



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 07:41 PM EDT

PDB ID : 8G6Y / pdb_00008g6y
EMDB ID : EMD-29788
Title : Structure of WT E.coli ribosome 50S subunit with complexed with mRNA, P-site fMet-NH-tRNA^{fMet} and A-site 3-aminopyridine-4-carboxylic acid charged NH-tRNA^{Phe}
Authors : Majumdar, C.; Cate, J.H.D.
Deposited on : 2023-02-16
Resolution : 2.09 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:

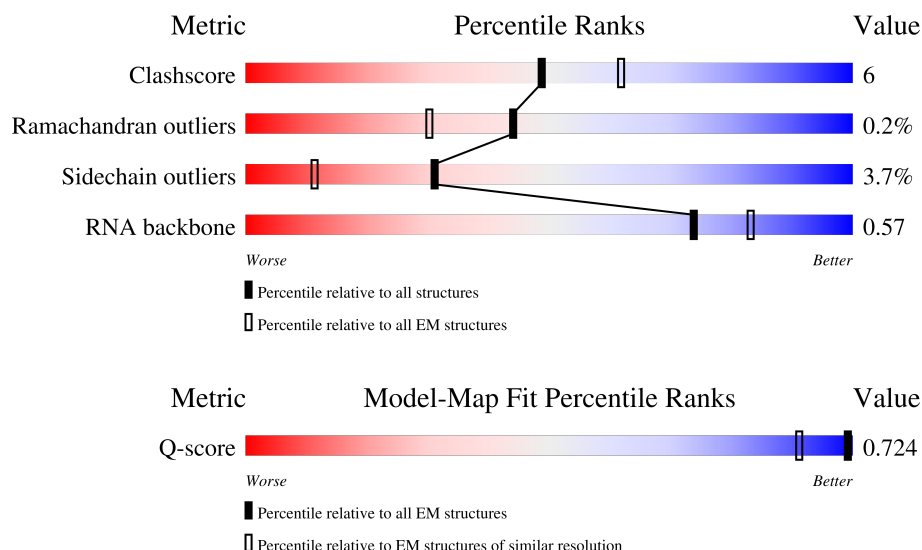
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.09 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	2022 (1.60 - 2.59)

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	55	
2	1	46	
3	2	65	

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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	X	28	
7	Y	76	
8	Z	76	
9	a	2904	
10	b	120	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	i	142	
18	j	123	
19	k	144	
20	l	136	
21	m	127	
22	n	117	
23	o	115	
24	p	118	
25	q	103	
26	r	110	
27	s	100	
28	t	104	

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Mol	Chain	Length	Quality of chain
29	u	94	84%16%
30	v	85	76%13%11%
31	w	78	82%17%.
32	x	63	5% 86%11%. .
33	y	59	5% 92%7%. .
34	z	57	72%26%. .

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 93683 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	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- 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
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	15	Total	C	N	O	P	0	0
			317	143	56	103	15		

- Molecule 7 is a RNA chain called A-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	74	Total	C	N	O	P	0	0
			1578	705	285	515	73		

- Molecule 8 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	75	Total	C	N	O	P	0	0
			1601	713	289	524	75		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP A1AGK1

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called Ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	76	Total	C	N	O	S	0	0
			576	357	114	104	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

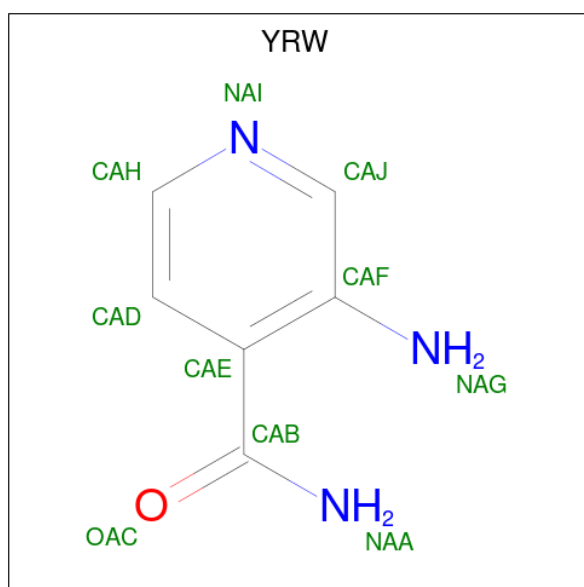
- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

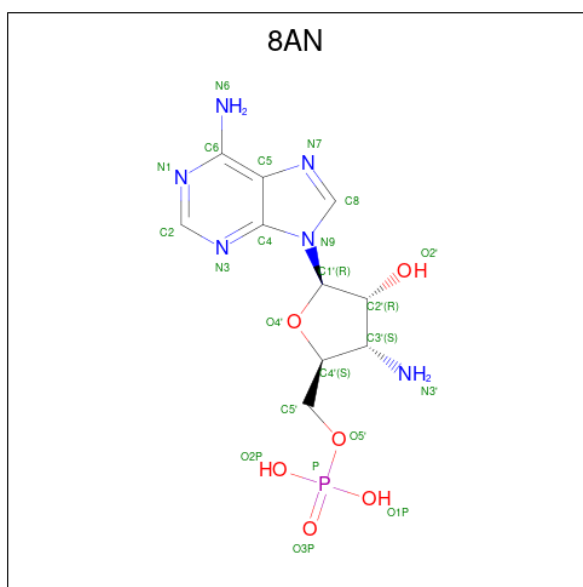
Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total	Zn	0
			1	1	
35	4	1	Total	Zn	0
			1	1	

- Molecule 36 is 3-aminopyridine-4-carboxamide (CCD ID: YRW) (formula: C₆H₇N₃O) (labeled as "Ligand of Interest" by depositor).



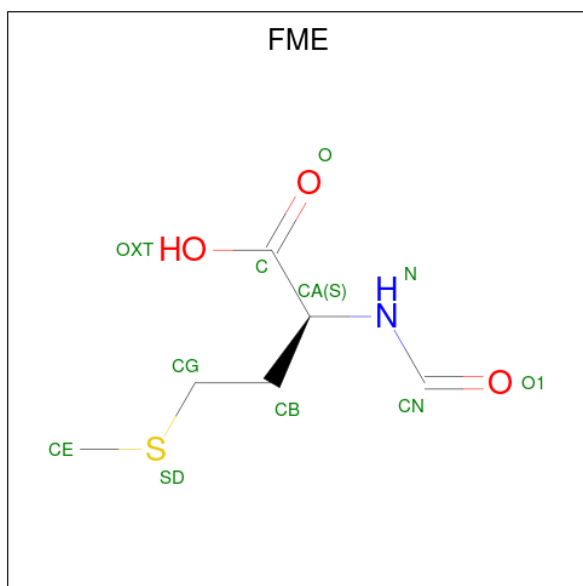
Mol	Chain	Residues	Atoms				AltConf
36	Y	1	Total	C	N	O	0
			10	6	3	1	

- Molecule 37 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (CCD ID: 8AN) (formula: C₁₀H₁₅N₆O₆P).



Mol	Chain	Residues	Atoms					AltConf
37	Z	1	Total	C	N	O	P	0
			22	10	6	5	1	

- Molecule 38 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
38	Z	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	a	224	Total 224	Mg 224	0
39	b	5	Total 5	Mg 5	0
39	d	1	Total 1	Mg 1	0
39	z	1	Total 1	Mg 1	0

- Molecule 40 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
40	a	13	Total 13	K 13	0
40	c	2	Total 2	K 2	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	0	1	Total 1	O 1	0
41	1	16	Total 16	O 16	0
41	2	22	Total 22	O 22	0
41	3	2	Total 2	O 2	0
41	Z	1	Total 1	O 1	0
41	a	3019	Total 3019	O 3019	0
41	b	38	Total 38	O 38	0
41	c	84	Total 84	O 84	0
41	d	36	Total 36	O 36	0
41	e	28	Total 28	O 28	0
41	i	9	Total 9	O 9	0
41	j	12	Total 12	O 12	0

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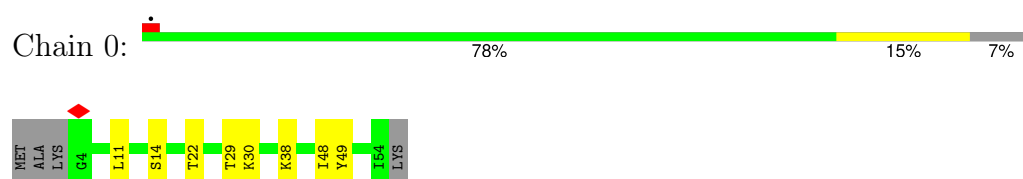
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Mol	Chain	Residues	Atoms		AltConf
41	k	26	Total 26	O 26	0
41	l	24	Total 24	O 24	0
41	m	21	Total 21	O 21	0
41	o	9	Total 9	O 9	0
41	p	20	Total 20	O 20	0
41	q	12	Total 12	O 12	0
41	r	24	Total 24	O 24	0
41	s	7	Total 7	O 7	0
41	t	1	Total 1	O 1	0
41	u	4	Total 4	O 4	0
41	v	10	Total 10	O 10	0
41	w	9	Total 9	O 9	0
41	x	1	Total 1	O 1	0
41	z	24	Total 24	O 24	0

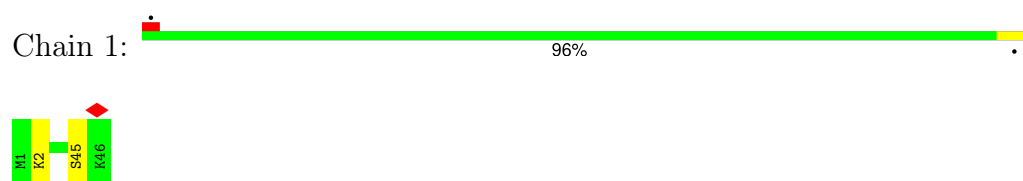
3 Residue-property plots [i](#)

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

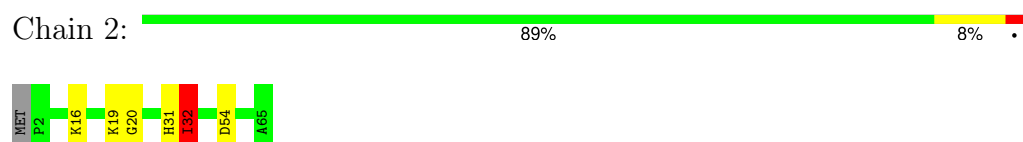
- Molecule 1: 50S ribosomal protein L33



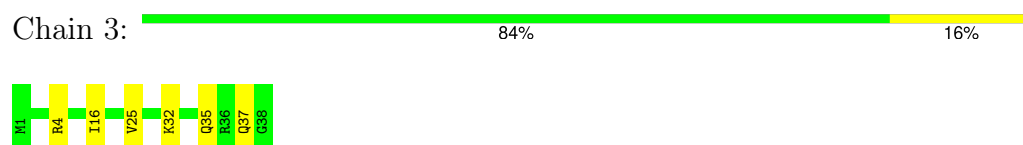
- Molecule 2: 50S ribosomal protein L34



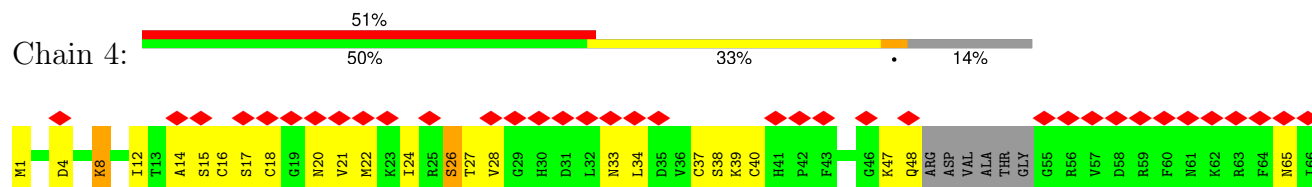
- Molecule 3: 50S ribosomal protein L35



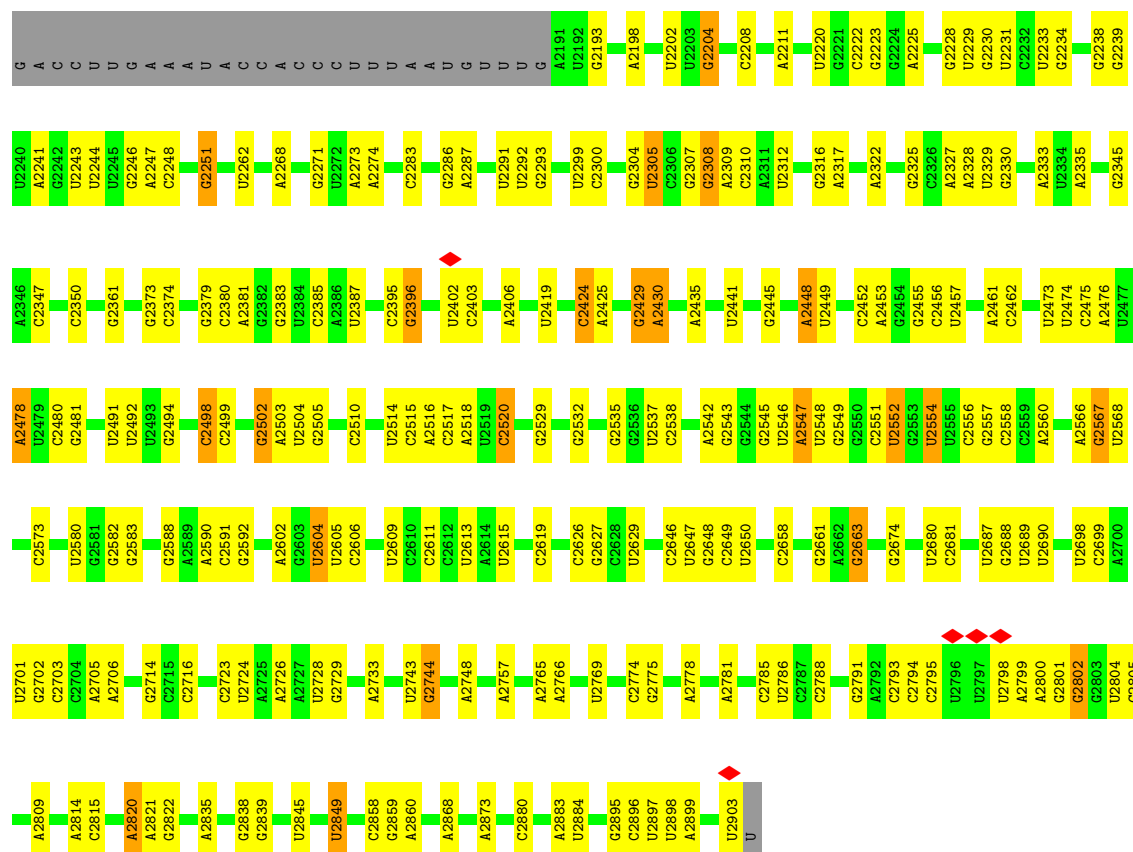
- Molecule 4: 50S ribosomal protein L36



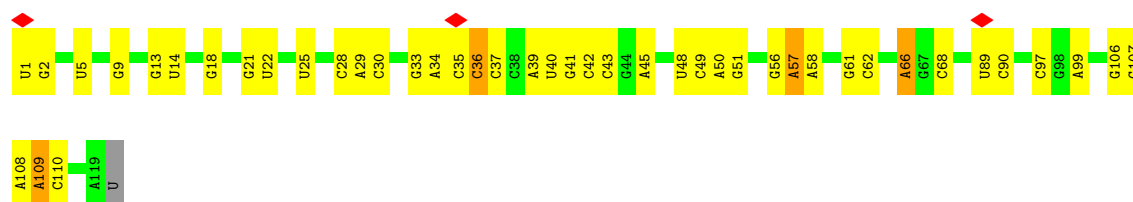
- Molecule 5: 50S ribosomal protein L31



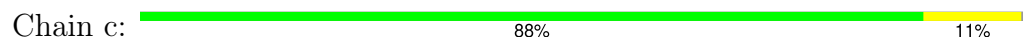
G	U1991	G1869	A1744	C1592	C1498	U1400	G1187	A	U999	G881	U755	A613	A502
C	G1992	C1870	A1745	A1593	A1504	U1405	G1197	A	A1000	G882	G760	A614	A503
U	U1993	A1871	U1746	U1594	A1505	U1406	G1198	C	G1001	G883	A761	U615	A504
C	C1997	G1872	U1747	U1599	U1506	G1407	U1199	G	C1002	U884	G775	A626	A505
U	U1998	C1873	C1748	C1600	U1507	G1408	C1200	U	U1005	C885	G776	C509	C509
A	G2012	C1874	A1754	A1603	A1508	U1412	U1224	A	U1012	A886	A782	C634	C530
U	A2013	G1875	A1762	C1604	A1509	A1413	G1225	U	C1013	U887	G783	C635	C531
G	A2014	A1876	G1763	A1604	G1510	U1414	A1226	A	G1026	C888	G784	G636	A532
U	A2015	C1877	C1764	C1607	G1511	U1415	A1226	G	U1027	C889	G785	A637	G533
C	G2020	A1878	A1773	A1608	U1513	G1416	G1250	C	A1028	C990	U638	U534	U534
U	C2021	G1884	U1774	A1614	G1514	C1417	A1253	U	A1029	G891	A788	U639	G537
G	U2022	A1889	U1778	A1618	A1515	G1418	A1253	A	U1033	A892	A789	C640	A538
A	G2023	A1900	U1782	G1622	U1523	A1419	G1256	C	U1040	C893	U790	A644	A538
U	U2026	G1906	A1783	G1622	C1526	A1427	G1256	U	A1045	U894	G791	U646	C544
C	A2030	C1907	U1784	U1647	G1527	C1428	U1263	G	C1046	U895	A792	G647	U545
U	G2031	G1907	A1785	U1648	A1528	A1432	A1268	U	A1046	A896	G805	U646	U546
U	G2032	U1786	A1786	G1649	A1529	A1433	A1269	U	G1047	C897	U651	A547	A547
G	A2033	C1788	A1787	U1684	G1533	A1434	C1270	U	C1052	C898	U652	G548	G548
G	G2038	A1789	A1788	G1653	U1534	G1435	G1271	U	C	A899	U653	G549	G549
A	U1917	A1916	C1789	G1660	A1535	G1436	A1272	U	G	A900	A654	C550	C550
G	G1922	U1917	A1791	U1800	C1536	G1437	U1438	U	A	A901	A655	A563	A563
G	U1923	U1917	A1794	A1664	G1537	U1438	C1289	U	C	G907	U657	U568	U568
U	C2043	U1923	C1795	A1664	U1538	U1442	C1290	U	G	C908	U657	U568	U568
U	C2055	C1924	U1796	A1672	G1538	U1443	G1300	U	A	A909	U657	U568	U568
U	G2056	C1925	G1797	G1673	U1539	G1444	A1301	U	U	A910	U657	U568	U568
G	U2039	U1917	A1791	G1674	U1539	G1445	A1301	U	U	A911	U657	U568	U568
A	A2060	G1929	C1800	U1800	A1544	G1452	C1306	U	U	A912	U657	U568	U568
A	G2061	G1930	A1801	A1681	A1545	A1453	A1307	U	U	A913	U657	U568	U568
G	A2062	U1931	A1802	G1682	A1546	A1453	A1307	U	U	A914	U657	U568	U568
U	C2063	A1932	A1803	U1683	C1547	U1460	U1329	U	U	A915	U657	U568	U568
U	G2064	G1933	C1804	G1684	A1548	C1461	U1352	U	U	A916	U657	U568	U568
U	C2065	A1937	A1805	G1703	A1549	U1461	A1352	U	U	A917	U657	U568	U568
G	C2066	U1938	A1808	C1704	C1550	U1466	A1353	U	U	A918	U657	U568	U568
A	G2069	U1939	C1816	G1710	C1561	U1466	A1353	U	U	A919	U657	U568	U568
C	A2070	C1947	A1829	U1714	U1562	U1469	A1354	U	U	A920	U657	U568	U568
C	A2071	U1946	G1835	G1715	U1563	A1470	G1355	U	U	A921	U657	U568	U568
C	C2072	C1947	A1829	U1715	C1564	G1478	G1357	U	U	A922	U657	U568	U568
C	C2073	U1955	A1835	G1715	C1565	G1478	G1358	U	U	A923	U657	U568	U568
A	U2074	U1956	A1835	U1720	A1566	G1478	G1358	U	U	A924	U657	U568	U568
G	U2075	C1957	C1842	G1721	A1566	G1478	G1358	U	U	A925	U657	U568	U568
U	U2076	C1958	C1843	A1722	A1566	G1478	G1358	U	U	A926	U657	U568	U568
U	U2077	C1959	C1843	A1722	A1566	G1478	G1358	U	U	A927	U657	U568	U568
U	U2078	C1960	C1843	A1722	A1566	G1478	G1358	U	U	A928	U657	U568	U568
U	U2079	C1961	C1843	A1722	A1566	G1478	G1358	U	U	A929	U657	U568	U568
U	U2080	C1962	C1843	A1722	A1566	G1478	G1358	U	U	A930	U657	U568	U568
U	U2081	C1963	C1843	A1722	A1566	G1478	G1358	U	U	A931	U657	U568	U568
U	U2082	C1964	C1843	A1722	A1566	G1478	G1358	U	U	A932	U657	U568	U568
U	U2083	C1965	C1843	A1722	A1566	G1478	G1358	U	U	A933	U657	U568	U568
U	U2084	C1966	C1843	A1722	A1566	G1478	G1358	U	U	A934	U657	U568	U568
U	U2085	C1967	C1843	A1722	A1566	G1478	G1358	U	U	A935	U657	U568	U568
U	U2086	C1968	C1843	A1722	A1566	G1478	G1358	U	U	A936	U657	U568	U568
U	U2087	C1969	C1843	A1722	A1566	G1478	G1358	U	U	A937	U657	U568	U568
U	U2088	C1970	C1843	A1722	A1566	G1478	G1358	U	U	A938	U657	U568	U568
U	U2089	C1971	C1843	A1722	A1566	G1478	G1358	U	U	A939	U657	U568	U568
U	U2090	C1972	C1843	A1722	A1566	G1478	G1358	U	U	A940	U657	U568	U568
U	U2091	C1973	C1843	A1722	A1566	G1478	G1358	U	U	A941	U657	U568	U568
U	U2092	C1974	C1843	A1722	A1566	G1478	G1358	U	U	A942	U657	U568	U568
U	U2093	C1975	C1843	A1722	A1566	G1478	G1358	U	U	A943	U657	U568	U568
U	U2094	C1976	C1843	A1722	A1566	G1478	G1358	U	U	A944	U657	U568	U568
U	U2095	C1977	C1843	A1722	A1566	G1478	G1358	U	U	A945	U657	U568	U568
U	U2096	C1978	C1843	A1722	A1566	G1478	G1358	U	U	A946	U657	U568	U568
U	U2097	C1979	C1843	A1722	A1566	G1478	G1358	U	U	A947	U657	U568	U568
U	U2098	C1980	C1843	A1722	A1566	G1478	G1358	U	U	A948	U657	U568	U568
U	U2099	C1981	C1843	A1722	A1566	G1478	G1358	U	U	A949	U657	U568	U568
U	U2100	C1982	C1843	A1722	A1566	G1478	G1358	U	U	A950	U657	U568	U568
U	U2101	C1983	C1843	A1722	A1566	G1478	G1358	U	U	A951	U657	U568	U568
U	U2102	C1984	C1843	A1722	A1566	G1478	G1358	U	U	A952	U657	U568	U568
U	U2103	C1985	C1843	A1722	A1566	G1478	G1358	U	U	A953	U657	U568	U568
U	U2104	C1986	C1843	A1722	A1566	G1478	G1358	U	U	A954	U657	U568	U568
U	U2105	C1987	C1843	A1722	A1566	G1478	G1358	U	U	A955	U657	U568	U568
U	U2106	C1988	C1843	A1722	A1566	G1478	G1358	U	U	A956	U657	U568	U568
U	U2107	C1989	C1843	A1722	A1566	G1478	G1358	U	U	A957	U657	U568	U568
U	U2108	C1990	C1843	A1722	A1566	G1478	G1358	U	U	A958	U657	U568	U568
U	U2109	C1991	C1843	A1722	A1566	G1478	G1358	U	U	A959	U657	U568	U568
U	U2110	C1992	C1843	A1722	A1566	G1478	G1358	U	U	A960	U657	U568	U568
U	U2111	C1993	C1843	A1722	A1566	G1478	G1358	U	U	A961	U657	U568	U568
U	U2112	C1994	C1843	A1722	A1566	G1478	G1358	U	U	A962	U657	U568	U568
U	U2113	C1995	C1843	A1722	A1566	G1478	G1358	U	U	A963	U657	U568	U568
U	U2114	C1996	C1843	A1722	A1566	G1478	G1358	U	U	A964	U657	U568	U568
U	U2115	C1997	C1843	A1722	A1566	G1478	G1358	U	U	A965	U657	U568	U568
U	U2116	C1998	C1843	A1722	A1566	G1478	G1358	U	U	A966	U657	U568	U568
U	U2117	C1999	C1843	A1722	A1566	G1478	G1358	U	U	A967	U657	U568	U568
U	U2118	C2000	C1843	A1722	A1566	G1478	G1358	U	U	A968	U657	U568	U568
U	U2119	C2001	C1843	A1722	A1566	G1478	G1358	U	U	A969	U657	U568	U568
U	U2120	C2002	C1843	A1722	A1566	G1478	G1358	U	U	A970	U657	U568	U568
U	U2121	C2003	C1843	A1722	A1566	G1478	G1358	U	U	A971	U657	U568	U568
U	U2122	C2004	C1843	A1722	A1566	G1478	G1358	U	U	A972	U657	U568	U568
U	U2123	C2005	C1843	A1722	A1566	G1478	G1358	U	U	A973	U657	U568	U568
U	U2124	C2006	C1843	A1722	A1566	G1478	G1358	U	U	A974	U657	U568	U568
U	U2125	C2007	C1843	A1722	A1566	G1478	G1358	U	U	A975	U657	U568	U568
U	U2126	C2008	C1843	A1722	A1566	G1478	G1358	U	U	A976	U657	U568	U568
U	U2127	C2009	C1843	A1722	A1566	G1478	G1358	U	U	A977	U657	U568	U568
U	U2128	C2010	C1843	A1722	A1566	G1478	G1358	U	U	A978	U657	U568	U568
U	U2129	C2011	C1843	A1722	A1566	G1478	G1358	U	U	A979	U657	U568	U568
U	U2130	C2012	C1843	A1722	A1566	G1478	G1358	U	U	A980	U657	U568	U568
U	U2131	C2013	C1843	A1722	A1566	G1478	G1358	U	U	A981	U657	U568	U568
U	U2132	C2014	C1843	A1722	A1566	G1478	G1358	U	U	A982	U657	U568	U568
U	U2133	C2015	C1843	A1722	A1566	G1478	G1358	U	U	A983	U657	U568	U568
U	U2134	C2016	C1843	A1722	A1566	G1478	G1358	U	U	A984	U657	U568	U568
U	U2135	C2017	C1843	A1722	A1566	G1478	G1358	U	U	A985	U657	U568	U568
U	U2136	C2018	C1843	A1722	A1566	G1478	G1358	U	U	A986	U657	U568	U568
U	U2137	C2019											



