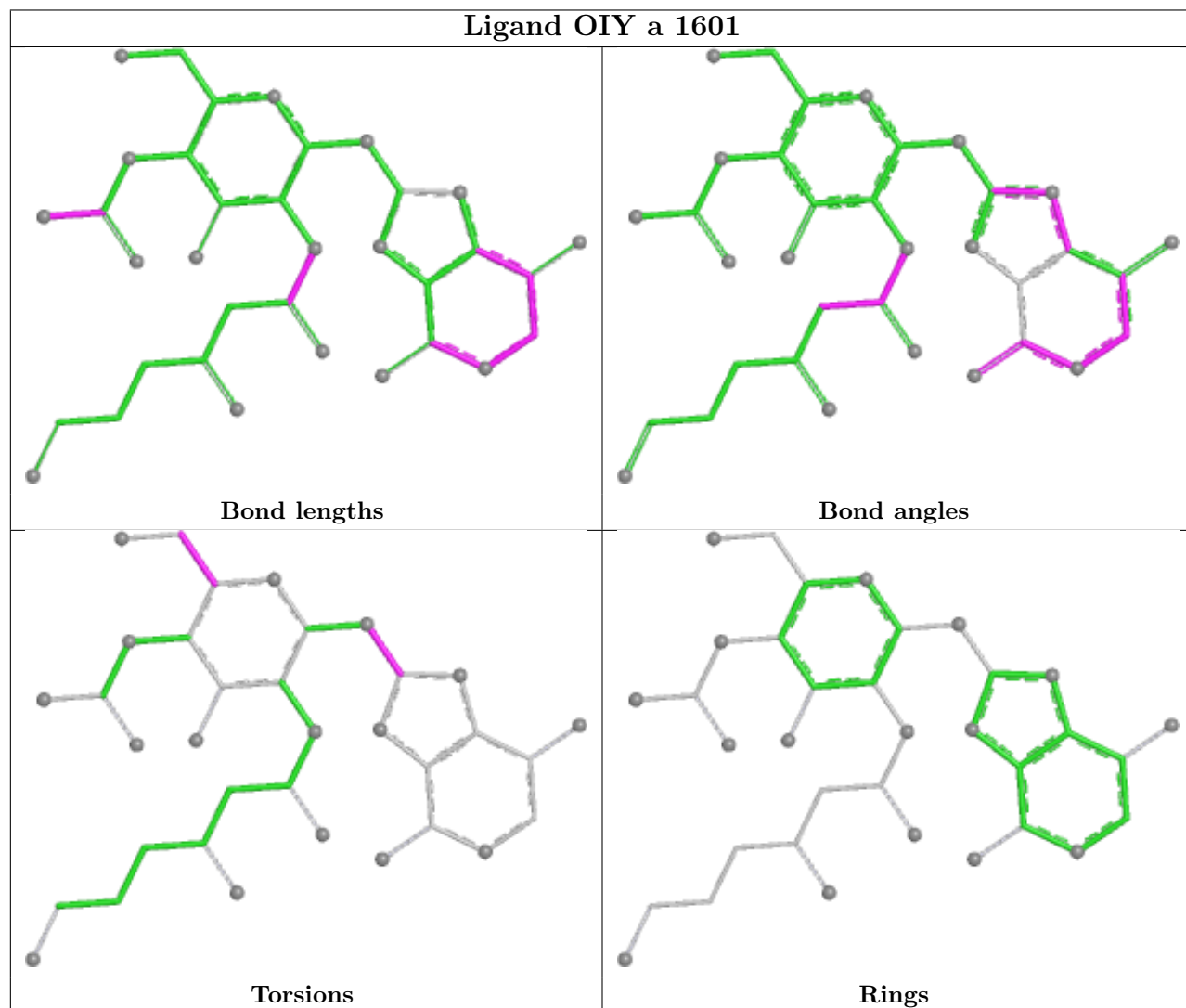
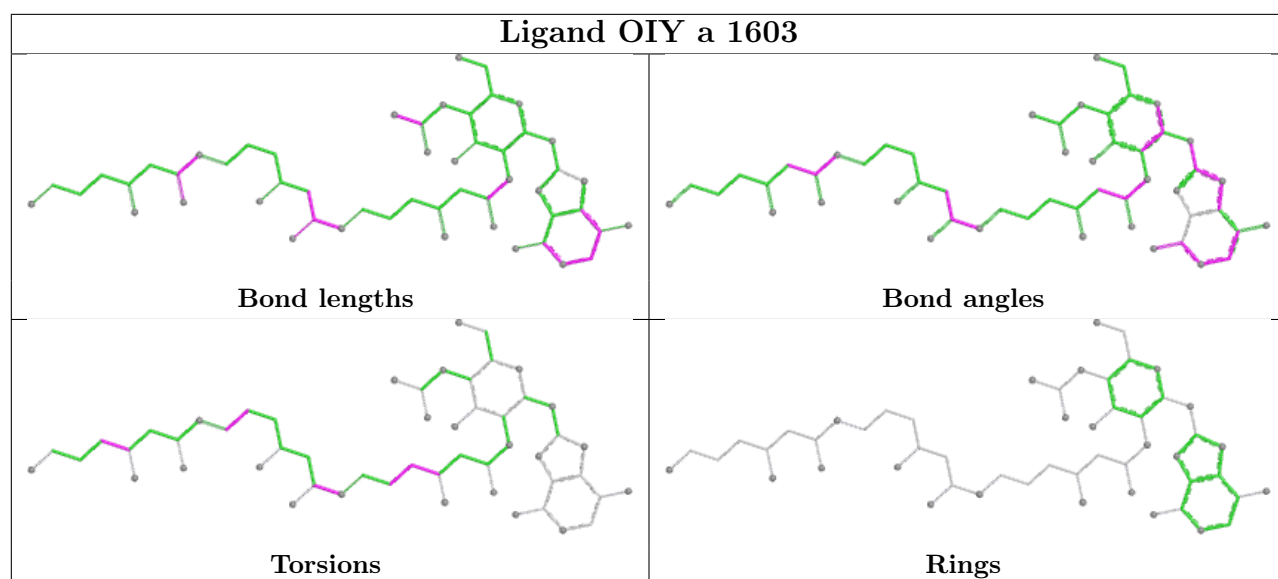
Mol	Chain	Res	Type	Atoms
55	A	3004	OIY	N08-C09-N11-C12
55	A	3005	OIY	N08-C09-N11-C12
55	A	3006	OIY	N08-C09-N11-C12
55	N	201	OIY	N08-C09-N11-C12
55	a	1601	OIY	N08-C09-N11-C12
55	a	1604	OIY	N08-C09-N11-C12
55	A	3002	OIY	N33-C34-C36-C37
55	A	3004	OIY	C29-C30-C31-C32
55	A	3005	OIY	C14-C13-N25-C26

