



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:53 AM UTC

PDB ID : 6WQN / pdb_00006wqn
EMDB ID : EMD-21872
Title : Structure of the 50S subunit of the ribosome from Methicillin Resistant Staphylococcus aureus in complex with the antibiotic, contezolid
Authors : Belousoff, M.J.
Deposited on : 2020-04-29
Resolution : 2.90 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

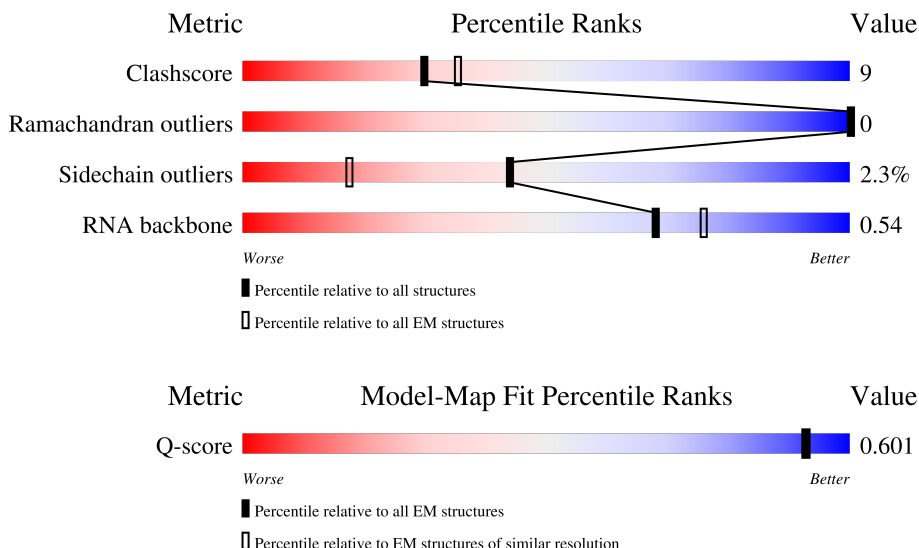
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



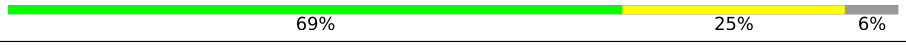
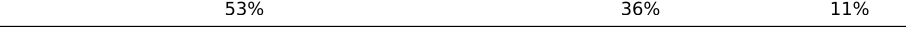
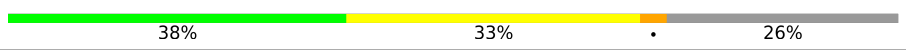
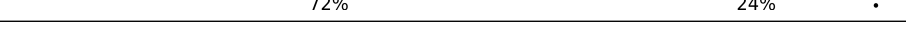
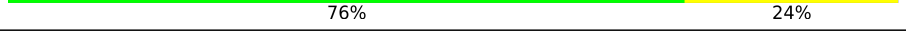
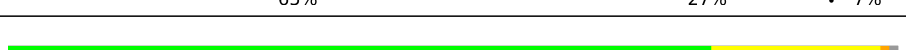
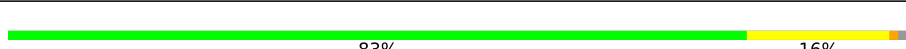
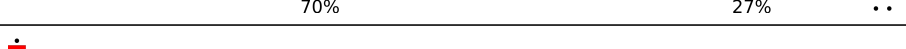
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	A	116	
2	B	277	
3	C	118	

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Mol	Chain	Length	Quality of chain
4	D	105	
5	E	117	
6	F	91	
7	G	105	
8	H	107	
9	J	62	
10	K	72	
11	L	217	
12	M	58	
13	N	57	
14	O	49	
15	P	50	
16	Q	65	
17	R	37	
18	S	207	
19	V	145	
20	W	122	
21	X	146	
22	Y	144	
23	Z	122	
24	a	119	
25	1	2923	
26	2	115	
27	I	85	

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 80715 atoms, of which 15 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 L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	112	Total	C	N	O	0	0
			907	572	182	153		

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 3 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 4 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			785	499	139	146	1		

- Molecule 5 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	110	Total	C	N	O	S	0	0
			845	527	162	154	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	GLY	variant	UNP A0A077UKF9

- Molecule 6 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	81	Total	C	N	O	S	0	0
			654	410	116	125	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	87	ASP	ILE	variant	UNP W8TUB4

- Molecule 7 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	91	Total	C	N	O	S	0	0
			702	444	129	128	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	54	SER	GLY	variant	UNP W8TRD5

- Molecule 8 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			727	465	129	132	1		

- Molecule 9 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	62	ALA	-	insertion	UNP A0A077URJ8

- Molecule 10 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	53	Total	C	N	O	0	0
			436	269	82	85		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	215	Total	C	N	O	S	0	0
			1621	1015	299	303	4		

- Molecule 12 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	56	Total	C	N	O	0	0
			432	269	82	81		

- Molecule 13 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	50	Total	C	N	O	S	0	0
			397	241	83	68	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	54	ALA	VAL	variant	UNP A0A077UWR7

- Molecule 14 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	47	Total	C	N	O	S	0	0
			390	233	79	73	5		

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	44	Total	C	N	O	S	0	0
			372	228	90	53	1		

- Molecule 16 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 17 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 18 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	192	Total	C	N	O	S	0	0
			1472	924	271	275	2		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	143	Total	C	N	O	S	0	0
			1138	710	209	217	2		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			911	566	173	168	4		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	144	Total	C	N	O	0	0
			1082	669	213	200		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	120	Total	C	N	O	S	0	0
			951	584	182	184	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	110	Total	C	N	O	0	0
			857	536	165	156		

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	2687	Total	C	N	O	P	0	0
			57631	25735	10578	18635	2683		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1866	A	G	conflict	GB 1760383645

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	111	Total	C	N	O	P	0	0
			2358	1056	422	770	110		

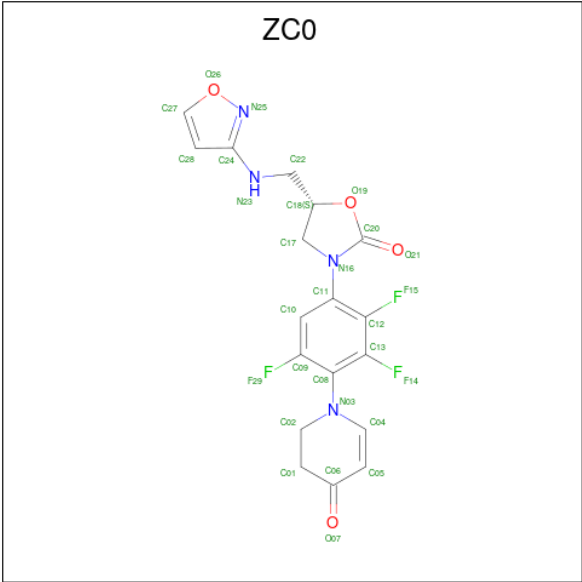
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	80	C	G	variant	GB 1750990749
2	109	C	G	variant	GB 1750990749
2	111	A	C	variant	GB 1750990749
2	112	G	A	variant	GB 1750990749

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	I	78	Total	C	N	O	0	0
			597	367	116	114		

- Molecule 28 is Contezolid (CCD ID: ZC0) (formula: C₁₈H₁₅F₃N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
28	1	1	44	18	3	15	4	4	0

3 Residue-property plots

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

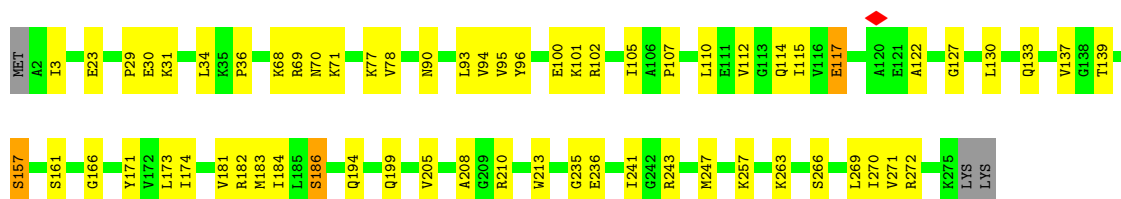
- Molecule 1: 50S ribosomal protein L19

Chain A: 



- Molecule 2: 50S ribosomal protein L2

Chain B: 



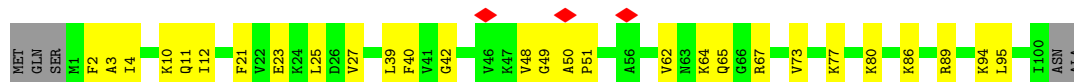
- Molecule 3: 50S ribosomal protein L20

Chain C: 



- Molecule 4: 50S ribosomal protein L21

Chain D: 



- Molecule 5: 50S ribosomal protein L22

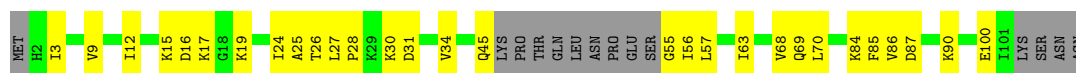
Chain E: 



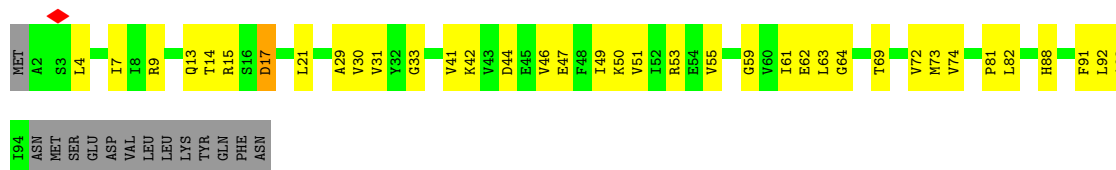
- Molecule 6: 50S ribosomal protein L23



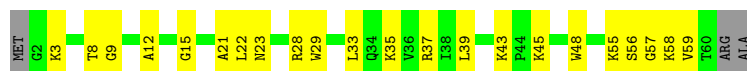
- Molecule 7: 50S ribosomal protein L24



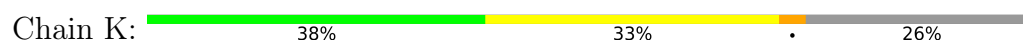
- Molecule 8: 50S ribosomal protein L25



- Molecule 9: 50S ribosomal protein L28

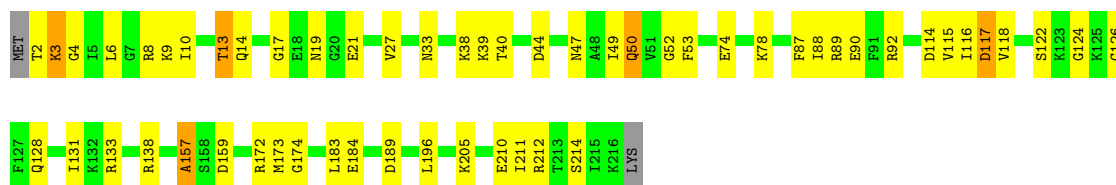


- Molecule 10: 50S ribosomal protein L29



- Molecule 11: 50S ribosomal protein L3





- Molecule 12: 50S ribosomal protein L30

Chain M: 72% 24% .



- Molecule 13: 50S ribosomal protein L32

Chain N: 77% 11% 12%



- Molecule 14: 50S ribosomal protein L33

Chain O: 55% 41% .



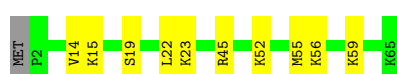
- Molecule 15: 50S ribosomal protein L34

Chain P: 68% 18% 12%



- Molecule 16: 50S ribosomal protein L35

Chain Q: 83% 15% .



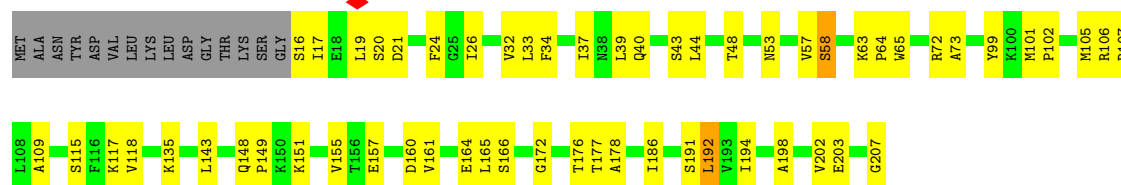
- Molecule 17: 50S ribosomal protein L36

Chain R: 76% 24%



- Molecule 18: 50S ribosomal protein L4

Chain S:  65% 27% 7%



- Molecule 19: 50S ribosomal protein L13

Chain V:  79% 19% 2%



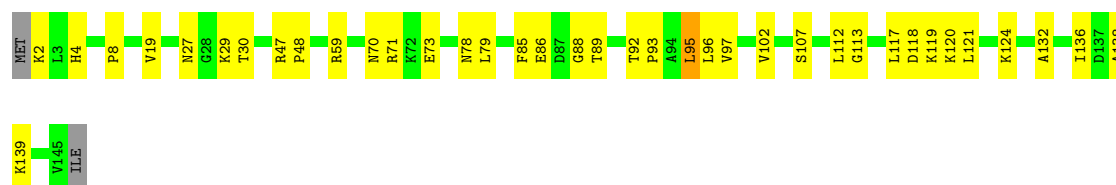
- Molecule 20: 50S ribosomal protein L14

Chain W:  83% 16% 1%



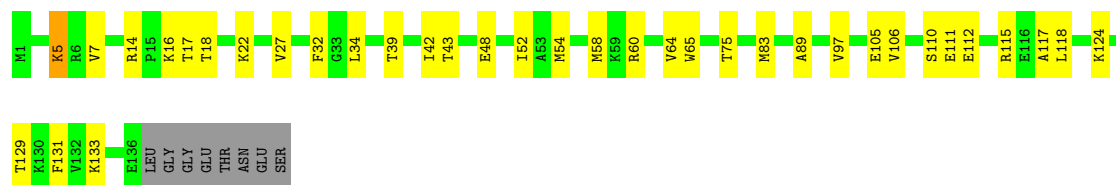
- Molecule 21: 50S ribosomal protein L15

Chain X:  73% 25% 2%



- Molecule 22: 50S ribosomal protein L16

Chain Y:  69% 24% 6%



- Molecule 23: 50S ribosomal protein L17

Chain Z:  70% 27% 3%



- Chain a: 
- 
- 68% 24% 8%
- MET
 ILE
 SER
 K4
 K9
 V10
 R11
 K28
 P29
 R30
 K38
 H39
 I45
 D46
 D47
 M48
 Q55
 Q59
 ASP
 SER
 ASP
 ILE
 ALA
 THR
 T66
 A67
 T68
 K69
 V70
 E71
 T74
 G77
 A85
 I89
 K90
 E91
 I92
 V93
 F94
 D95
 R96
 G97
 R104
 E110
 A111
 A112
 R113
- L117
 E118
 F119

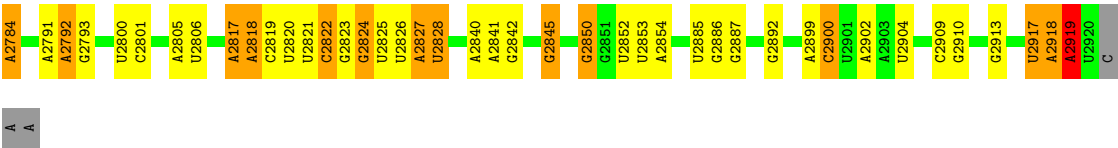
- Chain 1:

59% 25% 8% 8%

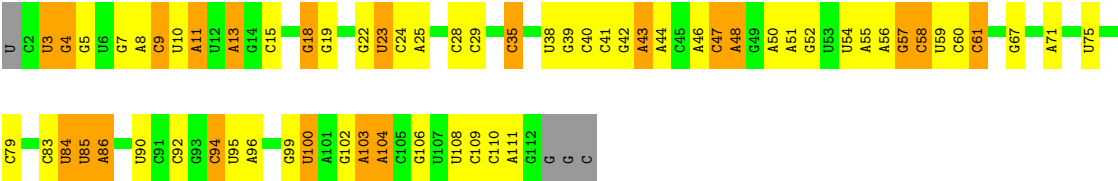
Chain 1: A sequence of 100 items, each represented by a colored square with a label. The items are arranged in a grid. The colors of the squares correspond to the distribution shown in the bar chart above. A red diamond marker is placed on the 100th item, labeled 'U298'.

Item Label	Color
A136	Grey
G137	Grey
U138	Grey
U139	Green
A140	Green
A150	Green
U151	Green
C152	Green
A156	Green
U157	Green
G158	Green
U159	Green
A161	Green
U162	Green
C163	Green
A164	Green
C165	Green
A166	Green
U167	Green
A168	Green
G169	Green
C170	Green
A171	Green
U174	Green
A175	Green
C176	Green
A177	Green
U178	Green
G179	Green
C180	Green
A184	Green
A185	Green
C186	Green
C187	Green
C188	Green
A194	Green
C195	Green
A199	Green
A200	Green
C201	Green
U202	Green
U205	Green
U206	Green
G208	Green
C213	Green
C214	Green
G215	Green
A216	Green
A219	Green
U299	Green
C300	Green
U301	Green
A302	Green
G303	Green
U309	Green
C310	Green
U311	Green
A	Green
U	Green
A	Green
C	Green
G	Green
A247	Green
C248	Green
U250	Green
U321	Green
C252	Green
C253	Green
C323	Green
A324	Green
A325	Green
A326	Green
C327	Green
G328	Green
A329	Green
C231	Green
C330	Green
C331	Green
A332	Green
C333	Green
A266	Green
G267	Green
A268	Green
C269	Green
A273	Green
A274	Green
A275	Green
C276	Green
C277	Green
C280	Green
A	Green
G	Green
C	Green
U	Green
U	Green
U	Green
G	Green
C	Green
U	Green
C	Green
A389	Green
A390	Green
A391	Green
C392	Green
C393	Green
U394	Green
U395	Green
C398	Green
U399	Green
A401	Green
U404	Green
G407	Green
U408	Green
C410	Green
A411	Green
C414	Green
U415	Green
G416	Green
A417	Green
C418	Green
U419	Green
A427	Green
G428	Green
G432	Green
U433	Green
G434	Green
A435	Green
A436	Green
A446	Green
G447	Green
G457	Green
A458	Green
C459	Green
A475	Green
A476	Green
U477	Green
C481	Green
U482	Green
C483	Green
U484	Green
A485	Green
G486	Green
G575	Green
U576	Green
A577	Green
G578	Green
U579	Green
A583	Green
U589	Green
U590	Green
A591	Green
A592	Green
U593	Green
G594	Green
U731	Green
C732	Green
U733	Green
A615	Green
G616	Green
A617	Green
A618	Green
A629	Green
G630	Green
U637	Green
U638	Green
U639	Green
A646	Green
U650	Green
A652	Green
A656	Green
G657	Green
A658	Green
A659	Green
A660	Green
U661	Green
G662	Green
A666	Green
G667	Green
C675	Green
A678	Green
G679	Green
C680	Green
G681	Green
A682	Green
G683	Green
C687	Green
U690	Green
A691	Green
G692	Green
G696	Green
C697	Green
U698	Green
A700	Green
G701	Green
U702	Green
A703	Green
A713	Green
G714	Green
A715	Green
A721	Green
U731	Green
C732	Green</