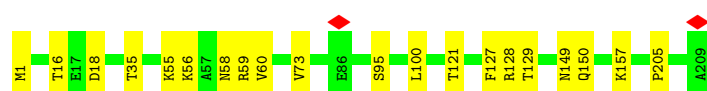
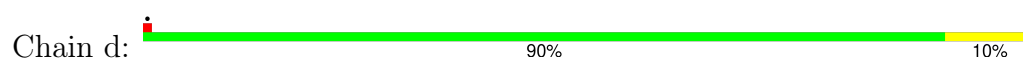
• Molecule 10: 5S rRNA



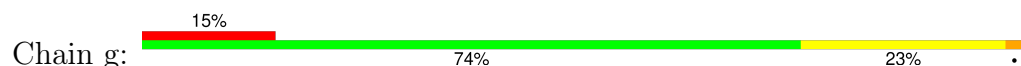
• Molecule 11: 50S ribosomal protein L2



• Molecule 12: 50S ribosomal protein L3



Chain e: 83% 17%



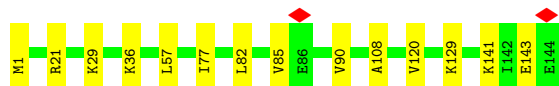
• Molecule 17: 50S ribosomal protein L13

Chain i:  85% 15%

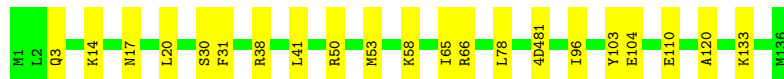
• Molecule 18: 50S ribosomal protein L14

Chain j:  79% 21%

• Molecule 19: 50S ribosomal protein L15

Chain k:  90% 10%

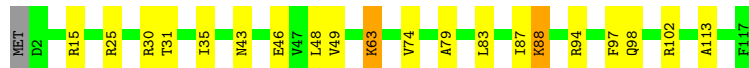
• Molecule 20: 50S ribosomal protein L16

Chain l:  85% 15%

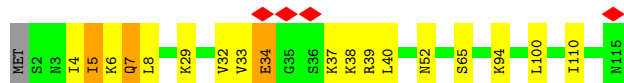
• Molecule 21: 50S ribosomal protein L17

Chain m:  83% 10% 7%

• Molecule 22: 50S ribosomal protein L18

Chain n:  82% 15%

• Molecule 23: 50S ribosomal protein L19

Chain o:  83% 13%

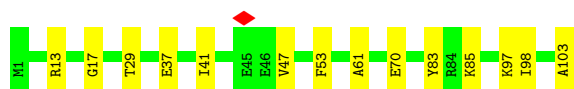
- Molecule 24: 50S ribosomal protein L20

Chain p:  87% 12%



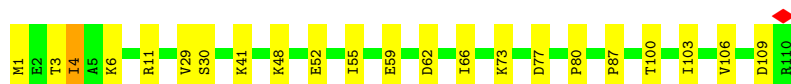
- Molecule 25: Ribosomal protein L21

Chain q:  86% 14%



- Molecule 26: 50S ribosomal protein L22

Chain r:  80% 19%



- Molecule 27: 50S ribosomal protein L23

Chain s:  84% 9% 7%



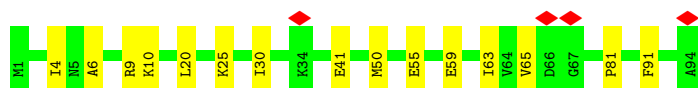
- Molecule 28: 50S ribosomal protein L24

Chain t:  5% 79% 15%



- Molecule 29: 50S ribosomal protein L25

Chain u:  84% 16%

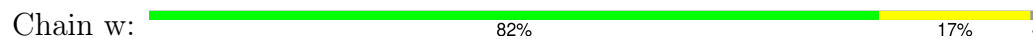


- Molecule 30: 50S ribosomal protein L27

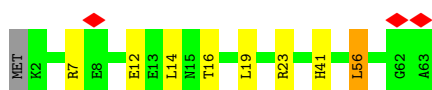
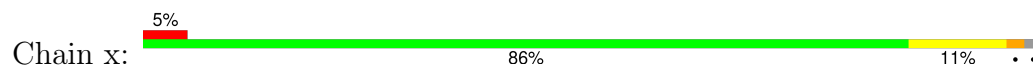
Chain v:  76% 13% 11%



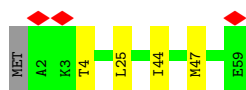
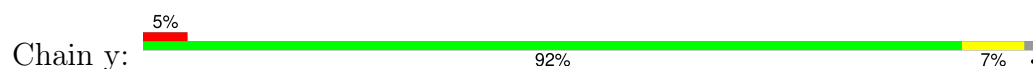
- Molecule 31: 50S ribosomal protein L28



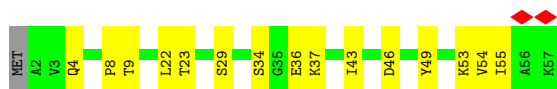
- Molecule 32: 50S ribosomal protein L29



- Molecule 33: 50S ribosomal protein L30



- Molecule 34: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288552	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.377	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0265	Depositor
Map size (Å)	408.704, 408.704, 408.704	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, YRW, 1MG, 4D4, FME, MEQ, ZN, MS6, 6MZ, K, 2MA, 2MG, MG, 5MC, G7M, OMC, 5MU, PSU, H2U, OMG, 3TD, OMU

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	0.26	0/424	0.50	0/565
2	1	0.27	0/380	0.51	0/498
3	2	0.28	0/513	0.50	0/676
4	3	0.30	0/303	0.53	0/397
5	4	0.24	0/488	0.60	0/649
6	X	0.44	1/354 (0.3%)	0.43	0/548
7	Y	0.72	4/1763 (0.2%)	0.74	4/2745 (0.1%)
8	Z	0.22	0/1788	0.45	2/2786 (0.1%)
9	a	0.31	7/65651 (0.0%)	0.41	3/102413 (0.0%)
10	b	0.24	0/2850	0.36	0/4444
11	c	0.27	0/2121	0.51	0/2852
12	d	0.27	0/1576	0.49	0/2119
13	e	0.26	0/1571	0.48	0/2113
14	f	0.22	0/1434	0.56	0/1926
15	g	0.25	0/1343	0.61	0/1816
16	h	0.26	0/306	0.76	0/413
17	i	0.26	0/1152	0.47	0/1551
18	j	0.27	0/955	0.46	0/1279
19	k	0.30	0/1062	0.57	0/1413
20	l	0.26	0/1073	0.47	0/1433
21	m	0.29	0/958	0.57	0/1281
22	n	0.23	0/902	0.54	0/1209
23	o	0.31	0/929	0.52	0/1242
24	p	0.28	0/960	0.50	0/1278
25	q	0.27	0/829	0.53	0/1107
26	r	0.28	0/864	0.46	0/1156
27	s	0.24	0/744	0.49	0/994
28	t	0.26	0/787	0.58	2/1051 (0.2%)
29	u	0.25	0/766	0.50	0/1025
30	v	0.25	0/583	0.46	0/772
31	w	0.27	0/635	0.51	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	x	0.22	0/502	0.49	0/667
33	y	0.25	0/453	0.46	0/605
34	z	0.26	0/450	0.44	0/599
All	All	0.31	12/97469 (0.0%)	0.45	11/146470 (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
3	2	0	1
15	g	0	1
31	w	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	8	U	C4-O4	17.84	1.59	1.23
7	Y	73	A	P-OP2	-13.11	1.22	1.49
9	a	2588	G	O3'-P	-10.76	1.45	1.61
7	Y	73	A	P-O5'	10.54	1.75	1.59
9	a	2510	C	O3'-P	9.26	1.75	1.61
9	a	2611	C	O3'-P	8.93	1.74	1.61
9	a	2056	G	O3'-P	7.52	1.72	1.61
9	a	2549	G	O3'-P	7.46	1.72	1.61
9	a	2246	G	O3'-P	6.25	1.70	1.61
9	a	2560	A	O3'-P	5.90	1.70	1.61
6	X	19	U	C1'-N1	5.08	1.56	1.48
7	Y	32	U	N1-C2	5.06	1.48	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	72	C	O3'-P-O5'	-26.09	64.86	104.00
7	Y	73	A	P-O5'-C5'	-9.58	106.53	120.90
7	Y	73	A	OP1-P-OP2	8.59	145.38	119.60
9	a	2605	PSU	P-O3'-C3'	-8.23	107.86	120.20
9	a	2606	C	P-O3'-C3'	-7.70	108.65	120.20
8	Z	72	A	P-O3'-C3'	-7.57	108.85	120.20
7	Y	72	C	OP1-P-O3'	-7.53	85.42	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	2445	2MG	P-O3'-C3'	-6.80	110.00	120.20
8	Z	71	C	P-O3'-C3'	-5.41	112.09	120.20
28	t	98	SER	CA-C-N	5.01	131.12	121.54
28	t	98	SER	C-N-CA	5.01	131.12	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	31	HIS	Peptide
15	g	47	ASP	Peptide
31	w	16	ASN	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	417	0	451	5	0
2	1	377	0	418	2	0
3	2	504	0	572	4	0
4	3	302	0	340	6	0
5	4	480	0	478	15	0
6	X	317	0	161	5	0
7	Y	1578	0	800	54	0
8	Z	1601	0	813	29	0
9	a	59130	0	29764	483	0
10	b	2549	0	1290	26	0
11	c	2082	0	2154	19	0
12	d	1566	0	1618	15	0
13	e	1552	0	1619	21	0
14	f	1410	0	1444	44	0
15	g	1323	0	1371	21	0
16	h	303	0	327	5	0
17	i	1129	0	1162	12	0
18	j	946	0	1023	16	0
19	k	1053	0	1129	13	0
20	l	1075	0	1146	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	m	945	0	989	8	0
22	n	892	0	923	10	0
23	o	917	0	962	11	0
24	p	947	0	1019	13	0
25	q	816	0	839	9	0
26	r	857	0	922	14	0
27	s	738	0	807	3	0
28	t	779	0	831	13	0
29	u	753	0	780	9	0
30	v	576	0	588	8	0
31	w	625	0	652	9	0
32	x	501	0	531	5	0
33	y	449	0	488	2	0
34	z	444	0	458	10	0
35	3	1	0	0	0	0
35	4	1	0	0	0	0
36	Y	10	0	0	1	0
37	Z	22	0	11	1	0
38	Z	10	0	10	1	0
39	a	224	0	0	1	0
39	b	5	0	0	0	0
39	d	1	0	0	0	0
39	z	1	0	0	0	0
40	a	13	0	0	0	0
40	c	2	0	0	0	0
41	0	1	0	0	0	0
41	1	16	0	0	0	0
41	2	22	0	0	0	0
41	3	2	0	0	0	0
41	Z	1	0	0	0	0
41	a	3019	0	0	36	0
41	b	38	0	0	0	0
41	c	84	0	0	3	0
41	d	36	0	0	1	0
41	e	28	0	0	0	0
41	i	9	0	0	0	0
41	j	12	0	0	0	0
41	k	26	0	0	0	0
41	l	24	0	0	0	0
41	m	21	0	0	1	0
41	o	9	0	0	0	0
41	p	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	q	12	0	0	0	0
41	r	24	0	0	0	0
41	s	7	0	0	0	0
41	t	1	0	0	0	0
41	u	4	0	0	0	0
41	v	10	0	0	0	0
41	w	9	0	0	0	0
41	x	1	0	0	1	0
41	z	24	0	0	0	0
All	All	93683	0	58890	847	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 6.