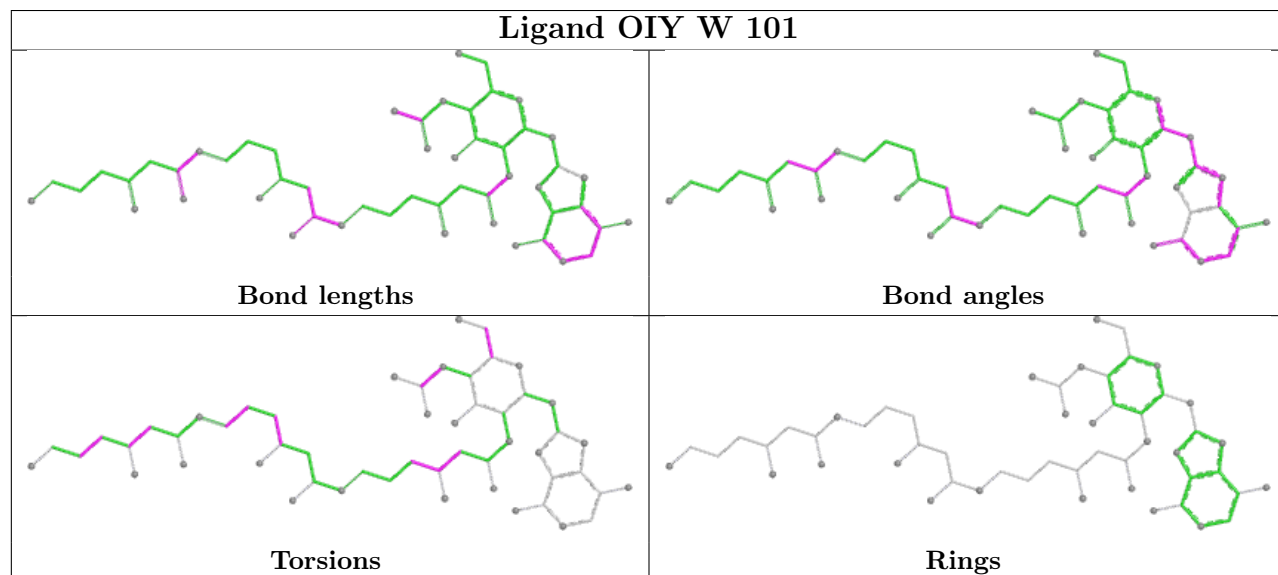
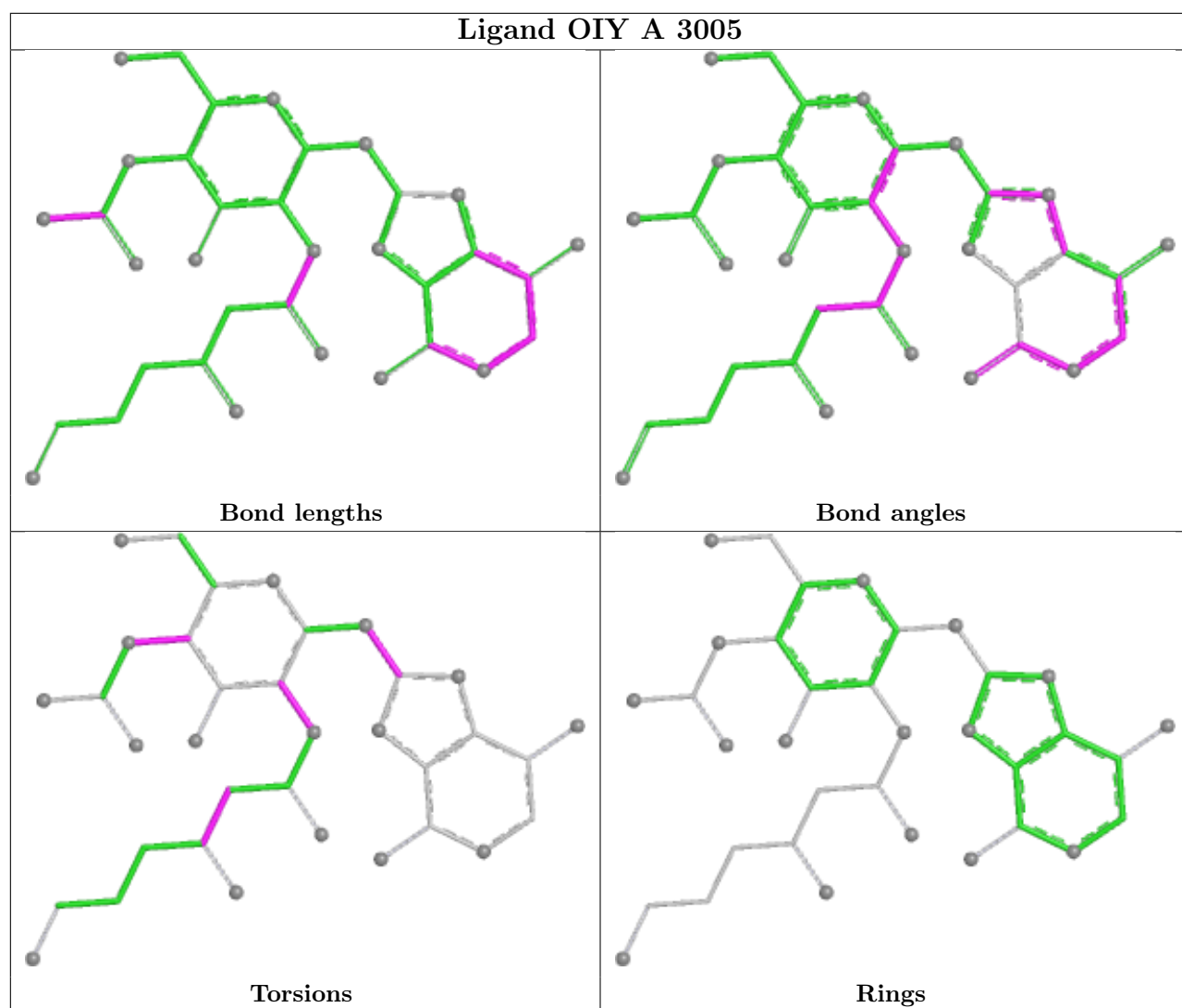
There are no ring outliers.

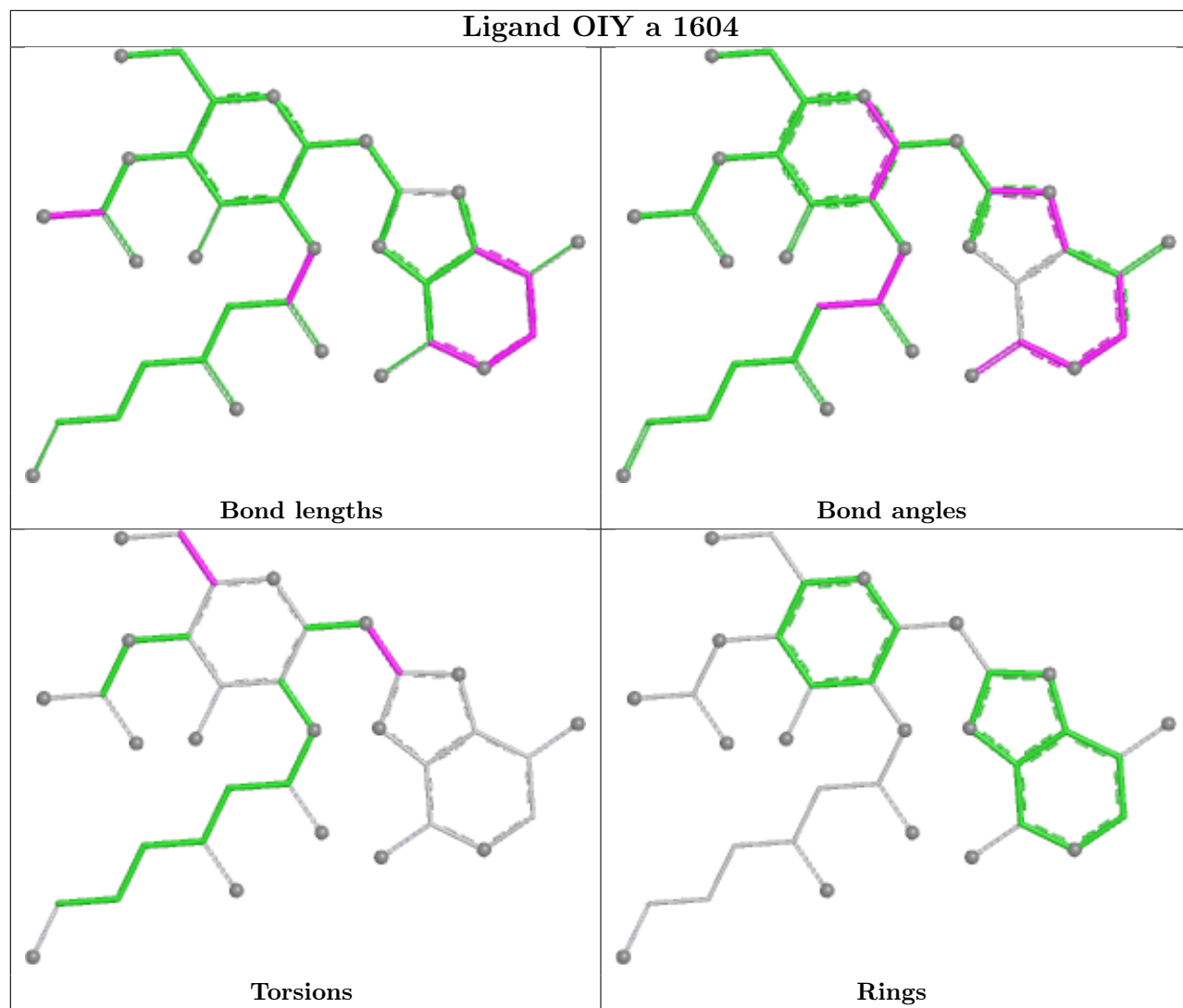
7 monomers are involved in 8 short contacts:

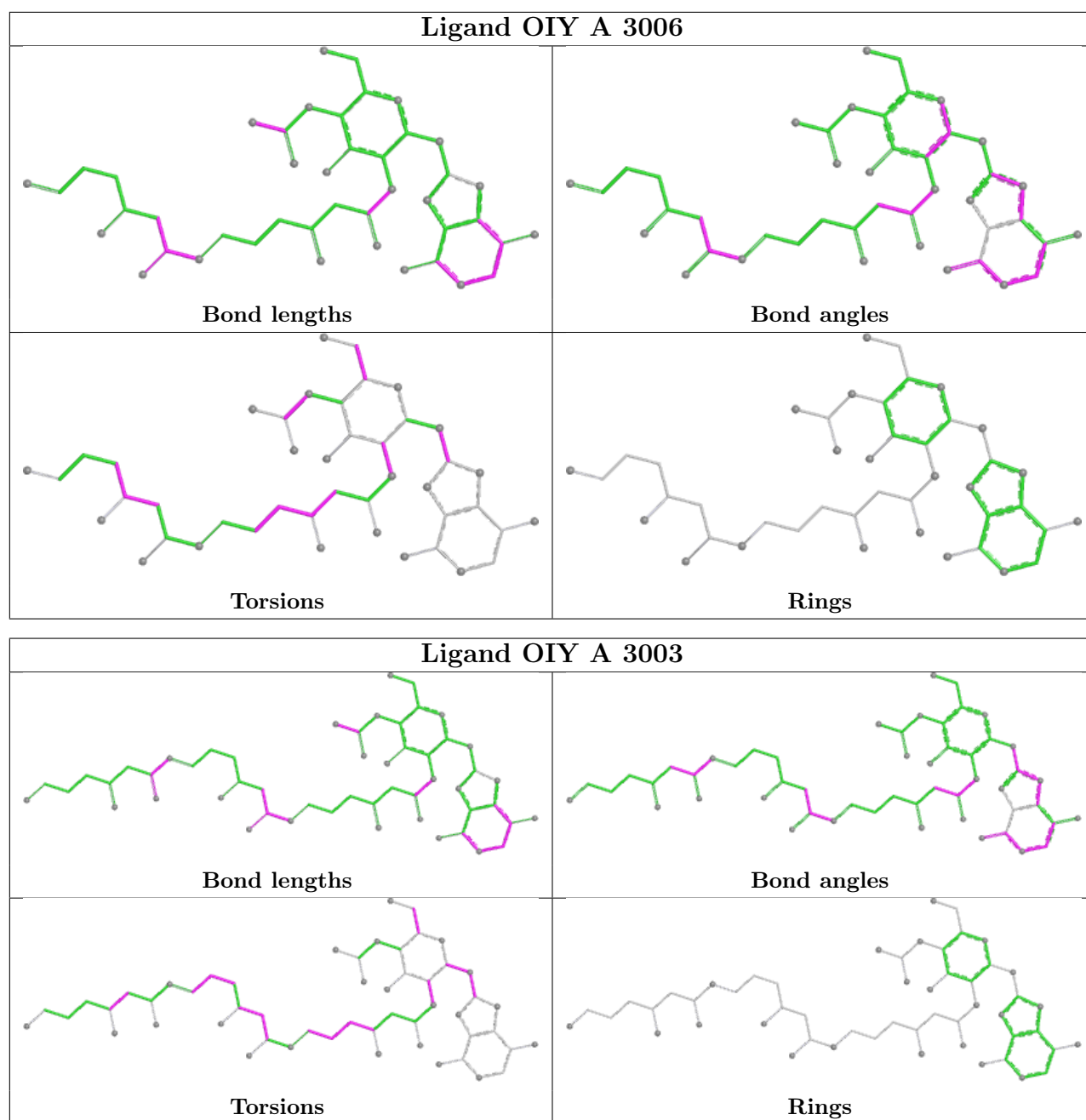
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A	3005	OIY	1	0
55	W	101	OIY	2	0
55	A	3006	OIY	1	0
55	N	201	OIY	1	0
55	A	3002	OIY	1	0
55	a	1602	OIY	1	0
55	A	3004	OIY	1	0

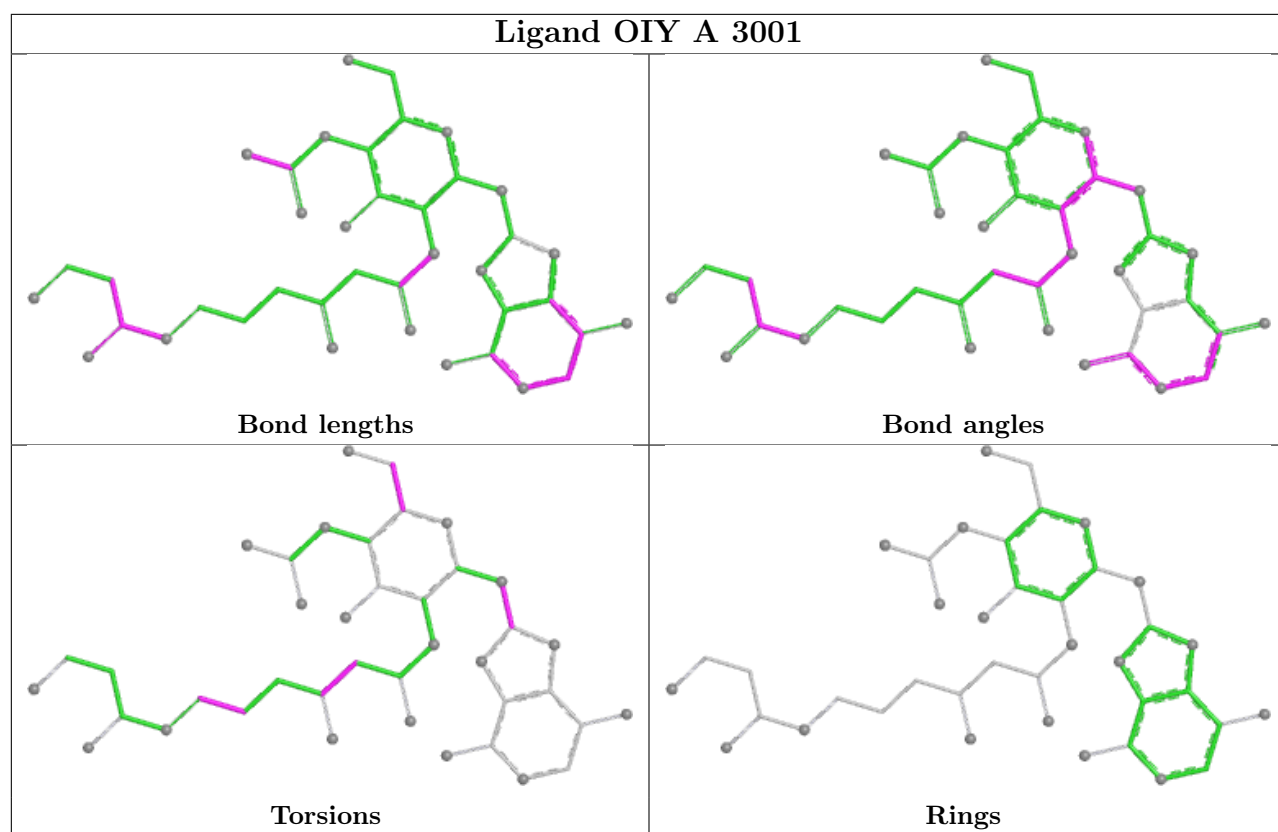
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