U2649	G2556	C2449	C2344	A2226	U	G2079	A1955	A1848	A1708	C1587	G1523	U	A1196	G1346	G1309	A
G2657	U2557	U2450	A2347	C2229	G	G2080	G1957	G1849	A1709	U1588	G1526	U	G1177	G1347	A1310	G
C2565	U2564	C2451	G2348	A2230	A	A2081	C2082	U1854	G1710	U1589	A	U	A1178	U1348	A1312	U
C2566	C2565	A2453	A2349	C2231	C	G2082	A1965	C1864	G1711	C1590	G	A	U1176	U1349	A1313	C
C2567	C2567	C2454	G2358	C2236	C	A2086	C1969	C1865	G1718	A1592	U	A1459	U1175	G1346	G1314	G1154
A2568	A2568	G2455	C2359	U2237	C	A2087	C2087	C1865	U1737	U1593	U	G1462	C1177	G1347	C1315	C1160
U2574	U2574	A2456	A2360	U2238	U	G2088	U1978	G1872	C1738	U1594	A	G1463	C1178	U1348	C1316	A1161
G2580	U2580	A2466	U2361	A2239	A	A2089	A1979	G1873	G1739	C1595	U	U1464	C1179	U1349	G1320	A1162
U2581	U2581	C2467	A2362	U2240	C	G2094	G1981	A1874	U1754	U1596	A	G1465	U1176	U1350	A1173	A1173
U2582	U2582	C2468	A2363	U2241	U	U2095	U1982	A1875	U1755	U1597	G	G1466	U1177	U1351	G1321	A1174
U2590	U2590	A2475	G2368	A2252	A	G2096	U1983	A1881	U1756	U1598	C	G1467	U1178	U1352	A1323	U1176
A2591	A2591	U2476	C2369	A2253	C	U2102	C1990	A1886	U1757	G1599	A	A1471	C1179	U1353	G1329	C1177
A2592	A2592	A2477	U2370	G2265	G	A2122	C1994	U1887	A1758	A1605	A	C1472	U1179	U1354	U1330	C1178
A2593	A2593	A2478	G2371	G2266	U	A2123	G1996	U1888	G1760	A1606	A	U	G1336	U1336	G1336	G1192
A2594	A2594	C2479	A2373	U2270	G	A2126	A1996	G1889	A1764	G1613	C	U	U1337	U1337	G1183	G1192
C2595	C2595	U2489	C2374	U2271	A	C2126	A1997	G1890	A1765	U1616	A1546	U	U1338	U1338	C1184	C1184
G2596	G2596	C2490	C2377	U2272	G	G	A1998	U1891	C1766	U1617	C	U	U1339	U1339	U1195	U1195
U2597	U2597	A2496	C2378	A2294	C	G	G1999	U1892	A1771	A1626	A1547	U	U1340	U1340	U1196	U1196
A2598	A2598	U2500	C2391	A2295	C	C	G2007	C	G1780	U1629	U	U	U1341	U1341	A1199	A1199
U2599	U2599	U2501	G2397	A2296	U	C	A2008	U	G1781	A1630	U	U	U1342	U1342	A1200	A1200
C2600	C2600	C2502	G2398	C2308	G	C	U2009	C	G1782	U1631	U	U	U1343	U1343	C1351	C1351
G2601	G2601	A2503	G2399	G2309	G	A	U2010	U	G1783	A1632	U	U	U1344	U1344	C1352	C1352
C2602	C2602	C2504	U2400	U2311	U	U	G2011	C	G1784	A1633	U	U	U1345	U1345	G1354	G1354
A2604	A2604	A2505	C2401	C2312	G	U	G2012	G1900	G1790	A1634	G	U	U1346	U1346	U1212	U1212
U2606	U2606	C2506	C2402	A2313	G	U	U2013	C1901	G1791	A1635	U	U	U1347	U1347	G1357	G1357
C2607	C2607	G2507	C2403	A2314	G	G	U2014	A1904	A1800	U1636	C1557	U	U1348	U1348	C1213	C1213
U2608	U2608	U2508	G2404	U2315	A	U	G2015	A1905	A1801	C1558	U1557	U	U1349	U1349	C1214	C1214
G2609	G2609	C2509	U2410	U2316	U	C	U2016	C1906	U1806	A1562	U1558	U	U1350	U1350	U1215	U1215
U2611	U2611	G2511	A2411	U2317	C	A	C2023	C	U1807	A1563	A1560	U	U1351	U1351	U1216	U1216
A2515	A2515	A2512	G2412	C2320	U	G	G2024	G1910	A1810	A1564	G1561	U	U1352	U1352	U1217	U1217
G2529	G2529	C2513	U2413	C2321	A	G	G2025	A1911	A1811	U1565	G1562	U	U1353	U1353	G1218	G1218
A2530	A2530	U2514	C2414	C2322	C	U	U2026	A1912	A1812	C1566	U1563	U	U1354	U1354	A1220	A1220
U2531	U2531	C2515	U2415	U2323	C	U	G2027	U1913	A1813	U1567	U1564	U	U1355	U1355	C1221	C1221
G2532	G2532	U2516	C2416	C2324	C	A	A2040	G1914	G1817	G1568	U1565	U	U1356	U1356	U1224	U1224
U2533	U2533	C2517	U2417	U2325	U	G	G2041	G1915	U1818	A1569	G1566	U	U1357	U1357	U1225	U1225
G2534	G2534	U2518	C2418	C2326	U	G	U2042	G1916	U1819	C1567	U1567	U	U1358	U1358	G1226	G1226
A2535	A2535	C2519	U2419	A2327	A	U	G2043	C1922	C1821	A1570	G1568	U	U1359	U1359	U1227	U1227
U2536	U2536	U2520	C2420	C2328	C	A	U2044	G1923	C1822	C1571	U1570	U	U1360	U1360	U1238	U1238
C2537	C2537	C2521	U2421	U2329	U	G	U2045	G1924	U1823	G1574	G1571	U	U1361	U1361	C1239	C1239
U2538	U2538	U2522	C2422	C2330	G	G	G2046	C1925	C1823	A1575	U1571	U	U1362	U1362	A1421	A1421
C2539	C2539	A2523	U2423	U2331	U	A	U2047	G1926	C1824	C1576	U1572	U	U1363	U1363	A1240	A1240
U2540	U2540	C2524	C2424	U2332	C	G	G2048	A1927	C1825	G1577	U1573	U	U1364	U1364	A1242	A1242
A2541	A2541	U2525	U2425	U2333	U	C	U2049	C1928	U1826	A1578	G1574	U	U1365	U1365	U1287	U1287
C2542	C2542	C2526	C2426	C2334	C	U	G2050	C1929	C1827	C1579	U1574	U	U1366	U1366	G1288	G1288
U2543	U2543	U2527	U2427	U2335	U	C	U2051	C1930	U1828	A1580	G1575	U	U1367	U1367	A1289	A1289
A2544	A2544	C2528	C2428	U2336	U	U	G2052	C1931	C1829	C1581	U1576	U	U1368	U1368	A1291	A1291
U2545	U2545	U2529	U2429	C2337	C	G	U2053	C1932	C1830	G1582	U1577	U	U1369	U1369	A1292	A1292
C2546	C2546	C2530	C2430	U2338	U	A	G2054	C1933	U1831	A1583	U1578	U	U1370	U1370	U1293	U1293
U2547	U2547	U2531	U2431	U2339	U	G	U2055	G1934	C1832	C1584	U1579	U	U1371	U1371	G1294	G1294
A2548	A2548	C2532	C2432	U2340	C	U	G2056	C1935	C1833	A1585	G1580	U	U1372	U1372	U1451	U1451
U2549	U2549	U2533	U2433	U2341	U	C	U2057	C1936	U1834	C1581	U1581	U	U1373	U1373	C1452	C1452
G2553	G2553	C2534	C2434	U2342	A	A	G2058	C1937	U1835	A1582	U1582	U	U1374	U1374	G1453	G1453
C2554	C2554	U2535	U2435	U2343	C	G	U2059	C1938	C1836	C1583	U1583	U	U1375	U1375	U1454	U1454
U2555	U2555	U2536	U2436	U2344	U	U	G2060	C1939	U1837	A1584	G1584	U	U1376	U1376		
		C2537	C2437	U2345	U	C	U2061	C1940	C1838	A1585	G1585	U	U1377	U1377		
		U2538	U2438	U2346	U	U	G2062	C1941	U1839	A1586	G1586	U	U1378	U1378		
		C2539	C2439	U2347	U	C	U2063	C1942	U1840	A1587	G1587	U	U1379	U1379		
		U2540	U2440	U2348	U	U	G2064	C1943	U1841	A1588	G1588	U	U1380	U1380		
		C2541	C2441	U2349	U	U	U2065	C1944	U1842	A1589	G1589	U	U1381	U1381		
		U2542	U2442	U2350	U	U	G2066	C1945	U1843	A1590	G1590	U	U1382	U1382		
		C2543	C2443	U2351	U	U	U2067	C1946	U1844	A1591	G1591	U	U1383	U1383		
		U2544	U2444	U2352	U	U	G2068	C1947	U1845	A1592	G1592	U	U1384	U1384		
		C2545	C2445	U2353	U	U	U2069	C1948	U1846	A1593	G1593	U	U1385	U1385		
		U2546	U2446	U2354	U	U	G2070	C1949	U1847	A1594	G1594	U	U1386	U1386		
		C2547	C2447	U2355	U	U	U2071	C1950				U	U1387	U1387		
		U2548	U2448	U2356	U	U	G2072	C1951				U	U1388	U1388		
		C2549	C2449	U2357	U	U	U2073	C1952				U	U1389	U1389		
		U2550	U2450	U2358	U	U	G2074	C1953				U	U1390	U1390		
		C2551	C2451	U2359	U	U	U2075	C1954				U	U1391	U1391		
		U2552	U2452	U2360	U	U	G2076	C1955				U	U1392	U1392		
		C2553	C2453	U2361	U	U	U2077	C1956				U	U1393	U1393		
		U2554	U2454	U2362	U	U	G2078	C1957				U	U1394	U1394		
		C2555	C2455	U2363	U	U						U	U1395	U1395		
		U2556	U2456	U2364	U	U						U	U1396	U1396		
		C2557	C2457	U2365	U	U						U	U1397	U1397		
		U2558	U2458	U2366	U	U						U	U1398	U1398		
		C2559	C2459	U2367	U	U						U	U1399	U1399		
		U2560	U2460	U2368	U	U						U	U1400	U1400		
		C2561	C2461	U2369	U	U						U	U1401	U1401		
		U2562	U2462	U2370	U	U						U	U1402	U1402		
		C2563	C2463	U2371	U	U						U	U1403	U1403		
		U2564	U2464	U2372	U	U						U	U1404	U1404		
		C2565	C2465	U2373	U	U						U	U1405	U1405		
		U2566	U2466	U2374	U	U						U	U1406	U1406		
		C2567	C2467	U2375	U	U						U	U1407	U1407		
		U2568	U2468	U2376	U	U						U	U1408	U1408		
		C2569	C2469	U2377	U	U						U	U1409	U1409		
		U2570	U2470	U2378	U	U						U	U1410	U1410		
		C2571	C2471	U2379	U	U						U				



• Molecule 26: 5S rRNA



• Molecule 27: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.435	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	372.32, 372.32, 372.32	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89500004, 0.89500004, 0.89500004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZC0

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	A	0.74	0/919	0.85	0/1228
2	B	0.24	0/2129	0.37	0/2858
3	C	0.08	0/955	0.26	0/1265
4	D	0.30	0/795	0.44	0/1062
5	E	0.30	0/853	0.42	0/1149
6	F	0.32	0/659	0.45	0/879
7	G	0.75	0/708	0.86	1/943 (0.1%)
8	H	0.62	0/735	0.75	0/986
9	J	0.36	0/469	0.51	0/625
10	K	0.09	0/437	0.31	0/583
11	L	0.43	0/1645	0.66	3/2208 (0.1%)
12	M	0.07	0/434	0.24	0/585
13	N	0.66	2/404 (0.5%)	0.68	1/537 (0.2%)
14	O	0.09	0/393	0.27	0/523
15	P	0.49	0/376	0.72	0/491
16	Q	0.35	0/526	0.53	0/690
17	R	0.75	0/299	0.96	0/393
18	S	0.22	0/1494	0.37	0/2018
19	V	0.30	0/1160	0.39	0/1563
20	W	0.51	0/918	0.69	0/1232
21	X	0.38	2/1096 (0.2%)	0.48	0/1461
22	Y	0.22	0/1113	0.36	0/1493
23	Z	0.08	0/955	0.28	0/1277
24	a	0.55	0/865	0.68	0/1154
25	1	0.09	0/64545	0.30	36/100652 (0.0%)
26	2	0.04	0/2636	0.09	0/4105
27	I	0.08	0/603	0.27	0/801
All	All	0.21	4/88121 (0.0%)	0.36	41/132761 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	5	LYS	C-N	8.48	1.45	1.33
21	X	71	ARG	C-N	6.63	1.42	1.33
13	N	6	ARG	C-N	6.58	1.42	1.33
21	X	70	ASN	C-N	5.86	1.42	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	254	A	C4'-C3'-O3'	10.59	128.88	113.00
11	L	159	ASP	N-CA-C	-10.55	99.78	111.07
25	1	2078	A	C4'-C3'-O3'	-8.37	96.84	109.40
25	1	1405	G	C4'-C3'-O3'	7.67	124.51	113.00
25	1	2850	G	C4'-C3'-O3'	7.66	124.48	113.00
25	1	2506	U	C1'-C2'-O2'	-7.39	97.32	108.40
25	1	2567	C	C1'-C2'-O2'	-7.25	97.53	108.40
25	1	2421	C	C4'-C3'-O3'	6.90	123.35	113.00
25	1	2506	U	C4'-C3'-O3'	6.81	123.21	113.00
25	1	2323	U	C2'-C3'-O3'	-6.81	99.29	109.50
25	1	1466	G	C4'-C3'-O3'	6.66	122.99	113.00
25	1	915	U	C4'-C3'-O3'	6.62	122.93	113.00
25	1	2539	C	C4'-C3'-O3'	6.56	122.84	113.00
25	1	2597	G	C4'-C3'-O3'	6.52	122.78	113.00
25	1	2567	C	C4'-C3'-O3'	6.49	122.74	113.00
13	N	5	LYS	O-C-N	6.41	129.01	122.09
25	1	1516	C	C4'-C3'-O3'	6.40	122.60	113.00
25	1	834	A	C2'-C3'-O3'	-6.39	99.91	109.50
25	1	2079	G	C4'-C3'-O3'	6.30	122.45	113.00
25	1	2554	C	C4'-C3'-O3'	6.28	122.42	113.00
25	1	2538	U	C4'-C3'-O3'	6.21	122.31	113.00
25	1	1362	C	C2'-C3'-O3'	-6.06	100.41	109.50
25	1	1657	G	C4'-C3'-O3'	6.01	122.01	113.00
25	1	732	C	C4'-C3'-O3'	5.91	121.86	113.00
25	1	254	A	C2'-C3'-O3'	-5.83	104.95	113.70
25	1	65	A	C4'-C3'-O3'	5.83	121.74	113.00
25	1	2542	C	C4'-C3'-O3'	5.76	121.63	113.00
11	L	157	ALA	N-CA-C	5.74	119.31	111.39
7	G	24	ILE	N-CA-C	-5.66	107.77	113.20
25	1	254	A	N9-C1'-C2'	-5.64	103.54	112.00
25	1	2566	C	C1'-C2'-O2'	-5.61	99.98	108.40
11	L	157	ALA	CA-C-O	-5.59	115.36	121.84
25	1	2919	A	C1'-C2'-O2'	-5.49	100.17	108.40
25	1	45	G	C4'-C3'-O3'	5.41	121.11	113.00
25	1	2557	U	C4'-C3'-O3'	5.32	120.97	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	2419	A	C4'-C3'-O3'	5.19	120.79	113.00
25	1	915	U	C1'-C2'-O2'	-5.13	100.71	108.40
25	1	2542	C	C1'-C2'-O2'	-5.12	100.72	108.40
25	1	914	G	C4'-C3'-O3'	5.05	120.58	113.00
25	1	484	U	C4'-C3'-O3'	5.03	120.55	113.00
25	1	916	U	C4'-C3'-O3'	5.02	120.53	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	907	0	981	24	0
2	B	2094	0	2205	47	0
3	C	943	0	1014	25	0
4	D	785	0	825	23	0
5	E	845	0	900	23	0
6	F	654	0	686	25	0
7	G	702	0	759	15	0
8	H	727	0	777	31	0
9	J	463	0	501	18	0
10	K	436	0	459	27	0
11	L	1621	0	1655	43	0
12	M	432	0	472	7	0
13	N	397	0	407	4	0
14	O	390	0	396	14	0
15	P	372	0	420	15	0
16	Q	521	0	586	7	0
17	R	296	0	340	8	0
18	S	1472	0	1520	46	0
19	V	1138	0	1130	24	0
20	W	911	0	970	25	0
21	X	1082	0	1119	33	0
22	Y	1089	0	1155	28	0
23	Z	951	0	999	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	857	0	903	32	0
25	1	57631	0	28986	612	0
26	2	2358	0	1198	54	0
27	I	597	0	607	8	0
28	1	29	15	0	0	0
All	All	80700	15	51970	1162	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 9.