All (847) 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)
28:t:49:VAL:O	28:t:54:GLN:HA	1.34	1.22
7:Y:26:A:N6	7:Y:44:G:H1	1.59	1.00
7:Y:26:A:H61	7:Y:44:G:H1	0.90	0.89
5:4:16:CYS:SG	5:4:37:CYS:HB3	2.15	0.86
9:a:1482:G:H1'	9:a:1509:A:H61	1.42	0.84
5:4:18:CYS:SG	5:4:40:CYS:HB2	2.17	0.84
9:a:1250:G:H5''	24:p:6:ARG:HD3	1.59	0.83
9:a:284:U:O2	9:a:356:G:N2	2.12	0.82
9:a:1478:G:H1	9:a:1513:U:H3	1.28	0.81
9:a:1047:G:HO2'	9:a:1110:G:H1	1.22	0.81
11:c:29:PRO:HG2	11:c:34:LEU:HD11	1.63	0.81
15:g:164:TYR:HB2	15:g:167:GLU:HB2	1.62	0.80
7:Y:55:U:C5	7:Y:57:G:OP2	2.35	0.80
9:a:2582:G:OP2	41:a:6301:HOH:O	2.00	0.78
7:Y:58:A:O2'	7:Y:61:C:N4	2.17	0.77
14:f:52:ASN:HB3	14:f:150:ARG:HH22	1.51	0.76
9:a:2012:G:OP1	26:r:11:ARG:NH2	2.18	0.75
14:f:29:PRO:HB2	14:f:169:LEU:HD22	1.69	0.74
29:u:9:ARG:HG2	29:u:41:GLU:HG3	1.70	0.74
7:Y:26:A:N1	7:Y:44:G:N2	2.35	0.73
7:Y:51:U:H3	7:Y:63:G:H1	1.34	0.73
9:a:1415:U:H3	9:a:1587:G:H1	1.35	0.73
10:b:66:A:OP2	10:b:108:A:N6	2.22	0.72
9:a:2658:C:OP1	15:g:158:LYS:NZ	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:215:G:OP2	41:a:6302:HOH:O	2.08	0.71
9:a:1136:G:N7	41:a:6316:HOH:O	2.22	0.71
12:d:128:ARG:NH2	41:d:401:HOH:O	2.23	0.71
9:a:340:A:O2'	13:e:162:ARG:NH1	2.24	0.70
18:j:121:GLU:OE1	23:o:65:SER:OG	2.07	0.70
9:a:2096:C:O2	9:a:2193:G:N2	2.16	0.70
9:a:46:G:OP2	41:a:6302:HOH:O	2.09	0.70
17:i:114:LEU:HG	17:i:118:MET:HE3	1.74	0.69
30:v:25:ARG:HH11	30:v:31:VAL:HG12	1.56	0.69
12:d:55:LYS:HD3	12:d:60:VAL:HG22	1.73	0.69
21:m:22:ARG:HG3	21:m:70:THR:HA	1.74	0.69
9:a:2766:A:OP1	41:a:6304:HOH:O	2.11	0.69
9:a:1586:A:H3'	9:a:1587:G:H8	1.57	0.69
17:i:1:MET:HE1	25:q:13:ARG:H	1.57	0.69
9:a:278:A:N1	9:a:361:G:O2'	2.26	0.69
9:a:2396:G:N7	41:a:6333:HOH:O	2.27	0.68
29:u:4:ILE:HG12	29:u:50:MET:HE1	1.74	0.68
9:a:549:G:H2'	9:a:550:C:H6	1.58	0.68
9:a:1157:G:OP1	41:a:6303:HOH:O	2.11	0.68
9:a:2502:G:OP2	41:a:6305:HOH:O	2.11	0.67
9:a:856:G:H2'	9:a:857:G:C8	2.29	0.67
7:Y:63:G:H2'	7:Y:64:A:C8	2.29	0.67
8:Z:24:U:O2'	9:a:1923:U:OP1	2.12	0.67
9:a:54:G:N7	41:a:6348:HOH:O	2.28	0.67
9:a:288:U:H2'	9:a:289:G:C8	2.29	0.67
9:a:1434:A:H2'	9:a:1435:G:H8	1.58	0.67
7:Y:43:C:H2'	7:Y:44:G:C8	2.30	0.66
9:a:499:U:H5''	28:t:43:LYS:HE3	1.76	0.66
14:f:17:MET:HG3	14:f:22:TYR:HB2	1.77	0.66
18:j:105:ARG:NH1	18:j:122:VAL:O	2.29	0.66
6:X:23:A:H4'	6:X:24:A:O4'	1.96	0.66
9:a:370:G:OP2	41:a:6306:HOH:O	2.14	0.65
9:a:1434:A:H2'	9:a:1435:G:C8	2.32	0.65
10:b:108:A:O2'	10:b:109:A:OP2	2.15	0.65
15:g:94:TYR:HA	15:g:106:SER:O	1.96	0.65
14:f:158:THR:HG22	14:f:160:ALA:H	1.60	0.65
20:l:50:ARG:HG3	20:l:65:ILE:HD11	1.78	0.65
29:u:20:LEU:HD11	29:u:41:GLU:HG2	1.77	0.65
9:a:447:A:OP2	41:a:6307:HOH:O	2.14	0.65
9:a:2547:A:H2'	9:a:2548:U:C6	2.30	0.65
9:a:2327:A:H2'	9:a:2328:A:C8	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:22:G:H2'	7:Y:23:A:H8	1.62	0.64
9:a:2537:U:H2'	9:a:2538:C:C6	2.33	0.64
9:a:278:A:N6	9:a:362:A:N7	2.46	0.64
9:a:538:A:H5''	17:i:7:LYS:HE3	1.79	0.64
9:a:1968:G:OP1	41:a:6308:HOH:O	2.15	0.64
9:a:639:U:H2'	9:a:640:C:C6	2.32	0.64
7:Y:15:G:H22	7:Y:48:C:H42	1.43	0.64
9:a:2592:G:OP1	41:a:6308:HOH:O	2.15	0.64
19:k:29:LYS:O	19:k:29:LYS:HG2	1.96	0.64
5:4:37:CYS:N	5:4:40:CYS:SG	2.67	0.63
7:Y:18:G:N2	7:Y:58:A:OP1	2.32	0.63
7:Y:19:G:C6	9:a:896:A:N6	2.66	0.63
38:Z:102:FME:SD	38:Z:102:FME:N	2.72	0.62
20:l:53:MET:HE1	20:l:103:TYR:CG	2.34	0.62
9:a:1115:G:O2'	9:a:1116:G:O5'	2.17	0.62
10:b:5:U:OP1	10:b:61:G:O2'	2.16	0.61
10:b:51:G:OP1	22:n:63:LYS:NZ	2.27	0.61
3:2:16:LYS:HE3	3:2:20:GLY:HA2	1.81	0.61
5:4:38:SER:HB3	14:f:105:THR:HA	1.81	0.61
9:a:1874:C:H2'	9:a:1875:G:O4'	2.00	0.61
9:a:568:U:H1'	9:a:2030:6MZ:H9C1	1.82	0.61
9:a:626:A:N7	41:a:6363:HOH:O	2.31	0.61
9:a:2243:U:H2'	9:a:2244:U:C6	2.35	0.61
28:t:49:VAL:O	28:t:54:GLN:CA	2.29	0.61
14:f:112:ARG:NH1	14:f:134:GLU:OE2	2.33	0.61
9:a:1197:G:H2'	9:a:1198:U:H6	1.66	0.60
17:i:96:ARG:HD2	17:i:99:ARG:HG3	1.83	0.60
7:Y:23:A:H2'	7:Y:24:G:H8	1.66	0.60
9:a:422:A:OP2	41:a:6306:HOH:O	2.16	0.60
39:a:6235:MG:MG	41:a:8407:HOH:O	1.45	0.60
9:a:1028:A:N6	9:a:1125:G:H2'	2.16	0.60
9:a:286:U:H2'	9:a:287:G:H8	1.66	0.60
7:Y:23:A:H2'	7:Y:24:G:C8	2.37	0.60
9:a:585:G:N7	24:p:6:ARG:NH1	2.49	0.60
9:a:634:C:H2'	9:a:635:C:C6	2.36	0.60
9:a:792:A:N1	41:a:6368:HOH:O	2.31	0.60
9:a:2430:A:OP1	41:a:6309:HOH:O	2.17	0.60
33:y:44:ILE:HD13	33:y:47:MET:HE3	1.84	0.60
14:f:108:VAL:HG12	14:f:109:PRO:HD3	1.84	0.60
20:l:66:ARG:NH1	20:l:104:GLU:OE2	2.34	0.60
34:z:46:ASP:O	34:z:53:LYS:NZ	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:44:A:H2'	8:Z:45:G:O4'	2.02	0.60
9:a:549:G:H2'	9:a:550:C:C6	2.36	0.60
10:b:29:A:H2'	10:b:30:C:C6	2.37	0.60
9:a:813:U:H2'	9:a:814:C:C6	2.37	0.59
8:Z:15:G:OP2	8:Z:16:C:N4	2.35	0.59
7:Y:19:G:C5	9:a:896:A:N6	2.70	0.59
10:b:1:U:H2'	10:b:2:G:C8	2.38	0.59
9:a:307:G:N1	9:a:310:A:OP2	2.36	0.59
19:k:77:ILE:HD13	19:k:108:ALA:HB1	1.83	0.59
26:r:3:THR:OG1	26:r:62:ASP:OD2	2.20	0.59
25:q:41:ILE:HD13	25:q:103:ALA:HA	1.85	0.59
7:Y:60:U:OP1	7:Y:62:C:N4	2.23	0.59
24:p:86:ALA:HB2	24:p:116:ALA:HB2	1.85	0.59
8:Z:15:G:H22	8:Z:48:C:H42	1.51	0.58
9:a:139:U:O2'	9:a:141:G:N7	2.29	0.58
9:a:586:A:N1	9:a:809:G:O2'	2.36	0.58
9:a:1794:A:H2'	9:a:1795:C:C6	2.39	0.58
10:b:48:U:H2'	10:b:49:C:C6	2.38	0.58
9:a:2291:U:H2'	9:a:2292:U:C6	2.39	0.58
7:Y:55:U:C4	7:Y:57:G:H5'	2.38	0.58
10:b:1:U:H2'	10:b:2:G:H8	1.68	0.58
12:d:1:MET:HE1	12:d:100:LEU:HD11	1.85	0.58
7:Y:21:A:N6	7:Y:46:G:O2'	2.37	0.58
9:a:1386:C:H2'	9:a:1387:A:C8	2.38	0.58
9:a:284:U:H3	9:a:356:G:H1	1.52	0.58
9:a:286:U:H2'	9:a:287:G:C8	2.38	0.58
9:a:1868:C:O2	9:a:1873:G:N2	2.18	0.58
6:X:24:A:H4'	6:X:25:C:OP2	2.03	0.58
18:j:7:MET:HE1	18:j:44:LYS:HG3	1.85	0.58
24:p:97:ASP:OD2	25:q:13:ARG:NE	2.34	0.58
9:a:152:A:H2'	9:a:153:U:C6	2.39	0.58
9:a:2064:C:H2'	9:a:2065:C:C6	2.39	0.58
9:a:64:A:H2'	9:a:65:U:C6	2.39	0.57
9:a:581:C:H2'	9:a:582:A:C8	2.39	0.57
3:2:54:ASP:HB3	19:k:57:LEU:HD22	1.85	0.57
7:Y:30:G:H2'	7:Y:31:A:H8	1.70	0.57
9:a:1469:A:H2'	9:a:1470:A:C8	2.39	0.57
20:l:20:LEU:HD13	29:u:81:PRO:HG2	1.86	0.57
9:a:145:C:H2'	9:a:146:A:C8	2.40	0.57
9:a:353:C:H2'	9:a:354:A:H8	1.68	0.57
9:a:2328:A:H2'	9:a:2329:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:105:ARG:NH2	23:o:32:VAL:HG11	2.19	0.57
8:Z:51:C:H2'	8:Z:52:G:H8	1.70	0.57
9:a:2312:U:H5'	14:f:85:ILE:HD11	1.87	0.57
8:Z:9:G:H21	8:Z:45:G:H3'	1.69	0.57
9:a:534:U:O2'	24:p:49:ASP:OD2	2.18	0.56
14:f:40:VAL:HG11	14:f:50:LEU:HA	1.87	0.56
18:j:43:ILE:HD12	18:j:56:ASP:HB2	1.88	0.56
9:a:3:U:H2'	9:a:4:U:C6	2.40	0.56
9:a:871:U:H2'	9:a:872:U:C6	2.40	0.56
7:Y:75:C:H2'	7:Y:76:A:C8	2.40	0.56
4:3:32:LYS:HE2	9:a:2478:A:H5'	1.87	0.56
7:Y:58:A:O2'	7:Y:60:U:OP2	2.21	0.56
5:4:16:CYS:SG	5:4:17:SER:N	2.79	0.56
9:a:1482:G:H1'	9:a:1509:A:N6	2.17	0.56
9:a:1868:C:N3	9:a:1873:G:N1	2.38	0.56
15:g:24:ILE:HD13	15:g:37:LEU:HG	1.87	0.56
15:g:24:ILE:HG21	15:g:72:LEU:HD21	1.88	0.56
9:a:851:C:H2'	9:a:852:U:C6	2.41	0.56
9:a:1538:G:H2'	9:a:1539:U:H6	1.70	0.55
16:h:34:GLY:O	16:h:36:ALA:N	2.39	0.55
34:z:54:VAL:HG23	34:z:55:ILE:HG12	1.88	0.55
6:X:22:U:O4	6:X:23:A:N6	2.36	0.55
9:a:2014:A:H2'	9:a:2015:A:C8	2.41	0.55
9:a:143:C:H2'	9:a:144:A:C8	2.41	0.55
8:Z:51:C:H2'	8:Z:52:G:C8	2.42	0.55
9:a:358:U:H2'	9:a:359:G:C8	2.41	0.55
20:l:53:MET:HE1	20:l:103:TYR:CD1	2.41	0.55
29:u:20:LEU:HD22	29:u:25:LYS:HB2	1.88	0.55
9:a:2096:C:H2'	9:a:2097:A:C8	2.42	0.55
10:b:41:G:O6	14:f:69:LYS:HE2	2.07	0.55
14:f:29:PRO:HB3	14:f:160:ALA:HB2	1.89	0.55
9:a:1141:U:H4'	9:a:1142:A:O4'	2.07	0.55
14:f:140:GLU:OE1	14:f:140:GLU:N	2.35	0.55
9:a:1800:C:H5'	11:c:146:MET:HE1	1.88	0.55
9:a:1946:U:H2'	9:a:1947:C:C6	2.42	0.54
32:x:7:ARG:HG3	32:x:56:LEU:HD11	1.89	0.54
8:Z:67:C:H2'	8:Z:68:C:C6	2.42	0.54
9:a:2086:U:H2'	9:a:2087:G:C8	2.42	0.54
9:a:1816:C:N4	11:c:35:GLU:OE1	2.34	0.54
15:g:84:THR:HB	15:g:134:LYS:HG2	1.89	0.54
34:z:34:SER:OG	34:z:36:GLU:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:2066:C:OP1	41:a:6310:HOH:O	2.18	0.54
9:a:1871:A:H2'	9:a:1872:A:C8	2.43	0.54
24:p:49:ASP:HA	24:p:52:GLN:HB2	1.89	0.54
10:b:106:G:H2'	10:b:107:G:O4'	2.07	0.54
18:j:1:MET:HE3	18:j:32:TYR:CZ	2.43	0.54
26:r:29:VAL:HB	26:r:55:ILE:HD11	1.88	0.54
30:v:38:VAL:HG12	30:v:59:LEU:HB2	1.90	0.54
9:a:593:U:H2'	9:a:594:U:C6	2.43	0.54
10:b:61:G:H2'	10:b:62:C:C6	2.43	0.54
31:w:3:ARG:O	31:w:12:PRO:HD3	2.08	0.54
17:i:34:ARG:HG3	17:i:39:LYS:HB2	1.90	0.54
17:i:28:LEU:HD12	17:i:142:ILE:HG21	1.90	0.54
9:a:1486:U:H2'	9:a:1487:U:H6	1.73	0.53
4:3:25:VAL:HB	4:3:35:GLN:CG	2.38	0.53
9:a:1405:U:H2'	9:a:1406:U:C6	2.43	0.53
9:a:1590:A:H2'	9:a:1591:A:C8	2.43	0.53
9:a:2698:U:H2'	9:a:2699:C:C6	2.43	0.53
24:p:76:TYR:CZ	24:p:80:ILE:HG13	2.44	0.53
10:b:40:U:O2'	10:b:43:C:OP2	2.25	0.53
20:l:30:SER:HA	20:l:133:LYS:HE3	1.91	0.53
23:o:29:LYS:HD3	23:o:40:LEU:HD23	1.91	0.53
9:a:2591:C:H2'	9:a:2592:G:C8	2.43	0.53
9:a:2822:G:N3	41:a:6383:HOH:O	2.33	0.53
14:f:142:ASP:HB3	14:f:145:LYS:HB3	1.91	0.53
1:0:14:SER:OG	1:0:48:ILE:O	2.22	0.53
8:Z:3:C:H2'	8:Z:4:G:C8	2.44	0.53
9:a:1746:A:H2'	9:a:1747:U:C6	2.44	0.53
9:a:2728:U:HO2'	9:a:2729:G:H8	1.55	0.53
13:e:190:ALA:O	13:e:194:LYS:HD2	2.09	0.53
30:v:37:ILE:HG21	30:v:80:ILE:HG21	1.89	0.53
36:Y:101:YRW:NAG	36:Y:101:YRW:OAC	2.38	0.53
8:Z:31:G:H2'	8:Z:32:C:H6	1.74	0.53
9:a:483:A:H5''	28:t:47:LYS:HD3	1.91	0.53
9:a:1178:C:H2'	9:a:1179:G:C8	2.44	0.53
9:a:1537:G:H3'	9:a:1537:G:N3	2.24	0.53
2:1:2:LYS:HE3	9:a:687:C:H5''	1.90	0.53
9:a:357:C:H2'	9:a:358:U:C6	2.44	0.53
14:f:40:VAL:HG23	14:f:86:GLY:HA2	1.90	0.53
34:z:43:ILE:HG22	34:z:49:TYR:HB2	1.92	0.53
9:a:1802:A:H2'	9:a:1803:A:C8	2.44	0.52
9:a:353:C:H2'	9:a:354:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:63:ALA:O	15:g:67:THR:HG22	2.09	0.52
9:a:851:C:H2'	9:a:852:U:H6	1.75	0.52
9:a:1722:A:N6	9:a:1738:G:O2'	2.41	0.52
9:a:1794:A:H2'	9:a:1795:C:H6	1.74	0.52
9:a:1932:A:H2'	9:a:1933:G:O4'	2.10	0.52
8:Z:23:C:H2'	8:Z:24:U:C6	2.45	0.52
9:a:645:C:H2'	9:a:647:G:C8	2.44	0.52
9:a:930:G:H1'	33:y:25:LEU:HD11	1.91	0.52
5:4:26:SER:OG	5:4:27:THR:N	2.41	0.52
9:a:1226:A:OP1	24:p:16:LYS:NZ	2.38	0.52
9:a:2498:OMC:HM22	9:a:2499:C:H5'	1.92	0.52
14:f:33:LYS:HG2	14:f:157:THR:HB	1.91	0.52
18:j:99:ILE:HD13	18:j:118:LEU:HB2	1.92	0.52
28:t:49:VAL:HG12	28:t:52:LEU:H	1.74	0.52
9:a:883:G:N2	9:a:894:U:O2	2.43	0.52
30:v:59:LEU:HD12	30:v:80:ILE:HD12	1.91	0.52
7:Y:15:G:O6	7:Y:48:C:O2	2.28	0.52
9:a:2233:U:H2'	9:a:2234:G:C8	2.45	0.52
16:h:5:LEU:O	16:h:16:GLY:N	2.40	0.52
9:a:271:G:O2'	9:a:272:A:O5'	2.22	0.51
9:a:416:U:OP1	41:a:6311:HOH:O	2.19	0.51
9:a:897:C:H2'	9:a:898:C:H6	1.74	0.51
9:a:1660:G:N7	41:a:6388:HOH:O	2.34	0.51
9:a:1946:U:H2'	9:a:1947:C:H6	1.75	0.51
9:a:1179:G:H2'	9:a:1180:U:C6	2.44	0.51
9:a:1587:G:H2'	9:a:1588:G:H8	1.75	0.51
9:a:1607:C:N4	9:a:1622:G:OP2	2.32	0.51
9:a:1939:5MU:OP1	9:a:2604:PSU:O2'	2.26	0.51
9:a:139:U:H5'	9:a:140:C:H5	1.75	0.51
9:a:594:U:H2'	9:a:595:C:C6	2.44	0.51
9:a:636:G:OP1	19:k:129:LYS:NZ	2.37	0.51
30:v:25:ARG:NH1	30:v:31:VAL:HG12	2.26	0.51
9:a:2455:G:H2'	9:a:2456:C:C6	2.45	0.51
8:Z:61:C:H2'	8:Z:62:C:C6	2.46	0.51
9:a:1506:U:H2'	9:a:1507:C:H6	1.75	0.51
18:j:58:LEU:HA	18:j:89:ASN:ND2	2.26	0.51
7:Y:70:G:H2'	7:Y:71:G:H8	1.74	0.51
8:Z:55:U:H2'	8:Z:57:A:OP2	2.11	0.51
9:a:1842:G:H2'	9:a:1843:C:C6	2.45	0.51
18:j:58:LEU:HD11	18:j:86:LEU:HD13	1.92	0.51
9:a:279:A:H2'	9:a:280:U:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:152:GLU:HG2	13:e:153:LEU:N	2.24	0.51
9:a:1183:U:H2'	9:a:1184:U:C6	2.46	0.51
9:a:1412:U:H2'	9:a:1413:A:H8	1.75	0.51
9:a:1664:A:N3	18:j:67:LYS:NZ	2.58	0.51
25:q:37:GLU:HG2	25:q:53:PHE:CD2	2.46	0.51
26:r:41:LYS:HZ2	34:z:22:LEU:HD11	1.74	0.51
9:a:811:U:H2'	19:k:21:ARG:HA	1.92	0.51
9:a:1859:U:H2'	9:a:1860:G:C8	2.46	0.51
10:b:34:A:N3	10:b:36:C:N4	2.57	0.51
21:m:4:ARG:NH1	41:m:202:HOH:O	2.43	0.51
31:w:74:ARG:NH2	31:w:76:GLU:OE2	2.44	0.51
9:a:2674:G:H4'	18:j:30:ARG:HD2	1.93	0.50
13:e:153:LEU:HG	13:e:171:ASP:HB3	1.92	0.50
9:a:95:A:O2'	32:x:41:HIS:ND1	2.40	0.50
9:a:892:A:H2'	9:a:893:C:C6	2.46	0.50
9:a:290:U:H2'	9:a:291:G:C8	2.46	0.50
9:a:2646:C:OP1	41:a:6312:HOH:O	2.19	0.50
13:e:1:MET:HB2	13:e:16:GLU:CD	2.37	0.50
14:f:5:HIS:HB2	14:f:97:TRP:CD1	2.47	0.50
5:4:20:ASN:HD22	5:4:37:CYS:HB2	1.75	0.50
9:a:936:A:H2'	9:a:937:C:C6	2.46	0.50
9:a:1149:G:H2'	9:a:1150:C:C6	2.47	0.50
9:a:1790:C:H2'	9:a:1791:A:C5	2.46	0.50
9:a:2025:C:H2'	9:a:2026:U:C6	2.46	0.50
9:a:191:A:H2'	9:a:192:C:C6	2.47	0.50
9:a:2316:G:H2'	9:a:2317:A:H8	1.77	0.50
17:i:13:ARG:NH1	17:i:49:ASP:O	2.38	0.50
32:x:12:GLU:O	32:x:16:THR:HG22	2.12	0.50
7:Y:63:G:H2'	7:Y:64:A:H8	1.72	0.50
9:a:788:A:OP1	9:a:790:U:H5	1.95	0.50
9:a:1412:U:H2'	9:a:1413:A:C8	2.46	0.50
32:x:19:LEU:HB3	32:x:23:ARG:NH2	2.26	0.50
7:Y:26:A:H2'	7:Y:27:G:H8	1.76	0.50
7:Y:70:G:H2'	7:Y:71:G:C8	2.47	0.50
9:a:150:U:H2'	9:a:151:C:C6	2.47	0.50
9:a:351:C:H2'	9:a:352:A:C8	2.47	0.50
9:a:1703:G:H2'	9:a:1704:C:C6	2.47	0.50
9:a:2557:G:H2'	9:a:2558:C:C6	2.47	0.50
17:i:11:VAL:HG21	17:i:50:THR:HA	1.94	0.50
7:Y:43:C:O2'	7:Y:44:G:H5'	2.10	0.49
9:a:1538:G:H2'	9:a:1539:U:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:7:GLN:HG2	23:o:8:LEU:N	2.27	0.49
7:Y:55:U:H3'	7:Y:56:C:H5''	1.93	0.49
22:n:35:ILE:HB	22:n:102:ARG:HH11	1.76	0.49
23:o:4:ILE:HA	23:o:7:GLN:NE2	2.28	0.49
29:u:6:ALA:HB3	29:u:65:VAL:HG22	1.92	0.49
8:Z:15:G:H3'	8:Z:16:C:H6	1.77	0.49
9:a:877:A:O2'	9:a:900:A:N6	2.46	0.49
9:a:1506:U:H2'	9:a:1507:C:C6	2.47	0.49
9:a:1747:U:H2'	9:a:1748:C:C6	2.47	0.49
9:a:2096:C:H2'	9:a:2097:A:H8	1.77	0.49
9:a:2305:U:H5''	14:f:131:GLY:HA3	1.94	0.49
9:a:145:C:H2'	9:a:146:A:H8	1.75	0.49
9:a:2799:A:O2'	9:a:2800:A:H5''	2.13	0.49
9:a:581:C:H2'	9:a:582:A:H8	1.78	0.49
9:a:685:A:H5''	9:a:788:A:H62	1.77	0.49
11:c:36:LYS:NZ	11:c:38:SER:OG	2.45	0.49
19:k:77:ILE:CD1	19:k:108:ALA:HB1	2.42	0.49
9:a:1873:G:H2'	9:a:1874:C:C6	2.47	0.49
7:Y:60:U:H2'	7:Y:61:C:H5	1.78	0.49
8:Z:22:G:H2'	8:Z:23:C:H6	1.77	0.49
9:a:1485:U:H2'	9:a:1486:U:C6	2.48	0.49
9:a:1548:A:H2'	9:a:1549:A:C8	2.47	0.49
9:a:832:U:H2'	9:a:833:A:C8	2.48	0.49
9:a:1158:C:OP2	41:a:6303:HOH:O	2.19	0.49
9:a:2012:G:P	26:r:11:ARG:HH22	2.36	0.49
9:a:2649:C:H2'	9:a:2650:U:H6	1.77	0.49
13:e:149:ILE:HG22	13:e:192:ALA:HB1	1.95	0.49
16:h:8:LYS:HA	16:h:14:SER:HA	1.93	0.49
9:a:328:U:O3'	28:t:66:GLN:HG3	2.13	0.49
9:a:784:G:H5'	9:a:785:G:OP1	2.13	0.49
9:a:2801:G:H2'	9:a:2802:G:C8	2.48	0.49
15:g:85:LYS:HG3	15:g:141:ILE:HG12	1.94	0.49
1:0:22:THR:HG21	9:a:2419:U:H4'	1.95	0.48
9:a:852:U:H2'	9:a:853:C:C6	2.48	0.48
9:a:1178:C:H2'	9:a:1179:G:H8	1.77	0.48
9:a:1923:U:H2'	9:a:1924:C:C6	2.48	0.48
9:a:2583:G:OP2	41:a:6301:HOH:O	2.20	0.48
14:f:11:GLU:O	14:f:15:LYS:HG3	2.13	0.48
7:Y:15:G:H22	7:Y:48:C:N4	2.11	0.48
9:a:909:A:H2'	9:a:912:C:H5	1.78	0.48
9:a:1028:A:H2'	9:a:1029:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:43:ASN:HD21	22:n:46:GLU:HG3	1.78	0.48
7:Y:19:G:C2	9:a:882:G:H1'	2.49	0.48
9:a:1443:U:H2'	9:a:1444:G:H8	1.78	0.48
9:a:1796:U:H2'	9:a:1797:G:H8	1.77	0.48
9:a:187:G:N7	41:a:6398:HOH:O	2.35	0.48
9:a:355:U:H2'	9:a:356:G:H8	1.78	0.48
31:w:51:VAL:HG22	31:w:52:SER:O	2.14	0.48
7:Y:37:A:H2'	7:Y:38:A:O4'	2.14	0.48
9:a:1197:G:H2'	9:a:1198:U:C6	2.47	0.48
9:a:2514:U:H2'	9:a:2515:C:C6	2.49	0.48
18:j:102:PRO:HB3	18:j:121:GLU:HB3	1.96	0.48
9:a:813:U:H2'	9:a:814:C:H6	1.78	0.48
9:a:998:C:OP1	24:p:84:LYS:NZ	2.41	0.48
26:r:1:MET:HE3	26:r:109:ASP:OD2	2.14	0.48
7:Y:57:G:C2	9:a:896:A:C2	3.02	0.48
23:o:34:GLU:OE2	23:o:39:ARG:NE	2.44	0.48
9:a:64:A:H2'	9:a:65:U:H6	1.78	0.48
9:a:151:C:H2'	9:a:152:A:H8	1.78	0.48
9:a:1788:C:OP2	41:a:6314:HOH:O	2.20	0.48
9:a:2769:U:OP1	17:i:95:ARG:NH2	2.47	0.48
12:d:1:MET:HB3	12:d:205:PRO:HG2	1.95	0.48
25:q:83:TYR:OH	25:q:85:LYS:HE3	2.14	0.48
9:a:12:U:O2	9:a:2626:C:H4'	2.14	0.48
9:a:639:U:H2'	9:a:640:C:H6	1.77	0.48
9:a:1199:U:H2'	9:a:1200:C:H6	1.78	0.48
9:a:2859:G:H2'	9:a:2860:A:C8	2.49	0.48
9:a:590:A:H2'	9:a:591:U:C6	2.49	0.47
9:a:947:A:H2'	9:a:948:C:C6	2.49	0.47
11:c:162:VAL:HG22	11:c:176:LEU:HA	1.96	0.47
12:d:149:ASN:OD1	12:d:150:MEQ:N	2.44	0.47
13:e:23:PHE:HA	13:e:107:SER:OG	2.14	0.47
14:f:134:GLU:HB3	14:f:136:ILE:HG12	1.94	0.47
16:h:9:VAL:HG21	16:h:12:LEU:HD12	1.96	0.47
26:r:73:LYS:HB2	26:r:106:VAL:HB	1.95	0.47
9:a:1181:U:H2'	9:a:1182:G:C8	2.49	0.47
9:a:1653:G:H3'	21:m:2:ARG:HG2	1.94	0.47
4:3:4:ARG:O	4:3:37:GLN:HA	2.15	0.47
9:a:413:C:H2'	9:a:414:C:C6	2.48	0.47
20:l:53:MET:HG3	20:l:120:ALA:HB2	1.96	0.47
34:z:29:SER:O	34:z:37:LYS:HA	2.14	0.47
9:a:2897:U:H2'	9:a:2898:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:36:LEU:O	14:f:88:LYS:HA	2.15	0.47
5:4:14:ALA:HB2	5:4:24:ILE:HD13	1.97	0.47
7:Y:5:G:H2'	7:Y:6:G:H8	1.79	0.47
9:a:1496:A:H2'	9:a:1498:C:C5	2.49	0.47
9:a:2020:A:H5'	34:z:9:THR:CG2	2.44	0.47
5:4:28:VAL:HB	14:f:140:GLU:HA	1.96	0.47
9:a:144:A:H2'	9:a:145:C:O4'	2.15	0.47
9:a:414:C:H2'	9:a:415:A:C8	2.50	0.47
9:a:634:C:H2'	9:a:635:C:H6	1.78	0.47
9:a:893:C:H2'	9:a:894:U:C6	2.49	0.47
9:a:1357:C:H2'	9:a:1358:G:O4'	2.15	0.47
9:a:1365:A:OP1	31:w:3:ARG:NH2	2.45	0.47
9:a:1599:U:H2'	9:a:1600:C:C6	2.50	0.47
9:a:2291:U:OP1	9:a:2380:C:O2'	2.28	0.47
9:a:2849:U:H4'	9:a:2868:A:C2	2.49	0.47
11:c:100:GLU:OE1	41:c:601:HOH:O	2.20	0.47
9:a:157:C:H2'	9:a:158:U:O4'	2.15	0.47
9:a:1361:G:H2'	9:a:1362:C:C6	2.50	0.47
9:a:2074:U:H2'	9:a:2075:U:C6	2.49	0.47
29:u:30:ILE:HD11	29:u:63:ILE:HD12	1.96	0.47
9:a:278:A:C6	9:a:362:A:C8	3.02	0.47
9:a:742:A:H2'	9:a:743:A:C8	2.49	0.47
13:e:136:GLN:O	13:e:136:GLN:NE2	2.47	0.47
13:e:153:LEU:HD23	13:e:153:LEU:HA	1.78	0.47
7:Y:19:G:N1	9:a:882:G:H1'	2.30	0.47
7:Y:31:A:C4	7:Y:32:U:C5	3.03	0.47
9:a:2615:U:C2	34:z:4:GLN:HA	2.50	0.47
8:Z:42:G:H2'	8:Z:43:A:O4'	2.15	0.46
9:a:570:G:H2'	9:a:2030:6MZ:N7	2.30	0.46
9:a:645:C:O2'	9:a:646:U:H5''	2.14	0.46
9:a:1957:C:H2'	9:a:1958:C:C6	2.50	0.46
9:a:2723:C:H2'	9:a:2724:U:O4'	2.15	0.46
28:t:47:LYS:HD2	28:t:48:PRO:HD2	1.97	0.46
8:Z:48:C:C4	8:Z:59:A:C8	3.04	0.46
9:a:55:G:O2'	9:a:127:A:N1	2.44	0.46
9:a:479:A:N3	9:a:481:G:H5''	2.30	0.46
9:a:645:C:H2'	9:a:647:G:N7	2.30	0.46
9:a:2071:A:H2'	9:a:2072:C:C6	2.50	0.46
41:a:7260:HOH:O	12:d:128:ARG:HD2	2.15	0.46
14:f:47:LYS:NZ	14:f:84:PRO:HG2	2.31	0.46
27:s:6:ARG:O	27:s:10:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:143:C:H2'	9:a:144:A:H8	1.77	0.46
9:a:322:A:OP2	13:e:163:ASN:HB2	2.16	0.46
9:a:364:C:H2'	9:a:365:U:C6	2.51	0.46
9:a:1786:A:H1'	9:a:1938:A:N6	2.30	0.46
9:a:2461:A:H2'	9:a:2462:C:C6	2.50	0.46
13:e:168:ASP:HB2	13:e:183:PHE:CZ	2.51	0.46
7:Y:19:G:C4	9:a:896:A:N1	2.84	0.46
9:a:65:U:O2'	9:a:456:C:N3	2.48	0.46
9:a:833:A:H2'	9:a:834:G:C8	2.50	0.46
9:a:1796:U:H2'	9:a:1797:G:C8	2.50	0.46
14:f:36:LEU:HB2	14:f:89:VAL:HG22	1.97	0.46
9:a:1443:U:H2'	9:a:1444:G:C8	2.50	0.46
9:a:1859:U:H2'	9:a:1860:G:H8	1.81	0.46
28:t:18:ASP:HB3	28:t:21:LYS:HD2	1.96	0.46
8:Z:3:C:H2'	8:Z:4:G:H8	1.81	0.46
9:a:580:U:H2'	9:a:581:C:C6	2.51	0.46
9:a:1180:U:H2'	9:a:1181:U:C6	2.50	0.46
9:a:2646:C:H2'	9:a:2647:U:O4'	2.15	0.46
26:r:48:LYS:HE2	26:r:52:GLU:OE2	2.16	0.46
7:Y:22:G:H2'	7:Y:23:A:C8	2.45	0.46
8:Z:19:G:H4'	8:Z:20:U:OP2	2.15	0.46
9:a:588:U:H2'	9:a:589:U:C6	2.51	0.46
9:a:1486:U:H2'	9:a:1487:U:C6	2.51	0.46
9:a:1842:G:H2'	9:a:1843:C:H6	1.81	0.46
14:f:13:VAL:HG13	14:f:14:LYS:HD3	1.98	0.46
29:u:55:GLU:HB3	29:u:59:GLU:OE1	2.15	0.46
9:a:40:U:H2'	9:a:41:C:C6	2.51	0.46
9:a:1045:C:O2	9:a:1111:A:N6	2.49	0.46
9:a:1182:G:H2'	9:a:1183:U:O4'	2.15	0.46
9:a:1354:A:H2'	9:a:1355:G:O4'	2.16	0.46
11:c:87:ARG:NH1	41:c:602:HOH:O	2.26	0.46
15:g:176:LYS:HA	15:g:176:LYS:HD3	1.59	0.46
7:Y:15:G:N2	7:Y:48:C:H42	2.13	0.46
9:a:983:A:OP1	41:a:6315:HOH:O	2.21	0.46
9:a:2273:A:H2'	9:a:2274:A:C8	2.51	0.46
11:c:97:LYS:HD2	11:c:97:LYS:HA	1.65	0.46
25:q:37:GLU:HG2	25:q:53:PHE:CE2	2.51	0.46
9:a:30:G:H2'	9:a:31:C:C6	2.51	0.45
9:a:1485:U:H2'	9:a:1486:U:H6	1.81	0.45
9:a:2038:G:H2'	9:a:2039:U:O4'	2.15	0.45
14:f:32:GLU:HG3	14:f:33:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:304:U:H2'	9:a:305:C:C6	2.51	0.45
13:e:21:ARG:HD3	13:e:106:LYS:HB3	1.97	0.45
5:4:28:VAL:HB	14:f:140:GLU:HG3	1.97	0.45
8:Z:62:C:H2'	8:Z:63:G:H8	1.82	0.45
6:X:20:U:H2'	6:X:21:C:C6	2.51	0.45
7:Y:30:G:C4	7:Y:31:A:C8	3.04	0.45
9:a:839:U:H2'	9:a:840:C:C6	2.50	0.45
9:a:1997:C:OP2	12:d:129:THR:OG1	2.26	0.45
9:a:2516:A:O2'	9:a:2517:C:H5'	2.17	0.45
9:a:2680:U:O2'	9:a:2681:C:H5'	2.17	0.45
10:b:41:G:OP1	10:b:43:C:N4	2.47	0.45
13:e:49:ARG:O	13:e:74:LYS:HD2	2.16	0.45
24:p:81:ASN:HD21	24:p:85:LYS:HE3	1.81	0.45
27:s:14:PRO:HA	27:s:32:LEU:HD23	1.98	0.45
7:Y:55:U:H5	7:Y:57:G:OP2	1.95	0.45
7:Y:61:C:H3'	7:Y:62:C:O4'	2.16	0.45
9:a:927:A:H2'	9:a:928:A:C8	2.52	0.45
9:a:1442:U:H2'	9:a:1443:U:C6	2.51	0.45
9:a:2473:U:O2	9:a:2473:U:H2'	2.15	0.45
12:d:59:ARG:HA	12:d:59:ARG:HD3	1.71	0.45
14:f:78:LYS:O	14:f:79:ILE:HD13	2.16	0.45
31:w:66:THR:O	31:w:70:GLU:HG3	2.16	0.45
9:a:1224:U:H2'	9:a:1225:G:C8	2.51	0.45
9:a:2228:G:H2'	9:a:2229:U:C6	2.51	0.45
9:a:2309:A:H2'	9:a:2310:C:C6	2.51	0.45
9:a:2793:C:H2'	9:a:2794:C:H6	1.81	0.45
15:g:105:LEU:HB2	15:g:113:VAL:HB	1.98	0.45
21:m:30:ARG:HH12	21:m:74:GLU:CD	2.24	0.45
31:w:68:LEU:HD22	31:w:78:TYR:CE2	2.52	0.45
9:a:150:U:H2'	9:a:151:C:H6	1.82	0.45
9:a:909:A:H2'	9:a:912:C:C5	2.52	0.45
9:a:1187:G:H5''	25:q:83:TYR:CE1	2.52	0.45
9:a:1494:A:H2'	9:a:1495:A:C8	2.52	0.45
9:a:1710:G:H4'	9:a:2858:C:O2	2.17	0.45
9:a:1754:A:C8	23:o:94:LYS:HE2	2.52	0.45
20:l:31:PHE:CE1	20:l:110:GLU:HG3	2.52	0.45
7:Y:46:G:H3'	7:Y:47:U:H5''	1.98	0.45
9:a:197:A:N6	9:a:2430:A:H2'	2.32	0.45
9:a:933:A:H5'	9:a:934:U:OP2	2.17	0.45
9:a:1198:U:H2'	9:a:1199:U:C6	2.52	0.45
9:a:2065:C:H2'	9:a:2066:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:2532:G:N2	9:a:2663:G:O2'	2.49	0.45
9:a:2801:G:H2'	9:a:2802:G:H8	1.82	0.45
10:b:108:A:HO2'	10:b:109:A:P	2.38	0.45
14:f:22:TYR:OH	14:f:165:GLU:OE2	2.35	0.45
23:o:5:ILE:HA	23:o:8:LEU:HD12	1.98	0.45
9:a:476:G:H4'	9:a:502:A:N1	2.32	0.45
9:a:2804:U:H2'	9:a:2805:C:O4'	2.17	0.45
9:a:2820:A:C5	21:m:4:ARG:HD2	2.52	0.45
9:a:57:C:H2'	9:a:58:G:O4'	2.17	0.45
9:a:277:G:H5'	9:a:278:A:OP1	2.16	0.45
9:a:500:G:N1	9:a:503:A:OP2	2.50	0.45
9:a:1877:A:H2'	9:a:1878:G:O4'	2.17	0.45
9:a:2395:C:H2'	9:a:2396:G:O4'	2.17	0.45
9:a:2537:U:H2'	9:a:2538:C:H6	1.81	0.45
9:a:2648:G:H2'	9:a:2649:C:C6	2.52	0.45
26:r:80:PRO:O	26:r:100:THR:OG1	2.33	0.45
1:0:11:LEU:HB3	1:0:49:TYR:HB3	1.99	0.44
9:a:572:A:H5''	9:a:573:U:OP2	2.17	0.44
41:a:7771:HOH:O	19:k:29:LYS:HG3	2.15	0.44
10:b:61:G:H2'	10:b:62:C:H6	1.82	0.44
19:k:141:LYS:HZ3	19:k:143:GLU:HG2	1.82	0.44
28:t:49:VAL:HG12	28:t:51:ALA:H	1.82	0.44
8:Z:9:G:N2	8:Z:45:G:H3'	2.31	0.44
9:a:95:A:H2'	9:a:96:C:O4'	2.17	0.44
9:a:308:G:H2'	9:a:309:A:C8	2.53	0.44
9:a:2649:C:H2'	9:a:2650:U:C6	2.53	0.44
9:a:2705:A:H2'	9:a:2706:A:O4'	2.18	0.44
11:c:29:PRO:HG3	11:c:63:ARG:NH1	2.32	0.44
15:g:73:ASN:O	15:g:77:ILE:HG13	2.17	0.44
9:a:657:U:H2'	9:a:658:U:C6	2.52	0.44
9:a:945:A:C4	9:a:2448:A:C2	3.05	0.44
9:a:1115:G:C4	9:a:1116:G:C8	3.05	0.44
9:a:1268:A:H2'	9:a:1269:A:O4'	2.18	0.44
9:a:1407:G:O2'	9:a:1408:G:H5'	2.18	0.44
14:f:35:THR:HA	14:f:89:VAL:O	2.17	0.44
9:a:91:A:H1'	9:a:92:U:C6	2.52	0.44
9:a:247:G:H4'	9:a:386:G:C5	2.53	0.44
9:a:287:G:H2'	9:a:288:U:O4'	2.17	0.44
9:a:1135:C:N3	41:a:6403:HOH:O	2.36	0.44
12:d:121:THR:HB	12:d:127:PHE:CD2	2.52	0.44
14:f:135:GLN:HB2	14:f:141:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:30:ILE:HG12	29:u:91:PHE:HB2	2.00	0.44
14:f:2:ALA:HB2	14:f:94:GLU:OE2	2.18	0.44
4:3:25:VAL:HB	4:3:35:GLN:HG2	1.99	0.44
8:Z:45:G:H8	8:Z:45:G:OP2	2.00	0.44
9:a:151:C:H2'	9:a:152:A:C8	2.53	0.44
9:a:476:G:N1	9:a:479:A:OP2	2.49	0.44
9:a:609:A:H2'	9:a:610:C:O4'	2.18	0.44
9:a:1001:A:H2'	9:a:1002:G:O4'	2.17	0.44
9:a:1199:U:H2'	9:a:1200:C:C6	2.52	0.44
9:a:1957:C:H2'	9:a:1958:C:H6	1.82	0.44
9:a:2069:G7M:H8	41:a:7600:HOH:O	2.17	0.44
9:a:2743:U:H2'	9:a:2744:G:O4'	2.18	0.44
9:a:327:G:H2'	9:a:328:U:O4'	2.18	0.44
9:a:714:U:H1'	9:a:717:C:H5	1.82	0.44
9:a:918:A:H5''	10:b:97:C:O2'	2.17	0.44
13:e:189:THR:O	13:e:193:VAL:HG23	2.18	0.44
21:m:66:ALA:O	21:m:69:ARG:O	2.35	0.44
3:2:32:ILE:H	3:2:32:ILE:HG13	1.36	0.44
9:a:208:C:H2'	9:a:209:C:C6	2.53	0.44
9:a:1508:A:H2	9:a:1509:A:C6	2.35	0.44
9:a:2627:G:O2'	9:a:2781:A:N1	2.44	0.44
41:a:7794:HOH:O	11:c:39:LYS:HD2	2.18	0.44
10:b:9:G:OP1	22:n:15:ARG:HD3	2.18	0.44
10:b:41:G:P	10:b:43:C:H41	2.40	0.44
9:a:349:U:H2'	9:a:350:G:C8	2.53	0.44
9:a:2316:G:H2'	9:a:2317:A:C8	2.53	0.44
9:a:2520:C:C6	9:a:2567:G:H1'	2.53	0.44
7:Y:19:G:C4	9:a:896:A:C6	3.06	0.43
8:Z:25:C:O2'	9:a:1922:G:H4'	2.18	0.43
9:a:163:C:H2'	9:a:164:C:O4'	2.18	0.43
9:a:391:A:H1'	9:a:411:G:O4'	2.18	0.43
9:a:636:G:OP1	19:k:129:LYS:HG2	2.17	0.43
9:a:2552:OMU:HM23	9:a:2554:U:C6	2.53	0.43
12:d:56:LYS:O	12:d:60:VAL:HG23	2.17	0.43
13:e:119:ILE:O	13:e:187:VAL:HA	2.18	0.43
14:f:8:TYR:HB2	14:f:173:PHE:HZ	1.83	0.43
18:j:63:VAL:HG12	18:j:107:LEU:HD11	2.00	0.43
9:a:146:A:H2'	9:a:147:C:C6	2.53	0.43
9:a:1715:G:N2	9:a:1744:A:OP2	2.50	0.43
28:t:86:ARG:NH1	28:t:100:SER:O	2.35	0.43
9:a:2299:U:H2'	9:a:2300:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:54:U:O2	7:Y:58:A:C8	2.71	0.43
9:a:644:A:H2'	9:a:645:C:O4'	2.18	0.43
9:a:849:A:H2'	9:a:850:U:C6	2.54	0.43
9:a:1778:U:H2'	9:a:1784:A:N6	2.32	0.43
9:a:2480:C:H2'	9:a:2481:G:O4'	2.18	0.43
9:a:2701:U:OP2	41:a:6313:HOH:O	2.20	0.43
9:a:2814:A:H2'	9:a:2815:C:H6	1.83	0.43
13:e:185:LYS:HA	13:e:185:LYS:HD3	1.82	0.43
28:t:99:ASN:O	28:t:101:GLU:HG2	2.17	0.43
31:w:68:LEU:O	31:w:72:ARG:HG3	2.18	0.43
9:a:1889:A:H2'	9:a:1890:A:C8	2.54	0.43
9:a:2838:G:H2'	9:a:2839:G:O4'	2.19	0.43
7:Y:27:G:C4	7:Y:28:G:C8	3.07	0.43
8:Z:67:C:H2'	8:Z:68:C:H6	1.83	0.43
9:a:857:G:H2'	9:a:858:G:O4'	2.18	0.43
11:c:37:ASN:OD1	11:c:37:ASN:N	2.52	0.43
15:g:26:ILE:HD11	15:g:72:LEU:HD23	2.01	0.43
25:q:17:GLY:O	25:q:97:LYS:NZ	2.44	0.43
7:Y:19:G:C2	9:a:896:A:C5	3.06	0.43
9:a:1178:C:C2	9:a:1179:G:C8	3.06	0.43
9:a:1805:A:N3	11:c:50:THR:HB	2.34	0.43
9:a:2291:U:H2'	9:a:2292:U:H6	1.83	0.43
9:a:2845:U:H5''	23:o:52:ASN:O	2.18	0.43
13:e:118:LEU:HD11	13:e:188:MET:SD	2.59	0.43
9:a:169:G:H2'	9:a:170:U:C6	2.54	0.43
9:a:594:U:H2'	9:a:595:C:H6	1.83	0.43
9:a:1289:C:H2'	9:a:1290:C:H6	1.84	0.43
9:a:1386:C:H2'	9:a:1387:A:H8	1.84	0.43
9:a:2329:U:H2'	9:a:2330:G:C8	2.54	0.43
9:a:2788:C:O2'	9:a:2809:A:N3	2.49	0.43
10:b:14:U:O2	10:b:107:G:H4'	2.19	0.43
12:d:149:ASN:CG	12:d:150:MEQ:H	2.26	0.43
14:f:38:MET:HG3	14:f:57:LEU:HD22	2.00	0.43
25:q:61:ALA:HB2	25:q:98:ILE:HD13	2.00	0.43
7:Y:25:C:C2	7:Y:26:A:C8	3.07	0.43
7:Y:57:G:N1	9:a:896:A:C2	2.87	0.43
9:a:1432:G:O2'	9:a:1433:A:H5'	2.18	0.43
9:a:1720:U:H2'	9:a:1721:G:O4'	2.19	0.43
9:a:1924:C:H2'	9:a:1925:C:O4'	2.19	0.43
11:c:72:ASP:OD2	11:c:189:ARG:NH1	2.47	0.43
22:n:79:ALA:HB3	22:n:113:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:25:VAL:HB	4:3:35:GLN:HG3	2.00	0.43
9:a:1435:G:H2'	9:a:1436:G:C8	2.54	0.43
9:a:1604:C:H5'	41:a:7246:HOH:O	2.19	0.43
10:b:39:A:H2'	10:b:40:U:C6	2.54	0.43
10:b:66:A:H61	10:b:107:G:H2'	1.84	0.43
11:c:145:GLU:HG2	11:c:151:GLY:C	2.43	0.43
9:a:170:U:H2'	9:a:171:U:C6	2.54	0.42
9:a:271:G:HO2'	9:a:272:A:P	2.42	0.42
9:a:1672:A:C2	9:a:2582:G:H5'	2.54	0.42
9:a:1683:U:H2'	9:a:1684:G:C8	2.54	0.42
9:a:2702:G:H2'	9:a:2703:C:H6	1.83	0.42
14:f:69:LYS:HB3	14:f:82:GLY:HA2	2.01	0.42
15:g:137:ASP:O	15:g:141:ILE:HG22	2.19	0.42
22:n:30:ARG:HG3	22:n:35:ILE:HD12	2.00	0.42
7:Y:69:G:H8	7:Y:69:G:OP2	2.02	0.42
9:a:155:A:H2'	9:a:156:A:C8	2.54	0.42
9:a:208:C:H2'	9:a:209:C:H6	1.85	0.42
9:a:708:G:H2'	9:a:709:U:C6	2.54	0.42
9:a:1000:A:H2'	9:a:1001:A:C8	2.54	0.42
9:a:1306:C:H2'	9:a:1307:A:H8	1.83	0.42
9:a:1437:C:H2'	9:a:1438:U:C6	2.54	0.42
15:g:33:LEU:HB2	15:g:75:MET:HG3	2.00	0.42
8:Z:54:U:H2'	8:Z:55:U:O4'	2.19	0.42
9:a:1853:A:N1	9:a:2087:G:H1'	2.34	0.42
9:a:1923:U:H2'	9:a:1924:C:H6	1.83	0.42
9:a:2590:A:H2'	9:a:2591:C:H6	1.83	0.42
9:a:544:C:H5'	9:a:545:U:OP1	2.19	0.42
9:a:580:U:O3'	24:p:31:VAL:HG13	2.19	0.42
9:a:1399:C:H2'	9:a:1400:U:C6	2.55	0.42
9:a:1591:A:H2'	9:a:1592:C:C6	2.54	0.42
9:a:2241:A:N3	41:a:6413:HOH:O	2.37	0.42
9:a:2304:G:H22	9:a:2312:U:H3	1.66	0.42
20:l:17:ASN:O	20:l:38:ARG:NH1	2.52	0.42
30:v:37:ILE:HD11	30:v:82:ILE:HD11	2.02	0.42
9:a:39:G:H2'	9:a:40:U:C6	2.55	0.42
9:a:714:U:O2'	9:a:716:A:N7	2.45	0.42
19:k:85:VAL:HG21	19:k:90:VAL:HG22	2.01	0.42
3:2:19:LYS:HG3	9:a:651:G:H5'	2.01	0.42
4:3:16:ILE:CD1	4:3:25:VAL:HG22	2.49	0.42
5:4:8:LYS:O	5:4:27:THR:HA	2.20	0.42
5:4:15:SER:O	5:4:33:ASN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:600:G:H2'	9:a:601:C:C6	2.54	0.42
9:a:729:G:OP1	11:c:10:SER:OG	2.37	0.42
9:a:1444:G:H2'	9:a:1445:G:H8	1.84	0.42
9:a:1495:A:H2'	9:a:1496:A:C8	2.54	0.42
9:a:1867:G:H2'	9:a:1868:C:O4'	2.20	0.42
14:f:135:GLN:HG3	14:f:141:ILE:HG21	2.00	0.42
14:f:141:ILE:HD13	14:f:141:ILE:HA	1.84	0.42
18:j:66:LYS:HA	18:j:79:PHE:O	2.19	0.42
23:o:100:LEU:HD11	23:o:110:ILE:HD11	2.02	0.42
9:a:118:A:N3	9:a:178:G:H1'	2.34	0.42
9:a:1250:G:C5'	24:p:6:ARG:HD3	2.40	0.42
9:a:1511:G:H2'	9:a:1512:C:H6	1.85	0.42
9:a:1528:A:C4	9:a:1544:A:C6	3.08	0.42
9:a:3:U:H2'	9:a:4:U:H6	1.84	0.42
9:a:413:C:H2'	9:a:414:C:H6	1.82	0.42
9:a:810:U:C4	19:k:29:LYS:O	2.72	0.42
9:a:2222:C:H4'	11:c:185:GLU:OE2	2.20	0.42
9:a:2262:U:OP1	9:a:2387:U:O2'	2.37	0.42
9:a:2292:U:H2'	9:a:2293:G:C8	2.55	0.42
9:a:2452:C:H2'	9:a:2453:A:C8	2.55	0.42
12:d:16:THR:OG1	12:d:18:ASP:OD1	2.37	0.42
17:i:58:ASN:N	17:i:127:GLY:O	2.45	0.42
34:z:37:LYS:HB2	34:z:37:LYS:HE2	1.86	0.42
9:a:360:U:H3'	9:a:361:G:C8	2.54	0.42
9:a:589:U:H2'	9:a:590:A:C8	2.54	0.42
9:a:760:G:H2'	9:a:761:A:O4'	2.20	0.42
13:e:46:GLN:O	13:e:88:ARG:NH1	2.53	0.42
13:e:115:GLN:HE22	19:k:1:MET:N	2.18	0.42
22:n:94:ARG:HD2	22:n:97:PHE:O	2.19	0.42
28:t:14:LEU:HD11	28:t:71:ALA:HB2	2.01	0.42
1:0:38:LYS:HB2	1:0:49:TYR:CD1	2.55	0.42
9:a:290:U:H2'	9:a:291:G:H8	1.84	0.42
9:a:484:C:H2'	9:a:485:C:H6	1.84	0.42
9:a:503:A:H4'	9:a:505:A:H5'	2.01	0.42
9:a:878:A:N7	9:a:899:A:H2	2.17	0.42
9:a:1263:U:O2'	34:z:8:PRO:HD2	2.20	0.42
9:a:2345:G:N3	9:a:2381:A:H2'	2.34	0.42
9:a:2556:C:H2'	9:a:2557:G:O4'	2.20	0.42
9:a:2567:G:H2'	9:a:2568:U:C6	2.54	0.42
9:a:2619:C:OP1	12:d:157:LYS:NZ	2.52	0.42
9:a:2895:G:H2'	9:a:2896:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:5:HIS:HB2	14:f:97:TRP:CG	2.55	0.42
22:n:87:ILE:O	22:n:88:LYS:HG2	2.20	0.42
6:X:19:U:O5'	6:X:19:U:H6	2.03	0.41
9:a:703:U:H2'	9:a:704:G:O4'	2.20	0.41
9:a:2545:G:H2'	9:a:2546:U:O4'	2.20	0.41
9:a:2793:C:H2'	9:a:2794:C:C6	2.54	0.41
14:f:175:PHE:O	14:f:177:PHE:N	2.53	0.41
8:Z:26:G:N3	8:Z:26:G:H2'	2.36	0.41
9:a:537:G:H5''	17:i:5:THR:HG21	2.01	0.41
9:a:1028:A:H61	9:a:1125:G:H2'	1.84	0.41
15:g:60:ASP:OD1	15:g:60:ASP:N	2.47	0.41
2:l:45:SER:OG	9:a:126:A:OP1	2.24	0.41
5:4:8:LYS:HD2	5:4:8:LYS:HA	1.59	0.41
8:Z:11:A:H2'	8:Z:12:G:C8	2.56	0.41
10:b:28:C:H5''	22:n:31:THR:HG21	2.02	0.41
13:e:21:ARG:HD3	13:e:106:LYS:CB	2.50	0.41
32:x:14:LEU:HG	41:x:101:HOH:O	2.21	0.41
7:Y:72:C:H2'	7:Y:73:A:O4'	2.20	0.41
9:a:303:G:H2'	9:a:304:U:C6	2.55	0.41
9:a:373:U:OP1	31:w:54:LYS:NZ	2.29	0.41
9:a:754:U:H2'	9:a:755:U:C6	2.55	0.41
9:a:1484:U:H2'	9:a:1485:U:H6	1.86	0.41
9:a:2373:G:H2'	9:a:2374:C:C6	2.55	0.41
10:b:57:A:H2'	10:b:58:A:C8	2.56	0.41
12:d:35:THR:HG22	12:d:73:VAL:HG21	2.03	0.41
15:g:24:ILE:HD11	15:g:43:VAL:HG11	2.03	0.41
20:l:41:LEU:HG	20:l:96:ILE:HG13	2.02	0.41
30:v:72:LYS:HE3	30:v:72:LYS:HB3	1.76	0.41
8:Z:28:C:H2'	8:Z:29:G:H8	1.84	0.41
9:a:12:U:O2	9:a:12:U:H2'	2.21	0.41
9:a:176:A:O2'	9:a:177:G:H5'	2.20	0.41
9:a:263:G:H2'	9:a:264:C:O4'	2.20	0.41
9:a:2661:G:H8	9:a:2661:G:OP2	2.04	0.41
15:g:84:THR:HA	15:g:133:LEU:O	2.21	0.41
18:j:109:SER:O	18:j:113:MET:HG2	2.20	0.41
26:r:4:ILE:HG12	26:r:106:VAL:HG22	2.03	0.41
27:s:4:GLU:CD	27:s:49:LYS:HE3	2.46	0.41
5:4:37:CYS:SG	5:4:39:LYS:HG2	2.61	0.41
9:a:852:U:H2'	9:a:853:C:H6	1.83	0.41
9:a:1563:U:H2'	9:a:1564:C:C6	2.55	0.41
9:a:2065:C:H4'	9:a:2251:OMG:HM22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:45:HIS:O	15:g:46:ALA:HB3	2.21	0.41
15:g:86:LYS:HB2	15:g:165:ALA:HB2	2.02	0.41
5:4:1:MET:HE2	5:4:1:MET:HB3	1.95	0.41
9:a:1682:G:H2'	9:a:1683:U:C6	2.55	0.41
9:a:2271:G:OP1	30:v:18:ALA:HB1	2.19	0.41
9:a:2591:C:H2'	9:a:2592:G:H8	1.86	0.41
26:r:55:ILE:O	26:r:59:GLU:HG3	2.21	0.41
9:a:1955:U:H2'	9:a:2551:C:O2'	2.20	0.41
9:a:2065:C:H2'	9:a:2066:C:C6	2.56	0.41
11:c:29:PRO:HB3	41:c:604:HOH:O	2.21	0.41
14:f:64:LYS:HG2	14:f:65:PRO:HD2	2.02	0.41
14:f:145:LYS:HA	14:f:145:LYS:HD2	1.87	0.41
21:m:47:VAL:O	21:m:51:LEU:HD23	2.21	0.41
21:m:55:ALA:HA	21:m:80:PHE:CE2	2.55	0.41
24:p:17:ILE:HD13	24:p:17:ILE:HA	1.88	0.41
7:Y:41:C:H2'	7:Y:42:C:H6	1.86	0.41
9:a:120:U:H5''	9:a:122:G:OP2	2.21	0.41
9:a:298:G:N1	9:a:339:U:OP2	2.35	0.41
9:a:349:U:H2'	9:a:350:G:H8	1.86	0.41
9:a:880:G:C6	9:a:881:G:N7	2.89	0.41
9:a:1394:U:H4'	9:a:1603:A:H4'	2.02	0.41
9:a:1561:C:H2'	9:a:1562:U:C6	2.56	0.41
9:a:1733:G:H2'	9:a:1734:G:H8	1.86	0.41
9:a:2095:A:H5'	16:h:11:ASN:OD1	2.20	0.41
9:a:2202:U:O2'	9:a:2204:G:OP1	2.33	0.41
9:a:2646:C:H6	9:a:2646:C:O5'	2.03	0.41
9:a:2687:U:H2'	9:a:2688:G:O4'	2.20	0.41
7:Y:24:G:C6	7:Y:25:C:C4	3.09	0.41
9:a:44:A:H2'	9:a:45:G:O4'	2.21	0.41
9:a:219:A:N3	9:a:234:U:O2'	2.46	0.41
9:a:419:U:H2'	9:a:420:C:C6	2.56	0.41
9:a:1593:A:H2'	9:a:1594:U:C6	2.56	0.41
9:a:1614:A:C6	26:r:87:PRO:HB3	2.55	0.41
9:a:2424:C:O2	9:a:2429:G:O2'	2.24	0.41
11:c:141:VAL:HB	11:c:190:ALA:HB1	2.02	0.41
7:Y:35:A:H2'	7:Y:36:A:O4'	2.20	0.40
9:a:250:G:H2'	9:a:251:A:C8	2.56	0.40
9:a:532:A:N1	9:a:2020:A:H1'	2.35	0.40
9:a:532:A:N7	9:a:2021:C:O2'	2.48	0.40
9:a:608:A:H2'	9:a:609:A:C8	2.56	0.40
9:a:839:U:H2'	9:a:840:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:5:ALA:HB2	15:g:66:GLY:HA2	2.03	0.40
17:i:110:PRO:O	17:i:115:GLY:HA3	2.21	0.40
26:r:6:LYS:HA	26:r:103:ILE:O	2.21	0.40
9:a:613:A:H3'	9:a:614:A:H8	1.85	0.40
9:a:2032:G:C5	12:d:150:MEQ:HE3	2.56	0.40
9:a:2590:A:H2'	9:a:2591:C:C6	2.56	0.40
13:e:194:LYS:O	13:e:197:GLU:HG3	2.21	0.40
14:f:63:GLN:NE2	14:f:90:THR:O	2.54	0.40
23:o:33:VAL:HG22	23:o:38:LYS:HG3	2.03	0.40
31:w:68:LEU:HD13	31:w:78:TYR:CE1	2.56	0.40
9:a:493:G:H2'	9:a:494:G:O4'	2.22	0.40
9:a:1526:C:H2'	9:a:1527:G:O4'	2.21	0.40
9:a:1545:A:H2'	9:a:1546:G:O4'	2.21	0.40
9:a:1681:G:N3	9:a:1762:A:H2'	2.36	0.40
9:a:2293:G:O3'	22:n:98:GLN:NE2	2.53	0.40
9:a:2814:A:H2'	9:a:2815:C:C6	2.56	0.40
10:b:21:G:H2'	10:b:22:U:O4'	2.22	0.40
19:k:82:LEU:O	19:k:85:VAL:HG22	2.21	0.40
1:0:30:LYS:HE2	9:a:2286:G:OP1	2.20	0.40
8:Z:75:C:H5''	37:Z:101:8AN:O2P	2.21	0.40
9:a:24:G:O2'	26:r:77:ASP:HB3	2.20	0.40
9:a:753:A:H2'	9:a:754:U:H6	1.87	0.40
9:a:894:U:H2'	9:a:895:U:H4'	2.03	0.40
9:a:1289:C:H2'	9:a:1290:C:C6	2.56	0.40
9:a:1435:G:H2'	9:a:1436:G:H8	1.85	0.40
9:a:1465:G:H2'	9:a:1466:U:O4'	2.21	0.40
9:a:1746:A:H2'	9:a:1747:U:H6	1.84	0.40
9:a:2230:G:H2'	9:a:2231:U:C6	2.56	0.40
9:a:2307:G:H4'	9:a:2308:G:O5'	2.21	0.40
9:a:2542:A:H4'	9:a:2543:G:C8	2.56	0.40
9:a:2774:C:H2'	9:a:2775:G:O4'	2.21	0.40
11:c:105:LEU:O	11:c:107:PRO:HD3	2.22	0.40
14:f:4:LEU:HG	14:f:101:GLU:HG3	2.03	0.40
14:f:111:ILE:HD13	14:f:137:ILE:HG21	2.02	0.40
15:g:98:VAL:HG22	15:g:103:ILE:HG12	2.03	0.40
18:j:34:GLY:N	18:j:37:ASP:OD2	2.47	0.40
9:a:160:A:N3	9:a:2208:C:O2'	2.45	0.40
9:a:322:A:H5'	9:a:340:A:H1'	2.03	0.40
9:a:1549:A:H2'	9:a:1550:C:C6	2.57	0.40
9:a:2247:A:H2'	9:a:2248:C:H6	1.87	0.40
9:a:2305:U:C2	14:f:151:GLY:HA3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:2785:C:H2'	9:a:2786:U:C6	2.57	0.40
10:b:48:U:H2'	10:b:49:C:H6	1.85	0.40
28:t:26:LYS:HB3	28:t:26:LYS:HE2	1.83	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	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	4
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	50 (89%)	6 (11%)	0	100	100
11	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
12	d	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
13	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
14	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
15	g	174/177 (98%)	153 (88%)	20 (12%)	1 (1%)	21	18
16	h	39/149 (26%)	33 (85%)	5 (13%)	1 (3%)	4	1
17	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
18	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
19	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	18	15
20	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
21	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
22	n	114/117 (97%)	111 (97%)	2 (2%)	1 (1%)	14	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
24	p	115/118 (98%)	115 (100%)	0	0	100	100
25	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
26	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
27	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
28	t	100/104 (96%)	91 (91%)	8 (8%)	1 (1%)	12	9
29	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	v	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
31	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
32	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
33	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
34	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	3112/3337 (93%)	2997 (96%)	109 (4%)	6 (0%)	44	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	32	ILE
15	g	47	ASP
19	k	36	LYS
16	h	35	LYS
22	n	88	LYS
28	t	99	ASN