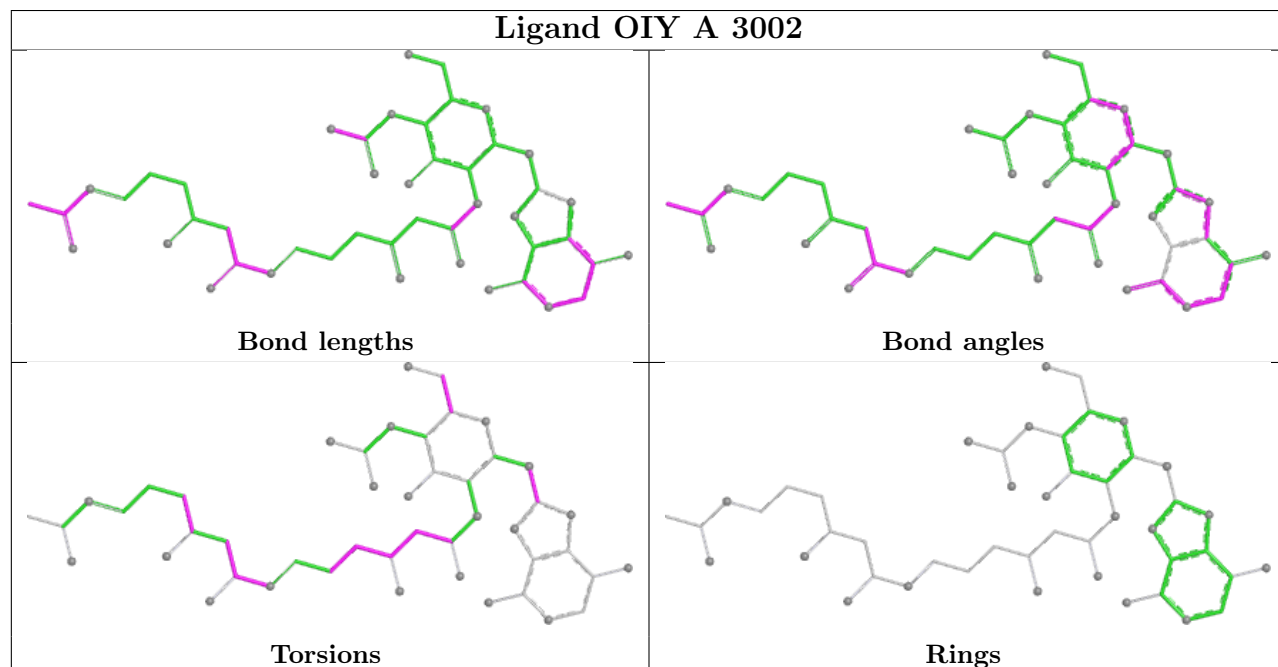
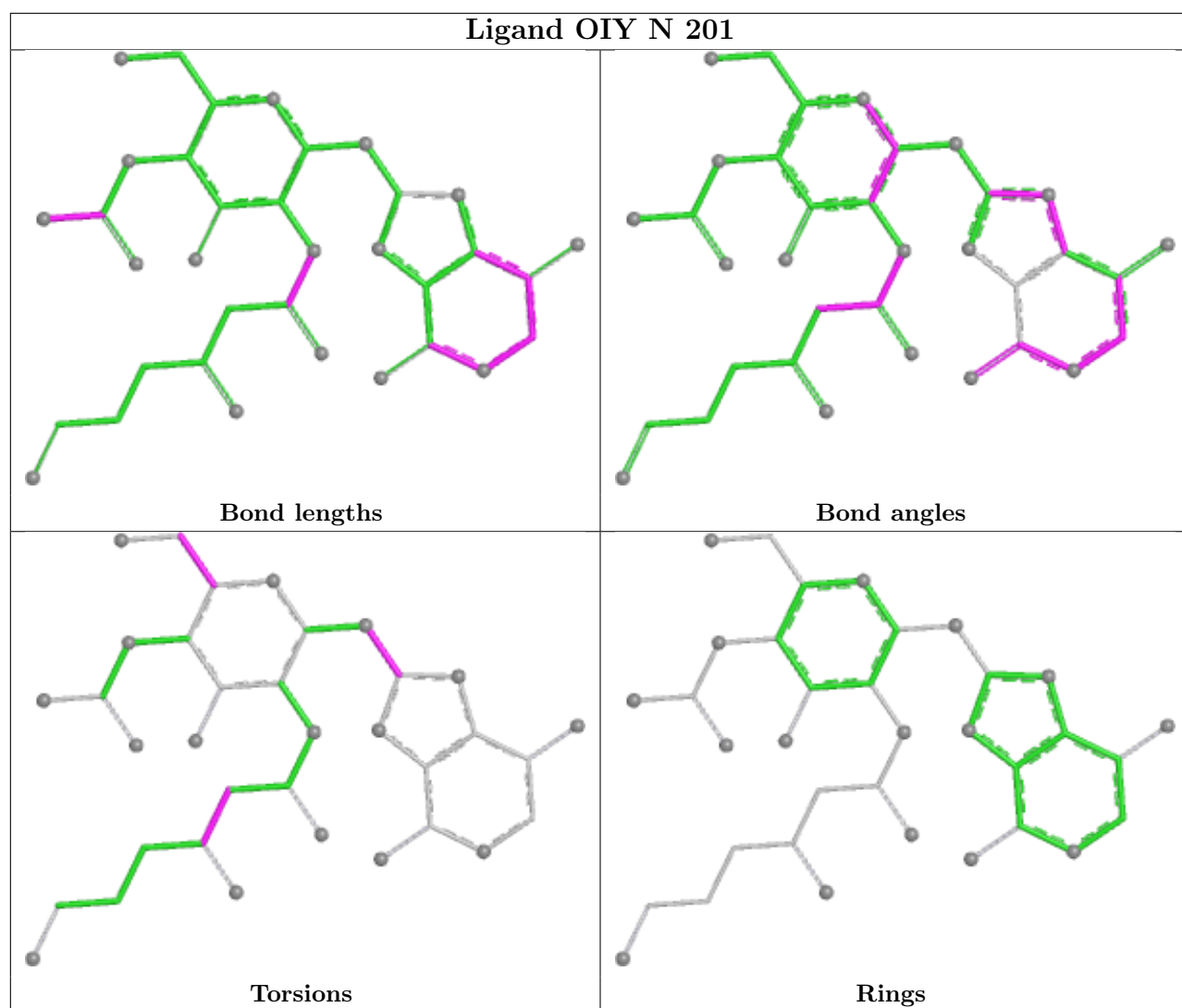