All (1162) 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)
25:1:1914:C:H2'	25:1:1915:G:H5''	1.48	0.94
25:1:1083:G:H2'	25:1:1084:U:H5''	1.53	0.91
25:1:1625:U:H2'	25:1:1626:A:H5''	1.53	0.90
20:W:112:MET:HE2	20:W:112:MET:HA	1.53	0.90
15:P:41:LYS:HD2	25:1:505:U:H5''	1.52	0.89
4:D:50:ALA:HB1	4:D:51:PRO:HA	1.54	0.88
25:1:1320:G:N2	25:1:1323:A:OP2	2.08	0.87
25:1:1449:A:H61	25:1:1632:A:H1'	1.39	0.86
25:1:757:G:H3'	25:1:758:G:H5''	1.56	0.86
25:1:1806:U:OP2	25:1:1811:A:N6	2.09	0.85
25:1:899:U:H2'	25:1:900:G:H5''	1.56	0.85
25:1:1491:C:O2	25:1:1574:G:N2	2.08	0.85
14:O:15:ARG:HA	14:O:15:ARG:HH11	1.40	0.84
24:a:68:THR:OG1	26:2:48:A:OP2	1.95	0.84
25:1:923:A:H2'	25:1:924:G:H5''	1.58	0.84
8:H:4:LEU:HD23	8:H:4:LEU:H	1.42	0.84
25:1:764:C:H2'	25:1:765:U:H5''	1.60	0.84
26:2:67:G:O6	26:2:102:G:N2	2.10	0.84
3:C:88:ILE:HG22	3:C:90:ILE:HG13	1.60	0.83
3:C:4:VAL:HG22	25:1:1238:U:H1'	1.60	0.83
26:2:46:A:O2'	26:2:47:C:O4'	1.96	0.83
21:X:85:PHE:HB3	21:X:89:THR:HG21	1.60	0.83
25:1:2397:G:H2'	25:1:2398:G:H5''	1.61	0.83
26:2:99:G:H3'	26:2:100:U:H5''	1.58	0.82
25:1:157:U:H3	25:1:171:A:H61	1.27	0.82
21:X:79:LEU:HD12	21:X:113:GLY:HA2	1.62	0.82
26:2:7:G:O6	26:2:106:G:N2	2.11	0.82
3:C:31:LEU:HB2	3:C:34:VAL:HG12	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:131:ILE:HD13	11:L:138:ARG:HG2	1.62	0.81
6:F:4:ARG:HG2	6:F:5:ASP:H	1.46	0.80
24:a:68:THR:HG21	26:2:47:C:H5''	1.64	0.80
25:1:169:G:H2'	25:1:170:C:H5'	1.64	0.80
25:1:1357:G:OP2	25:1:1357:G:N2	2.15	0.80
25:1:1865:C:OP1	25:1:1954:A:O2'	2.00	0.80
2:B:171:TYR:HB3	2:B:183:MET:HB3	1.64	0.80
12:M:6:ILE:HG12	12:M:56:VAL:HG12	1.62	0.79
25:1:1513:A:H2'	25:1:1514:A:C8	2.17	0.79
25:1:2649:U:O2'	25:1:2845:G:N2	2.15	0.79
18:S:155:VAL:HB	18:S:194:ILE:HG13	1.63	0.79
25:1:101:G:O2'	25:1:102:A:OP2	2.01	0.79
25:1:1493:U:H3	25:1:1505:G:H22	1.30	0.78
2:B:174:ILE:HD12	2:B:184:ILE:HD12	1.65	0.78
18:S:19:LEU:HD13	18:S:21:ASP:OD2	1.84	0.78
20:W:2:ILE:HG23	20:W:32:THR:HB	1.64	0.78
10:K:18:ILE:HG22	10:K:19:LYS:HD3	1.64	0.78
25:1:1675:G:N2	25:1:1678:A:OP2	2.16	0.78
10:K:31:GLN:HG2	10:K:37:LEU:HB2	1.64	0.78
25:1:589:U:O4	25:1:592:A:N6	2.17	0.77
8:H:72:VAL:HG12	8:H:93:ALA:HB2	1.65	0.77
22:Y:16:LYS:HG2	22:Y:18:THR:HG22	1.64	0.77
25:1:2507:C:H2'	25:1:2508:G:H5'	1.65	0.77
25:1:2603:G:N3	25:1:2603:G:H2'	2.00	0.77
1:A:53:ARG:HB2	1:A:60:THR:HG22	1.64	0.76
25:1:1185:U:H4'	25:1:1186:A:O4'	1.86	0.76
25:1:169:G:OP2	25:1:169:G:N2	2.16	0.76
11:L:157:ALA:HB2	25:1:2602:C:C5'	2.16	0.76
6:F:17:SER:OG	6:F:18:GLU:OE1	2.05	0.75
8:H:7:ILE:HB	8:H:42:LYS:HB3	1.67	0.75
25:1:158:G:H2'	25:1:159:U:H5'	1.68	0.75
25:1:229:A:O2'	25:1:230:A:OP1	2.04	0.75
25:1:1632:A:O2'	25:1:1635:A:N6	2.18	0.75
11:L:157:ALA:HB2	25:1:2602:C:H5'	1.67	0.75
20:W:1:MET:N	20:W:21:THR:OG1	2.19	0.74
25:1:592:A:O2'	25:1:593:U:H5''	1.87	0.74
25:1:293:U:H2'	25:1:294:G:H5''	1.69	0.74
24:a:77:GLY:HA3	24:a:111:ALA:HB3	1.68	0.74
25:1:1711:G:O2'	25:1:2018:U:O4	2.06	0.74
2:B:78:VAL:HB	2:B:112:VAL:HA	1.70	0.73
18:S:102:PRO:HD2	18:S:105:MET:HE3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:93:LEU:HD23	19:V:101:LEU:HD13	1.70	0.73
25:1:909:G:H21	25:1:911:A:H61	1.35	0.73
26:2:5:G:H1	26:2:108:U:H3	1.34	0.73
25:1:205:U:O2'	25:1:206:U:OP1	2.07	0.73
3:C:88:ILE:HA	4:D:50:ALA:CB	2.19	0.73
22:Y:48:GLU:O	22:Y:52:ILE:HG13	1.89	0.73
25:1:200:A:N6	25:1:2457:A:O2'	2.22	0.73
11:L:117:ASP:OD1	11:L:214:SER:HA	1.89	0.72
25:1:150:A:H61	25:1:179:A:H2	1.36	0.72
25:1:1834:G:H3'	25:1:1835:U:H5''	1.71	0.72
10:K:38:GLU:HG2	10:K:39:GLU:H	1.50	0.72
25:1:2918:A:H2'	25:1:2919:A:C8	2.24	0.72
25:1:1066:G:H4'	25:1:1067:U:O5'	1.89	0.72
25:1:1596:G:H2'	25:1:1597:U:H5'	1.72	0.72
25:1:1625:U:C2'	25:1:1626:A:H5''	2.20	0.72
6:F:20:MET:HG2	6:F:24:LYS:HB2	1.71	0.72
5:E:42:ALA:HB2	25:1:2037:G:H5''	1.72	0.71
17:R:31:LYS:HD2	25:1:2505:A:H5'	1.71	0.71
23:Z:72:LEU:HA	23:Z:78:THR:HG22	1.73	0.71
8:H:46:VAL:O	8:H:49:ILE:HG22	1.90	0.71
10:K:16:GLU:O	10:K:20:SER:OG	2.04	0.71
2:B:133:GLN:HG2	2:B:186:SER:HB3	1.72	0.71
7:G:45:GLN:O	7:G:55:GLY:N	2.23	0.71
18:S:16:SER:OG	18:S:17:ILE:HD12	1.90	0.71
25:1:253:G:H2'	25:1:254:A:C8	2.25	0.70
25:1:274:A:N3	25:1:415:U:O2'	2.24	0.70
25:1:1083:G:C2'	25:1:1084:U:H5''	2.21	0.70
25:1:2060:A:O2'	25:1:2062:G:OP2	2.08	0.70
25:1:2335:G:N2	25:1:2335:G:OP2	2.23	0.70
25:1:2370:U:O2'	25:1:2400:U:O2'	2.07	0.70
5:E:35:ILE:O	5:E:39:THR:OG1	2.08	0.70
5:E:78:GLU:OE2	25:1:24:G:N2	2.24	0.70
18:S:19:LEU:CD1	18:S:21:ASP:OD2	2.39	0.70
15:P:41:LYS:CD	25:1:505:U:H5''	2.22	0.70
25:1:2337:A:O2'	25:1:2338:A:OP1	2.09	0.70
18:S:43:SER:HB2	25:1:660:A:OP2	1.92	0.69
21:X:93:PRO:O	21:X:97:VAL:HG22	1.92	0.69
25:1:254:A:H2'	25:1:255:G:O4'	1.92	0.69
25:1:2465:U:O2'	25:1:2467:C:OP1	2.08	0.69
25:1:1886:A:H62	25:1:1910:G:H8	1.40	0.69
25:1:1891:U:OP1	25:1:2437:G:O2'	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:692:G:N2	25:1:2378:G:OP1	2.25	0.69
26:2:60:C:H2'	26:2:61:C:H5''	1.75	0.69
7:G:84:LYS:HE2	7:G:84:LYS:HA	1.74	0.69
18:S:19:LEU:HD13	18:S:21:ASP:CG	2.16	0.69
25:1:514:G:H2'	25:1:515:G:H5'	1.75	0.69
25:1:2715:G:N1	25:1:2747:U:OP2	2.18	0.69
25:1:2917:U:H2'	25:1:2918:A:C8	2.28	0.69
25:1:1780:G:N2	25:1:1783:G:OP2	2.21	0.68
8:H:55:VAL:HB	8:H:59:GLY:HA3	1.74	0.68
25:1:137:G:O2'	25:1:138:U:OP1	2.09	0.68
18:S:160:ASP:O	18:S:164:GLU:HG3	1.93	0.68
25:1:2333:U:H4'	25:1:2334:G:O5'	1.94	0.68
25:1:2622:G:N2	25:1:2625:A:OP2	2.27	0.68
25:1:2314:A:H62	25:1:2371:U:H3	1.40	0.68
1:A:60:THR:HG21	25:1:2711:U:OP1	1.94	0.67
10:K:17:GLN:O	10:K:22:LYS:HG3	1.93	0.67
25:1:1492:G:H1	25:1:1506:C:H42	1.43	0.67
6:F:89:LEU:HD22	10:K:30:PHE:HZ	1.60	0.67
20:W:2:ILE:O	20:W:32:THR:HA	1.94	0.67
25:1:1914:C:C2'	25:1:1915:G:H5''	2.22	0.67
8:H:33:GLY:HA3	8:H:93:ALA:H	1.60	0.67
9:J:37:ARG:HG2	9:J:37:ARG:HH21	1.60	0.67
25:1:764:C:C2'	25:1:765:U:H5''	2.24	0.67
10:K:9:LEU:HD13	10:K:10:THR:N	2.10	0.67
23:Z:32:THR:HG22	23:Z:33:THR:H	1.60	0.67
25:1:360:A:C3'	25:1:361:U:H5''	2.25	0.67
16:Q:19:SER:HB3	25:1:696:G:OP1	1.96	0.66
2:B:236:GLU:HG3	25:1:2627:A:C2	2.31	0.66
25:1:2507:C:C2'	25:1:2508:G:H5'	2.25	0.66
9:J:57:GLY:O	9:J:58:LYS:HE2	1.94	0.66
25:1:1210:U:H2'	25:1:1211:G:O4'	1.95	0.66
25:1:268:A:H2'	25:1:269:G:C4'	2.25	0.66
22:Y:58:MET:HE1	22:Y:64:VAL:CG2	2.26	0.66
25:1:1518:G:O2'	25:1:1519:U:H5'	1.96	0.66
25:1:2397:G:C2'	25:1:2398:G:H5''	2.25	0.66
8:H:9:ARG:HD2	8:H:13:GLN:OE1	1.96	0.66
22:Y:34:LEU:HD11	22:Y:129:THR:HB	1.76	0.66
25:1:2612:U:O2'	25:1:2613:C:H5'	1.96	0.66
24:a:39:HIS:ND1	24:a:59:LYS:HB3	2.11	0.66
25:1:152:C:OP1	25:1:1396:A:O2'	2.13	0.66
25:1:273:A:OP2	25:1:297:G:N1	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:1:MET:SD	20:W:2:ILE:HG13	2.37	0.65
25:1:2007:G:O2'	25:1:2009:U:OP2	2.14	0.65
23:Z:74:GLU:HG2	23:Z:79:GLN:NE2	2.12	0.65
25:1:2501:U:H5''	25:1:2502:C:C5	2.31	0.65
6:F:48:VAL:HB	6:F:82:LEU:HD22	1.76	0.65
15:P:41:LYS:HE3	25:1:505:U:H5'	1.78	0.65
25:1:49:A:H4'	25:1:50:U:H5''	1.78	0.65
25:1:490:C:H2'	25:1:491:C:H5'	1.79	0.65
25:1:682:A:H4'	25:1:683:G:O5'	1.96	0.65
25:1:234:C:O2'	25:1:235:G:OP1	2.14	0.65
25:1:899:U:C2'	25:1:900:G:H5''	2.25	0.65
25:1:372:A:O4'	25:1:523:A:H1'	1.97	0.65
25:1:2825:U:H2'	25:1:2826:U:C6	2.32	0.65
20:W:1:MET:HG2	20:W:8:LEU:HD21	1.76	0.65
25:1:1514:A:H2'	25:1:1515:G:C8	2.31	0.65
25:1:1881:A:H62	25:1:1915:G:H8	1.44	0.65
20:W:1:MET:N	20:W:8:LEU:HD11	2.12	0.65
2:B:122:ALA:HB3	2:B:130:LEU:HD21	1.79	0.65
7:G:16:ASP:HB3	7:G:19:LYS:HD2	1.78	0.65
25:1:509:G:N2	25:1:512:A:OP2	2.29	0.65
1:A:28:LEU:HD22	1:A:86:ILE:CG2	2.27	0.64
3:C:31:LEU:HB2	3:C:34:VAL:CG1	2.27	0.64
11:L:114:ASP:O	11:L:184:GLU:HA	1.98	0.64
25:1:545:G:H22	25:1:548:A:H5'	1.60	0.64
25:1:1754:C:O2'	25:1:1755:U:H5'	1.97	0.64
16:Q:55:MET:O	16:Q:59:LYS:HG3	1.98	0.64
10:K:60:ARG:O	10:K:61:GLU:HG2	1.98	0.64
26:2:46:A:N3	26:2:47:C:H1'	2.13	0.64
4:D:21:PHE:CE2	4:D:94:LYS:HG3	2.31	0.64
4:D:27:VAL:CG2	4:D:62:VAL:HG21	2.28	0.64
8:H:4:LEU:H	8:H:4:LEU:CD2	2.10	0.64
7:G:85:PHE:CD1	7:G:90:LYS:HG2	2.33	0.64
24:a:74:THR:HG23	24:a:111:ALA:HB2	1.78	0.64
25:1:721:A:H8	25:1:2096:G:H21	1.42	0.64
25:1:2056:G:OP2	25:1:2056:G:N2	2.27	0.64
2:B:112:VAL:HG23	2:B:112:VAL:O	1.98	0.64
21:X:120:LYS:O	21:X:121:LEU:HD13	1.97	0.64
25:1:2377:C:O2'	25:1:2378:G:OP1	2.16	0.64
25:1:2429:U:H2'	25:1:2430:C:H5'	1.80	0.64
25:1:2822:C:O2'	25:1:2824:G:O4'	2.16	0.64
15:P:41:LYS:NZ	25:1:505:U:H4'	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:184:C:H3'	25:1:185:A:H5''	1.80	0.64
8:H:9:ARG:NH1	8:H:13:GLN:OE1	2.28	0.64
25:1:2626:G:O2'	25:1:2627:A:H5'	1.97	0.64
26:2:108:U:H2'	26:2:109:C:O4'	1.98	0.64
25:1:1431:U:H2'	25:1:1432:A:H5''	1.80	0.63
26:2:84:U:O2'	26:2:85:U:O5'	2.16	0.63
25:1:1765:A:H2'	25:1:1766:C:O4'	1.98	0.63
24:a:70:VAL:HG22	24:a:104:ARG:HG2	1.79	0.63
26:2:22:G:O2'	26:2:23:U:H5''	1.98	0.63
9:J:8:THR:HG22	9:J:9:GLY:H	1.64	0.63
14:O:36:CYS:SG	14:O:39:GLU:HG3	2.38	0.63
25:1:268:A:H2'	25:1:269:G:H4'	1.81	0.63
10:K:9:LEU:HD13	10:K:11:THR:H	1.62	0.63
12:M:40:ASN:CG	12:M:41:PRO:HD2	2.23	0.63
25:1:1512:U:H2'	25:1:1513:A:C8	2.33	0.63
25:1:2852:U:H1'	25:1:2854:A:C4	2.33	0.63
8:H:61:ILE:HG13	8:H:91:PHE:HE1	1.62	0.63
19:V:63:ILE:HD11	19:V:94:ARG:HG3	1.81	0.63
25:1:414:C:C2'	25:1:415:U:H4'	2.29	0.63
4:D:2:PHE:CZ	4:D:42:GLY:HA3	2.34	0.63
25:1:1578:A:H3'	25:1:1579:C:H5'	1.81	0.63
25:1:2783:U:H4'	25:1:2784:A:OP1	1.98	0.63
3:C:88:ILE:HA	4:D:50:ALA:HB3	1.80	0.62
25:1:920:A:N6	25:1:944:G:OP2	2.31	0.62
22:Y:83:MET:HE2	22:Y:83:MET:HA	1.82	0.62
8:H:33:GLY:HA2	8:H:92:LEU:HD12	1.81	0.62
25:1:2433:C:H4'	25:1:2434:A:O5'	1.99	0.62
26:2:18:G:H1	26:2:61:C:H42	1.47	0.62
18:S:34:PHE:CZ	21:X:8:PRO:HG3	2.33	0.62
25:1:1834:G:H3'	25:1:1835:U:C5'	2.30	0.62
25:1:1910:G:O2'	25:1:1911:A:H5'	1.99	0.62
9:J:12:ALA:HB3	9:J:28:ARG:HH21	1.64	0.62
21:X:93:PRO:HD3	21:X:124:LYS:O	1.98	0.62
26:2:3:U:H3	26:2:110:C:H42	1.48	0.62
26:2:40:C:H2'	26:2:41:C:H5'	1.82	0.62
25:1:84:A:N6	25:1:101:G:H1'	2.14	0.62
25:1:327:G:O6	25:1:401:U:O2'	2.14	0.62
18:S:107:ARG:HH22	18:S:207:GLY:H	1.48	0.62
19:V:22:GLU:OE1	19:V:62:LYS:HD2	2.00	0.62
25:1:753:U:H3	25:1:768:A:H61	1.48	0.62
8:H:44:ASP:HB3	8:H:47:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:14:ILE:O	10:K:17:GLN:HG2	2.00	0.61
25:1:2457:A:N3	25:1:2457:A:H2'	2.15	0.61
25:1:329:A:C2	25:1:399:U:H1'	2.35	0.61
25:1:675:G:N2	25:1:678:A:OP2	2.25	0.61
25:1:1488:A:H61	25:1:1595:C:H42	1.47	0.61
6:F:8:LYS:O	6:F:9:ARG:HG3	1.99	0.61
18:S:53:ASN:O	18:S:57:VAL:HG23	2.00	0.61
25:1:333:C:H42	25:1:393:G:H1	1.47	0.61
25:1:343:A:H1'	25:1:362:C:H1'	1.82	0.61
3:C:27:SER:HA	3:C:30:THR:CG2	2.29	0.61
2:B:208:ALA:HB2	25:1:1817:C:O2'	2.00	0.61
18:S:117:LYS:NZ	18:S:186:ILE:O	2.34	0.61
25:1:2580:G:H3'	25:1:2581:U:H5''	1.82	0.61
18:S:63:LYS:HD3	18:S:65:TRP:O	2.01	0.61
25:1:1521:A:H61	25:1:1559:G:H1	1.49	0.61
1:A:53:ARG:HB2	1:A:60:THR:CG2	2.31	0.61
20:W:112:MET:HE2	20:W:112:MET:CA	2.30	0.61
25:1:499:A:O2'	25:1:501:C:N4	2.32	0.61
25:1:659:A:O2'	25:1:660:A:OP1	2.15	0.61
2:B:236:GLU:HG3	25:1:2627:A:H2	1.66	0.61
3:C:83:LEU:CD2	3:C:88:ILE:HD12	2.30	0.61
10:K:21:SER:O	10:K:50:ILE:HD11	2.01	0.61
11:L:92:ARG:HH21	25:1:2664:U:H5''	1.65	0.61
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.66	0.61
24:a:11:ARG:C	24:a:11:ARG:HD2	2.25	0.61
25:1:2827:A:H2'	25:1:2828:U:O4'	2.01	0.61
19:V:115:LEU:O	19:V:119:GLN:HG3	2.00	0.60
25:1:1854:U:O2'	25:1:1997:A:N3	2.32	0.60
25:1:2336:A:H3'	25:1:2337:A:H5'	1.83	0.60
22:Y:111:GLU:OE1	22:Y:115:ARG:NH1	2.33	0.60
25:1:117:A:OP2	25:1:118:A:H2'	2.01	0.60
9:J:37:ARG:HA	9:J:45:LYS:O	2.01	0.60
24:a:96:ARG:HH11	24:a:96:ARG:HB2	1.66	0.60
25:1:1632:A:H5''	25:1:1633:A:OP1	2.01	0.60
8:H:21:LEU:HD11	8:H:42:LYS:HD3	1.82	0.60
21:X:78:ASN:ND2	21:X:112:LEU:HB2	2.16	0.60
24:a:113:ARG:HD3	24:a:119:PHE:CD1	2.36	0.60
25:1:360:A:H3'	25:1:361:U:H5''	1.83	0.60
25:1:552:A:H1'	25:1:554:C:C4	2.36	0.60
25:1:1449:A:N6	25:1:1632:A:H1'	2.14	0.60
8:H:64:GLY:HA2	8:H:69:THR:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:74:GLU:O	11:L:78:LYS:HG3	2.01	0.60
25:1:184:C:H3'	25:1:185:A:C5'	2.32	0.60
25:1:360:A:H2'	25:1:361:U:H5''	1.83	0.60
3:C:27:SER:HB3	3:C:31:LEU:CD1	2.32	0.60
1:A:39:ARG:HD2	1:A:40:GLU:N	2.16	0.60
20:W:1:MET:CE	20:W:2:ILE:HG13	2.32	0.60
11:L:92:ARG:NH2	25:1:2664:U:H5''	2.17	0.60
23:Z:103:ILE:HG23	23:Z:117:VAL:CG1	2.32	0.60
24:a:30:ARG:HA	24:a:93:VAL:HG23	1.84	0.60
25:1:754:U:H2'	25:1:755:C:C6	2.36	0.59
25:1:2321:C:H2'	25:1:2322:C:C6	2.37	0.59
25:1:2917:U:H2'	25:1:2918:A:H8	1.67	0.59
24:a:77:GLY:HA3	24:a:111:ALA:CB	2.32	0.59
25:1:409:G:H3'	25:1:410:G:H8	1.67	0.59
25:1:914:G:H2'	25:1:915:U:C6	2.37	0.59
4:D:4:ILE:HG12	4:D:40:PHE:HB3	1.84	0.59
9:J:55:LYS:O	9:J:56:SER:OG	2.19	0.59
25:1:91:A:O2'	25:1:92:G:H5'	2.02	0.59
25:1:328:G:N1	25:1:400:C:H1'	2.17	0.59
5:E:14:PRO:O	5:E:18:ARG:HG3	2.03	0.59
9:J:3:LYS:HE2	9:J:33:LEU:HD12	1.83	0.59
6:F:86:SER:HB3	6:F:88:ASP:OD1	2.02	0.59
21:X:29:LYS:HG3	21:X:30:THR:H	1.67	0.59
3:C:74:MET:HE1	3:C:110:VAL:HG13	1.84	0.59
24:a:94:PHE:HB2	24:a:119:PHE:HE2	1.68	0.59
25:1:793:G:N3	25:1:793:G:H2'	2.17	0.59
25:1:1978:U:H2'	25:1:1980:A:OP2	2.03	0.59
25:1:2541:U:H2'	25:1:2542:C:C6	2.38	0.59
25:1:262:G:H21	25:1:666:A:H8	1.49	0.59