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	46/49 (94%)	45 (98%)	1 (2%)	45	53
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	48	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	45 (82%)	10 (18%)	2	1
11	c	216/218 (99%)	210 (97%)	6 (3%)	38	43
12	d	163/163 (100%)	161 (99%)	2 (1%)	63	72
13	e	165/165 (100%)	160 (97%)	5 (3%)	36	41
14	f	148/150 (99%)	132 (89%)	16 (11%)	6	4
15	g	137/138 (99%)	124 (90%)	13 (10%)	8	5
16	h	32/114 (28%)	31 (97%)	1 (3%)	35	39
17	i	116/116 (100%)	113 (97%)	3 (3%)	40	46
18	j	104/104 (100%)	103 (99%)	1 (1%)	68	76
19	k	103/103 (100%)	102 (99%)	1 (1%)	68	76
20	l	107/107 (100%)	103 (96%)	4 (4%)	30	33
21	m	98/103 (95%)	97 (99%)	1 (1%)	68	76
22	n	86/87 (99%)	80 (93%)	6 (7%)	14	11
23	o	99/100 (99%)	94 (95%)	5 (5%)	21	21
24	p	89/90 (99%)	89 (100%)	0	100	100
25	q	84/84 (100%)	81 (96%)	3 (4%)	31	34
26	r	93/93 (100%)	90 (97%)	3 (3%)	34	38
27	s	80/84 (95%)	77 (96%)	3 (4%)	29	32
28	t	83/85 (98%)	78 (94%)	5 (6%)	17	15
29	u	78/78 (100%)	77 (99%)	1 (1%)	61	69
30	v	57/63 (90%)	55 (96%)	2 (4%)	32	35
31	w	67/68 (98%)	67 (100%)	0	100	100
32	x	54/55 (98%)	53 (98%)	1 (2%)	50	58
33	y	48/49 (98%)	47 (98%)	1 (2%)	47	54
34	z	47/48 (98%)	46 (98%)	1 (2%)	47	54
All	All	2578/2700 (96%)	2482 (96%)	96 (4%)	31	33