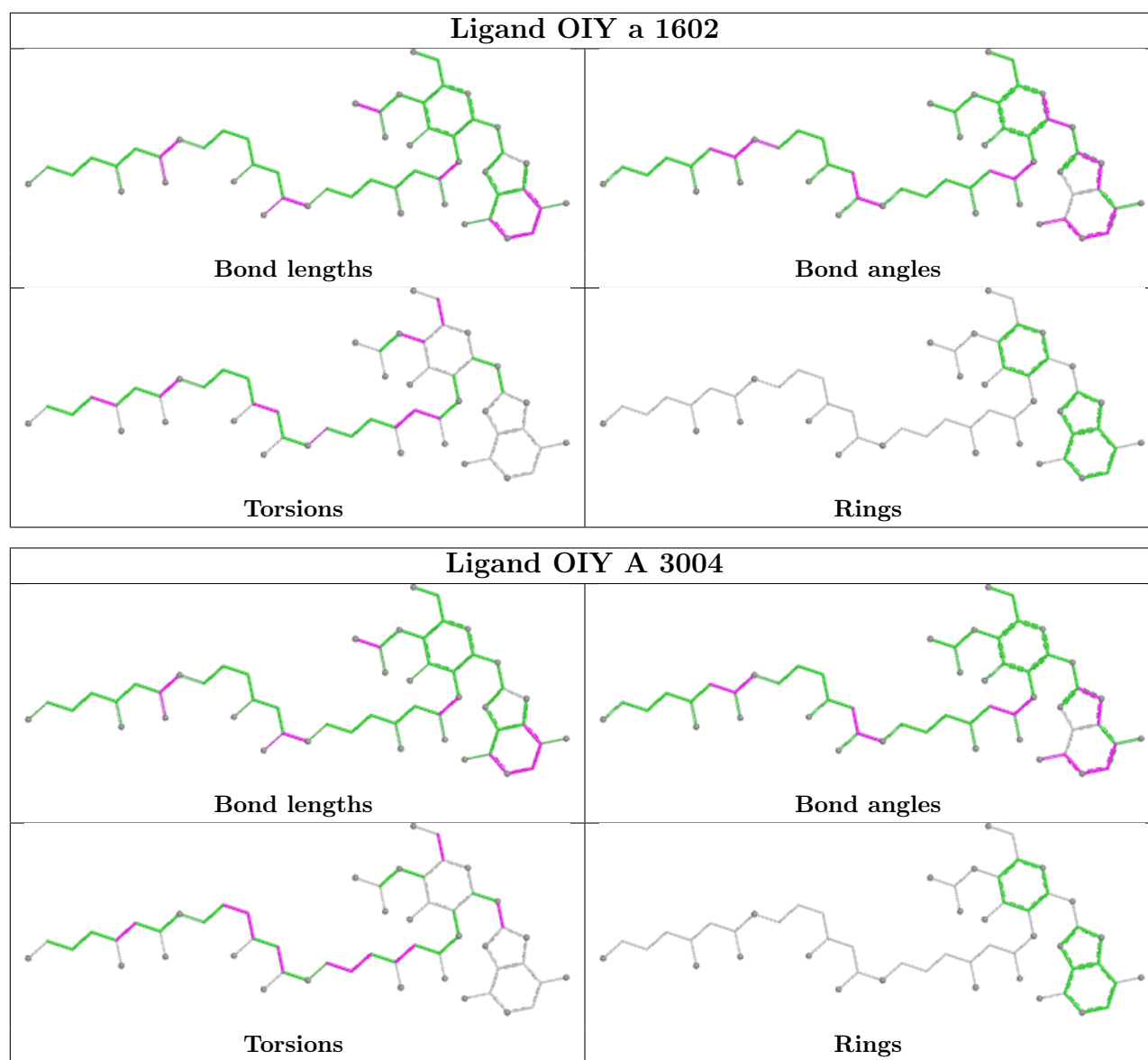












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

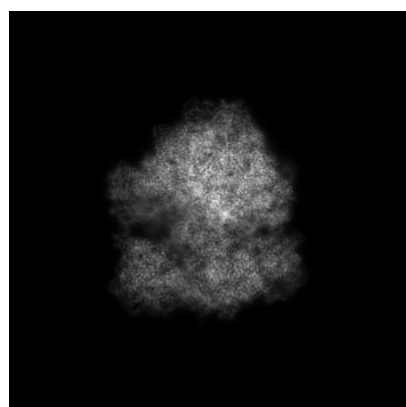
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26820. These allow visual inspection of the internal detail of the map and identification of artifacts.

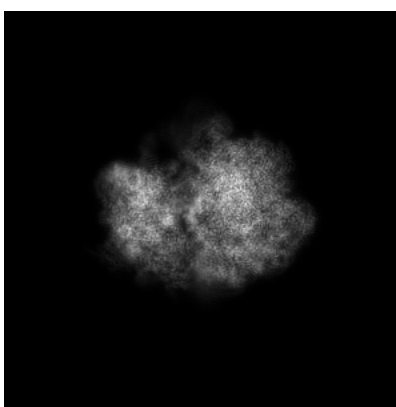
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

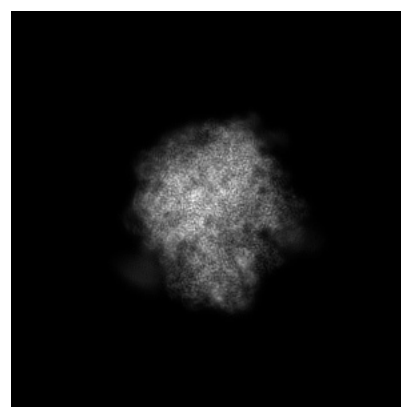
6.1.1 Primary map



X



Y

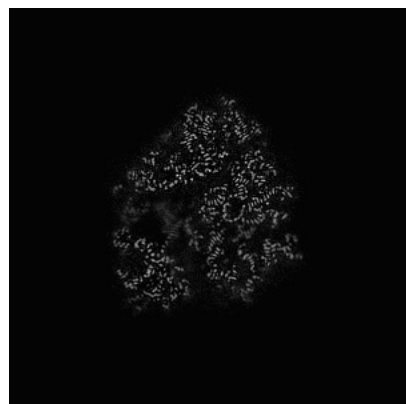


Z

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

6.2 Central slices [i](#)

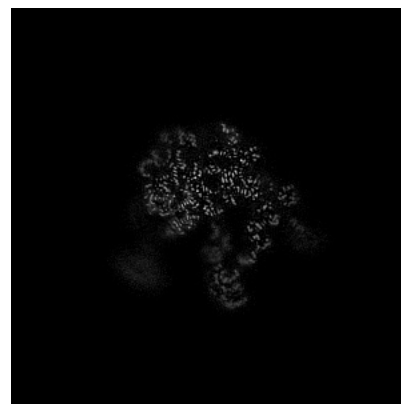
6.2.1 Primary map



X Index: 320



Y Index: 320

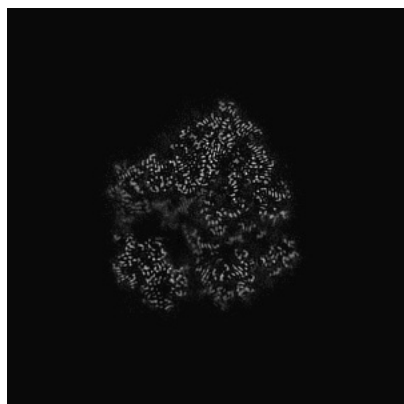


Z Index: 320

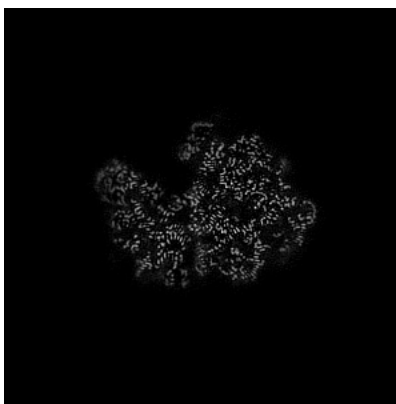
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

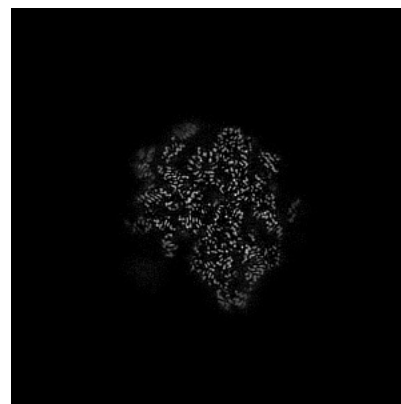
6.3.1 Primary map



X Index: 329



Y Index: 341

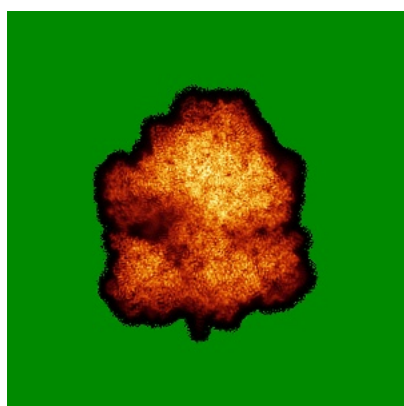


Z Index: 364

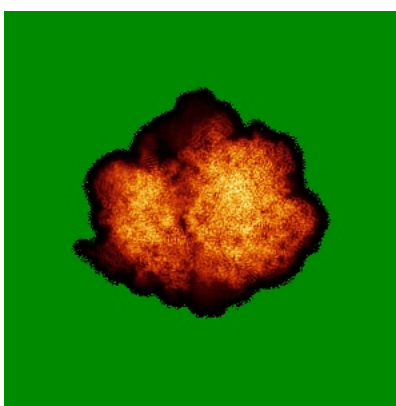
The images above show the largest variance slices of the map in three orthogonal directions.