25:1:2537:C:H2'	25:1:2538:U:C6	2.38	0.59
4:D:50:ALA:HB1	4:D:51:PRO:CA	2.31	0.59
11:L:13:THR:HG22	11:L:14:GLN:H	1.68	0.58
17:R:31:LYS:HD3	25:1:2555:U:H5'	1.85	0.58
23:Z:51:GLY:HA2	23:Z:86:PHE:CE2	2.38	0.58
25:1:514:G:C2'	25:1:515:G:H5'	2.33	0.58
25:1:894:A:H2'	25:1:895:U:O2	2.02	0.58
25:1:2008:A:H5''	25:1:2009:U:OP2	2.03	0.58
25:1:2327:A:O2'	25:1:2344:C:N4	2.35	0.58
4:D:10:LYS:NZ	4:D:23:GLU:OE2	2.36	0.58
14:O:31:GLU:HG3	14:O:46:ARG:HG3	1.85	0.58
23:Z:5:LYS:HA	23:Z:13:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1293:U:O5'	25:1:1294:G:H5'	2.04	0.58
25:1:1493:U:H2'	25:1:1494:G:H5'	1.85	0.58
25:1:1864:C:O2'	25:1:1865:C:OP1	2.22	0.58
7:G:12:ILE:HG13	7:G:69:GLN:HG3	1.86	0.58
20:W:44:LYS:O	20:W:54:LYS:HD2	2.04	0.58
25:1:1493:U:OP1	25:1:1576:A:H4'	2.04	0.58
25:1:2421:C:H2'	25:1:2422:C:C6	2.38	0.58
19:V:63:ILE:HD12	19:V:94:ARG:HE	1.67	0.58
25:1:84:A:H61	25:1:101:G:H1'	1.67	0.58
25:1:1758:A:H3'	25:1:1758:A:N3	2.19	0.58
25:1:2549:U:O2'	25:1:2674:U:OP1	2.17	0.58
24:a:30:ARG:NH2	24:a:47:ASP:OD2	2.37	0.58
25:1:732:C:H2'	25:1:733:U:C6	2.39	0.58
8:H:4:LEU:HD23	8:H:4:LEU:N	2.15	0.57
5:E:33:ILE:O	5:E:37:LYS:HG3	2.04	0.57
25:1:629:A:H62	25:1:1289:A:H2	1.51	0.57
10:K:25:LEU:HD11	10:K:43:ILE:HG23	1.86	0.57
22:Y:27:VAL:HA	22:Y:105:GLU:OE2	2.04	0.57
24:a:68:THR:OG1	26:2:48:A:H5''	2.03	0.57
24:a:94:PHE:HB2	24:a:119:PHE:CE2	2.39	0.57
25:1:156:A:H2'	25:1:157:U:O4'	2.05	0.57
15:P:41:LYS:HE3	25:1:505:U:C5'	2.35	0.57
22:Y:22:LYS:NZ	25:1:909:G:N7	2.53	0.57
25:1:2429:U:C2'	25:1:2430:C:H5'	2.34	0.57
26:2:75:U:H3	26:2:94:C:H5	1.52	0.57
18:S:32:VAL:HG12	18:S:109:ALA:HB2	1.86	0.57
18:S:157:GLU:HG3	18:S:198:ALA:HB2	1.87	0.57
23:Z:48:ILE:O	23:Z:52:LYS:HG3	2.04	0.57
25:1:1708:A:H61	25:1:2023:C:H42	1.52	0.57
21:X:117:LEU:HD21	21:X:121:LEU:HD23	1.85	0.57
25:1:43:A:H2'	25:1:44:A:O4'	2.04	0.57
25:1:2079:G:O2'	25:1:2080:G:H5'	2.04	0.57
3:C:49:ASP:OD2	25:1:579:U:O2'	2.12	0.57
4:D:80:LYS:HD2	25:1:1017:A:H5''	1.86	0.57
5:E:23:LEU:HD22	13:N:24:VAL:HG22	1.86	0.57
10:K:32:LEU:HA	10:K:37:LEU:HB3	1.86	0.57
25:1:2308:C:O2'	25:1:2309:G:H5'	2.04	0.57
18:S:157:GLU:HG3	18:S:198:ALA:CA	2.34	0.57
11:L:157:ALA:HB2	25:1:2602:C:H5''	1.86	0.57
18:S:73:ALA:HB2	25:1:1294:G:H5''	1.87	0.57
18:S:44:LEU:HG	25:1:660:A:OP1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:329:A:H61	25:1:398:C:H42	1.53	0.56
27:I:80:LYS:HB2	27:I:86:GLN:CD	2.30	0.56
19:V:46:THR:HB	19:V:49:VAL:HG22	1.86	0.56
25:1:418:G:O2'	25:1:446:G:O6	2.13	0.56
25:1:697:U:H3'	25:1:698:U:C5'	2.34	0.56
25:1:1823:U:H2'	25:1:1824:C:C6	2.40	0.56
25:1:2420:U:H2'	25:1:2421:C:C6	2.40	0.56
4:D:4:ILE:HA	4:D:12:ILE:O	2.06	0.56
8:H:50:LYS:O	8:H:53:ARG:HB2	2.05	0.56
20:W:1:MET:CG	20:W:8:LEU:HD21	2.35	0.56
23:Z:103:ILE:HG23	23:Z:117:VAL:HG11	1.87	0.56
25:1:1518:G:H22	25:1:1562:C:H42	1.53	0.56
25:1:1575:A:O2'	25:1:1576:A:H5'	2.05	0.56
25:1:1651:C:H4'	25:1:1652:A:O5'	2.05	0.56
25:1:2601:G:H2'	25:1:2602:C:C6	2.39	0.56
25:1:273:A:C2	25:1:415:U:H2'	2.40	0.56
25:1:2536:G:H2'	25:1:2537:C:C6	2.40	0.56
2:B:69:ARG:HH21	2:B:117:GLU:HG2	1.70	0.56
22:Y:64:VAL:HG22	22:Y:106:VAL:HG12	1.87	0.56
26:2:38:U:O2'	26:2:41:C:OP2	2.24	0.56
11:L:116:ILE:HD12	11:L:211:ILE:CG2	2.36	0.56
25:1:161:A:H61	25:1:168:A:P	2.29	0.56
25:1:1996:A:H5'	25:1:1997:A:OP1	2.05	0.56
10:K:10:THR:O	10:K:14:ILE:HG13	2.06	0.56
10:K:44:ARG:NH1	10:K:48:LYS:HD2	2.20	0.56
15:P:8:PRO:HB2	25:1:1346:G:H4'	1.88	0.56
25:1:1480:G:H1'	25:1:1520:A:H8	1.70	0.56
25:1:1588:U:H2'	25:1:1589:U:C6	2.41	0.56
25:1:2605:G:H4'	25:1:2605:G:OP2	2.05	0.56
1:A:11:THR:HG21	11:L:13:THR:HG21	1.87	0.55
2:B:137:VAL:HG21	2:B:166:GLY:HA2	1.87	0.55
3:C:8:THR:HG22	3:C:8:THR:O	2.06	0.55
23:Z:42:SER:O	23:Z:46:LYS:HG3	2.06	0.55
25:1:302:A:O2'	25:1:303:G:OP2	2.19	0.55
25:1:525:A:H4'	25:1:526:A:OP1	2.04	0.55
23:Z:85:LEU:O	23:Z:86:PHE:HB2	2.06	0.55
25:1:99:U:OP1	25:1:100:U:H2'	2.06	0.55
20:W:1:MET:HB3	20:W:6:THR:HG21	1.88	0.55
23:Z:59:ARG:CZ	25:1:1498:U:H5'	2.36	0.55
25:1:1596:G:C2'	25:1:1597:U:H5'	2.35	0.55
2:B:105:ILE:O	2:B:107:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:LYS:HB2	6:F:84:GLU:HG3	1.88	0.55
8:H:47:GLU:O	8:H:51:VAL:HG23	2.07	0.55
9:J:15:GLY:HA3	9:J:29:TRP:HZ3	1.71	0.55
9:J:37:ARG:HG2	9:J:37:ARG:NH2	2.22	0.55
12:M:4:LEU:HD11	12:M:44:ARG:HE	1.72	0.55
19:V:28:ARG:HH22	25:1:1186:A:H4'	1.72	0.55
25:1:750:A:C2	25:1:772:A:H1'	2.42	0.55
1:A:4:HIS:O	1:A:8:GLU:HG2	2.06	0.55
8:H:81:PRO:HG2	8:H:82:LEU:HD12	1.87	0.55
22:Y:17:THR:O	22:Y:17:THR:HG22	2.07	0.55
25:1:158:G:C2'	25:1:159:U:H5'	2.36	0.55
25:1:2770:U:H2'	25:1:2771:G:C4'	2.37	0.55
26:2:57:G:H2'	26:2:58:C:C5'	2.37	0.55
26:2:57:G:H2'	26:2:58:C:H5'	1.87	0.55
7:G:9:VAL:HG12	7:G:70:LEU:HD23	1.87	0.55
18:S:19:LEU:C	18:S:19:LEU:HD12	2.32	0.55
25:1:2359:C:OP1	27:I:54:TYR:OH	2.25	0.55
25:1:2822:C:HO2'	25:1:2824:G:C1'	2.19	0.55
3:C:83:LEU:HD22	3:C:88:ILE:HD12	1.89	0.55
14:O:46:ARG:HG2	14:O:47:GLU:H	1.71	0.55
21:X:92:THR:HG23	21:X:93:PRO:HD2	1.88	0.55
25:1:525:A:H1'	25:1:526:A:H5''	1.87	0.55
25:1:2626:G:HO2'	25:1:2627:A:H5'	1.72	0.55
11:L:50:GLN:HG2	11:L:88:ILE:CG2	2.36	0.55
11:L:52:GLY:HA2	11:L:87:PHE:O	2.07	0.55
11:L:124:GLY:HA2	11:L:174:GLY:HA3	1.88	0.55
25:1:1522:G:H1	25:1:1558:U:H3	1.55	0.55
25:1:1821:U:H2'	25:1:1822:C:C6	2.42	0.55
2:B:36:PRO:HB3	25:1:1616:A:O2'	2.06	0.54
25:1:1847:U:H4'	25:1:1848:A:OP2	2.07	0.54
11:L:2:THR:O	11:L:3:LYS:HG3	2.07	0.54
25:1:169:G:C2'	25:1:170:C:H5'	2.35	0.54
25:1:915:U:H2'	25:1:916:U:C6	2.42	0.54
11:L:4:GLY:HA2	11:L:211:ILE:O	2.08	0.54
25:1:435:A:H2'	25:1:436:A:H5''	1.89	0.54
25:1:1498:U:HO2'	25:1:1499:U:H5	1.56	0.54
25:1:2348:G:N3	25:1:2348:G:H3'	2.22	0.54
25:1:199:A:N3	25:1:199:A:H2'	2.23	0.54
25:1:1754:C:C2'	25:1:1755:U:H5'	2.37	0.54
5:E:33:ILE:HG22	5:E:37:LYS:HE3	1.89	0.54
15:P:38:LYS:NZ	25:1:515:G:H1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:48:ASN:N	24:a:48:ASN:OD1	2.39	0.54
25:1:229:A:O2'	25:1:230:A:P	2.66	0.54
25:1:1956:G:H4'	25:1:1957:G:OP1	2.08	0.54
25:1:2705:U:H2'	25:1:2706:A:C8	2.42	0.54
4:D:27:VAL:HG23	4:D:62:VAL:HG21	1.90	0.54
5:E:65:ASN:OD1	5:E:65:ASN:N	2.41	0.54
25:1:923:A:C2'	25:1:924:G:H5''	2.33	0.54
11:L:126:GLY:O	11:L:172:ARG:HA	2.08	0.54
21:X:138:ALA:C	21:X:139:LYS:HE2	2.33	0.54
25:1:360:A:C2'	25:1:361:U:H5''	2.36	0.54
25:1:1493:U:C2'	25:1:1494:G:H5'	2.38	0.54
25:1:101:G:O2'	25:1:102:A:H5'	2.07	0.54
11:L:131:ILE:CD1	11:L:138:ARG:HG2	2.37	0.54
22:Y:5:LYS:HE3	25:1:945:A:H61	1.72	0.54
25:1:1353:A:H2'	25:1:1354:G:C8	2.42	0.54
26:2:28:C:H2'	26:2:29:C:H5'	1.90	0.54
19:V:63:ILE:CD1	19:V:94:ARG:HE	2.21	0.54
21:X:79:LEU:HD12	21:X:113:GLY:CA	2.37	0.54
25:1:1218:G:H3'	25:1:1218:G:N3	2.23	0.54
25:1:127:C:H2'	25:1:128:C:C6	2.44	0.53
10:K:9:LEU:CD1	10:K:11:THR:H	2.21	0.53
23:Z:112:ASP:OD1	25:1:1693:G:O2'	2.16	0.53
25:1:247:A:H2'	25:1:248:G:O4'	2.08	0.53
25:1:458:A:O2'	25:1:459:C:OP1	2.26	0.53
25:1:2372:G:N3	25:1:2408:C:H2'	2.24	0.53
25:1:2431:C:H2'	25:1:2432:G:O4'	2.08	0.53
18:S:161:VAL:O	18:S:165:LEU:HG	2.09	0.53
24:a:69:LYS:HD3	24:a:69:LYS:N	2.24	0.53
25:1:2529:G:H5''	25:1:2530:A:H5'	1.91	0.53
25:1:2694:C:H3'	25:1:2695:G:H5'	1.90	0.53
2:B:68:LYS:HE3	2:B:70:ASN:ND2	2.23	0.53
22:Y:42:ILE:HD11	22:Y:97:VAL:HG21	1.91	0.53
25:1:1578:A:H3'	25:1:1579:C:C5'	2.37	0.53
24:a:68:THR:C	24:a:69:LYS:HD3	2.32	0.53
1:A:28:LEU:HD12	1:A:49:VAL:CG2	2.38	0.53
19:V:30:SER:HB3	19:V:106:ILE:HG12	1.90	0.53
25:1:414:C:H2'	25:1:415:U:H4'	1.89	0.53
25:1:2590:U:H2'	25:1:2592:A:OP2	2.08	0.53
18:S:39:LEU:HD13	18:S:101:MET:HE2	1.91	0.53
25:1:138:U:H2'	25:1:139:U:H5''	1.90	0.53
23:Z:4:ARG:HB2	23:Z:39:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:407:G:H3'	25:1:407:G:N3	2.23	0.53
25:1:515:G:OP2	25:1:515:G:N2	2.37	0.53
25:1:666:A:H2'	25:1:667:G:H5'	1.91	0.53
25:1:697:U:H3'	25:1:698:U:H5''	1.91	0.53
26:2:83:C:H2'	26:2:84:U:O4'	2.09	0.53
11:L:90:GLU:OE2	25:1:2663:U:H4'	2.08	0.53
7:G:26:THR:HG22	7:G:28:PRO:HD3	1.91	0.52
25:1:389:A:H5'	25:1:390:A:OP2	2.09	0.52
25:1:2397:G:C3'	25:1:2398:G:H5''	2.39	0.52
25:1:2553:G:H2'	25:1:2554:C:C6	2.44	0.52
11:L:40:THR:HA	11:L:47:ASN:OD1	2.09	0.52
18:S:40:GLN:HG3	25:1:660:A:C5'	2.38	0.52
19:V:66:THR:HG21	25:1:1185:U:H2'	1.91	0.52
20:W:1:MET:CA	20:W:8:LEU:HD11	2.40	0.52
25:1:793:G:N2	25:1:796:A:OP2	2.42	0.52
25:1:1940:A:H62	25:1:1946:A:H2	1.57	0.52
25:1:2792:A:H5'	25:1:2793:G:OP2	2.09	0.52
26:2:9:C:H42	26:2:104:A:H61	1.57	0.52
23:Z:72:LEU:HD22	23:Z:72:LEU:O	2.09	0.52
25:1:1493:U:H3	25:1:1505:G:N2	2.05	0.52
26:2:3:U:H4'	26:2:4:G:OP1	2.09	0.52
21:X:86:GLU:O	21:X:121:LEU:HD11	2.09	0.52
24:a:68:THR:HB	24:a:70:VAL:HG23	1.92	0.52
25:1:963:A:H62	25:1:2295:A:H2	1.55	0.52
25:1:1320:G:H2'	25:1:1321:A:H5''	1.91	0.52
25:1:2340:C:H2'	25:1:2341:A:H8	1.74	0.52
25:1:2694:C:H2'	25:1:2695:G:H5'	1.91	0.52
25:1:234:C:HO2'	25:1:235:G:P	2.32	0.52
25:1:321:U:H5'	25:1:322:A:OP1	2.10	0.52
25:1:615:A:H61	25:1:2056:G:H8	1.56	0.52
25:1:2817:A:O2'	25:1:2818:A:OP2	2.21	0.52
11:L:210:GLU:OE2	11:L:212:ARG:NH2	2.42	0.52
19:V:8:ASN:O	19:V:12:ILE:HG13	2.09	0.52
25:1:679:G:H2'	25:1:680:C:C6	2.44	0.52
25:1:1058:U:H3	25:1:1192:A:H61	1.57	0.52
26:2:56:A:H2'	26:2:57:G:H5''	1.91	0.52
7:G:45:GLN:OE1	7:G:57:LEU:HD12	2.10	0.52
25:1:50:U:H4'	25:1:51:G:OP2	2.08	0.52
25:1:490:C:C2'	25:1:491:C:H5'	2.40	0.52
25:1:1471:A:H4'	25:1:1472:C:O5'	2.09	0.52
25:1:2505:A:H2'	25:1:2506:U:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:2649:U:O3'	25:1:2845:G:N2	2.43	0.52
5:E:10:ILE:CG2	5:E:12:ILE:HD12	2.40	0.52
7:G:26:THR:C	7:G:27:LEU:HD12	2.34	0.52
10:K:32:LEU:HB2	10:K:37:LEU:HD12	1.92	0.52
11:L:38:LYS:HG2	11:L:49:ILE:HG22	1.92	0.52
19:V:46:THR:HB	19:V:49:VAL:CG2	2.40	0.52
21:X:86:GLU:O	21:X:89:THR:HG22	2.10	0.52
22:Y:60:ARG:HB3	22:Y:60:ARG:HH21	1.75	0.52
24:a:28:LYS:HD2	24:a:91:GLU:HB3	1.91	0.52
25:1:1854:U:OP1	25:1:1998:A:O2'	2.27	0.51
26:2:38:U:H1'	26:2:43:A:N6	2.24	0.51
6:F:23:ASP:N	6:F:23:ASP:OD1	2.43	0.51
18:S:48:THR:HB	25:1:38:A:N3	2.25	0.51
22:Y:124:LYS:O	25:1:2511:G:O2'	2.28	0.51
25:1:914:G:H2'	25:1:915:U:H6	1.75	0.51
4:D:67:ARG:NH2	4:D:89:ARG:HD3	2.24	0.51
24:a:39:HIS:CE1	24:a:59:LYS:HB3	2.45	0.51
25:1:136:A:H3'	25:1:137:G:H5''	1.92	0.51
25:1:921:C:N4	25:1:943:C:H3'	2.25	0.51
21:X:73:GLU:O	21:X:107:SER:OG	2.25	0.51
25:1:491:C:O2'	25:1:492:G:H5'	2.10	0.51
5:E:72:LYS:HE2	5:E:73:GLU:OE1	2.11	0.51
15:P:41:LYS:HZ1	25:1:505:U:H4'	1.76	0.51
23:Z:32:THR:HG23	25:1:1315:C:OP1	2.10	0.51
25:1:762:C:H2'	25:1:763:A:O4'	2.11	0.51
26:2:15:C:H42	26:2:103:A:H2	1.56	0.51
21:X:124:LYS:HD3	21:X:124:LYS:C	2.35	0.51
23:Z:55:ASP:OD1	23:Z:55:ASP:N	2.43	0.51
25:1:591:A:H4'	25:1:592:A:H5'	1.93	0.51
25:1:1756:U:H2'	25:1:1757:U:C6	2.46	0.51
18:S:64:PRO:HB2	18:S:65:TRP:CE3	2.46	0.51
20:W:6:THR:HG1	25:1:1710:G:HO2'	1.59	0.51
25:1:909:G:H21	25:1:911:A:N6	2.05	0.51
25:1:1160:C:H2'	25:1:1161:A:C8	2.45	0.51
25:1:2419:A:H2	25:1:2451:C:H42	1.59	0.51
25:1:2842:G:H4'	25:1:2845:G:O6	2.10	0.51
26:2:110:C:H2'	26:2:111:A:O4'	2.10	0.51
12:M:47:ILE:HG21	12:M:56:VAL:HG11	1.93	0.51
17:R:36:GLN:O	17:R:36:GLN:HG2	2.10	0.51
25:1:319:G:H1	25:1:401:U:H3	1.58	0.51
25:1:517:A:H2'	25:1:518:A:H5'	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:2821:U:H4'	25:1:2822:C:OP1	2.09	0.51
1:A:28:LEU:HD22	1:A:86:ILE:HG23	1.93	0.51
23:Z:72:LEU:HD23	23:Z:78:THR:CG2	2.41	0.51
25:1:320:U:H2'	25:1:320:U:O2	2.10	0.51
13:N:10:LYS:HE2	25:1:562:C:OP2	2.10	0.51
25:1:764:C:C3'	25:1:765:U:H5''	2.40	0.51
25:1:101:G:C2'	25:1:102:A:OP2	2.59	0.50
25:1:434:G:H2'	25:1:436:A:C2	2.46	0.50
25:1:1514:A:H61	25:1:1566:G:H1	1.59	0.50
25:1:2692:A:O2'	25:1:2693:C:H5'	2.12	0.50
15:P:35:ARG:NH1	15:P:42:VAL:O	2.44	0.50
21:X:29:LYS:HG3	21:X:30:THR:N	2.27	0.50
25:1:805:G:H2'	25:1:806:A:O4'	2.11	0.50
25:1:1336:G:N1	25:1:1684:A:OP2	2.29	0.50
26:2:85:U:H5'	26:2:86:A:OP1	2.11	0.50
18:S:151:LYS:HA	18:S:172:GLY:O	2.11	0.50
22:Y:14:ARG:HH11	25:1:1002:U:H5'	1.76	0.50
25:1:1569:G:P	25:1:1569:G:H21	2.35	0.50
2:B:210:ARG:HA	2:B:213:TRP:CE2	2.46	0.50
9:J:43:LYS:HB3	25:1:167:U:H1'	1.94	0.50
10:K:39:GLU:OE2	10:K:42:ARG:HD2	2.11	0.50
25:1:1312:A:H4'	25:1:1313:G:OP1	2.11	0.50
3:C:27:SER:HA	3:C:30:THR:HG22	1.93	0.50
23:Z:11:ASP:OD1	23:Z:12:GLN:HG3	2.10	0.50
23:Z:39:GLU:OE1	25:1:2717:A:N6	2.45	0.50
25:1:101:G:H4'	25:1:102:A:H5''	1.92	0.50
25:1:1183:G:O2'	25:1:1184:C:H5'	2.11	0.50
25:1:1449:A:N3	25:1:1449:A:H3'	2.26	0.50
25:1:2536:G:H2'	25:1:2537:C:H6	1.76	0.50
6:F:20:MET:HG2	6:F:20:MET:O	2.12	0.50
8:H:61:ILE:HB	8:H:72:VAL:HG23	1.93	0.50
25:1:161:A:N3	25:1:161:A:H2'	2.26	0.50
21:X:88:GLY:H	21:X:121:LEU:HD13	1.75	0.50
22:Y:14:ARG:NH1	25:1:1002:U:H5'	2.26	0.50
25:1:1063:U:HO2'	25:1:1065:A:H2	1.57	0.50
25:1:1071:A:C2	25:1:2515:A:H5'	2.47	0.50
3:C:100:ILE:HG12	19:V:43:VAL:HG22	1.93	0.50
6:F:56:MET:SD	6:F:77:LYS:HE2	2.52	0.50
22:Y:54:MET:HG2	22:Y:58:MET:HE2	1.92	0.50
25:1:2885:U:OP2	25:1:2886:G:O2'	2.24	0.50
26:2:60:C:C2'	26:2:61:C:H5''	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HG2	1:A:46:GLU:HG3	1.93	0.50
4:D:27:VAL:HG21	4:D:62:VAL:HG21	1.93	0.50
8:H:13:GLN:HB3	8:H:17:ASP:HB2	1.93	0.50
15:P:31:VAL:O	15:P:35:ARG:HG3	2.12	0.50
18:S:20:SER:HB2	18:S:203:GLU:OE1	2.10	0.50
25:1:1616:A:H2'	25:1:1617:A:O4'	2.12	0.50