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	29	THR
3	2	32	ILE

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Mol	Chain	Res	Type
5	4	4	ASP
5	4	8	LYS
5	4	12	ILE
5	4	21	VAL
5	4	22	MET
5	4	26	SER
5	4	34	LEU
5	4	47	LYS
5	4	48	GLN
5	4	65	ASN
11	c	5	LYS
11	c	125	LYS
11	c	156	ARG
11	c	162	VAL
11	c	182	ARG
11	c	259	SER
12	d	58	ASN
12	d	95	SER
13	e	17	THR
13	e	55	SER
13	e	123	LYS
13	e	125	SER
13	e	153	LEU
14	f	9	LYS
14	f	17	MET
14	f	21	ASN
14	f	32	GLU
14	f	40	VAL
14	f	57	LEU
14	f	68	THR
14	f	69	LYS
14	f	74	VAL
14	f	108	VAL
14	f	135	GLN
14	f	136	ILE
14	f	137	ILE
14	f	145	LYS
14	f	146	VAL
14	f	161	LYS
15	g	23	VAL
15	g	29	LYS
15	g	36	THR

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Mol	Chain	Res	Type
15	g	44	LYS
15	g	45	HIS
15	g	56	ASP
15	g	84	THR
15	g	90	VAL
15	g	105	LEU
15	g	122	THR
15	g	127	THR
15	g	129	THR
15	g	166	ASP
16	h	12	LEU
17	i	10	THR
17	i	11	VAL
17	i	12	LYS
18	j	76	VAL
19	k	120	VAL
20	l	3	GLN
20	l	14	LYS
20	l	58	LYS
20	l	78	LEU
21	m	96	ARG
22	n	25	ARG
22	n	48	LEU
22	n	49	VAL
22	n	63	LYS
22	n	74	VAL
22	n	83	LEU
23	o	5	ILE
23	o	6	LYS
23	o	7	GLN
23	o	34	GLU
23	o	37	LYS
25	q	29	THR
25	q	47	VAL
25	q	70	GLU
26	r	4	ILE
26	r	30	SER
26	r	66	ILE
27	s	25	GLU
27	s	28	ASN
27	s	64	LYS
28	t	26	LYS

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Mol	Chain	Res	Type
28	t	31	SER
28	t	54	GLN
28	t	58	ILE
28	t	100	SER
29	u	10	LYS
30	v	10	THR
30	v	70	GLU
32	x	56	LEU
33	y	4	THR
34	z	23	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	20	ASN
11	c	115	GLN
11	c	134	ASN
12	d	94	GLN
13	e	94	GLN
13	e	115	GLN
15	g	48	ASN
17	i	47	HIS
19	k	104	GLN
20	l	60	GLN
21	m	107	ASN
22	n	38	GLN
23	o	7	GLN
23	o	10	GLN
23	o	66	ASN
26	r	9	HIS
27	s	48	GLN
27	s	70	HIS
28	t	46	GLN
29	u	24	ASN
29	u	87	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	118/120 (98%)	19 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	X	14/28 (50%)	4 (28%)	1 (7%)
7	Y	71/76 (93%)	27 (38%)	1 (1%)
8	Z	74/76 (97%)	22 (29%)	0
9	a	2749/2904 (94%)	331 (12%)	0
All	All	3026/3204 (94%)	403 (13%)	2 (0%)

All (403) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	X	19	U
6	X	24	A
6	X	25	C
6	X	27	A
7	Y	13	C
7	Y	14	A
7	Y	19	G
7	Y	20	U
7	Y	22	G
7	Y	34	G
7	Y	42	C
7	Y	44	G
7	Y	45	U
7	Y	46	G
7	Y	47	U
7	Y	48	C
7	Y	49	C
7	Y	51	U
7	Y	55	U
7	Y	56	C
7	Y	57	G
7	Y	58	A
7	Y	59	U
7	Y	62	C
7	Y	63	G
7	Y	66	U
7	Y	68	C
7	Y	69	G
7	Y	70	G
7	Y	72	C
7	Y	74	C
8	Z	4	G
8	Z	8	U

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Mol	Chain	Res	Type
8	Z	9	G
8	Z	14	A
8	Z	15	G
8	Z	17	C
8	Z	18	G
8	Z	19	G
8	Z	20	U
8	Z	21	A
8	Z	44	A
8	Z	48	C
8	Z	56	C
8	Z	57	A
8	Z	58	A
8	Z	59	A
8	Z	61	C
8	Z	69	C
8	Z	70	G
8	Z	71	C
8	Z	72	A
8	Z	74	C
9	a	10	A
9	a	15	G
9	a	34	U
9	a	45	G
9	a	58	G
9	a	63	A
9	a	71	A
9	a	74	A
9	a	75	G
9	a	93	G
9	a	96	C
9	a	101	A
9	a	102	U
9	a	118	A
9	a	119	A
9	a	120	U
9	a	125	A
9	a	139	U
9	a	140	C
9	a	142	A
9	a	145	C
9	a	163	C

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Mol	Chain	Res	Type
9	a	165	A
9	a	181	A
9	a	196	A
9	a	215	G
9	a	216	A
9	a	221	A
9	a	222	A
9	a	248	G
9	a	272	A
9	a	273	G
9	a	276	U
9	a	278	A
9	a	279	A
9	a	282	A
9	a	287	G
9	a	289	G
9	a	311	A
9	a	329	G
9	a	330	A
9	a	343	C
9	a	353	C
9	a	355	U
9	a	356	G
9	a	361	G
9	a	362	A
9	a	386	G
9	a	396	G
9	a	404	A
9	a	405	U
9	a	411	G
9	a	455	C
9	a	456	C
9	a	481	G
9	a	490	C
9	a	491	G
9	a	504	A
9	a	505	A
9	a	509	C
9	a	530	G
9	a	531	C
9	a	532	A
9	a	544	C

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Mol	Chain	Res	Type
9	a	545	U
9	a	546	U
9	a	547	A
9	a	548	G
9	a	549	G
9	a	550	C
9	a	563	A
9	a	573	U
9	a	575	A
9	a	603	A
9	a	614	A
9	a	615	U
9	a	627	A
9	a	637	A
9	a	645	C
9	a	647	G
9	a	653	U
9	a	654	A
9	a	655	A
9	a	685	A
9	a	686	U
9	a	717	C
9	a	721	A
9	a	730	A
9	a	738	G
9	a	747	5MU
9	a	775	G
9	a	776	G
9	a	782	A
9	a	784	G
9	a	785	G
9	a	789	A
9	a	805	G
9	a	812	C
9	a	827	U
9	a	828	U
9	a	845	A
9	a	846	U
9	a	847	U
9	a	859	G
9	a	877	A
9	a	878	A

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Mol	Chain	Res	Type
9	a	883	G
9	a	884	U
9	a	885	C
9	a	887	U
9	a	888	C
9	a	889	C
9	a	890	C
9	a	891	G
9	a	893	C
9	a	895	U
9	a	896	A
9	a	897	C
9	a	907	G
9	a	910	A
9	a	914	G
9	a	932	U
9	a	946	C
9	a	961	C
9	a	974	G
9	a	983	A
9	a	996	A
9	a	1005	C
9	a	1012	U
9	a	1013	C
9	a	1026	G
9	a	1033	U
9	a	1040	A
9	a	1045	C
9	a	1046	A
9	a	1047	G
9	a	1108	U
9	a	1111	A
9	a	1112	G
9	a	1115	G
9	a	1116	G
9	a	1117	C
9	a	1132	U
9	a	1133	A
9	a	1135	C
9	a	1142	A
9	a	1171	G
9	a	1250	G

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Mol	Chain	Res	Type
9	a	1253	A
9	a	1256	G
9	a	1271	G
9	a	1272	A
9	a	1300	G
9	a	1301	A
9	a	1306	C
9	a	1329	U
9	a	1352	U
9	a	1365	A
9	a	1379	U
9	a	1383	A
9	a	1415	U
9	a	1416	G
9	a	1417	C
9	a	1419	A
9	a	1427	A
9	a	1428	C
9	a	1452	G
9	a	1453	A
9	a	1460	U
9	a	1461	C
9	a	1482	G
9	a	1490	A
9	a	1493	C
9	a	1504	A
9	a	1508	A
9	a	1509	A
9	a	1510	G
9	a	1515	A
9	a	1523	U
9	a	1529	G
9	a	1533	C
9	a	1535	A
9	a	1536	C
9	a	1537	G
9	a	1566	A
9	a	1569	A
9	a	1578	U
9	a	1581	G
9	a	1583	A
9	a	1584	U

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Mol	Chain	Res	Type
9	a	1585	C
9	a	1586	A
9	a	1587	G
9	a	1608	A
9	a	1647	U
9	a	1648	U
9	a	1649	G
9	a	1674	G
9	a	1715	G
9	a	1729	U
9	a	1730	C
9	a	1732	C
9	a	1733	G
9	a	1738	G
9	a	1744	A
9	a	1764	C
9	a	1773	A
9	a	1782	U
9	a	1800	C
9	a	1801	A
9	a	1808	A
9	a	1816	C
9	a	1829	A
9	a	1847	A
9	a	1858	A
9	a	1869	G
9	a	1870	C
9	a	1871	A
9	a	1872	A
9	a	1873	G
9	a	1874	C
9	a	1876	A
9	a	1884	G
9	a	1906	G
9	a	1908	C
9	a	1929	G
9	a	1930	G
9	a	1937	A
9	a	1938	A
9	a	1955	U
9	a	1965	C
9	a	1967	C

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Mol	Chain	Res	Type
9	a	1970	A
9	a	1971	U
9	a	1972	G
9	a	1991	U
9	a	1993	U
9	a	2023	C
9	a	2031	A
9	a	2033	A
9	a	2043	C
9	a	2055	C
9	a	2056	G
9	a	2060	A
9	a	2061	G
9	a	2062	A
9	a	2069	G7M
9	a	2093	G
9	a	2097	A
9	a	2198	A
9	a	2204	G
9	a	2211	A
9	a	2220	U
9	a	2223	G
9	a	2225	A
9	a	2238	G
9	a	2239	G
9	a	2268	A
9	a	2283	C
9	a	2287	A
9	a	2305	U
9	a	2308	G
9	a	2322	A
9	a	2325	G
9	a	2333	A
9	a	2335	A
9	a	2347	C
9	a	2350	C
9	a	2361	G
9	a	2379	G
9	a	2383	G
9	a	2385	C
9	a	2396	G
9	a	2402	U

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Mol	Chain	Res	Type
9	a	2403	C
9	a	2406	A
9	a	2424	C
9	a	2425	A
9	a	2429	G
9	a	2430	A
9	a	2435	A
9	a	2441	U
9	a	2448	A
9	a	2474	U
9	a	2475	C
9	a	2476	A
9	a	2478	A
9	a	2491	U
9	a	2492	U
9	a	2494	G
9	a	2502	G
9	a	2505	G
9	a	2518	A
9	a	2520	C
9	a	2529	G
9	a	2535	G
9	a	2547	A
9	a	2554	U
9	a	2566	A
9	a	2567	G
9	a	2573	C
9	a	2602	A
9	a	2609	U
9	a	2613	U
9	a	2629	U
9	a	2663	G
9	a	2689	U
9	a	2690	U
9	a	2714	G
9	a	2716	C
9	a	2726	A
9	a	2733	A
9	a	2744	G
9	a	2748	A
9	a	2757	A
9	a	2765	A