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

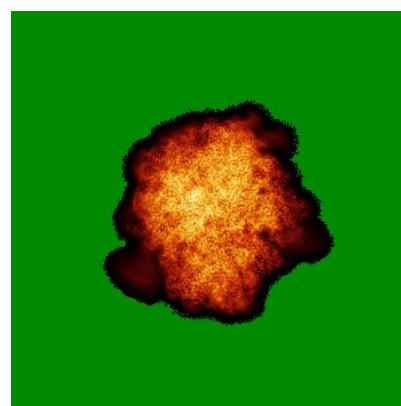
6.4.1 Primary map



X



Y

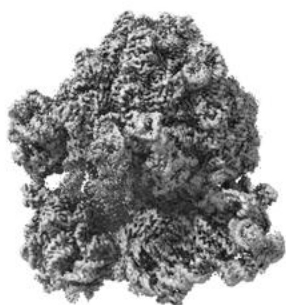


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

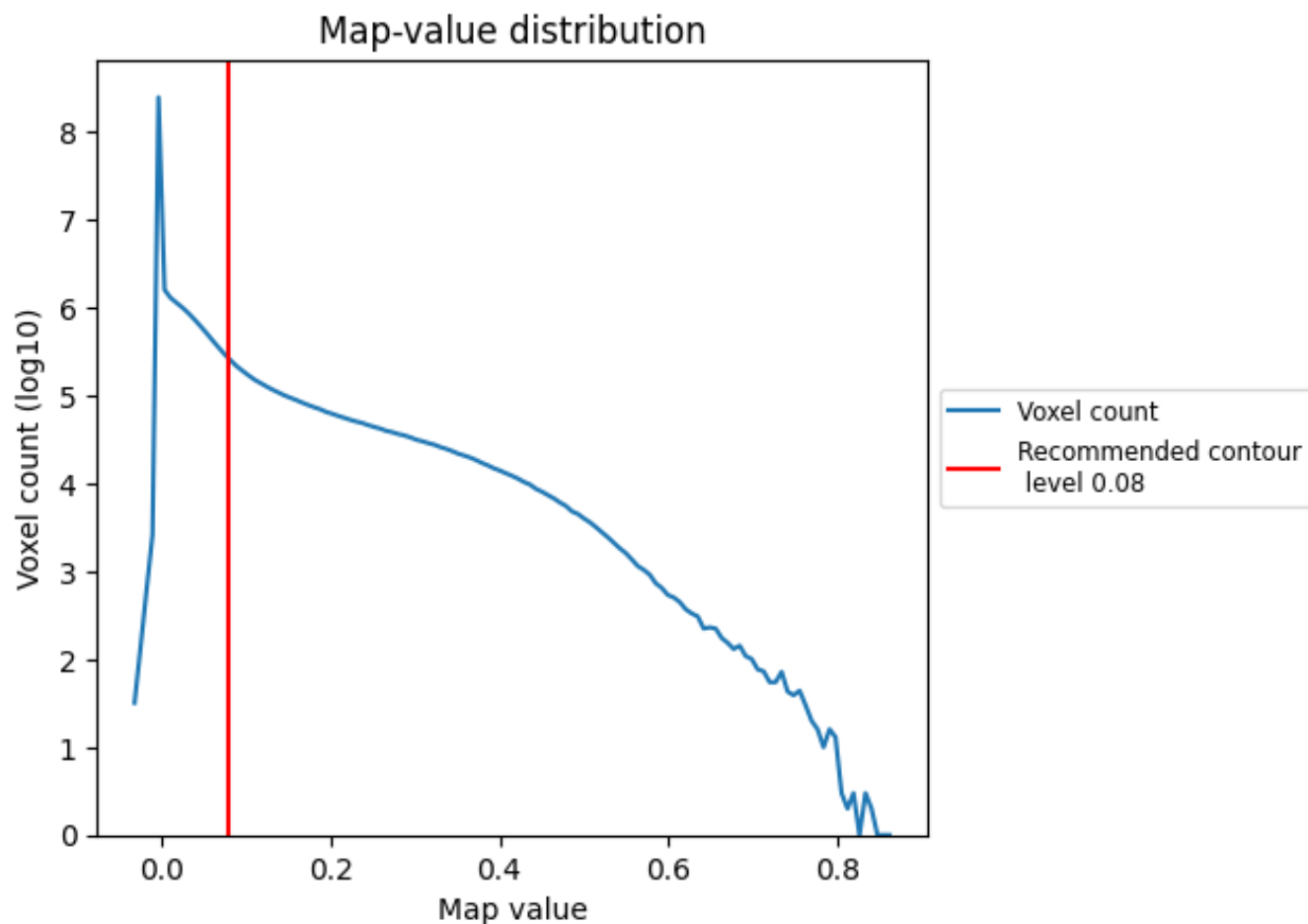
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

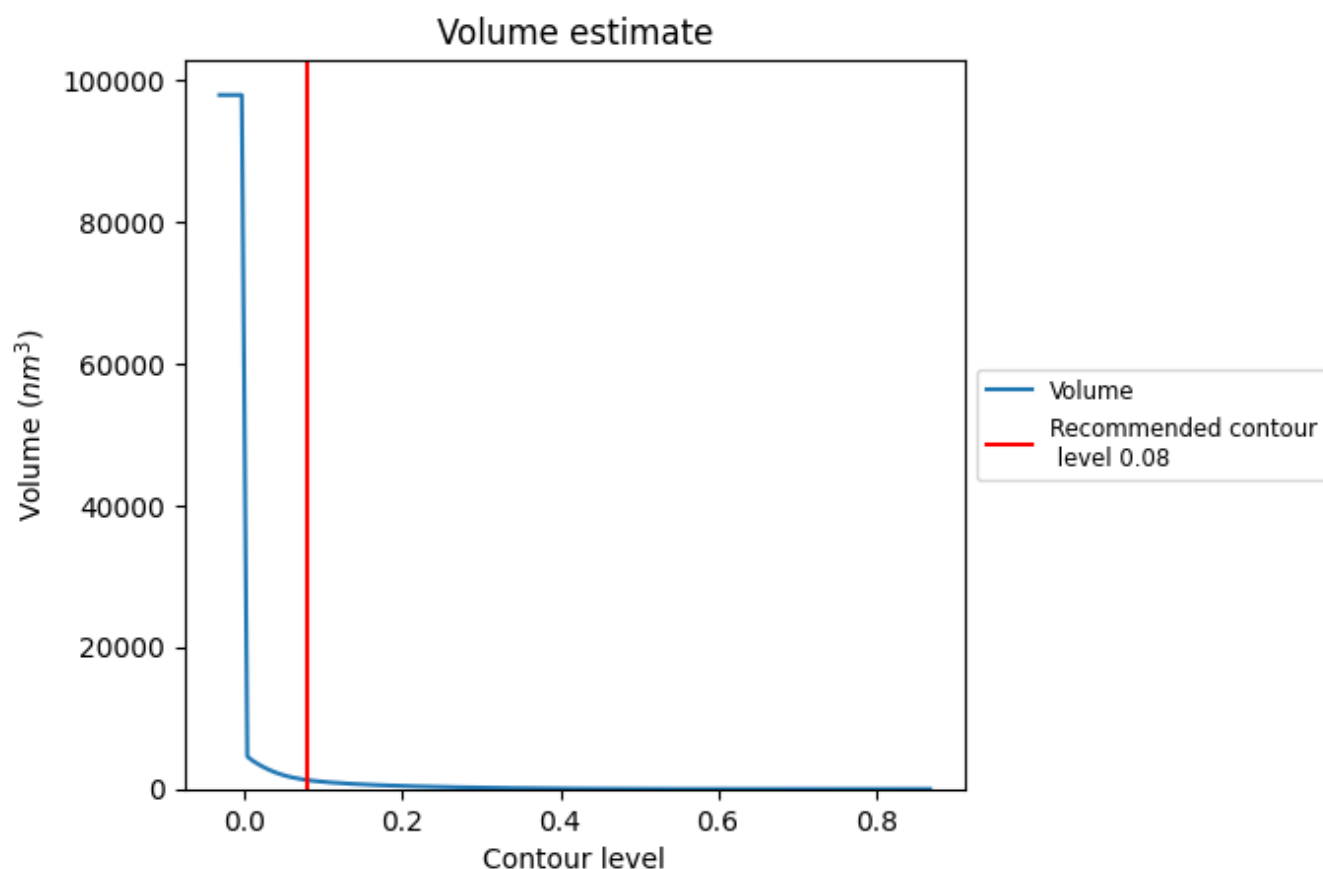
This section contains the results of statistical analysis of the map.