25:1:2309:G:H4'	25:1:2416:G:O2'	2.12	0.50
25:1:2321:C:H2'	25:1:2322:C:H6	1.76	0.50
11:L:8:ARG:HG3	11:L:53:PHE:HE2	1.76	0.49
11:L:33:ASN:HA	11:L:52:GLY:O	2.11	0.49
11:L:115:VAL:HG12	11:L:214:SER:HB3	1.94	0.49
18:S:157:GLU:HG3	18:S:198:ALA:HA	1.92	0.49
25:1:205:U:O2'	25:1:206:U:P	2.69	0.49
26:2:108:U:H2'	26:2:109:C:C4'	2.42	0.49
8:H:33:GLY:CA	8:H:92:LEU:HD12	2.41	0.49
11:L:39:LYS:HD3	11:L:44:ASP:OD2	2.12	0.49
25:1:615:A:H5''	25:1:616:G:OP2	2.11	0.49
25:1:1350:U:H5''	25:1:1351:C:OP2	2.12	0.49
25:1:2581:U:O2'	25:1:2582:U:H5'	2.12	0.49
24:a:74:THR:HG23	24:a:111:ALA:CB	2.41	0.49
25:1:1069:G:C4	25:1:1179:C:H1'	2.47	0.49
25:1:2038:U:H2'	25:1:2039:G:O4'	2.12	0.49
25:1:2336:A:H3'	25:1:2337:A:C5'	2.42	0.49
5:E:33:ILE:CG2	5:E:37:LYS:HE3	2.42	0.49
25:1:793:G:N2	25:1:795:A:H3'	2.27	0.49
25:1:1451:U:O4	25:1:1631:G:N1	2.46	0.49
25:1:2605:G:O2'	25:1:2606:C:H5'	2.12	0.49
25:1:2909:C:H2'	25:1:2910:G:O4'	2.12	0.49
10:K:20:SER:O	10:K:21:SER:HB2	2.12	0.49
25:1:393:G:O2'	25:1:394:U:H5'	2.13	0.49
25:1:1392:G:O2'	25:1:1393:C:H5'	2.12	0.49
3:C:88:ILE:CG2	3:C:90:ILE:HG13	2.36	0.49
6:F:51:ALA:HB2	6:F:83:LYS:HG3	1.93	0.49
10:K:25:LEU:CD1	10:K:43:ILE:HG23	2.43	0.49
18:S:102:PRO:O	18:S:106:ARG:HG3	2.13	0.49
23:Z:102:ARG:HD3	25:1:2902:A:OP1	2.12	0.49
26:2:3:U:H2'	26:2:4:G:C8	2.48	0.49
6:F:89:LEU:HD22	10:K:30:PHE:CZ	2.45	0.49
15:P:41:LYS:CE	25:1:505:U:C5'	2.89	0.49
19:V:70:GLU:HG2	19:V:91:GLY:HA3	1.93	0.49
25:1:275:A:H62	25:1:296:G:N2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:774:G:H3'	25:1:774:G:N3	2.28	0.49
25:1:2603:G:N3	25:1:2603:G:C2'	2.73	0.49
2:B:100:GLU:HA	2:B:100:GLU:OE1	2.12	0.49
18:S:143:LEU:HD13	18:S:148:GLN:HG3	1.94	0.49
25:1:992:A:H1'	25:1:1028:G:C8	2.48	0.49
16:Q:45:ARG:HD3	25:1:2445:A:OP1	2.13	0.49
25:1:661:U:H2'	25:1:662:G:C8	2.48	0.49
25:1:2335:G:H3'	25:1:2335:G:N3	2.28	0.49
25:1:2770:U:H3'	25:1:2771:G:H5''	1.94	0.49
2:B:30:GLU:O	2:B:34:LEU:HG	2.13	0.49
3:C:94:MET:HE3	4:D:11:GLN:O	2.13	0.49
25:1:41:A:H2'	25:1:42:G:C8	2.47	0.49
25:1:91:A:C2'	25:1:92:G:H5'	2.42	0.49
25:1:205:U:HO2'	25:1:206:U:P	2.33	0.49
27:I:18:THR:HG22	27:I:20:ASN:H	1.76	0.49
21:X:89:THR:HG22	21:X:121:LEU:HD12	1.95	0.48
25:1:1361:G:H1'	25:1:1660:A:N6	2.28	0.48
22:Y:58:MET:HE1	22:Y:64:VAL:HG21	1.94	0.48
25:1:427:A:O2'	25:1:428:G:H5'	2.13	0.48
25:1:903:G:O2'	25:1:2296:A:H5''	2.14	0.48
25:1:1872:G:O2'	25:1:1873:G:H5'	2.13	0.48
25:1:2237:U:H4'	25:1:2238:U:OP1	2.12	0.48
1:A:39:ARG:HD2	1:A:40:GLU:H	1.75	0.48
6:F:19:ALA:O	6:F:20:MET:HB3	2.14	0.48
8:H:7:ILE:HD12	8:H:42:LYS:O	2.13	0.48
25:1:2331:G:H3'	25:1:2333:U:H5	1.79	0.48
7:G:25:ALA:HB3	7:G:34:VAL:HB	1.94	0.48
22:Y:112:GLU:OE1	22:Y:112:GLU:HA	2.13	0.48
25:1:1771:A:N3	25:1:1771:A:H3'	2.27	0.48
25:1:2852:U:O4	25:1:2904:U:H5'	2.14	0.48
2:B:161:SER:HB3	2:B:194:GLN:HG3	1.95	0.48
10:K:31:GLN:CG	10:K:37:LEU:HB2	2.38	0.48
25:1:872:U:O2'	25:1:2095:U:N3	2.47	0.48
26:2:50:A:H3'	26:2:50:A:N3	2.29	0.48
4:D:48:VAL:HG12	4:D:49:GLY:H	1.77	0.48
25:1:2555:U:H2'	25:1:2557:U:C6	2.49	0.48
3:C:35:ALA:O	3:C:39:VAL:HG23	2.14	0.48
8:H:33:GLY:HA2	8:H:92:LEU:CD1	2.42	0.48
14:O:20:THR:HG22	14:O:21:LYS:H	1.78	0.48
25:1:517:A:C2'	25:1:518:A:H5'	2.43	0.48
18:S:157:GLU:HG3	18:S:198:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:38:LYS:O	24:a:69:LYS:HG2	2.13	0.48
24:a:96:ARG:HB2	24:a:96:ARG:NH1	2.29	0.48
25:1:251:G:H5'	25:1:253:G:N7	2.28	0.48
25:1:1065:A:H61	25:1:1186:A:H61	1.60	0.48
25:1:2313:A:H4'	25:1:2314:A:O4'	2.14	0.48
25:1:2535:G:H4'	25:1:2581:U:O2'	2.14	0.48
26:2:47:C:N4	26:2:48:A:H62	2.12	0.48
26:2:56:A:H2'	26:2:57:G:C5'	2.44	0.48
5:E:10:ILE:HG22	5:E:12:ILE:HD12	1.94	0.47
26:2:59:U:H2'	26:2:60:C:C6	2.49	0.47
11:L:116:ILE:HD12	11:L:211:ILE:HG23	1.96	0.47
25:1:1336:G:H4'	25:1:1338:U:C1'	2.44	0.47
25:1:367:A:N6	25:1:381:G:O2'	2.46	0.47
25:1:757:G:H3'	25:1:758:G:C5'	2.35	0.47
25:1:1508:C:C2'	25:1:1593:G:H22	2.26	0.47
26:2:99:G:C3'	26:2:100:U:H5''	2.38	0.47
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.29	0.47
25:1:1512:U:H2'	25:1:1513:A:H8	1.79	0.47
25:1:1806:U:O2	25:1:1810:A:N6	2.48	0.47
19:V:63:ILE:HD12	19:V:63:ILE:O	2.14	0.47
21:X:2:LYS:O	21:X:2:LYS:HG2	2.14	0.47
22:Y:34:LEU:CD1	22:Y:129:THR:HB	2.42	0.47
25:1:1028:G:N3	25:1:1028:G:H2'	2.30	0.47
25:1:1669:C:H2'	25:1:1670:A:H5'	1.96	0.47
4:D:73:VAL:HB	4:D:86:LYS:HB2	1.96	0.47
17:R:17:ILE:HG12	17:R:24:MET:O	2.13	0.47
22:Y:118:LEU:HD22	22:Y:131:PHE:HE1	1.80	0.47
25:1:904:G:O2'	25:1:961:G:O6	2.28	0.47
25:1:1625:U:C3'	25:1:1626:A:H5''	2.44	0.47
2:B:23:GLU:OE2	2:B:90:ASN:ND2	2.47	0.47
5:E:76:ALA:HA	5:E:102:HIS:O	2.15	0.47
11:L:10:ILE:HB	11:L:27:VAL:HB	1.97	0.47
18:S:178:ALA:HB1	18:S:202:VAL:CG2	2.45	0.47
19:V:27:GLY:HA3	25:1:1184:C:H5'	1.96	0.47
20:W:66:LYS:HE2	20:W:80:ASP:O	2.15	0.47
21:X:85:PHE:CE1	21:X:95:LEU:HD21	2.50	0.47
21:X:92:THR:CG2	21:X:93:PRO:HD2	2.45	0.47
23:Z:66:LEU:HD23	23:Z:82:LEU:HB2	1.95	0.47
25:1:483:C:H2'	25:1:484:U:C6	2.49	0.47
25:1:1486:C:H2'	25:1:1487:G:C8	2.50	0.47
25:1:1739:G:N3	25:1:1739:G:H3'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:2377:C:HO2'	25:1:2378:G:P	2.38	0.47
25:1:2608:G:H2'	25:1:2608:G:N3	2.30	0.47
25:1:2694:C:C2'	25:1:2695:G:H5'	2.45	0.47
26:2:28:C:C2'	26:2:29:C:H5'	2.44	0.47
2:B:94:VAL:HG23	2:B:96:TYR:HE1	1.80	0.47
7:G:63:ILE:HD11	7:G:68:VAL:CG1	2.45	0.47
25:1:638:U:H2'	25:1:639:U:C6	2.50	0.47
3:C:83:LEU:HD23	3:C:88:ILE:HD12	1.96	0.47
5:E:55:LEU:HD23	5:E:69:LEU:CD1	2.45	0.47
16:Q:14:VAL:HA	16:Q:23:LYS:O	2.15	0.47
18:S:39:LEU:HD12	18:S:99:TYR:CE2	2.50	0.47
19:V:60:ALA:HB1	19:V:102:ILE:HD12	1.97	0.47
25:1:2540:A:H2'	25:1:2541:U:C6	2.50	0.47
25:1:2626:G:C2'	25:1:2627:A:H5'	2.45	0.47
26:2:46:A:C4	26:2:47:C:H1'	2.50	0.47
4:D:3:ALA:HA	4:D:40:PHE:O	2.15	0.47
25:1:174:U:H2'	25:1:175:C:C6	2.50	0.47
25:1:616:G:O6	25:1:2056:G:O2'	2.29	0.47
25:1:863:G:N1	25:1:1227:U:OP2	2.37	0.47
25:1:1070:A:H1'	25:1:1178:C:N4	2.30	0.47
25:1:1313:G:OP2	25:1:1689:G:O2'	2.26	0.47
25:1:1514:A:H2'	25:1:1515:G:H8	1.79	0.47
25:1:1865:C:OP2	25:1:1865:C:H3'	2.14	0.47
27:I:50:GLY:O	27:I:65:ASP:HB3	2.14	0.47
2:B:69:ARG:NH2	2:B:117:GLU:HG2	2.30	0.46
6:F:4:ARG:HG2	6:F:5:ASP:N	2.24	0.46
6:F:36:THR:HG22	6:F:40:MET:HE2	1.96	0.46
20:W:1:MET:HE1	20:W:2:ILE:HG13	1.95	0.46
25:1:137:G:HO2'	25:1:138:U:P	2.35	0.46
25:1:1480:G:H1'	25:1:1520:A:C8	2.50	0.46
25:1:1981:G:O2'	25:1:1983:U:O4	2.16	0.46
25:1:2087:A:C4'	25:1:2088:G:OP2	2.62	0.46
25:1:2122:A:H2'	25:1:2123:A:C8	2.50	0.46
25:1:2419:A:H2'	25:1:2420:U:O4'	2.15	0.46
2:B:69:ARG:HE	2:B:117:GLU:CD	2.22	0.46
25:1:2489:U:O2'	25:1:2490:C:H5'	2.15	0.46
25:1:2694:C:C3'	25:1:2695:G:H5'	2.45	0.46
26:2:35:C:H42	26:2:47:C:H4'	1.79	0.46
15:P:10:LYS:HB2	25:1:1346:G:OP1	2.16	0.46
26:2:3:U:O2'	26:2:4:G:P	2.73	0.46
2:B:114:GLN:C	2:B:115:ILE:HG12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1065:A:H2'	25:1:1066:G:H5''	1.98	0.46
25:1:1160:C:H2'	25:1:1161:A:H8	1.80	0.46
25:1:2580:G:C3'	25:1:2581:U:H5''	2.44	0.46
2:B:70:ASN:O	2:B:71:LYS:HG3	2.14	0.46
25:1:522:G:N1	25:1:525:A:OP2	2.49	0.46
25:1:2501:U:H5''	25:1:2502:C:H5	1.78	0.46
25:1:2697:G:O2'	25:1:2698:A:H5'	2.16	0.46
5:E:55:LEU:HD23	5:E:69:LEU:HD12	1.96	0.46
25:1:762:C:C2'	25:1:763:A:H5'	2.46	0.46
25:1:2077:C:H2'	25:1:2078:A:O4'	2.16	0.46
25:1:2343:U:H2'	25:1:2344:C:H5''	1.98	0.46
25:1:1690:A:H3'	25:1:1691:G:C5'	2.46	0.46
25:1:1887:G:O2'	25:1:1888:U:H5'	2.14	0.46
25:1:2048:G:H2'	25:1:2048:G:N3	2.29	0.46
26:2:85:U:H4'	26:2:86:A:O5'	2.15	0.46
25:1:575:G:N3	25:1:575:G:H2'	2.30	0.46
25:1:2225:A:H4'	25:1:2226:A:OP1	2.16	0.46
25:1:2682:G:O2'	25:1:2683:U:OP2	2.33	0.46
6:F:89:LEU:HD13	10:K:30:PHE:CZ	2.50	0.46
9:J:15:GLY:HA3	9:J:29:TRP:CZ3	2.50	0.46
19:V:109:MET:HE2	25:1:1182:G:H21	1.81	0.46
22:Y:110:SER:OG	22:Y:111:GLU:N	2.49	0.46
25:1:213:C:H2'	25:1:214:G:H8	1.80	0.46
25:1:2338:A:H5''	25:1:2339:U:C5	2.51	0.46
22:Y:65:TRP:HE1	25:1:918:G:H4'	1.80	0.46
25:1:1347:G:H1'	25:1:1655:C:H5''	1.97	0.46
25:1:2358:G:O2'	25:1:2363:A:N1	2.45	0.46
25:1:2454:C:H5''	25:1:2455:G:OP1	2.16	0.46
25:1:2770:U:C3'	25:1:2771:G:H5''	2.46	0.46
2:B:77:LYS:O	2:B:94:VAL:HA	2.16	0.45
3:C:42:SER:HB2	25:1:579:U:H5'	1.98	0.45
6:F:38:VAL:O	6:F:42:VAL:HG23	2.16	0.45
7:G:86:VAL:HG23	7:G:87:ASP:H	1.81	0.45
12:M:31:THR:O	12:M:32:ASN:HB2	2.16	0.45
14:O:10:THR:HG23	14:O:44:LEU:O	2.16	0.45
17:R:16:VAL:HG22	17:R:25:VAL:HG22	1.97	0.45
18:S:135:LYS:N	18:S:166:SER:OG	2.49	0.45
25:1:101:G:O2'	25:1:102:A:P	2.74	0.45
27:I:83:ASP:O	27:I:84:LYS:HG3	2.16	0.45
2:B:107:PRO:HD2	2:B:110:LEU:HD22	1.98	0.45
21:X:120:LYS:HD3	21:X:120:LYS:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:55:GLN:HB2	26:2:110:C:OP1	2.16	0.45
24:a:89:ILE:O	24:a:89:ILE:HG13	2.16	0.45
26:2:8:A:H2'	26:2:9:C:O4'	2.16	0.45
3:C:74:MET:CE	3:C:110:VAL:HG13	2.46	0.45
5:E:111:LYS:HE3	5:E:111:LYS:HB2	1.70	0.45
8:H:62:GLU:O	8:H:62:GLU:HG2	2.16	0.45
9:J:35:LYS:HG2	9:J:48:TRP:CZ3	2.51	0.45
18:S:72:ARG:HD2	18:S:72:ARG:HA	1.76	0.45
24:a:70:VAL:HG22	24:a:104:ARG:CG	2.44	0.45
25:1:1065:A:H62	25:1:1185:U:H3	1.63	0.45
25:1:2740:A:O2'	25:1:2742:C:OP2	2.14	0.45
1:A:35:ILE:HD12	1:A:35:ILE:C	2.41	0.45
5:E:7:ALA:HB2	5:E:50:VAL:CG2	2.47	0.45
16:Q:15:LYS:O	16:Q:22:LEU:HA	2.17	0.45
20:W:15:GLY:O	20:W:46:ALA:HA	2.17	0.45
21:X:96:LEU:HB3	21:X:102:VAL:HG23	1.98	0.45
24:a:68:THR:O	24:a:104:ARG:HD3	2.16	0.45
25:1:690:U:H4'	25:1:691:A:H5''	1.99	0.45
25:1:743:C:O2'	25:1:779:A:N6	2.50	0.45
25:1:1220:A:H2'	25:1:1221:C:C6	2.51	0.45
25:1:1905:G:H2'	25:1:1906:C:O4'	2.15	0.45
25:1:2318:U:O2'	25:1:2401:C:H1'	2.17	0.45
25:1:2538:U:H2'	25:1:2539:C:C6	2.52	0.45
25:1:273:A:N1	25:1:415:U:H2'	2.32	0.45
25:1:476:A:H5''	25:1:477:U:OP2	2.16	0.45
25:1:1083:G:C3'	25:1:1084:U:H5''	2.45	0.45
25:1:1336:G:O2'	25:1:1684:A:N6	2.50	0.45
25:1:2564:U:H2'	25:1:2565:C:C6	2.52	0.45
2:B:210:ARG:HA	2:B:213:TRP:CZ2	2.51	0.45
25:1:2608:G:N2	25:1:2608:G:OP2	2.49	0.45
25:1:2739:U:H2'	25:1:2739:U:O2	2.15	0.45
21:X:88:GLY:N	21:X:120:LYS:O	2.46	0.45
25:1:661:U:H2'	25:1:662:G:H8	1.81	0.45
8:H:29:ALA:HB3	8:H:41:VAL:CG2	2.47	0.45
11:L:3:LYS:HE2	11:L:3:LYS:HB2	1.81	0.45
18:S:33:LEU:O	18:S:37:ILE:HG13	2.17	0.45
20:W:85:VAL:HG23	20:W:87:ILE:HG23	1.99	0.45
25:1:138:U:C2'	25:1:139:U:H5''	2.47	0.45
25:1:661:U:O2'	25:1:662:G:H5'	2.16	0.45
2:B:93:LEU:HD12	2:B:102:ARG:O	2.16	0.45
8:H:31:VAL:O	8:H:31:VAL:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:35:LYS:HG2	9:J:48:TRP:CH2	2.52	0.45
14:O:15:ARG:NE	14:O:37:SER:OG	2.50	0.45
19:V:28:ARG:NH2	25:1:1186:A:H4'	2.32	0.45
25:1:127:C:H2'	25:1:128:C:H6	1.81	0.45
25:1:253:G:H2'	25:1:254:A:H8	1.76	0.45
25:1:2221:U:H3'	25:1:2222:U:H5''	1.99	0.45
25:1:2418:G:O2'	25:1:2451:C:N4	2.50	0.45
27:I:64:ASP:OD1	27:I:66:THR:HG22	2.17	0.45
5:E:27:LYS:O	5:E:70:VAL:HG13	2.16	0.45
11:L:118:VAL:HG23	11:L:183:LEU:HD12	1.99	0.45
11:L:133:ARG:HG3	11:L:173:MET:HB3	1.98	0.45
21:X:117:LEU:O	21:X:118:ASP:HB2	2.17	0.45
23:Z:104:LEU:O	23:Z:117:VAL:HG13	2.17	0.45
25:1:526:A:N3	25:1:526:A:H2'	2.32	0.45
25:1:1431:U:C2'	25:1:1432:A:H5''	2.45	0.45
25:1:2618:C:H2'	25:1:2619:G:C8	2.51	0.45
25:1:2792:A:H3'	25:1:2792:A:N3	2.32	0.45
25:1:2800:U:O2'	25:1:2801:C:H5'	2.17	0.45
25:1:2828:U:H5''	25:1:2910:G:O6	2.16	0.45
2:B:247:MET:HE2	2:B:247:MET:HA	1.99	0.44
19:V:79:SER:HB3	19:V:86:LYS:HE2	1.99	0.44
25:1:2265:G:N3	25:1:2265:G:H2'	2.31	0.44
25:1:2340:C:H2'	25:1:2341:A:C8	2.52	0.44
25:1:83:G:H22	25:1:101:G:HO2'	1.65	0.44
25:1:102:A:H5'	25:1:102:A:N3	2.32	0.44
25:1:390:A:O2'	25:1:391:A:H5'	2.17	0.44
25:1:545:G:N1	25:1:548:A:OP2	2.50	0.44
25:1:899:U:C3'	25:1:900:G:H5''	2.46	0.44
25:1:1522:G:H2'	25:1:1523:G:C8	2.53	0.44
25:1:1931:G:H21	25:1:1955:A:H8	1.64	0.44
25:1:2529:G:H5''	25:1:2530:A:C5'	2.47	0.44
1:A:77:PRO:O	1:A:80:THR:HG22	2.17	0.44
14:O:25:ASN:ND2	25:1:2313:A:OP1	2.50	0.44
25:1:660:A:O2'	25:1:661:U:C6	2.68	0.44
25:1:963:A:H5''	26:2:92:C:O2'	2.17	0.44
25:1:1477:U:O2'	25:1:1478:A:H5'	2.17	0.44
14:O:6:THR:HA	14:O:17:TYR:O	2.17	0.44
20:W:15:GLY:HA3	20:W:50:GLY:HA3	1.98	0.44
25:1:2740:A:H3'	25:1:2741:G:H5''	1.99	0.44
2:B:183:MET:HE2	2:B:269:LEU:HD22	1.99	0.44
5:E:44:SER:HB2	5:E:45:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:ILE:N	7:G:56:ILE:HD12	2.32	0.44
20:W:2:ILE:HG23	20:W:32:THR:CB	2.40	0.44
25:1:687:G:N2	25:1:690:U:OP2	2.49	0.44
5:E:34:ALA:CB	13:N:27:MET:HE1	2.48	0.44
19:V:94:ARG:O	19:V:98:PRO:HG3	2.17	0.44
23:Z:72:LEU:O	23:Z:72:LEU:HD13	2.18	0.44
25:1:892:U:H5'	25:1:893:G:OP2	2.18	0.44
25:1:2094:G:O2'	25:1:2096:G:H5''	2.18	0.44
25:1:2555:U:O2'	25:1:2556:G:H3'	2.17	0.44
7:G:15:LYS:HB2	7:G:15:LYS:HE2	1.65	0.44
8:H:82:LEU:HD12	8:H:82:LEU:H	1.83	0.44
17:R:10:ILE:O	17:R:10:ILE:HG22	2.17	0.44
19:V:109:MET:HE2	25:1:1182:G:N2	2.33	0.44
25:1:194:A:H2'	25:1:195:C:C6	2.51	0.44
25:1:2347:A:H2'	25:1:2347:A:N3	2.32	0.44
25:1:2377:C:O2'	25:1:2378:G:P	2.75	0.44
25:1:2500:U:OP1	25:1:2556:G:N2	2.51	0.44
25:1:2554:C:H2'	25:1:2555:U:C6	2.53	0.44
25:1:2555:U:H2'	25:1:2557:U:H6	1.82	0.44
2:B:115:ILE:HD12	2:B:127:GLY:HA3	2.00	0.44
9:J:12:ALA:HB3	9:J:28:ARG:NH2	2.32	0.44
19:V:63:ILE:HD12	19:V:63:ILE:C	2.42	0.44
23:Z:47:LEU:HD21	23:Z:65:THR:OG1	2.18	0.44
25:1:489:A:H1'	25:1:1240:U:O4'	2.18	0.44