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Mol	Chain	Res	Type
9	a	2778	A
9	a	2791	G
9	a	2795	C
9	a	2798	U
9	a	2802	G
9	a	2820	A
9	a	2821	A
9	a	2835	A
9	a	2849	U
9	a	2873	A
9	a	2880	C
9	a	2883	A
9	a	2884	U
9	a	2899	A
9	a	2903	U
10	b	13	G
10	b	18	G
10	b	25	U
10	b	33	G
10	b	35	C
10	b	36	C
10	b	37	C
10	b	42	C
10	b	45	A
10	b	50	A
10	b	56	G
10	b	57	A
10	b	66	A
10	b	68	C
10	b	89	U
10	b	90	C
10	b	99	A
10	b	109	A
10	b	110	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	X	24	A
7	Y	13	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	2MG	a	2445	9	23,26,27	1.26	3 (13%)	33,38,41	2.19	7 (21%)
9	PSU	a	2504	40,9	18,21,22	1.42	3 (16%)	21,30,33	2.06	4 (19%)
9	3TD	a	1915	9	19,22,23	1.57	5 (26%)	23,32,35	2.15	3 (13%)
9	OMG	a	2251	8,40,9	23,26,27	1.19	3 (13%)	32,38,41	2.03	7 (21%)
12	MEQ	d	150	12	8,9,10	0.47	0	5,10,12	0.25	0
9	OMC	a	2498	39,9	19,22,23	0.76	1 (5%)	25,31,34	0.96	1 (4%)
9	PSU	a	1911	9	18,21,22	1.35	2 (11%)	21,30,33	2.11	3 (14%)
9	PSU	a	746	39,9	18,21,22	1.32	3 (16%)	21,30,33	1.94	4 (19%)
9	6MZ	a	1618	9	22,25,26	1.41	5 (22%)	29,36,39	2.30	11 (37%)
9	PSU	a	2457	9	18,21,22	1.48	4 (22%)	21,30,33	2.04	5 (23%)
9	PSU	a	2604	9	18,21,22	1.46	3 (16%)	21,30,33	2.06	5 (23%)
9	6MZ	a	2030	9	22,25,26	1.43	5 (22%)	29,36,39	2.46	12 (41%)
9	PSU	a	1917	9	18,21,22	1.46	2 (11%)	21,30,33	2.17	4 (19%)
9	2MG	a	1835	9	23,26,27	1.26	3 (13%)	33,38,41	2.27	9 (27%)
9	OMU	a	2552	39,9	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
9	G7M	a	2069	9	23,26,27	1.50	4 (17%)	34,39,42	1.67	5 (14%)
9	PSU	a	955	9	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
9	2MA	a	2503	39,40,9	22,25,26	1.45	4 (18%)	32,37,40	2.33	9 (28%)
9	PSU	a	2605	9	18,21,22	1.40	3 (16%)	21,30,33	2.18	4 (19%)
9	PSU	a	2580	9	18,21,22	1.36	3 (16%)	21,30,33	2.17	4 (19%)
9	5MU	a	747	9	19,22,23	1.39	5 (26%)	27,32,35	2.16	6 (22%)
9	H2U	a	2449	9	18,21,22	1.13	2 (11%)	19,30,33	1.07	2 (10%)
20	MS6	l	82	20	5,7,8	0.24	0	2,7,9	0.06	0
20	4D4	l	81	20	9,11,12	2.02	2 (22%)	7,13,15	1.05	0
9	5MU	a	1939	9	19,22,23	1.37	5 (26%)	27,32,35	2.14	6 (22%)
9	1MG	a	745	9	23,26,27	1.18	4 (17%)	33,39,42	1.71	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	5MC	a	1962	9	19,22,23	1.62	3 (15%)	26,32,35	1.09	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	2MG	a	2445	9	-	0/9/27/28	0/3/3/3
9	PSU	a	2504	40,9	-	0/7/25/26	0/2/2/2
9	3TD	a	1915	9	-	0/7/25/26	0/2/2/2
9	OMG	a	2251	8,40,9	-	0/9/27/28	0/3/3/3
12	MEQ	d	150	12	-	2/8/9/11	-
9	OMC	a	2498	39,9	-	0/9/27/28	0/2/2/2
9	PSU	a	1911	9	-	0/7/25/26	0/2/2/2
9	PSU	a	746	39,9	-	2/7/25/26	0/2/2/2
9	6MZ	a	1618	9	-	0/9/27/28	0/3/3/3
9	PSU	a	2457	9	-	0/7/25/26	0/2/2/2
9	PSU	a	2604	9	-	0/7/25/26	0/2/2/2
9	6MZ	a	2030	9	-	1/9/27/28	0/3/3/3
9	PSU	a	1917	9	-	0/7/25/26	0/2/2/2
9	2MG	a	1835	9	-	0/9/27/28	0/3/3/3
9	OMU	a	2552	39,9	-	1/9/27/28	0/2/2/2
9	G7M	a	2069	9	-	1/7/25/26	0/3/3/3
9	PSU	a	955	9	-	0/7/25/26	0/2/2/2
9	2MA	a	2503	39,40,9	-	1/7/25/26	0/3/3/3
9	PSU	a	2605	9	-	0/7/25/26	0/2/2/2
9	PSU	a	2580	9	-	0/7/25/26	0/2/2/2
9	5MU	a	747	9	-	1/7/25/26	0/2/2/2
9	H2U	a	2449	9	-	0/7/38/39	0/2/2/2
20	MS6	l	82	20	-	1/4/6/8	-
20	4D4	l	81	20	-	1/11/12/14	-
9	5MU	a	1939	9	-	0/7/25/26	0/2/2/2
9	1MG	a	745	9	-	0/7/25/26	0/3/3/3
9	5MC	a	1962	9	-	2/7/25/26	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	1962	5MC	C5-C4	6.01	1.48	1.44
9	a	2069	G7M	C5-N7	-4.88	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	2503	2MA	C5-C4	4.35	1.46	1.39
9	a	1618	6MZ	C5-C4	4.14	1.46	1.39
9	a	2030	6MZ	C5-C4	4.09	1.46	1.39
20	l	81	4D4	CZ-NE	4.04	1.41	1.33
9	a	2504	PSU	C6-C5	3.56	1.39	1.35
9	a	2457	PSU	C6-C5	3.45	1.39	1.35
9	a	955	PSU	C6-C5	3.43	1.39	1.35
9	a	1917	PSU	C6-C5	3.35	1.39	1.35
9	a	2605	PSU	C6-C5	3.26	1.38	1.35
9	a	2604	PSU	C4-N3	-3.26	1.32	1.38
9	a	2604	PSU	C6-C5	3.24	1.38	1.35
9	a	2580	PSU	C6-C5	3.23	1.38	1.35
9	a	1917	PSU	C4-N3	-3.15	1.33	1.38
9	a	1911	PSU	C6-C5	3.13	1.38	1.35
9	a	1915	3TD	C6-C5	3.13	1.38	1.35
9	a	1915	3TD	C4-N3	-3.12	1.33	1.40
9	a	745	1MG	C5-C4	3.07	1.47	1.38
9	a	2552	OMU	C4-N3	-3.03	1.33	1.38
9	a	1915	3TD	C10-N3	3.00	1.52	1.47
9	a	2445	2MG	C5-C4	2.99	1.46	1.38
9	a	2251	OMG	C5-C4	2.94	1.46	1.38
9	a	2449	H2U	C2-N3	-2.93	1.32	1.38
9	a	2605	PSU	C4-N3	-2.90	1.33	1.38
9	a	955	PSU	C4-N3	-2.88	1.33	1.38
9	a	2504	PSU	C4-N3	-2.88	1.33	1.38
9	a	2457	PSU	C4-N3	-2.87	1.33	1.38
9	a	1835	2MG	C5-C4	2.82	1.46	1.38
9	a	746	PSU	C4-N3	-2.82	1.33	1.38
9	a	2069	G7M	C5-C4	2.81	1.45	1.38
9	a	1618	6MZ	C5-N7	-2.81	1.34	1.39
20	l	81	4D4	CZ-NH2	2.77	1.42	1.32
9	a	1835	2MG	C6-N1	-2.75	1.33	1.38
9	a	747	5MU	C4-N3	-2.70	1.33	1.38
9	a	1939	5MU	C4-N3	-2.69	1.33	1.38
9	a	2580	PSU	C4-N3	-2.64	1.33	1.38
9	a	746	PSU	C6-C5	2.63	1.38	1.35
9	a	2030	6MZ	C4-N9	-2.58	1.32	1.37
9	a	2251	OMG	C6-N1	-2.56	1.34	1.38
9	a	2445	2MG	C6-N1	-2.56	1.34	1.38
9	a	747	5MU	C6-C5	2.56	1.38	1.34
9	a	1939	5MU	C6-C5	2.56	1.38	1.34
9	a	2030	6MZ	C5-N7	-2.55	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	2069	G7M	C6-N1	-2.54	1.34	1.38
9	a	2552	OMU	C2-N3	-2.54	1.33	1.38
9	a	2449	H2U	C4-N3	-2.54	1.33	1.37
9	a	1962	5MC	C6-C5	2.53	1.38	1.34
9	a	1915	3TD	C2-N1	-2.51	1.34	1.37
9	a	1835	2MG	C5-N7	-2.50	1.34	1.39
9	a	2503	2MA	C5-C6	2.50	1.48	1.41
9	a	1939	5MU	C4-C5	2.45	1.48	1.44
9	a	1911	PSU	C4-N3	-2.45	1.34	1.38
9	a	1939	5MU	C2-N3	-2.43	1.33	1.38
9	a	745	1MG	C2-N1	2.40	1.41	1.37
9	a	747	5MU	C4-C5	2.40	1.48	1.44
9	a	2604	PSU	C2-N3	-2.39	1.33	1.37
9	a	2030	6MZ	C5-C6	2.38	1.47	1.41
9	a	2503	2MA	C5-N7	-2.35	1.34	1.39
9	a	747	5MU	C6-N1	-2.32	1.34	1.38
9	a	1962	5MC	C6-N1	-2.32	1.34	1.38
9	a	1939	5MU	C6-N1	-2.30	1.34	1.38
9	a	2069	G7M	C4-N9	-2.27	1.32	1.38
9	a	2457	PSU	C2-N3	-2.27	1.33	1.37
9	a	2580	PSU	O4'-C1'	-2.27	1.40	1.43
9	a	2251	OMG	C5-N7	-2.26	1.34	1.39
9	a	745	1MG	C5-N7	-2.26	1.34	1.39
9	a	745	1MG	C4-N9	-2.25	1.32	1.38
9	a	747	5MU	C2-N1	2.23	1.42	1.38
9	a	1618	6MZ	C5-C6	2.22	1.47	1.41
9	a	2457	PSU	C2-N1	-2.16	1.33	1.36
9	a	955	PSU	C2-N3	-2.14	1.33	1.37
9	a	2030	6MZ	C8-N7	2.12	1.35	1.31
9	a	2504	PSU	C2-N3	-2.11	1.34	1.37
9	a	1915	3TD	C2-N3	-2.11	1.34	1.38
9	a	2445	2MG	C5-N7	-2.05	1.35	1.39
9	a	1618	6MZ	C8-N9	-2.04	1.34	1.37
9	a	2552	OMU	C5-C4	-2.04	1.39	1.43
9	a	1618	6MZ	C4-N9	-2.03	1.33	1.37
9	a	746	PSU	C2-N3	-2.02	1.34	1.37
9	a	2498	OMC	C6-C5	2.01	1.39	1.35
9	a	2605	PSU	C2-N3	-2.01	1.34	1.37
9	a	2503	2MA	C4-N9	-2.01	1.33	1.37

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	1915	3TD	N1-C2-N3	8.06	121.99	116.13
9	a	2503	2MA	C5-C4-N3	-7.84	118.92	127.18
9	a	1835	2MG	C2-N3-C4	7.35	121.20	112.00
9	a	2445	2MG	C2-N3-C4	6.98	120.73	112.00
9	a	1917	PSU	N1-C2-N3	6.84	122.38	115.17
9	a	2605	PSU	N1-C2-N3	6.80	122.34	115.17
9	a	2604	PSU	N1-C2-N3	6.69	122.22	115.17
9	a	2503	2MA	N3-C4-N9	6.59	135.35	126.99
9	a	2580	PSU	N1-C2-N3	6.56	122.09	115.17
9	a	955	PSU	N1-C2-N3	6.53	122.05	115.17
9	a	2504	PSU	N1-C2-N3	6.40	121.92	115.17
9	a	2457	PSU	N1-C2-N3	6.37	121.89	115.17
9	a	1911	PSU	N1-C2-N3	6.36	121.88	115.17
9	a	1835	2MG	C5-C4-N3	-6.28	118.39	128.39
9	a	746	PSU	N1-C2-N3	6.19	121.70	115.17
9	a	2251	OMG	C5-C4-N3	-6.07	118.73	128.39
9	a	2445	2MG	C5-C4-N3	-5.87	119.04	128.39
9	a	1618	6MZ	C5-C4-N3	-5.45	119.22	126.72
9	a	747	5MU	N3-C2-N1	5.37	121.88	114.89
9	a	2030	6MZ	C9-N6-C6	-5.35	117.89	122.85
9	a	747	5MU	C4-N3-C2	-5.29	120.41	127.34
9	a	2251	OMG	C2-N3-C4	5.26	121.37	112.30
9	a	1939	5MU	C4-N3-C2	-5.20	120.52	127.34
9	a	1618	6MZ	N3-C4-N9	5.04	135.75	127.17
9	a	2030	6MZ	C6-C5-N7	4.88	137.75	132.43
9	a	1939	5MU	N3-C2-N1	4.88	121.24	114.89
9	a	2069	G7M	N9-C4-N3	4.88	135.70	125.95
9	a	745	1MG	C5-C4-N3	-4.84	120.69	128.39
9	a	2251	OMG	N9-C4-N3	4.83	135.61	125.95
9	a	2030	6MZ	C5-C4-N3	-4.80	120.11	126.72
9	a	2552	OMU	C4-N3-C2	-4.71	120.76	126.61
9	a	2069	G7M	C5-C4-N3	-4.67	119.32	128.15
9	a	2069	G7M	C2-N3-C4	4.62	120.26	112.30
9	a	1939	5MU	C5-C4-N3	4.60	119.32	115.32
9	a	2552	OMU	N3-C2-N1	4.58	120.85	114.89
9	a	1835	2MG	N9-C4-N3	4.55	135.06	125.95
9	a	2605	PSU	C4-N3-C2	-4.52	120.14	126.37
9	a	2445	2MG	N9-C4-N3	4.39	134.73	125.95
9	a	2580	PSU	C4-N3-C2	-4.39	120.33	126.37
9	a	1911	PSU	C4-N3-C2	-4.38	120.34	126.37
9	a	1917	PSU	C4-N3-C2	-4.38	120.34	126.37
9	a	745	1MG	C2-N3-C4	4.36	121.78	111.98
9	a	2504	PSU	C4-N3-C2	-4.30	120.44	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	955	PSU	C4-N3-C2	-4.16	120.64	126.37
9	a	747	5MU	C5-C4-N3	4.14	118.92	115.32
9	a	2030	6MZ	C4-C5-N7	-4.11	105.88	110.58
9	a	746	PSU	C4-N3-C2	-4.10	120.72	126.37
9	a	2457	PSU	C4-N3-C2	-4.10	120.73	126.37
9	a	1618	6MZ	C9-N6-C6	-4.10	119.05	122.85
9	a	2604	PSU	C4-N3-C2	-4.04	120.80	126.37
9	a	1939	5MU	C5-C6-N1	-4.03	118.94	123.31
9	a	1915	3TD	C4-N3-C2	-3.99	120.39	124.61
9	a	1939	5MU	O4-C4-C5	-3.99	120.36	124.92
9	a	1911	PSU	O2-C2-N1	-3.93	118.73	122.79
9	a	747	5MU	O4-C4-C5	-3.90	120.45	124.92
9	a	1618	6MZ	N1-C2-N3	-3.89	122.70	128.58
9	a	1917	PSU	O2-C2-N1	-3.84	118.83	122.79
9	a	1618	6MZ	C2-N3-C4	3.72	120.91	111.83
9	a	2030	6MZ	N1-C2-N3	-3.69	122.99	128.58
9	a	2552	OMU	C5-C4-N3	3.67	119.95	114.80
9	a	2030	6MZ	N3-C4-N9	3.54	133.19	127.17
9	a	1618	6MZ	C4-N9-C8	3.53	109.44	105.74
9	a	2605	PSU	O2-C2-N1	-3.50	119.17	122.79
9	a	2030	6MZ	C2-N3-C4	3.50	120.38	111.83
9	a	745	1MG	N9-C4-N3	3.42	132.78	125.95
9	a	1939	5MU	O2-C2-N1	-3.37	118.40	122.80
9	a	747	5MU	C5-C6-N1	-3.37	119.65	123.31
9	a	2580	PSU	O2-C2-N1	-3.35	119.33	122.79
9	a	2445	2MG	C6-C5-N7	3.35	136.39	130.29
9	a	2457	PSU	O2-C2-N1	-3.34	119.35	122.79
9	a	2030	6MZ	C4-N9-C8	3.26	109.17	105.74
9	a	2503	2MA	C4-N9-C8	3.25	109.15	105.74
9	a	2251	OMG	C6-C5-N7	3.23	136.17	130.29
9	a	1962	5MC	C5-C6-N1	-3.22	119.81	123.31
9	a	2503	2MA	C4-C5-N7	-3.20	106.92	110.58
9	a	747	5MU	O2-C2-N1	-3.16	118.69	122.80
9	a	1835	2MG	C6-C5-N7	3.14	136.00	130.29
9	a	2504	PSU	O2-C2-N1	-3.10	119.60	122.79
9	a	745	1MG	C6-C5-N7	3.05	136.14	129.36
9	a	2030	6MZ	C5-N7-C8	3.03	108.22	103.45
9	a	2503	2MA	N6-C6-N1	3.01	121.09	117.03
9	a	2552	OMU	O2-C2-N1	-2.99	118.91	122.80
9	a	1618	6MZ	C6-C5-N7	2.98	135.68	132.43
9	a	1962	5MC	C5-C4-N3	-2.93	118.75	121.75
9	a	2503	2MA	C2-N1-C6	2.85	122.48	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	1618	6MZ	C4-C5-N7	-2.84	107.34	110.58
9	a	955	PSU	O2-C2-N1	-2.83	119.87	122.79
9	a	2552	OMU	O4-C4-C5	-2.82	120.30	125.16
9	a	745	1MG	C4-C5-N7	-2.76	106.29	110.67
9	a	2030	6MZ	N9-C8-N7	-2.76	110.02	113.94
9	a	746	PSU	O2-C2-N1	-2.60	120.10	122.79
9	a	1835	2MG	C4-C5-N7	-2.60	106.55	110.67
9	a	1618	6MZ	C5-N7-C8	2.57	107.49	103.45
9	a	2605	PSU	C5-C6-N1	-2.56	118.59	122.14
9	a	2503	2MA	C5-N7-C8	2.56	107.47	103.45
9	a	2457	PSU	C5-C6-N1	-2.53	118.63	122.14
9	a	2445	2MG	C4-C5-N7	-2.52	106.68	110.67
9	a	2498	OMC	O2-C2-N3	-2.47	118.43	122.33
9	a	2604	PSU	O2-C2-N1	-2.46	120.25	122.79
9	a	2604	PSU	O2-C2-N3	-2.44	117.53	121.86
9	a	1835	2MG	N1-C2-N2	2.39	119.00	116.56
9	a	2580	PSU	O4'-C1'-C2'	2.38	108.45	105.15
9	a	1835	2MG	O6-C6-C5	-2.37	120.27	126.53
9	a	2069	G7M	O6-C6-C5	-2.37	122.73	128.01
9	a	2251	OMG	O6-C6-C5	-2.34	120.35	126.53
9	a	1917	PSU	C5-C6-N1	-2.34	118.90	122.14
9	a	2030	6MZ	C2-N1-C6	2.32	122.92	115.24
9	a	1835	2MG	C2-N1-C6	-2.30	121.77	124.55
9	a	2504	PSU	C5-C6-N1	-2.30	118.95	122.14
9	a	1618	6MZ	N9-C8-N7	-2.29	110.68	113.94
9	a	2251	OMG	C4-C5-N7	-2.27	107.07	110.67
9	a	2503	2MA	N9-C8-N7	-2.25	110.74	113.94
9	a	2069	G7M	C5-C6-N1	2.24	116.47	111.84
9	a	2604	PSU	C5-C6-N1	-2.23	119.05	122.14
9	a	2449	H2U	O2-C2-N1	-2.22	120.44	123.10
9	a	2449	H2U	N3-C2-N1	2.18	118.84	116.65
9	a	1915	3TD	C1'-C5-C4	2.16	120.88	117.61
9	a	2251	OMG	C5-C6-N1	2.15	118.72	113.25
9	a	2503	2MA	C6-C5-N7	2.15	136.23	132.09
9	a	2030	6MZ	C4-N9-C1'	-2.14	121.62	126.63
9	a	2445	2MG	O6-C6-C5	-2.14	120.89	126.53
9	a	955	PSU	O2-C2-N3	-2.13	118.07	121.86
9	a	1835	2MG	N2-C2-N3	-2.13	117.80	120.51
9	a	745	1MG	C6-C5-C4	-2.12	117.57	119.97
9	a	1618	6MZ	C2-N1-C6	2.09	122.16	115.24
9	a	746	PSU	O2-C2-N3	-2.07	118.19	121.86
9	a	2457	PSU	O4'-C1'-C2'	2.03	107.95	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	2445	2MG	N1-C2-N2	2.01	118.61	116.56

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	d	150	MEQ	NE2-CD-CG-CB
12	d	150	MEQ	OE1-CD-CG-CB
9	a	747	5MU	C3'-C4'-C5'-O5'
20	l	81	4D4	NE-CD-CG-CB
9	a	1962	5MC	C2'-C1'-N1-C6
9	a	2030	6MZ	O4'-C4'-C5'-O5'
9	a	2552	OMU	C3'-C2'-O2'-CM2
9	a	1962	5MC	O4'-C1'-N1-C6
9	a	746	PSU	O4'-C1'-C5-C6
9	a	746	PSU	C2'-C1'-C5-C6
20	l	82	MS6	CB-CG-SD-CE
9	a	2069	G7M	O4'-C4'-C5'-O5'
9	a	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	2251	OMG	1	0
12	d	150	MEQ	3	0
9	a	2498	OMC	1	0
9	a	2604	PSU	1	0
9	a	2030	6MZ	2	0
9	a	2552	OMU	1	0
9	a	2069	G7M	1	0
9	a	1939	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 248 are monoatomic - leaving 3 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
36	YRW	Y	101	7	10,10,10	2.74	3 (30%)	12,13,13	1.70	1 (8%)
38	FME	Z	102	37	8,9,10	0.92	0	8,9,11	0.92	0
37	8AN	Z	101	38,8,39	21,24,25	0.71	1 (4%)	26,35,38	0.47	0

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
36	YRW	Y	101	7	-	0/4/4/4	0/1/1/1
38	FME	Z	102	37	-	4/7/9/11	-
37	8AN	Z	101	38,8,39	-	1/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	101	YRW	CAE-CAB	-7.48	1.39	1.50
36	Y	101	YRW	CAJ-NAI	2.91	1.40	1.34
37	Z	101	8AN	C3'-N3'	-2.83	1.43	1.47
36	Y	101	YRW	CAH-NAI	2.32	1.40	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Y	101	YRW	CAE-CAF-NAG	-4.41	116.53	122.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	Z	101	8AN	C4'-C5'-O5'-P
38	Z	102	FME	N-CA-CB-CG