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.

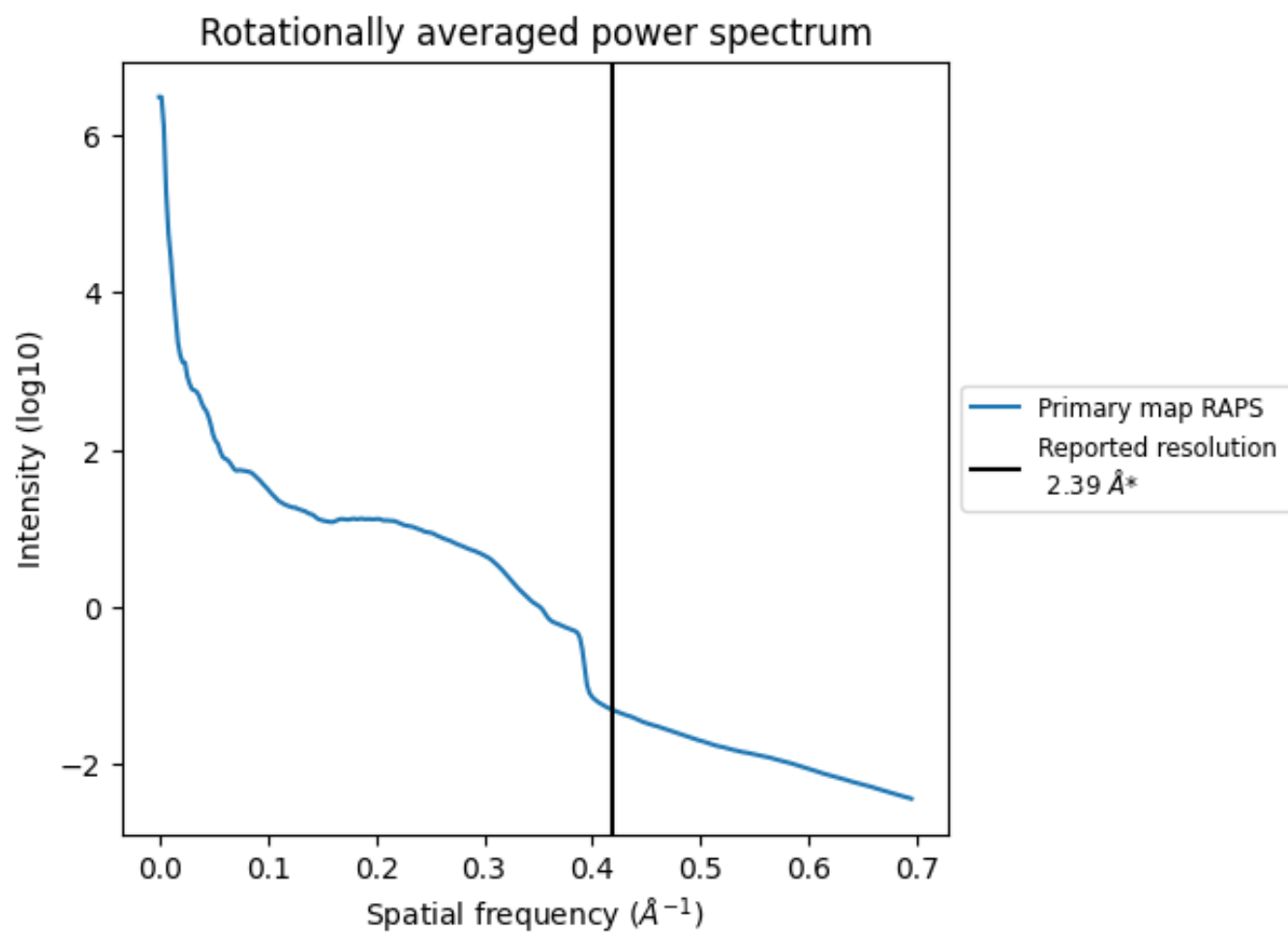
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1240 nm^3 ; this corresponds to an approximate mass of 1120 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 0.418 Å⁻¹

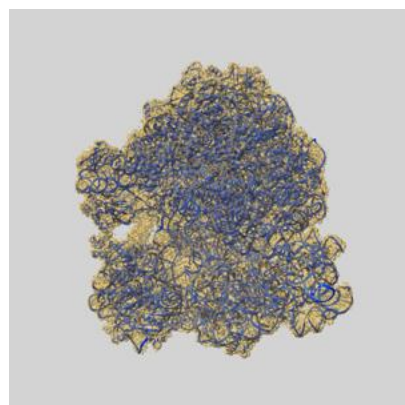
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

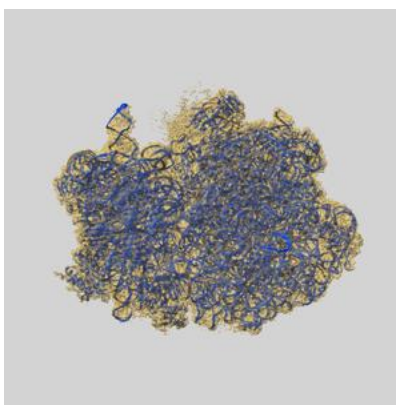
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26820 and PDB model 7UVY. Per-residue inclusion information can be found in section [3](#) on page [15](#).

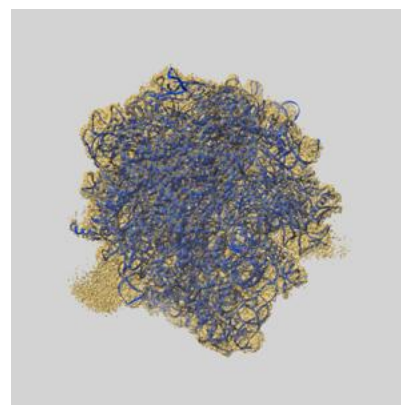
9.1 Map-model overlay [i](#)