25:1:774:G:H5'	25:1:775:A:H5''	1.99	0.44
25:1:1596:G:H2'	25:1:1597:U:C5'	2.46	0.44
25:1:1828:U:H3'	25:1:1829:A:H5'	2.00	0.44
2:B:263:LYS:HD2	25:1:2254:A:H5''	2.00	0.44
14:O:9:CYS:SG	14:O:10:THR:N	2.91	0.44
18:S:101:MET:HG3	18:S:102:PRO:HD2	2.00	0.44
23:Z:5:LYS:HA	23:Z:13:ARG:NE	2.33	0.44
1:A:57:VAL:HG22	1:A:57:VAL:O	2.17	0.43
2:B:173:LEU:HD12	2:B:181:VAL:HG12	2.00	0.43
25:1:1521:A:N6	25:1:1559:G:H1	2.13	0.43
25:1:2011:U:H2'	25:1:2012:G:C8	2.53	0.43
25:1:2825:U:H3'	25:1:2825:U:O2	2.18	0.43
26:2:99:G:H3'	26:2:100:U:C5'	2.40	0.43
11:L:88:ILE:O	11:L:89:ARG:HD3	2.18	0.43
25:1:1466:G:H2'	25:1:1467:G:C8	2.52	0.43
25:1:2594:G:H2'	25:1:2595:C:C6	2.54	0.43
20:W:1:MET:HB3	20:W:2:ILE:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:160:G:H3'	25:1:160:G:N3	2.33	0.43
25:1:878:C:H2'	25:1:879:U:C6	2.53	0.43
25:1:1063:U:O2'	25:1:1065:A:H2	2.01	0.43
25:1:1806:U:H5	25:1:1811:A:N7	2.17	0.43
25:1:2465:U:O3'	25:1:2466:A:H3'	2.18	0.43
25:1:904:G:O2'	25:1:905:U:OP2	2.36	0.43
25:1:1065:A:H61	25:1:1186:A:N6	2.16	0.43
26:2:110:C:H2'	26:2:111:A:C8	2.52	0.43
2:B:205:VAL:HG12	2:B:210:ARG:HB3	2.00	0.43
8:H:14:THR:HG22	8:H:15:ARG:N	2.34	0.43
11:L:115:VAL:HA	11:L:183:LEU:O	2.18	0.43
25:1:252:C:O2	25:1:252:C:C2'	2.65	0.43
25:1:1484:G:H1	25:1:1599:G:N2	2.15	0.43
25:1:1939:A:C6	25:1:1941:C:H2'	2.53	0.43
25:1:2567:C:H2'	25:1:2568:A:C8	2.54	0.43
2:B:3:ILE:HG13	2:B:199:GLN:OE1	2.19	0.43
4:D:64:LYS:HG2	4:D:65:GLN:N	2.33	0.43
11:L:38:LYS:HB2	11:L:38:LYS:HE2	1.75	0.43
23:Z:31:GLU:OE2	23:Z:118:ILE:HG12	2.18	0.43
25:1:698:U:H3'	25:1:699:U:C5'	2.48	0.43
25:1:857:C:O2'	25:1:858:U:H5'	2.18	0.43
25:1:2102:U:OP2	25:1:2265:G:O2'	2.31	0.43
25:1:2429:U:H2'	25:1:2430:C:C5'	2.48	0.43
2:B:29:PRO:HB2	2:B:34:LEU:HD21	1.99	0.43
5:E:7:ALA:HB2	5:E:50:VAL:HG22	2.01	0.43
6:F:89:LEU:HD13	10:K:30:PHE:CE1	2.53	0.43
8:H:30:VAL:HG12	8:H:88:HIS:HE1	1.84	0.43
11:L:19:ASN:OD1	11:L:19:ASN:N	2.51	0.43
18:S:115:SER:O	18:S:118:VAL:HG22	2.18	0.43
20:W:61:VAL:HG12	20:W:85:VAL:HG22	1.99	0.43
25:1:895:U:H5	25:1:973:A:N1	2.17	0.43
25:1:2325:A:H3'	25:1:2326:G:C8	2.53	0.43
25:1:2391:C:H4'	27:I:66:THR:HG21	2.00	0.43
9:J:58:LYS:HG3	9:J:59:VAL:H	1.84	0.43
18:S:117:LYS:HD2	18:S:192:LEU:HD12	2.01	0.43
20:W:108:GLU:OE2	20:W:108:GLU:N	2.52	0.43
25:1:250:G:C5	25:1:252:C:H1'	2.54	0.43
25:1:637:U:H2'	25:1:638:U:C6	2.54	0.43
25:1:915:U:H2'	25:1:916:U:H6	1.81	0.43
25:1:1309:G:N7	25:1:1362:C:H5	2.17	0.43
25:1:1504:U:H2'	25:1:1505:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:51:A:C2'	26:2:52:G:H5'	2.48	0.43
2:B:157:SER:HB2	25:1:1846:A:OP1	2.19	0.43
12:M:22:THR:O	12:M:26:LEU:HD12	2.19	0.43
14:O:7:LEU:O	14:O:16:ASN:HA	2.19	0.43
17:R:7:VAL:HG23	17:R:7:VAL:O	2.18	0.43
25:1:213:C:O2'	25:1:214:G:H5'	2.18	0.43
25:1:1423:C:O2'	25:1:1512:U:O2	2.26	0.43
25:1:2694:C:H3'	25:1:2695:G:C5'	2.48	0.43
5:E:10:ILE:O	5:E:100:THR:HA	2.19	0.43
25:1:1483:A:H3'	25:1:1484:G:H8	1.83	0.43
25:1:2580:G:C2	25:1:2610:G:H4'	2.54	0.43
25:1:2581:U:H2'	25:1:2582:U:H6	1.84	0.43
2:B:112:VAL:O	2:B:112:VAL:CG2	2.66	0.42
3:C:24:TYR:CE1	25:1:578:G:H5''	2.54	0.42
8:H:59:GLY:O	8:H:73:MET:HG2	2.18	0.42
9:J:21:ALA:O	9:J:22:LEU:HB2	2.17	0.42
12:M:17:GLU:OE2	12:M:20:ARG:HD3	2.19	0.42
22:Y:54:MET:HG3	22:Y:117:ALA:HB1	2.01	0.42
24:a:11:ARG:HD3	24:a:97:GLY:O	2.19	0.42
1:A:115:ILE:HD12	1:A:115:ILE:C	2.44	0.42
25:1:41:A:H2'	25:1:42:G:H8	1.83	0.42
25:1:2455:G:H5''	25:1:2456:G:P	2.59	0.42
2:B:235:GLY:HA2	25:1:2626:G:OP2	2.19	0.42
2:B:266:SER:O	2:B:270:ILE:HG13	2.19	0.42
9:J:22:LEU:HD23	9:J:22:LEU:HA	1.83	0.42
25:1:830:U:H2'	25:1:831:C:C6	2.54	0.42
25:1:1476:G:H2'	25:1:1477:U:C6	2.54	0.42
25:1:1510:U:H3	25:1:1571:G:H1	1.67	0.42
25:1:1578:A:H4'	25:1:1578:A:OP1	2.19	0.42
25:1:2343:U:H2'	25:1:2344:C:C5'	2.49	0.42
25:1:2597:G:H2'	25:1:2598:U:C6	2.53	0.42
1:A:53:ARG:CZ	1:A:53:ARG:HB3	2.50	0.42
11:L:6:LEU:H	11:L:33:ASN:HD21	1.66	0.42
25:1:578:G:H2'	25:1:579:U:C6	2.54	0.42
25:1:700:A:H4'	25:1:701:G:OP1	2.20	0.42
25:1:1066:G:H1'	25:1:1067:U:OP2	2.19	0.42
25:1:1498:U:O2	25:1:1498:U:H2'	2.20	0.42
25:1:2122:A:H2	25:1:2221:U:O4	2.02	0.42
25:1:2728:U:H3'	25:1:2729:G:C5'	2.48	0.42
1:A:51:LYS:HG3	1:A:98:LYS:HE3	2.00	0.42
11:L:19:ASN:HB2	11:L:21:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:34:ARG:HG2	15:P:37:ARG:NH2	2.35	0.42
21:X:132:ALA:O	21:X:136:ILE:HG13	2.20	0.42
23:Z:108:PRO:HA	23:Z:115:GLU:HA	2.01	0.42
25:1:44:A:O2'	25:1:45:G:H5'	2.18	0.42
1:A:66:ILE:HA	1:A:71:GLY:HA2	2.01	0.42
14:O:3:VAL:HG21	14:O:23:LYS:HD3	2.02	0.42
18:S:135:LYS:HA	18:S:135:LYS:HD2	1.93	0.42
21:X:119:LYS:HB2	21:X:121:LEU:HD21	2.02	0.42
25:1:187:C:H2'	25:1:188:C:C6	2.54	0.42
25:1:268:A:C2'	25:1:269:G:H4'	2.48	0.42
25:1:713:A:H2'	25:1:715:A:H62	1.84	0.42
25:1:1894:G:H1	25:1:1901:C:H42	1.67	0.42
25:1:2455:G:H5''	25:1:2456:G:OP1	2.20	0.42
1:A:12:LYS:HA	1:A:15:LEU:CD1	2.50	0.42
6:F:6:ILE:HG23	6:F:33:VAL:HG11	2.02	0.42
10:K:38:GLU:HG2	10:K:39:GLU:N	2.26	0.42
23:Z:117:VAL:HG12	23:Z:118:ILE:N	2.35	0.42
25:1:195:C:O2'	25:1:847:A:N3	2.46	0.42
26:2:95:U:H2'	26:2:96:A:O4'	2.20	0.42
3:C:112:LYS:HE3	3:C:112:LYS:HB2	1.69	0.42
20:W:66:LYS:HE3	20:W:66:LYS:HB2	1.79	0.42
21:X:47:ARG:HB2	21:X:48:PRO:HD2	2.01	0.42
25:1:85:G:H21	25:1:102:A:H8	1.68	0.42
25:1:229:A:HO2'	25:1:230:A:P	2.34	0.42
25:1:234:C:O2'	25:1:235:G:P	2.75	0.42
25:1:266:A:H2'	25:1:267:G:O4'	2.20	0.42
25:1:1565:U:H2'	25:1:1566:G:C8	2.55	0.42
2:B:241:ILE:HG22	2:B:243:ARG:H	1.84	0.42
6:F:43:GLU:HG2	6:F:48:VAL:O	2.20	0.42
11:L:128:GLN:OE1	11:L:128:GLN:HA	2.20	0.42
25:1:762:C:H2'	25:1:763:A:H5'	2.01	0.42
25:1:911:A:H2'	25:1:911:A:N3	2.35	0.42
25:1:1077:U:H5'	25:1:1078:G:P	2.60	0.42
5:E:66:THR:HA	5:E:69:LEU:HG	2.01	0.42
14:O:9:CYS:SG	14:O:43:THR:HG21	2.60	0.42
18:S:149:PRO:CG	18:S:191:SER:HB2	2.50	0.42
25:1:2899:A:H4'	25:1:2900:C:OP1	2.20	0.42
2:B:115:ILE:CD1	2:B:127:GLY:HA3	2.50	0.41
4:D:25:LEU:HD11	4:D:95:LEU:HD11	2.01	0.41
18:S:107:ARG:NH2	18:S:207:GLY:H	2.15	0.41
25:1:702:U:H2'	25:1:703:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:79:C:H42	26:2:90:U:H3	1.68	0.41
1:A:27:THR:HG23	1:A:47:GLY:O	2.20	0.41
3:C:33:LYS:HD3	25:1:1290:G:O4'	2.20	0.41
7:G:30:LYS:O	7:G:31:ASP:HB2	2.20	0.41
13:N:13:LYS:HB3	13:N:13:LYS:HE2	1.88	0.41
25:1:1182:G:H2'	25:1:1183:G:O4'	2.20	0.41
25:1:1518:G:O2'	25:1:1519:U:OP2	2.30	0.41
25:1:1828:U:O4	25:1:2229:C:H4'	2.20	0.41
25:1:2672:G:H3'	25:1:2673:C:C5'	2.49	0.41
6:F:11:VAL:CG2	6:F:26:THR:HG22	2.50	0.41
16:Q:52:LYS:HE2	16:Q:52:LYS:HB2	1.82	0.41
19:V:100:ARG:O	19:V:100:ARG:HG2	2.20	0.41
24:a:117:LEU:HD12	24:a:117:LEU:HA	1.86	0.41
25:1:2310:C:H2'	25:1:2311:U:O4'	2.19	0.41
4:D:39:LEU:HD12	4:D:39:LEU:N	2.35	0.41
4:D:64:LYS:HG2	4:D:65:GLN:H	1.85	0.41
25:1:207:A:H4'	25:1:208:G:OP1	2.20	0.41
25:1:458:A:N6	25:1:2439:A:O4'	2.53	0.41
25:1:503:A:H5'	25:1:505:U:H1'	2.02	0.41
25:1:922:G:O4'	25:1:943:C:N4	2.53	0.41
26:2:11:A:O2'	26:2:13:A:H2'	2.21	0.41
2:B:31:LYS:HA	2:B:34:LEU:HD12	2.03	0.41
18:S:148:GLN:HE21	18:S:148:GLN:HA	1.84	0.41
21:X:4:HIS:HB3	25:1:1242:A:N3	2.35	0.41
25:1:1497:A:H62	25:1:2730:C:H42	1.67	0.41
1:A:12:LYS:HA	1:A:15:LEU:HD13	2.02	0.41
11:L:50:GLN:HG2	11:L:88:ILE:HG22	2.02	0.41
25:1:1224:U:H5''	25:1:1225:G:OP1	2.20	0.41
25:1:2637:C:H4'	25:1:2638:C:O5'	2.20	0.41
2:B:182:ARG:HB2	2:B:269:LEU:O	2.20	0.41
25:1:213:C:H2'	25:1:214:G:C8	2.55	0.41
25:1:1848:A:H2'	25:1:1849:G:C8	2.56	0.41
25:1:2294:A:H3'	25:1:2294:A:N3	2.36	0.41
18:S:24:PHE:O	18:S:118:VAL:HG21	2.21	0.41
18:S:57:VAL:HG12	18:S:58:SER:N	2.36	0.41
25:1:1065:A:H2'	25:1:1066:G:C5'	2.51	0.41
25:1:1497:A:H2'	25:1:1498:U:O2	2.20	0.41
25:1:1660:A:H4'	25:1:1661:C:OP2	2.20	0.41
25:1:1865:C:O2	25:1:1865:C:C2'	2.68	0.41
25:1:2774:G:H21	25:1:2784:A:H62	1.69	0.41
27:I:80:LYS:HB2	27:I:86:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:VAL:HG12	2:B:272:ARG:HG3	2.03	0.41
6:F:25:TYR:CE1	6:F:82:LEU:HD12	2.56	0.41
6:F:59:LYS:HD2	25:1:1349:U:O4	2.20	0.41
10:K:18:ILE:O	10:K:22:LYS:HB2	2.20	0.41
15:P:41:LYS:CE	25:1:505:U:H5'	2.51	0.41
16:Q:56:LYS:HB3	16:Q:56:LYS:HE3	1.87	0.41
18:S:176:THR:OG1	18:S:177:THR:N	2.54	0.41
18:S:178:ALA:HB1	18:S:202:VAL:HG22	2.02	0.41
21:X:59:ARG:HB3	21:X:59:ARG:NH1	2.36	0.41
22:Y:58:MET:HE1	22:Y:64:VAL:HG22	2.01	0.41
25:1:262:G:H1'	25:1:666:A:O2'	2.21	0.41
25:1:841:C:H2'	25:1:842:U:C6	2.56	0.41
25:1:1518:G:H22	25:1:1562:C:N4	2.18	0.41
25:1:1813:A:H1'	25:1:1965:A:N6	2.36	0.41
25:1:1890:G:O3'	25:1:2438:A:H4'	2.20	0.41
26:2:18:G:H1	26:2:61:C:N4	2.16	0.41
9:J:21:ALA:HB3	9:J:23:ASN:ND2	2.36	0.41
21:X:19:VAL:HG12	21:X:27:ASN:HD22	1.86	0.41
21:X:89:THR:HG22	21:X:121:LEU:CD1	2.50	0.41
25:1:556:U:O2	25:1:556:U:O4'	2.39	0.41
2:B:77:LYS:HE3	2:B:77:LYS:HB3	1.79	0.40
8:H:74:VAL:O	8:H:74:VAL:HG23	2.20	0.40
11:L:17:GLY:HA3	11:L:21:GLU:HG2	2.04	0.40
14:O:23:LYS:HE2	14:O:23:LYS:HA	2.03	0.40
15:P:23:MET:HE3	15:P:23:MET:HB3	1.81	0.40
24:a:9:LYS:HA	24:a:9:LYS:HD2	1.76	0.40
25:1:259:A:H2'	25:1:260:A:C8	2.56	0.40
25:1:1329:G:H2'	25:1:1330:U:C6	2.56	0.40
25:1:2053:U:H2'	25:1:2054:G:O4'	2.20	0.40
25:1:2270:U:H2'	25:1:2271:U:C6	2.56	0.40
10:K:9:LEU:HD13	10:K:11:THR:N	2.33	0.40
11:L:116:ILE:HD12	11:L:211:ILE:HG21	2.02	0.40
20:W:9:LYS:HG2	20:W:10:VAL:N	2.36	0.40
25:1:276:C:H2'	25:1:277:C:C6	2.57	0.40
25:1:292:U:H3'	25:1:293:U:C5'	2.52	0.40
25:1:714:G:N3	25:1:714:G:C2'	2.85	0.40
25:1:2049:U:O2'	25:1:2644:C:H5'	2.20	0.40
25:1:2419:A:N3	25:1:2419:A:O4'	2.55	0.40
2:B:95:VAL:HG13	2:B:101:LYS:HD3	2.02	0.40
17:R:7:VAL:HG22	17:R:37:GLY:HA3	2.03	0.40
24:a:110:GLU:HA	24:a:110:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:79:U:O2'	25:1:389:A:H2'	2.22	0.40
25:1:215:G:H5'	25:1:216:A:OP2	2.20	0.40
25:1:244:A:H8	25:1:244:A:OP1	2.04	0.40
25:1:1483:A:H3'	25:1:1484:G:C8	2.56	0.40
25:1:1933:G:H1	25:1:1951:C:H42	1.67	0.40
25:1:1949:G:H2'	25:1:1950:U:O4'	2.21	0.40
25:1:2236:C:H5''	25:1:2237:U:OP2	2.20	0.40
26:2:3:U:H2'	26:2:4:G:H8	1.86	0.40
4:D:27:VAL:HG21	4:D:62:VAL:CG2	2.51	0.40
22:Y:16:LYS:CG	22:Y:18:THR:HG22	2.44	0.40
22:Y:32:PHE:HD1	22:Y:133:LYS:HG2	1.86	0.40
25:1:299:U:H4'	25:1:300:G:OP1	2.21	0.40
25:1:309:U:O4	25:1:407:G:H4'	2.21	0.40
25:1:528:C:H1'	25:1:543:G:N2	2.36	0.40
26:2:60:C:C3'	26:2:61:C:H5''	2.51	0.40
1:A:13:SER:O	1:A:13:SER:OG	2.36	0.40
3:C:74:MET:HE1	3:C:79:LEU:HD13	2.04	0.40
6:F:4:ARG:CG	6:F:5:ASP:H	2.26	0.40
11:L:9:LYS:HG2	11:L:205:LYS:HA	2.02	0.40
22:Y:75:THR:HA	22:Y:89:ALA:O	2.21	0.40
25:1:538:G:H2'	25:1:539:G:O4'	2.21	0.40
25:1:656:G:H5'	25:1:657:U:OP2	2.21	0.40
25:1:895:U:O2	25:1:895:U:O4'	2.40	0.40
25:1:1463:A:H2'	25:1:1465:G:C8	2.57	0.40
25:1:1497:A:H62	25:1:2730:C:N4	2.20	0.40
25:1:1562:C:O2'	25:1:1563:U:H5'	2.22	0.40
25:1:2725:U:H2'	25:1:2726:C:C6	2.56	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	A	110/116 (95%)	103 (94%)	7 (6%)	0	100	100
2	B	272/277 (98%)	264 (97%)	8 (3%)	0	100	100
3	C	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
4	D	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
5	E	108/117 (92%)	106 (98%)	2 (2%)	0	100	100
6	F	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
7	G	87/105 (83%)	85 (98%)	2 (2%)	0	100	100
8	H	91/107 (85%)	91 (100%)	0	0	100	100
9	J	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
10	K	51/72 (71%)	48 (94%)	3 (6%)	0	100	100
11	L	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
12	M	54/58 (93%)	54 (100%)	0	0	100	100
13	N	48/57 (84%)	48 (100%)	0	0	100	100
14	O	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
15	P	42/50 (84%)	42 (100%)	0	0	100	100
16	Q	62/65 (95%)	62 (100%)	0	0	100	100
17	R	35/37 (95%)	35 (100%)	0	0	100	100
18	S	190/207 (92%)	183 (96%)	7 (4%)	0	100	100
19	V	141/145 (97%)	140 (99%)	1 (1%)	0	100	100
20	W	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
21	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
22	Y	134/144 (93%)	129 (96%)	5 (4%)	0	100	100
23	Z	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
24	a	106/119 (89%)	103 (97%)	3 (3%)	0	100	100
27	I	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
All	All	2590/2793 (93%)	2515 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	98/102 (96%)	96 (98%)	2 (2%)	48	78
2	B	221/224 (99%)	216 (98%)	5 (2%)	44	76
3	C	96/98 (98%)	90 (94%)	6 (6%)	16	45
4	D	85/89 (96%)	84 (99%)	1 (1%)	63	86
5	E	89/94 (95%)	88 (99%)	1 (1%)	65	88
6	F	74/82 (90%)	73 (99%)	1 (1%)	59	85
7	G	77/91 (85%)	74 (96%)	3 (4%)	28	63
8	H	81/95 (85%)	79 (98%)	2 (2%)	42	74
9	J	49/51 (96%)	48 (98%)	1 (2%)	48	78
10	K	48/65 (74%)	45 (94%)	3 (6%)	16	45
11	L	170/175 (97%)	163 (96%)	7 (4%)	27	61
12	M	50/52 (96%)	49 (98%)	1 (2%)	48	78
13	N	45/49 (92%)	45 (100%)	0	100	100
14	O	45/47 (96%)	45 (100%)	0	100	100
15	P	39/45 (87%)	38 (97%)	1 (3%)	40	73
16	Q	55/56 (98%)	55 (100%)	0	100	100
17	R	35/35 (100%)	35 (100%)	0	100	100
18	S	158/170 (93%)	155 (98%)	3 (2%)	50	79
19	V	122/123 (99%)	120 (98%)	2 (2%)	55	83
20	W	99/100 (99%)	98 (99%)	1 (1%)	68	89
21	X	110/112 (98%)	109 (99%)	1 (1%)	70	90
22	Y	113/119 (95%)	109 (96%)	4 (4%)	32	66
23	Z	101/102 (99%)	100 (99%)	1 (1%)	68	89
24	a	87/95 (92%)	84 (97%)	3 (3%)	32	66
27	I	61/66 (92%)	59 (97%)	2 (3%)	33	67
All	All	2208/2337 (94%)	2157 (98%)	51 (2%)	44	76