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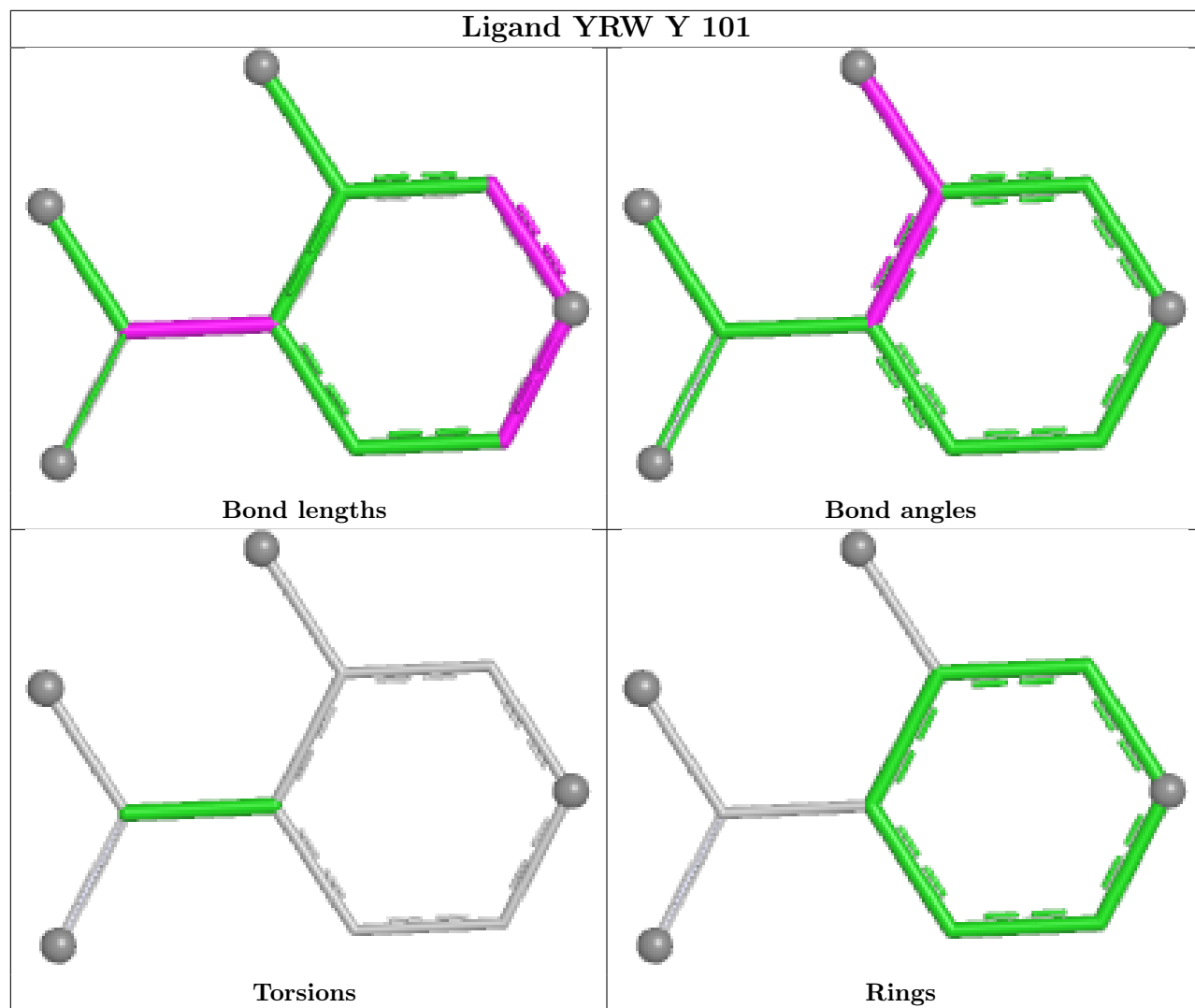
Mol	Chain	Res	Type	Atoms
38	Z	102	FME	C-CA-CB-CG
38	Z	102	FME	CB-CG-SD-CE
38	Z	102	FME	CA-CB-CG-SD

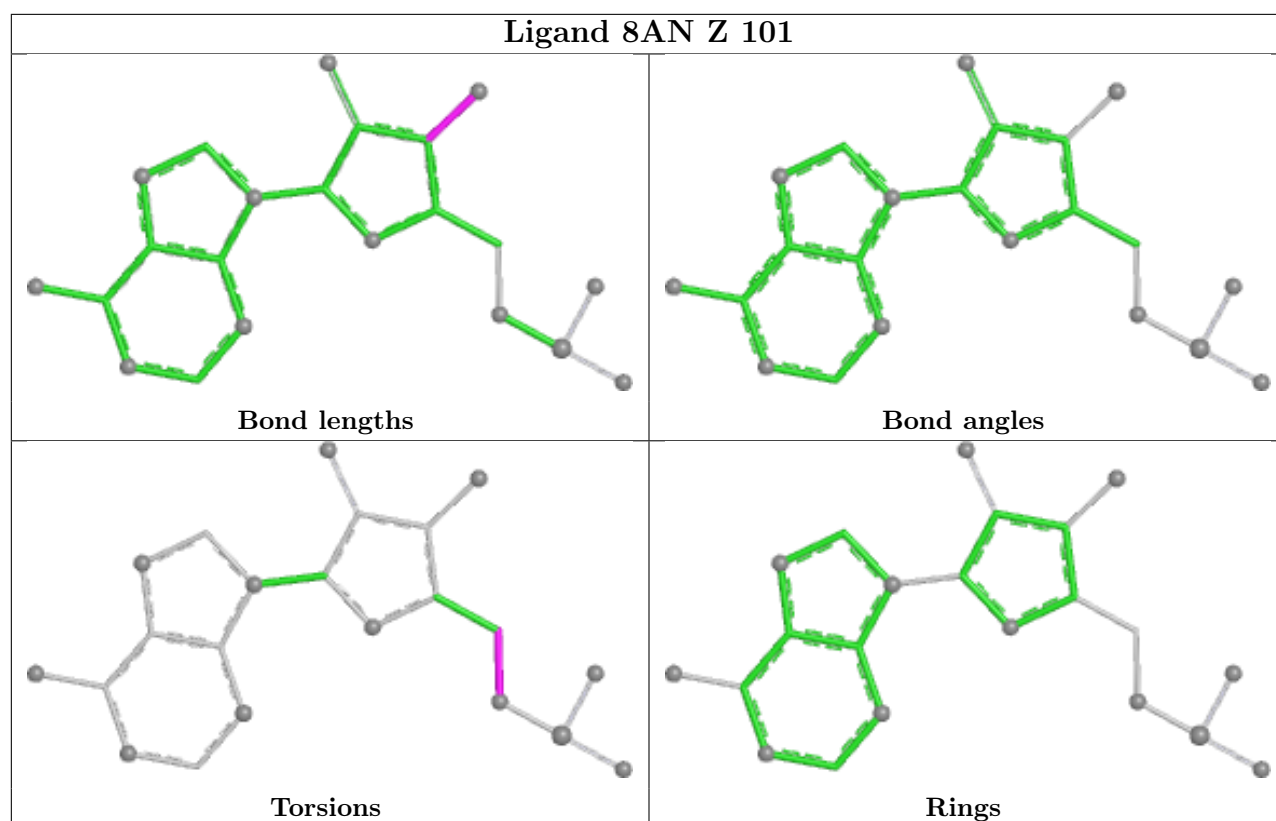
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	Y	101	YRW	1	0
38	Z	102	FME	1	0
37	Z	101	8AN	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.

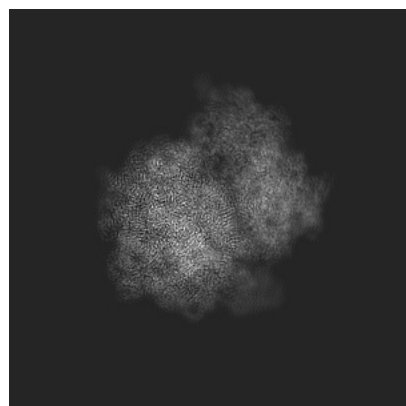
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29788. These allow visual inspection of the internal detail of the map and identification of artifacts.

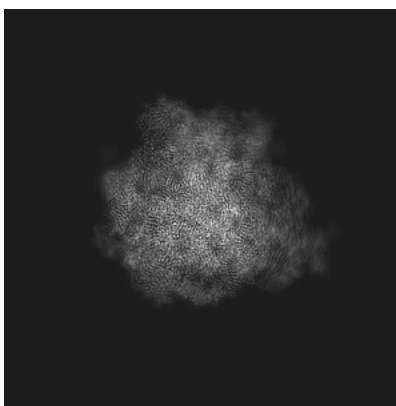
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

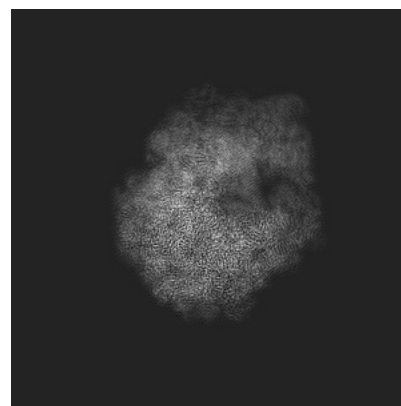
6.1.1 Primary map



X

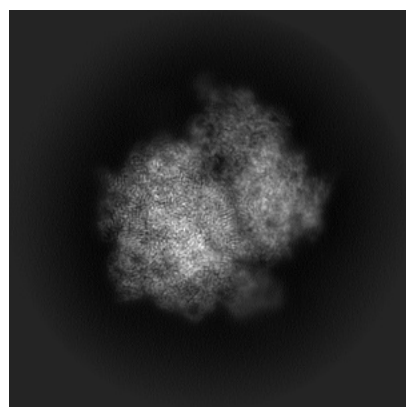


Y

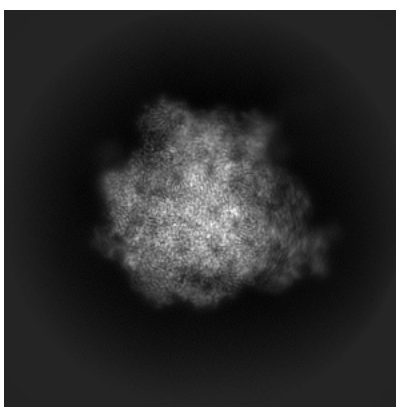


Z

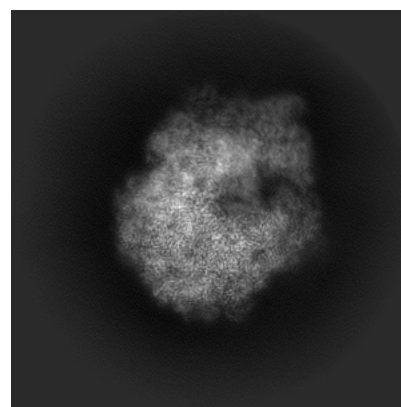
6.1.2 Raw map



X



Y

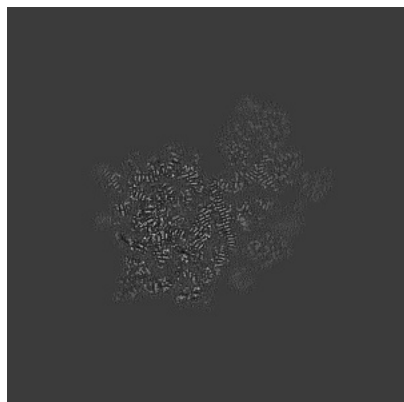


Z

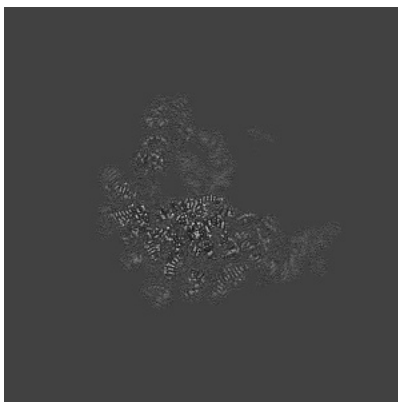
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

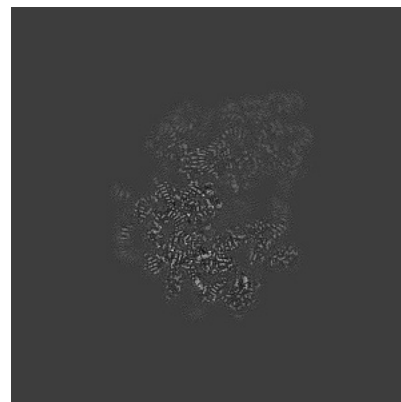
6.2.1 Primary map



X Index: 248

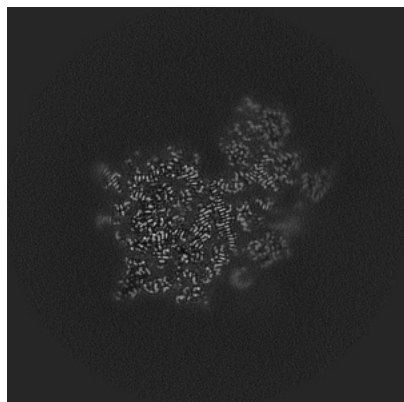


Y Index: 248

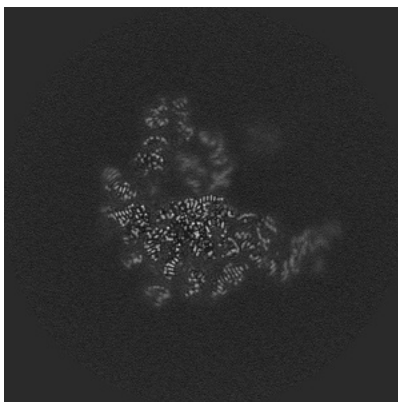


Z Index: 248

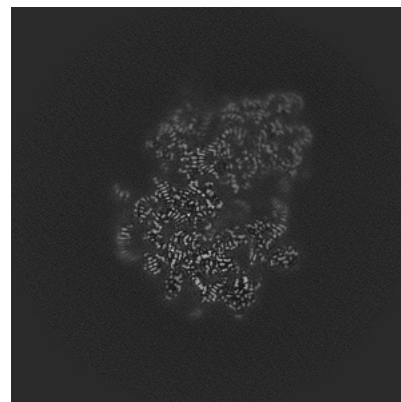
6.2.2 Raw map



X Index: 248



Y Index: 248



Z Index: 248

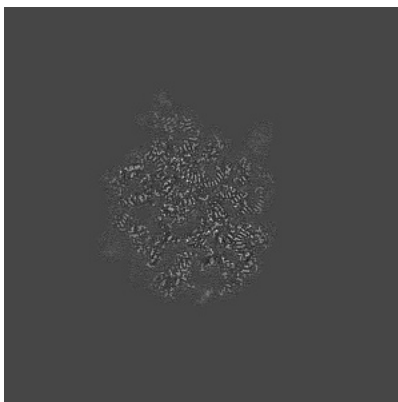
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 218

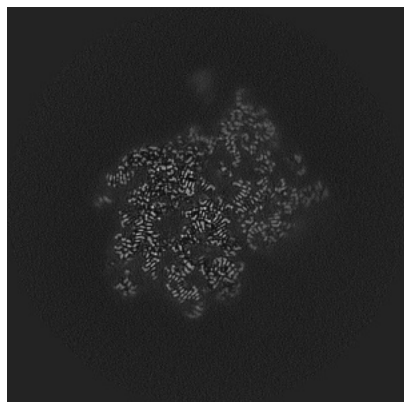


Y Index: 205

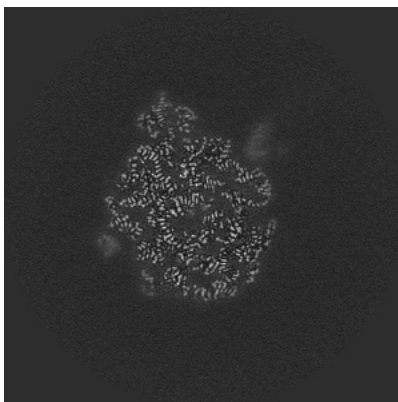


Z Index: 205

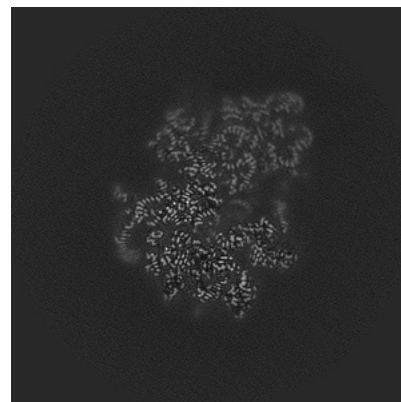
6.3.2 Raw map



X Index: 223



Y Index: 213

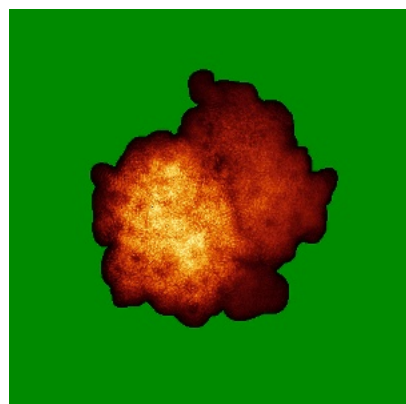


Z Index: 245

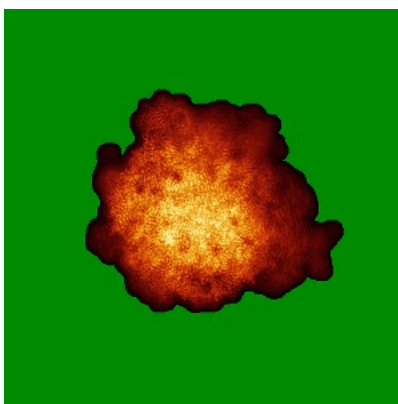
The images above show the largest variance slices of the map in three orthogonal directions.

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

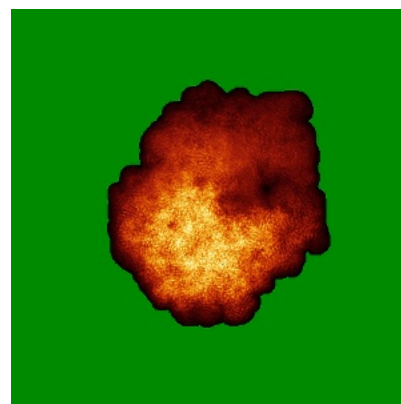
6.4.1 Primary map



X

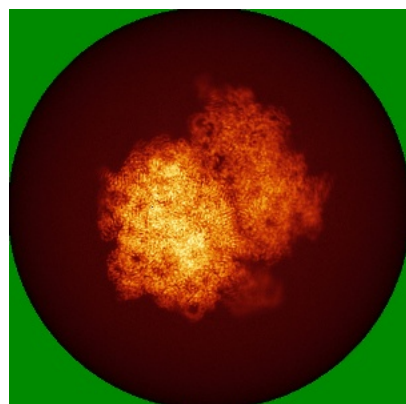


Y

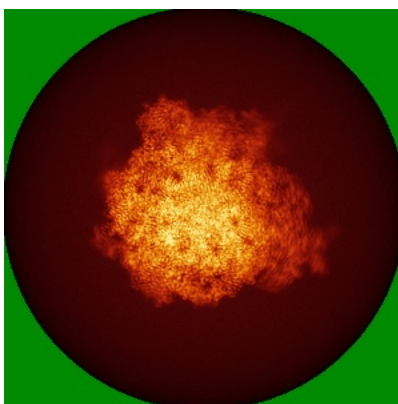


Z

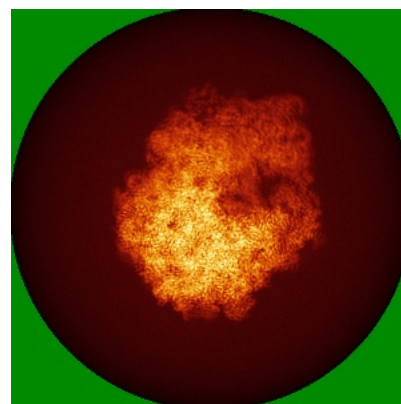
6.4.2 Raw map



X



Y

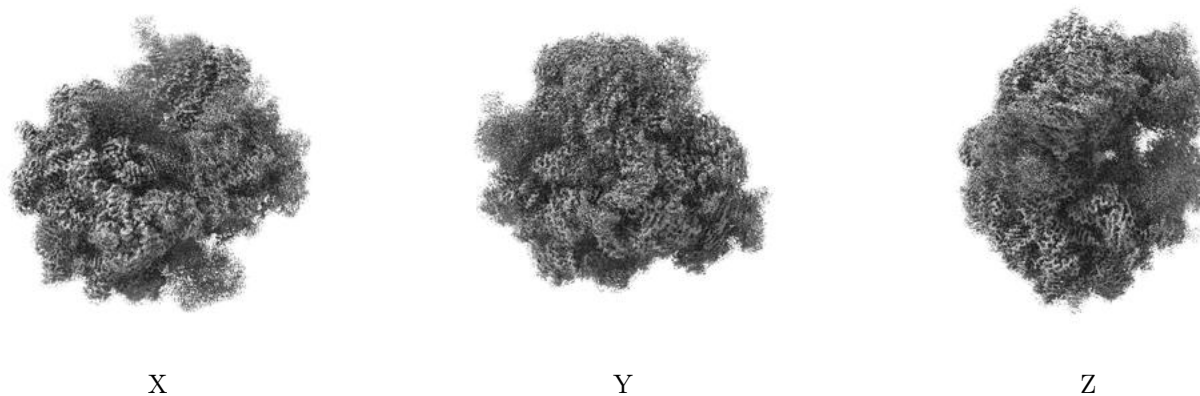


Z

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

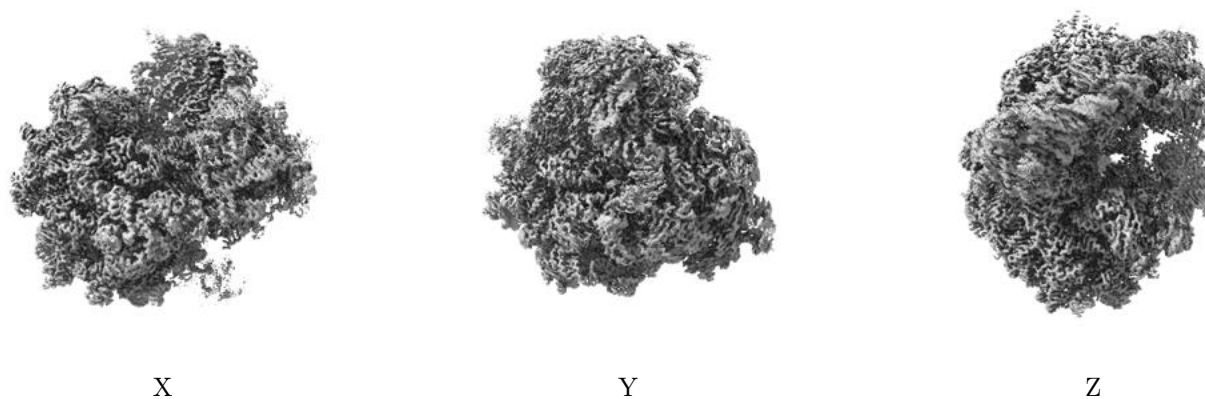
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0265. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