X



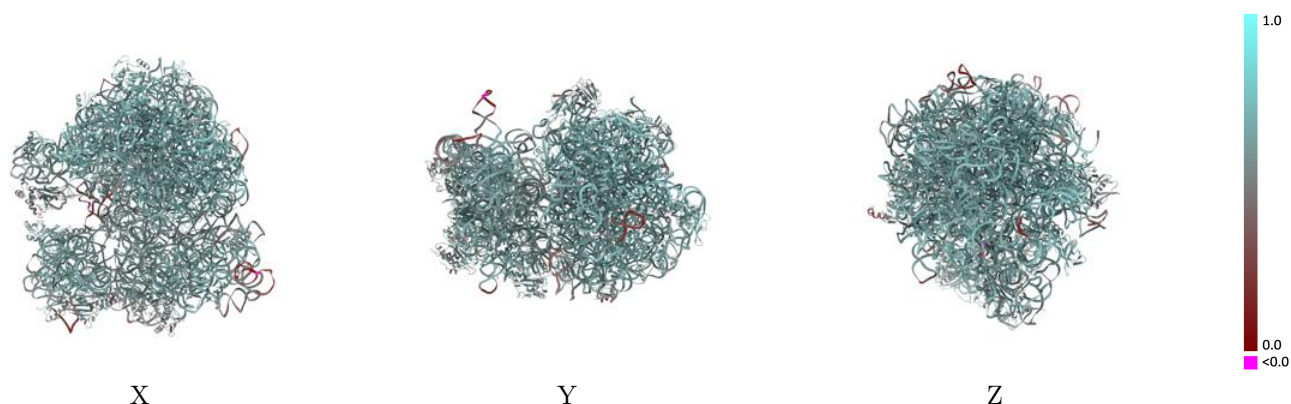
Y



Z

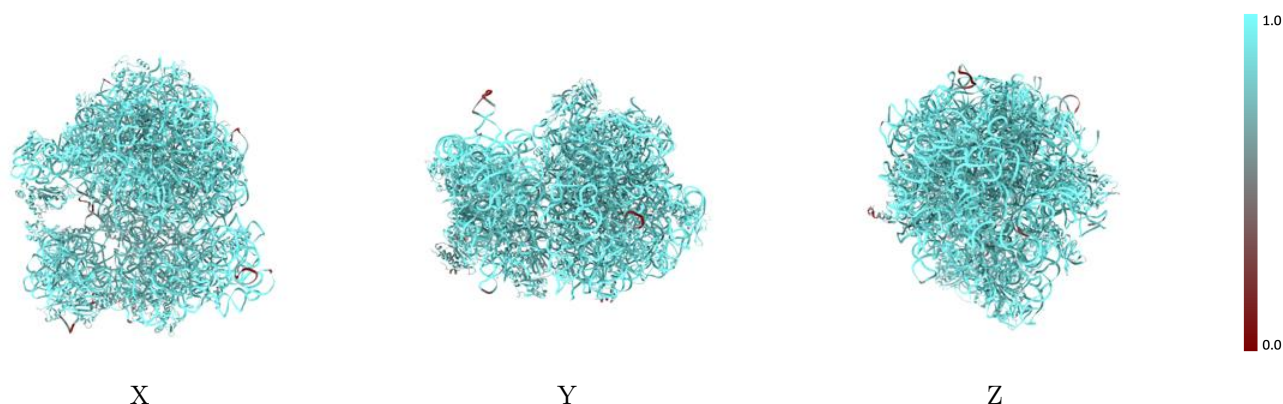
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



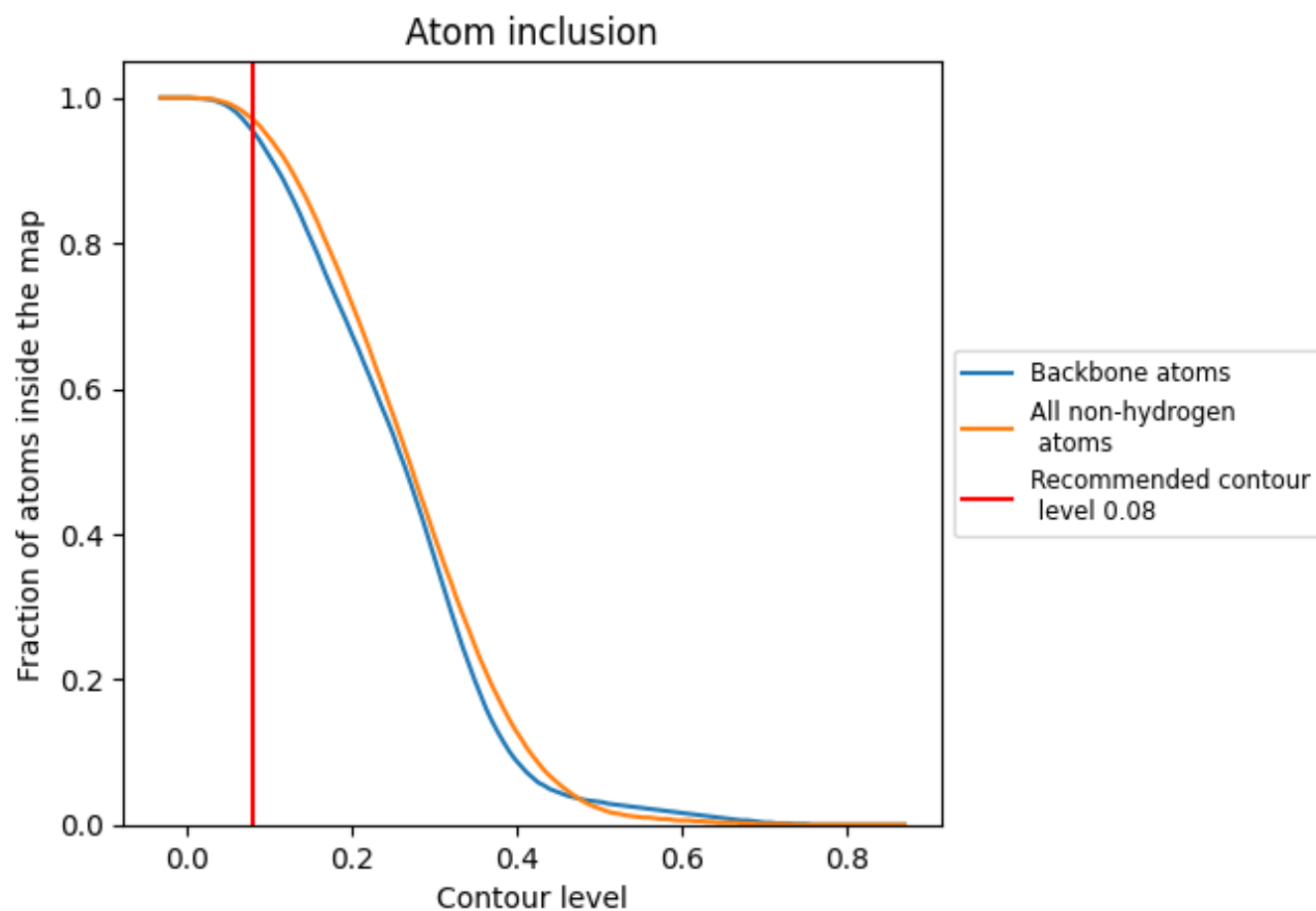
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 97% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.6220
0	 0.9260	 0.6420
1	 0.9880	 0.6980
2	 0.9960	 0.6850
3	 0.9830	 0.6550
A	 0.9900	 0.6450
B	 0.9960	 0.5940
C	 0.9850	 0.6670
D	 0.9820	 0.6790
E	 0.9740	 0.6600
F	 0.8410	 0.4750
G	 0.9170	 0.5690
H	 0.7110	 0.4750
I	 0.9860	 0.6760
J	 0.9770	 0.6620
K	 0.9830	 0.6710
L	 0.9730	 0.6600
M	 0.9950	 0.6880
N	 0.9610	 0.6060
O	 0.9770	 0.6530
P	 0.9970	 0.6900
Q	 0.9750	 0.6670
R	 0.9830	 0.6770
S	 0.9570	 0.6430
T	 0.9340	 0.6100
U	 0.9520	 0.6390
V	 0.9890	 0.6800
W	 0.9640	 0.6650
X	 0.9330	 0.5970
Y	 0.9710	 0.6680
Z	 0.9740	 0.6690
a	 0.9820	 0.6000
b	 0.6790	 0.4810
c	 0.9460	 0.6130
d	 0.9040	 0.5220



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Chain	Atom inclusion	Q-score
e	 0.9790	 0.6290
f	 0.9220	 0.5780
g	 0.8590	 0.5340
h	 0.9770	 0.6360
i	 0.9720	 0.6300
j	 0.9190	 0.6030
k	 0.9360	 0.5770
l	 0.9230	 0.6050
m	 0.9610	 0.6190
n	 0.9580	 0.6280
o	 0.9770	 0.6320
p	 0.9730	 0.6220
q	 0.9640	 0.6020
r	 0.9660	 0.6090
s	 0.9780	 0.6340
t	 0.9800	 0.6130
u	 0.6910	 0.5320
v	 0.8140	 0.4220
w	 0.9850	 0.6120