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN

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Mol	Chain	Res	Type
1	A	44	VAL
2	B	117	GLU
2	B	139	THR
2	B	157	SER
2	B	186	SER
2	B	257	LYS
3	C	18	ILE
3	C	30	THR
3	C	41	LYS
3	C	51	ARG
3	C	75	SER
3	C	84	LYS
4	D	77	LYS
5	E	82	LEU
6	F	62	LYS
7	G	3	ILE
7	G	17	LYS
7	G	100	GLU
8	H	17	ASP
8	H	63	LEU
9	J	39	LEU
10	K	15	GLU
10	K	16	GLU
10	K	48	LYS
11	L	3	LYS
11	L	13	THR
11	L	50	GLN
11	L	117	ASP
11	L	122	SER
11	L	189	ASP
11	L	196	LEU
12	M	29	LYS
15	P	10	LYS
18	S	26	ILE
18	S	58	SER
18	S	192	LEU
19	V	74	VAL
19	V	94	ARG
20	W	2	ILE
21	X	95	LEU
22	Y	5	LYS
22	Y	7	VAL

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Mol	Chain	Res	Type
22	Y	39	THR
22	Y	43	THR
23	Z	78	THR
24	a	45	ILE
24	a	71	GLU
24	a	93	VAL
27	I	16	SER
27	I	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
2	B	143	ASN
8	H	10	GLN
9	J	23	ASN
10	K	27	ASN
11	L	66	ASN
11	L	148	HIS
11	L	182	ASN
11	L	200	ASN
12	M	46	GLN
13	N	45	ASN
15	P	13	HIS
15	P	27	ASN
19	V	81	HIS
19	V	97	ASN
19	V	136	GLN
20	W	72	ASN
21	X	78	ASN
21	X	81	GLN
22	Y	13	HIS
24	a	37	ASN
27	I	58	ASN
27	I	86	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	1	2675/2923 (91%)	444 (16%)	48 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	2	110/115 (95%)	30 (27%)	4 (3%)
All	All	2785/3038 (91%)	474 (17%)	52 (1%)

All (474) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	1	5	A
25	1	13	A
25	1	28	A
25	1	35	G
25	1	42	G
25	1	43	A
25	1	45	G
25	1	63	U
25	1	64	A
25	1	71	A
25	1	75	G
25	1	84	A
25	1	88	G
25	1	91	A
25	1	94	A
25	1	95	A
25	1	100	U
25	1	101	G
25	1	102	A
25	1	117	A
25	1	119	U
25	1	136	A
25	1	137	G
25	1	138	U
25	1	139	U
25	1	140	A
25	1	158	G
25	1	160	G
25	1	161	A
25	1	162	A
25	1	164	A
25	1	165	C
25	1	166	A
25	1	167	U
25	1	168	A
25	1	171	A

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Mol	Chain	Res	Type
25	1	176	A
25	1	177	G
25	1	180	G
25	1	184	C
25	1	185	A
25	1	199	A
25	1	202	A
25	1	206	U
25	1	216	A
25	1	219	A
25	1	224	A
25	1	225	A
25	1	230	A
25	1	233	U
25	1	235	G
25	1	236	A
25	1	251	G
25	1	252	C
25	1	253	G
25	1	258	A
25	1	268	A
25	1	269	G
25	1	292	U
25	1	293	U
25	1	294	G
25	1	300	G
25	1	302	A
25	1	303	G
25	1	311	U
25	1	322	A
25	1	323	C
25	1	325	A
25	1	327	G
25	1	328	G
25	1	331	G
25	1	352	A
25	1	354	A
25	1	361	U
25	1	366	G
25	1	372	A
25	1	373	A
25	1	389	A

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Mol	Chain	Res	Type
25	1	395	U
25	1	398	C
25	1	401	U
25	1	404	U
25	1	407	G
25	1	411	A
25	1	415	U
25	1	416	G
25	1	419	U
25	1	432	G
25	1	447	A
25	1	457	G
25	1	459	C
25	1	475	A
25	1	481	C
25	1	482	U
25	1	483	C
25	1	484	U
25	1	486	G
25	1	491	C
25	1	502	C
25	1	519	G
25	1	526	A
25	1	527	G
25	1	529	A
25	1	546	A
25	1	549	U
25	1	550	A
25	1	552	A
25	1	553	A
25	1	554	C
25	1	567	G
25	1	575	G
25	1	576	U
25	1	577	A
25	1	578	G
25	1	583	A
25	1	592	A
25	1	594	G
25	1	606	G
25	1	615	A
25	1	616	G

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Mol	Chain	Res	Type
25	1	617	A
25	1	618	A
25	1	629	A
25	1	630	G
25	1	646	A
25	1	650	U
25	1	657	U
25	1	658	A
25	1	659	A
25	1	660	A
25	1	661	U
25	1	682	A
25	1	690	U
25	1	698	U
25	1	699	U
25	1	731	U
25	1	758	G
25	1	759	U
25	1	760	A
25	1	765	U
25	1	768	A
25	1	772	A
25	1	775	A
25	1	792	U
25	1	797	A
25	1	798	G
25	1	809	A
25	1	820	G
25	1	822	G
25	1	827	A
25	1	829	U
25	1	834	A
25	1	835	U
25	1	837	G
25	1	850	G
25	1	857	C
25	1	872	U
25	1	900	G
25	1	914	G
25	1	923	A
25	1	945	A
25	1	946	A

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Mol	Chain	Res	Type
25	1	948	U
25	1	955	A
25	1	970	U
25	1	977	A
25	1	985	A
25	1	989	A
25	1	990	G
25	1	1003	A
25	1	1005	G
25	1	1018	A
25	1	1024	A
25	1	1027	A
25	1	1040	A
25	1	1056	U
25	1	1057	A
25	1	1066	G
25	1	1067	U
25	1	1070	A
25	1	1077	U
25	1	1078	G
25	1	1084	U
25	1	1173	A
25	1	1176	U
25	1	1179	C
25	1	1192	A
25	1	1199	A
25	1	1200	A
25	1	1213	C
25	1	1214	C
25	1	1215	U
25	1	1216	U
25	1	1220	A
25	1	1287	U
25	1	1291	A
25	1	1309	G
25	1	1310	A
25	1	1312	A
25	1	1313	G
25	1	1321	A
25	1	1323	A
25	1	1337	A
25	1	1361	G

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Mol	Chain	Res	Type
25	1	1362	C
25	1	1363	U
25	1	1402	A
25	1	1405	G
25	1	1416	U
25	1	1421	A
25	1	1422	A
25	1	1431	U
25	1	1452	C
25	1	1453	G
25	1	1454	U
25	1	1462	G
25	1	1463	A
25	1	1464	U
25	1	1465	G
25	1	1466	G
25	1	1471	A
25	1	1472	C
25	1	1489	A
25	1	1490	G
25	1	1491	C
25	1	1492	G
25	1	1493	U
25	1	1497	A
25	1	1501	G
25	1	1514	A
25	1	1515	G
25	1	1516	C
25	1	1519	U
25	1	1557	C
25	1	1561	G
25	1	1564	G
25	1	1565	U
25	1	1566	G
25	1	1567	A
25	1	1568	U
25	1	1569	G
25	1	1570	G
25	1	1578	A
25	1	1579	C
25	1	1591	G
25	1	1593	G

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Mol	Chain	Res	Type
25	1	1595	C
25	1	1605	A
25	1	1606	C
25	1	1613	G
25	1	1616	A
25	1	1625	U
25	1	1626	A
25	1	1629	U
25	1	1630	A
25	1	1632	A
25	1	1635	A
25	1	1652	A
25	1	1654	A
25	1	1655	C
25	1	1657	G
25	1	1662	A
25	1	1690	A
25	1	1691	G
25	1	1692	C
25	1	1718	G
25	1	1737	U
25	1	1738	C
25	1	1755	U
25	1	1756	U
25	1	1758	A
25	1	1759	G
25	1	1760	G
25	1	1764	A
25	1	1765	A
25	1	1790	G
25	1	1791	G
25	1	1800	A
25	1	1827	C
25	1	1828	U
25	1	1835	U
25	1	1836	A
25	1	1843	U
25	1	1865	C
25	1	1875	A
25	1	1893	A
25	1	1904	A
25	1	1912	A