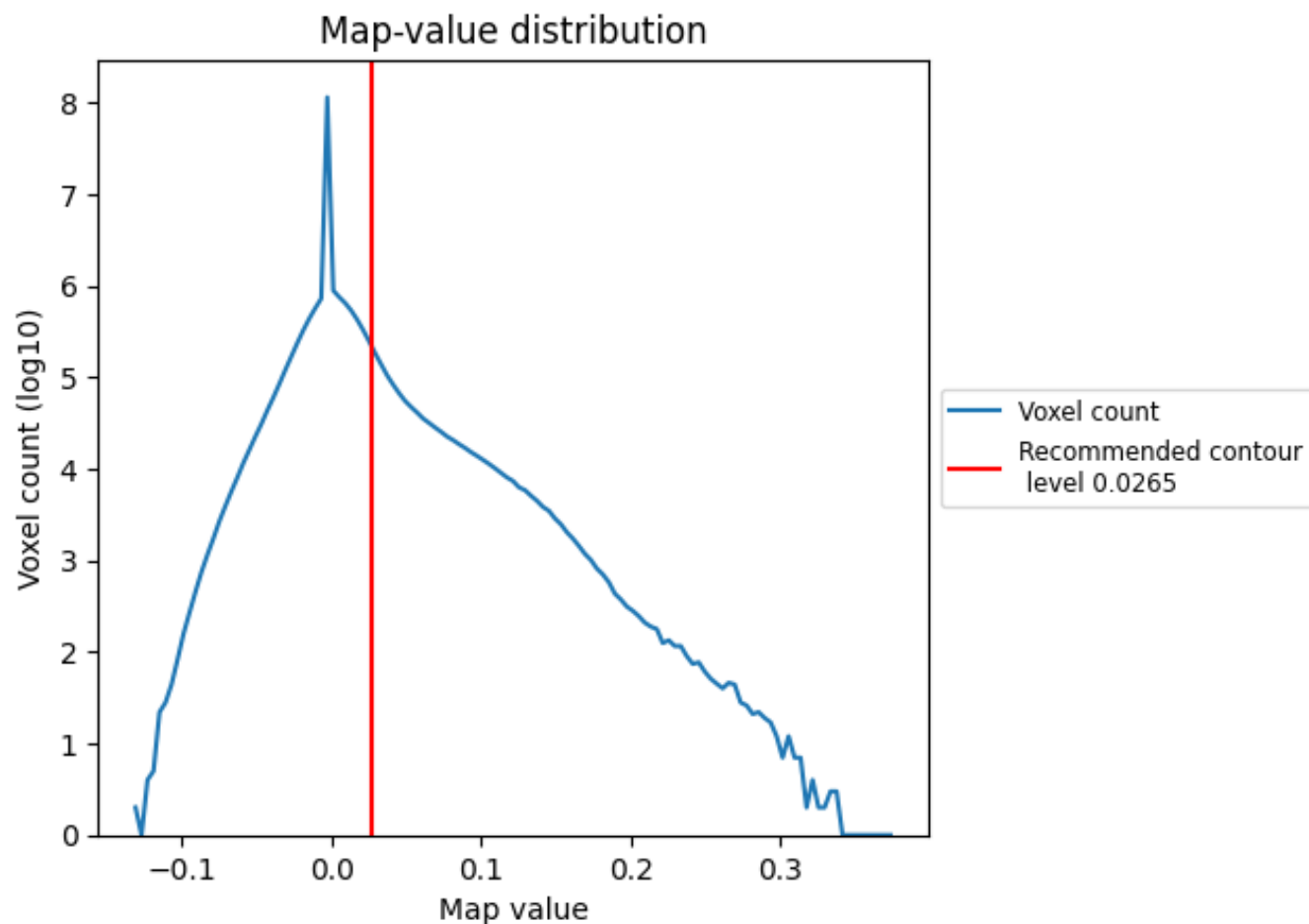
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

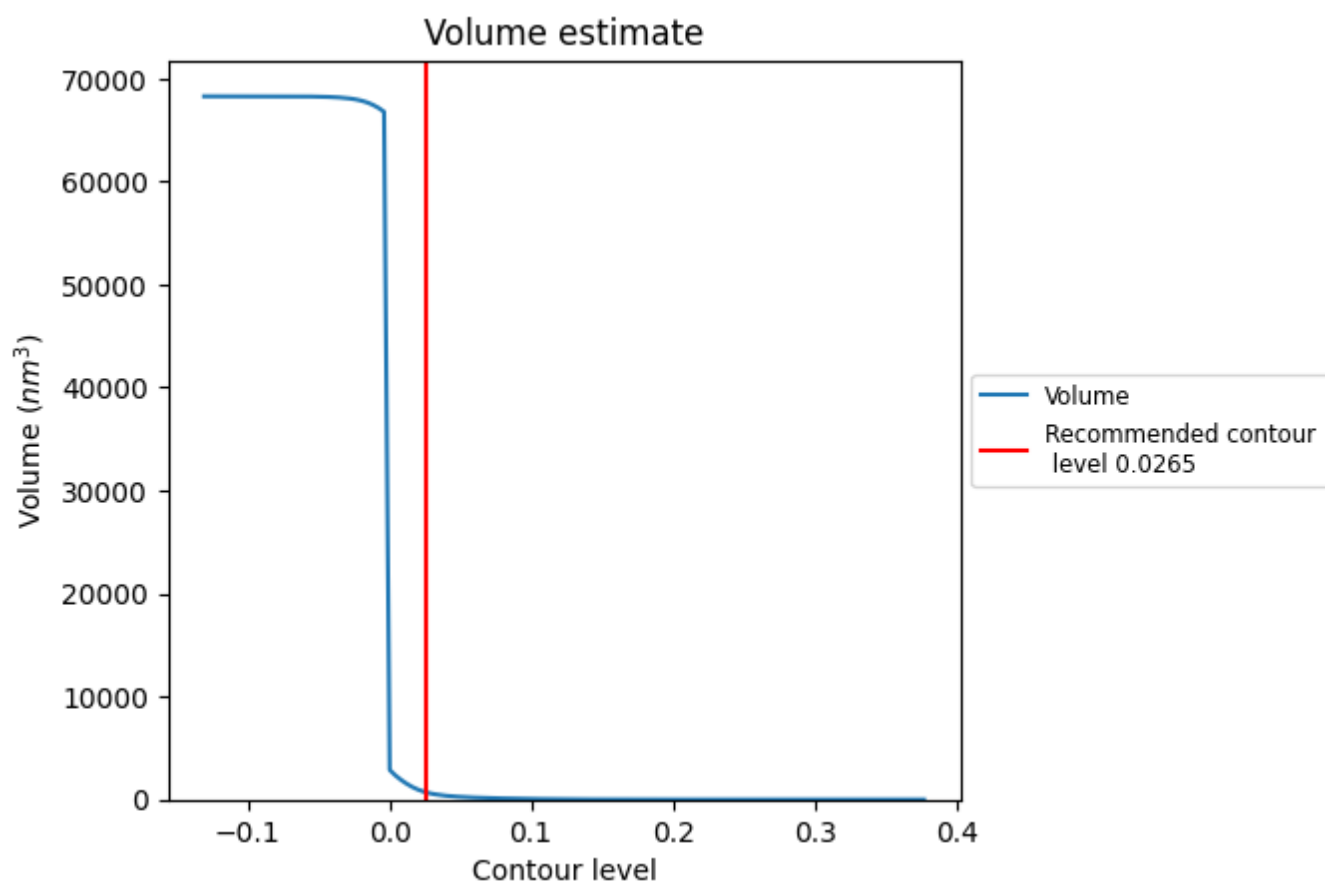
This section contains the results of statistical analysis of the map.

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.

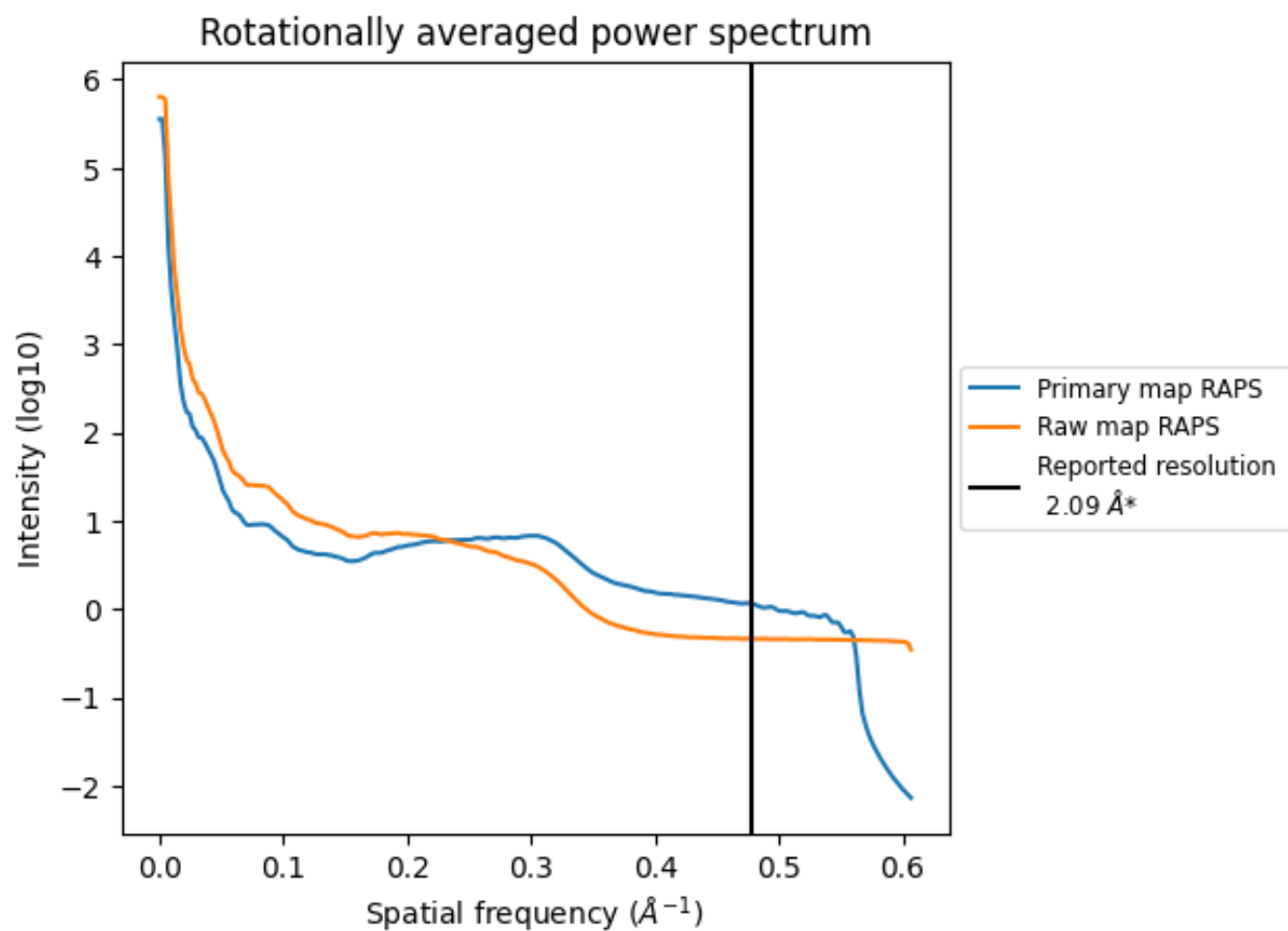
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 687 nm³; this corresponds to an approximate mass of 620 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 ⓘ

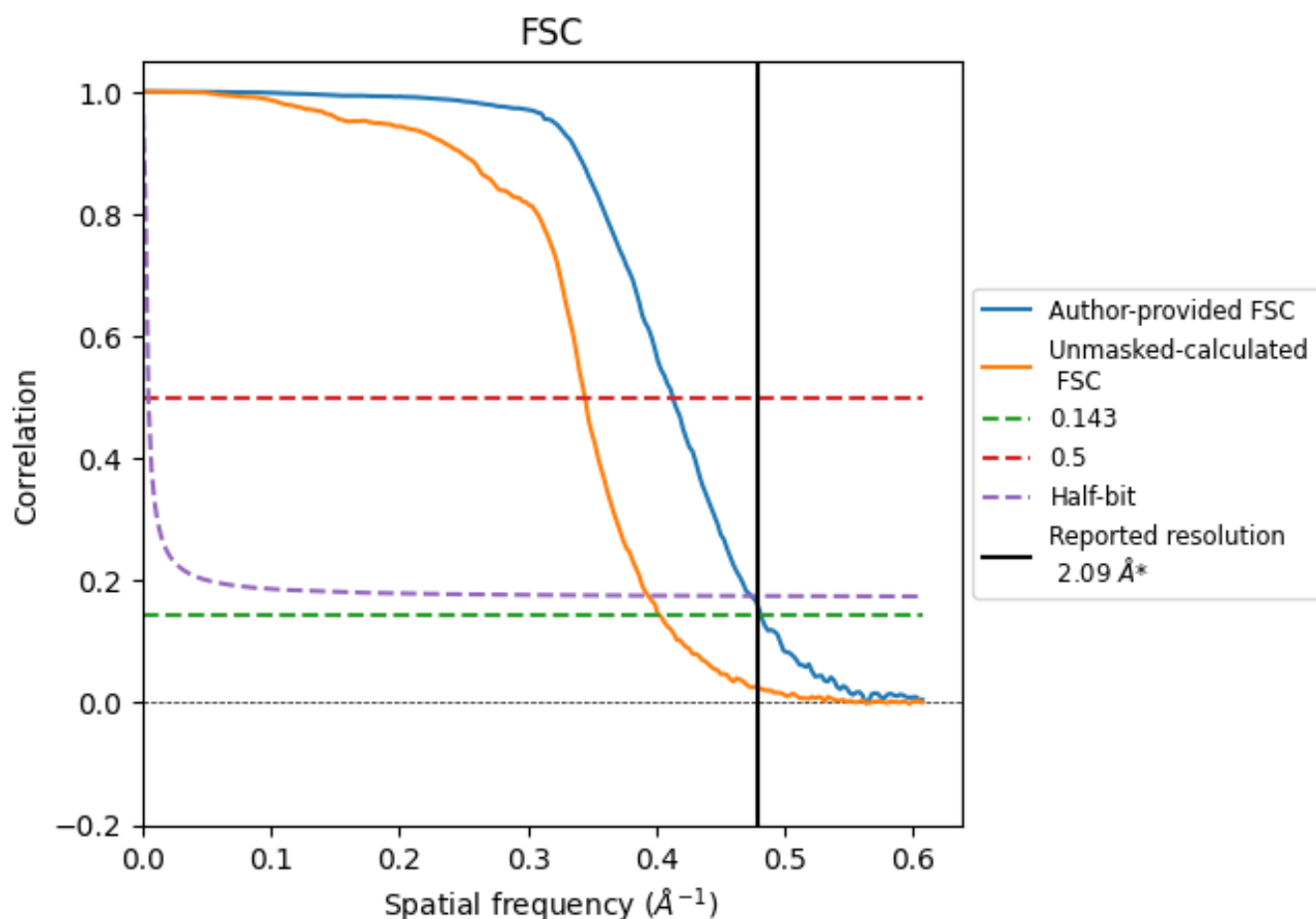


*Reported resolution corresponds to spatial frequency of 0.478 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.478 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

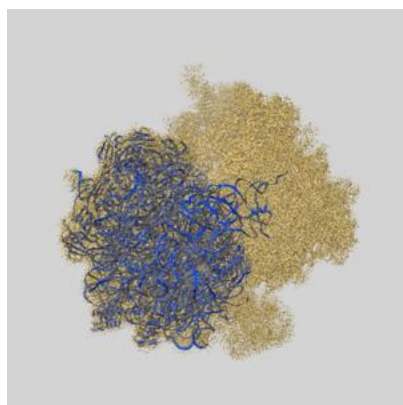
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.08	2.42	2.11
Unmasked-calculated*	2.49	2.90	2.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.49 differs from the reported value 2.09 by more than 10 %

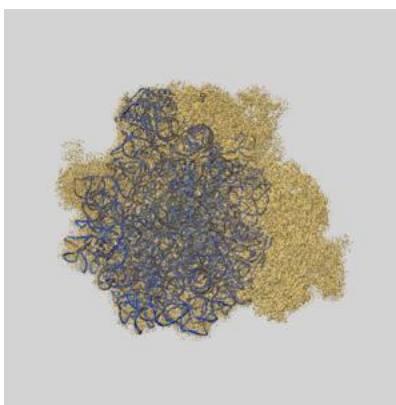
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29788 and PDB model 8G6Y. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

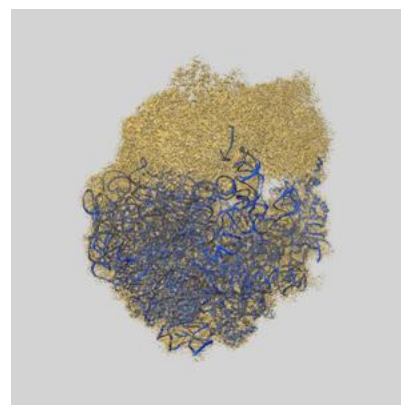
9.1 Map-model overlay [i](#)



X



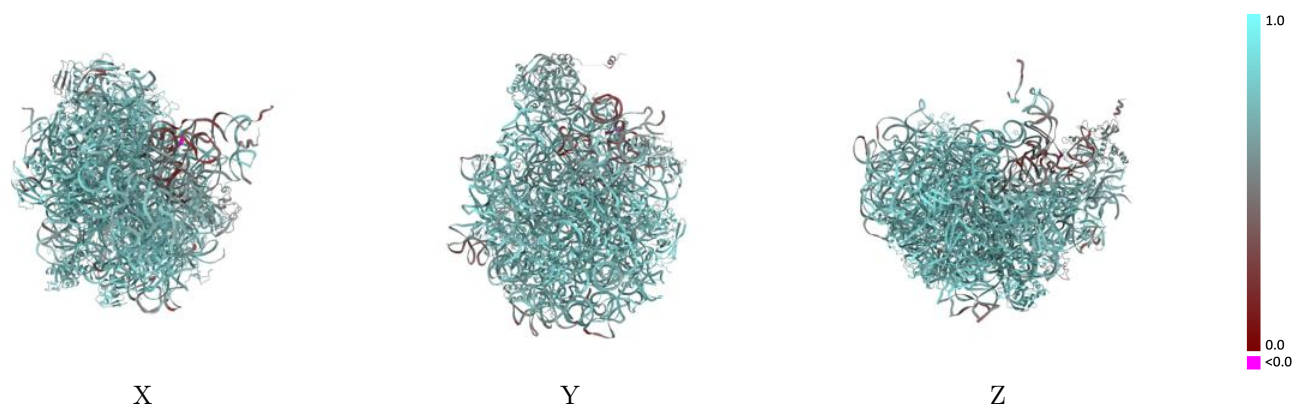
Y



Z

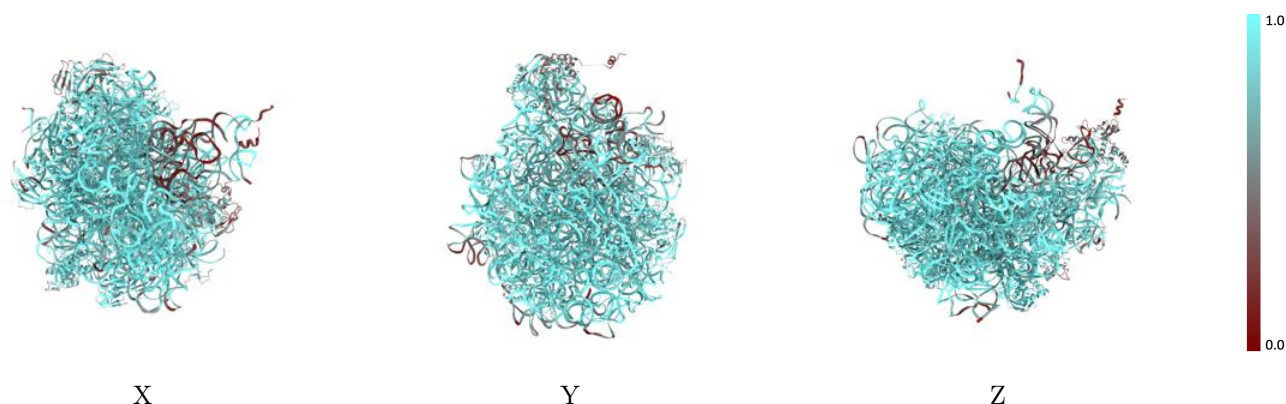
The images above show the 3D surface view of the map at the recommended contour level 0.0265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



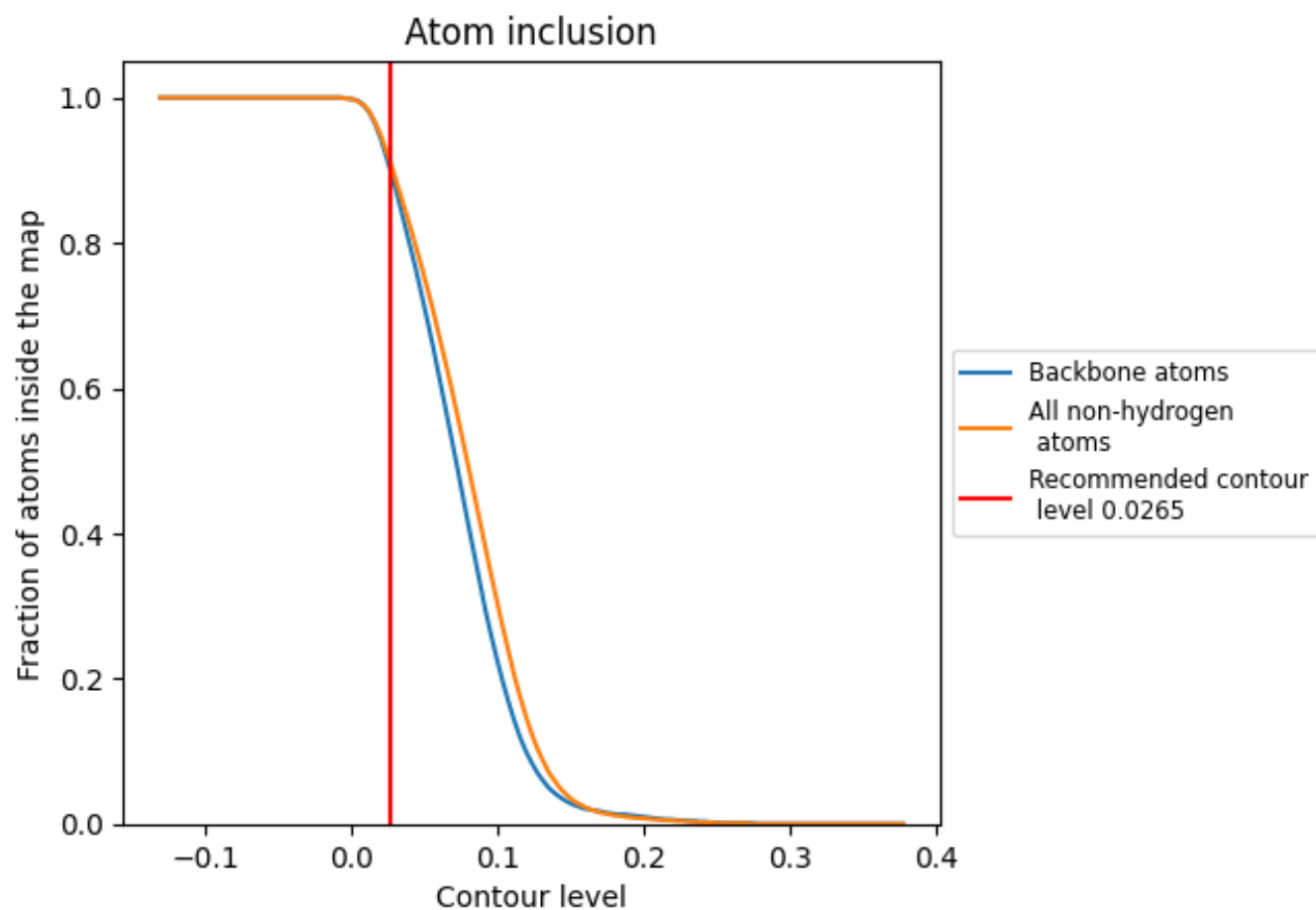
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0265).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.0265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.7240
0	 0.8920	 0.7380
1	 0.9690	 0.8000
2	 0.9860	 0.7970
3	 0.9490	 0.7580
4	 0.3880	 0.5030
X	 0.5650	 0.5140
Y	 0.4730	 0.4260
Z	 0.5100	 0.4750
a	 0.9460	 0.7360
b	 0.9060	 0.6800
c	 0.9720	 0.7820
d	 0.9500	 0.7820
e	 0.9000	 0.7420
f	 0.5990	 0.5890
g	 0.6930	 0.6070
h	 0.7270	 0.6540
i	 0.9620	 0.7840
j	 0.9490	 0.7730
k	 0.9430	 0.7620
l	 0.9470	 0.7680
m	 0.9900	 0.7930
n	 0.8970	 0.7120
o	 0.9260	 0.7630
p	 0.9760	 0.7950
q	 0.9250	 0.7510
r	 0.9350	 0.7730
s	 0.8880	 0.7270
t	 0.8610	 0.7000
u	 0.8750	 0.7190
v	 0.9400	 0.7790
w	 0.9470	 0.7560
x	 0.8180	 0.6840
y	 0.9150	 0.7540
z	 0.9230	 0.7660