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Mol	Chain	Res	Type
25	1	1915	G
25	1	1922	C
25	1	1933	G
25	1	1957	G
25	1	1965	A
25	1	1969	C
25	1	1982	U
25	1	1990	C
25	1	1994	C
25	1	1997	A
25	1	1998	A
25	1	1999	G
25	1	2009	U
25	1	2020	U
25	1	2040	A
25	1	2058	A
25	1	2059	G
25	1	2060	A
25	1	2070	C
25	1	2078	A
25	1	2079	G
25	1	2080	G
25	1	2082	C
25	1	2083	G
25	1	2086	A
25	1	2087	A
25	1	2088	G
25	1	2089	A
25	1	2096	G
25	1	2126	C
25	1	2218	G
25	1	2220	U
25	1	2222	U
25	1	2223	C
25	1	2230	G
25	1	2231	C
25	1	2237	U
25	1	2239	A
25	1	2240	U
25	1	2252	A
25	1	2265	G
25	1	2266	G

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Mol	Chain	Res	Type
25	1	2295	A
25	1	2310	C
25	1	2321	C
25	1	2322	C
25	1	2323	U
25	1	2324	C
25	1	2327	A
25	1	2328	A
25	1	2329	U
25	1	2332	U
25	1	2333	U
25	1	2334	G
25	1	2336	A
25	1	2337	A
25	1	2338	A
25	1	2339	U
25	1	2344	C
25	1	2347	A
25	1	2349	A
25	1	2361	U
25	1	2362	A
25	1	2368	G
25	1	2372	G
25	1	2374	C
25	1	2377	C
25	1	2378	G
25	1	2398	G
25	1	2410	G
25	1	2412	C
25	1	2418	G
25	1	2419	A
25	1	2420	U
25	1	2433	C
25	1	2434	A
25	1	2448	G
25	1	2449	C
25	1	2450	U
25	1	2452	A
25	1	2456	G
25	1	2457	A
25	1	2468	C
25	1	2475	A

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Mol	Chain	Res	Type
25	1	2477	A
25	1	2496	A
25	1	2501	U
25	1	2503	A
25	1	2509	A
25	1	2529	G
25	1	2530	A
25	1	2531	U
25	1	2532	G
25	1	2540	A
25	1	2541	U
25	1	2545	A
25	1	2553	G
25	1	2554	C
25	1	2556	G
25	1	2557	U
25	1	2574	U
25	1	2581	U
25	1	2593	A
25	1	2594	G
25	1	2599	A
25	1	2600	C
25	1	2601	G
25	1	2603	G
25	1	2604	A
25	1	2605	G
25	1	2606	C
25	1	2612	U
25	1	2613	C
25	1	2629	A
25	1	2630	G
25	1	2636	U
25	1	2637	C
25	1	2638	C
25	1	2640	U
25	1	2656	A
25	1	2657	G
25	1	2673	C
25	1	2695	G
25	1	2716	U
25	1	2718	C
25	1	2741	G

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Mol	Chain	Res	Type
25	1	2753	U
25	1	2760	A
25	1	2771	G
25	1	2775	A
25	1	2779	C
25	1	2784	A
25	1	2791	A
25	1	2792	A
25	1	2805	A
25	1	2806	U
25	1	2817	A
25	1	2818	A
25	1	2819	C
25	1	2820	U
25	1	2822	C
25	1	2823	G
25	1	2824	G
25	1	2828	U
25	1	2840	A
25	1	2841	A
25	1	2845	G
25	1	2850	G
25	1	2853	U
25	1	2887	G
25	1	2892	G
25	1	2900	C
25	1	2913	G
25	1	2917	U
25	1	2918	A
25	1	2919	A
26	2	3	U
26	2	4	G
26	2	9	C
26	2	10	U
26	2	11	A
26	2	13	A
26	2	18	G
26	2	19	G
26	2	23	U
26	2	24	C
26	2	25	A
26	2	35	C

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Mol	Chain	Res	Type
26	2	39	G
26	2	42	G
26	2	43	A
26	2	44	A
26	2	47	C
26	2	48	A
26	2	54	U
26	2	55	A
26	2	57	G
26	2	58	C
26	2	61	C
26	2	71	A
26	2	85	U
26	2	86	A
26	2	94	C
26	2	100	U
26	2	103	A
26	2	104	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1	41	A
25	1	63	U
25	1	101	G
25	1	137	G
25	1	205	U
25	1	229	A
25	1	234	C
25	1	252	C
25	1	458	A
25	1	482	U
25	1	525	A
25	1	659	A
25	1	660	A
25	1	797	A
25	1	834	A
25	1	1066	G
25	1	1077	U
25	1	1361	G
25	1	1362	C
25	1	1462	G

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Mol	Chain	Res	Type
25	1	1463	A
25	1	1464	U
25	1	1465	G
25	1	1514	A
25	1	1515	G
25	1	1564	G
25	1	1565	U
25	1	1566	G
25	1	1568	U
25	1	1864	C
25	1	2078	A
25	1	2087	A
25	1	2320	C
25	1	2322	C
25	1	2323	U
25	1	2337	A
25	1	2377	C
25	1	2418	G
25	1	2433	C
25	1	2449	C
25	1	2504	C
25	1	2556	G
25	1	2599	A
25	1	2600	C
25	1	2603	G
25	1	2637	C
25	1	2783	U
25	1	2827	A
26	2	3	U
26	2	57	G
26	2	84	U
26	2	85	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
28	ZC0	1	3001	-	30,32,32	3.02	10 (33%)	37,46,46	2.74	16 (43%)

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
28	ZC0	1	3001	-	-	6/13/35/35	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	3001	ZC0	C20-N16	8.99	1.46	1.36
28	1	3001	ZC0	C04-C05	7.34	1.52	1.35
28	1	3001	ZC0	O19-C20	6.64	1.44	1.35
28	1	3001	ZC0	C04-N03	4.91	1.50	1.36
28	1	3001	ZC0	O26-N25	-3.61	1.36	1.41
28	1	3001	ZC0	C17-N16	-3.34	1.41	1.47
28	1	3001	ZC0	C02-N03	3.16	1.50	1.47
28	1	3001	ZC0	O19-C18	-2.79	1.42	1.46
28	1	3001	ZC0	O07-C06	-2.71	1.18	1.23
28	1	3001	ZC0	C17-C18	-2.07	1.49	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	3001	ZC0	C17-C18-C22	-6.27	106.26	113.38
28	1	3001	ZC0	C17-N16-C20	-5.95	106.77	111.17
28	1	3001	ZC0	C18-C17-N16	5.38	106.93	101.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	3001	ZC0	C04-C05-C06	-4.83	117.53	120.89
28	1	3001	ZC0	C09-C08-C13	4.36	119.93	115.25
28	1	3001	ZC0	C18-O19-C20	-4.27	106.69	110.10
28	1	3001	ZC0	O19-C20-N16	-3.92	106.62	109.92
28	1	3001	ZC0	O19-C20-O21	3.81	126.86	122.40
28	1	3001	ZC0	C05-C04-N03	-3.60	118.92	123.40
28	1	3001	ZC0	N23-C24-N25	3.07	126.63	123.88
28	1	3001	ZC0	O19-C18-C17	3.05	107.45	104.50
28	1	3001	ZC0	C17-N16-C11	3.04	126.94	121.37
28	1	3001	ZC0	O26-N25-C24	3.03	106.87	103.71
28	1	3001	ZC0	C28-C24-N25	-2.84	107.65	112.20
28	1	3001	ZC0	O21-C20-N16	-2.47	126.52	128.80
28	1	3001	ZC0	C10-C09-C08	-2.29	119.94	123.34

There are no chirality outliers.

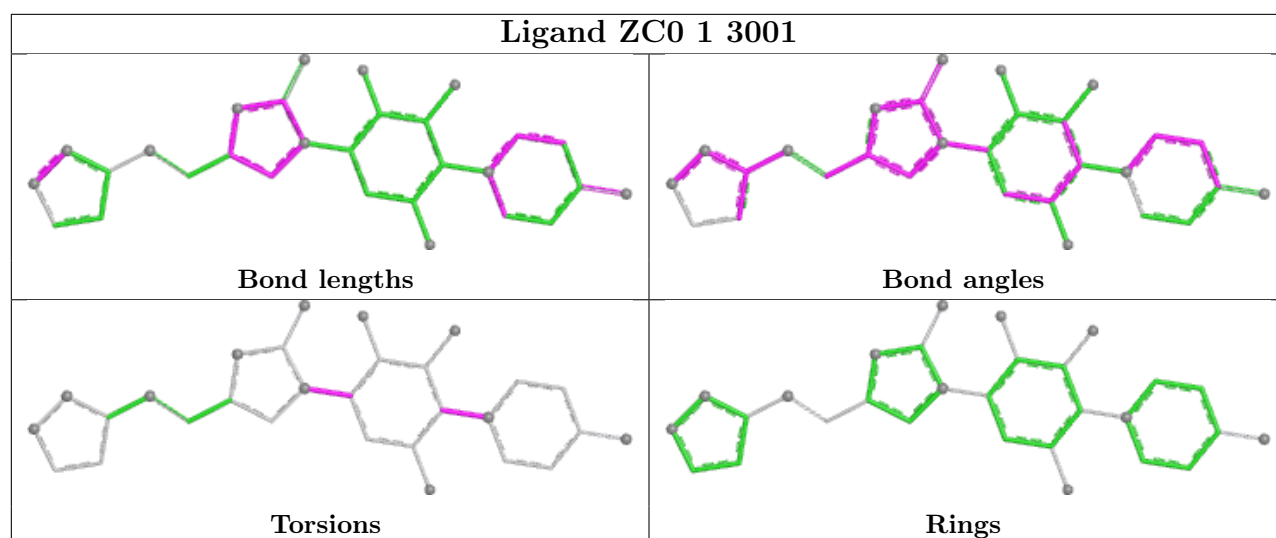
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	1	3001	ZC0	C09-C08-N03-C02
28	1	3001	ZC0	C13-C08-N03-C02
28	1	3001	ZC0	C10-C11-N16-C20
28	1	3001	ZC0	C12-C11-N16-C17
28	1	3001	ZC0	C12-C11-N16-C20
28	1	3001	ZC0	C10-C11-N16-C17

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

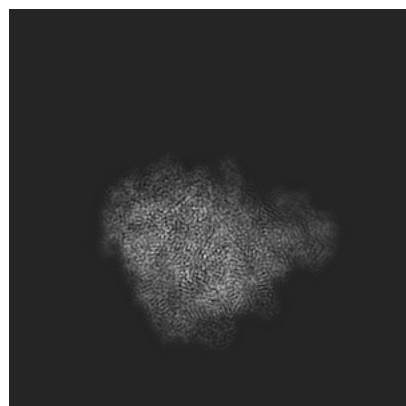
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21872. These allow visual inspection of the internal detail of the map and identification of artifacts.

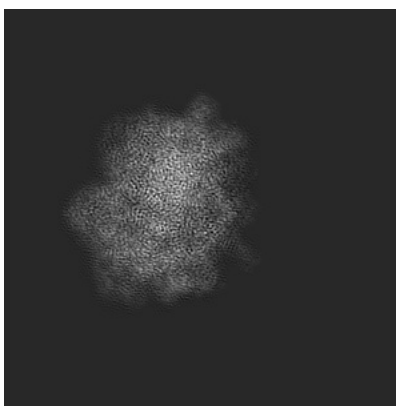
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

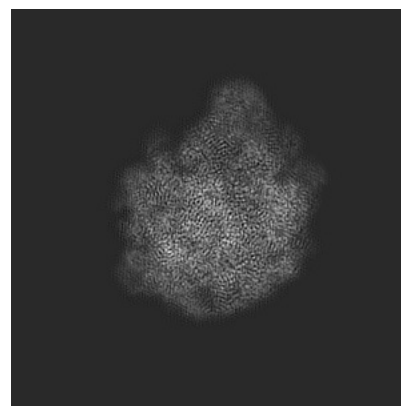
6.1.1 Primary map



X

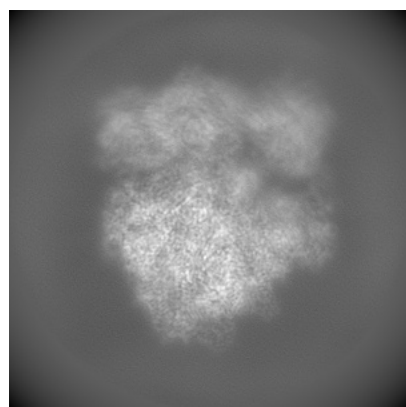


Y

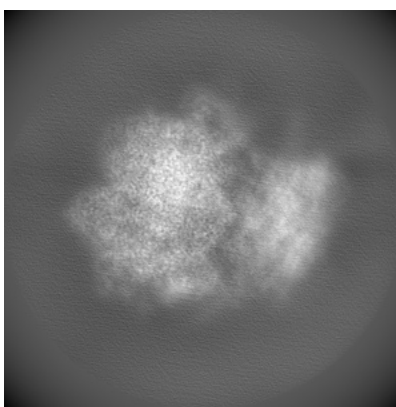


Z

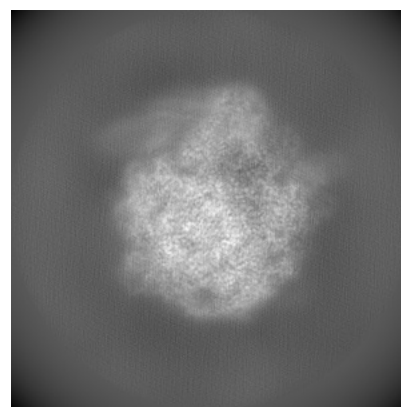
6.1.2 Raw map



X



Y

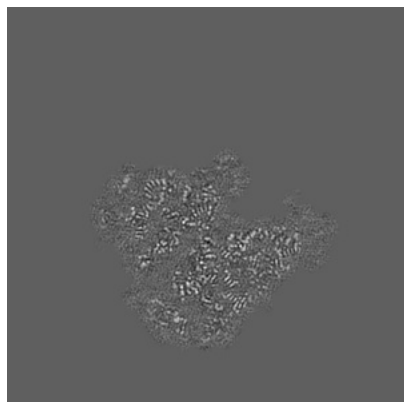


Z

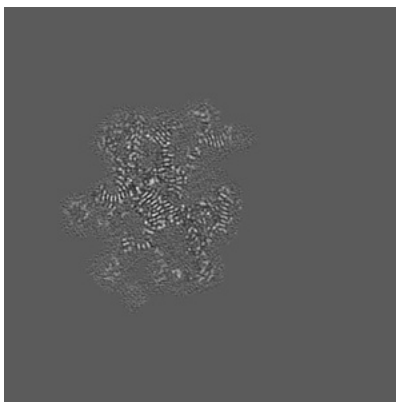
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

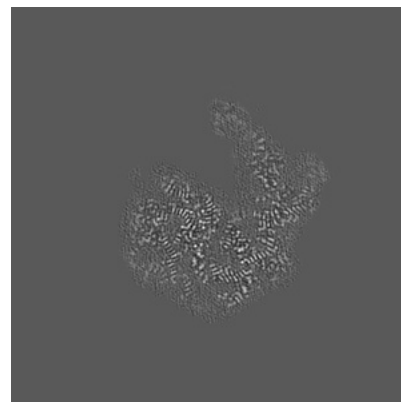
6.2.1 Primary map



X Index: 208

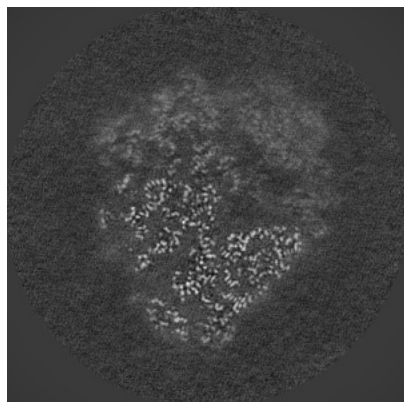


Y Index: 208

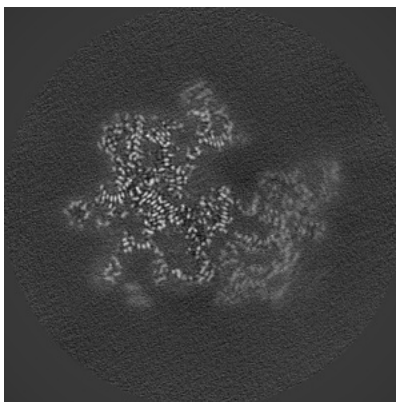


Z Index: 208

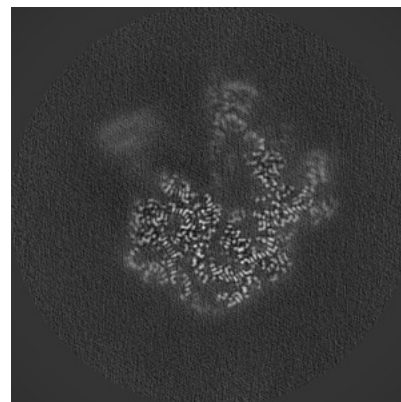
6.2.2 Raw map



X Index: 208



Y Index: 208

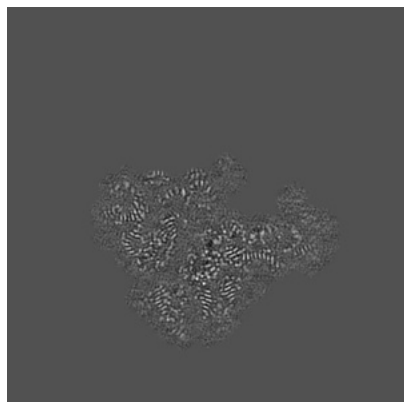


Z Index: 208

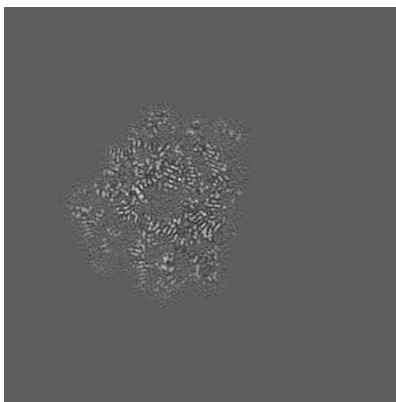
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

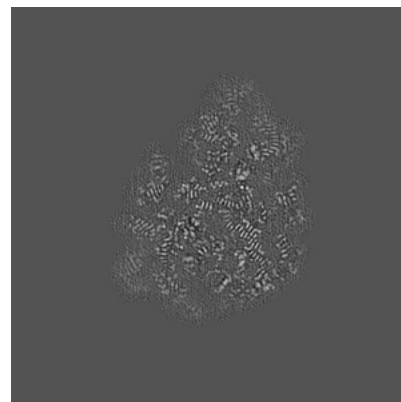
6.3.1 Primary map



X Index: 216

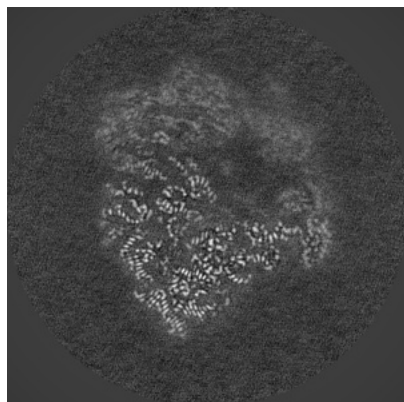


Y Index: 186

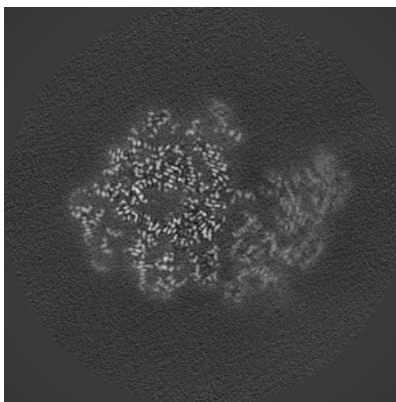


Z Index: 174

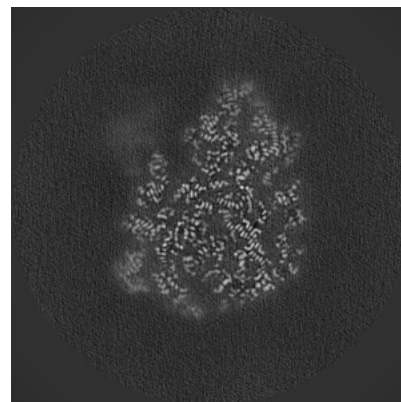
6.3.2 Raw map



X Index: 223



Y Index: 186

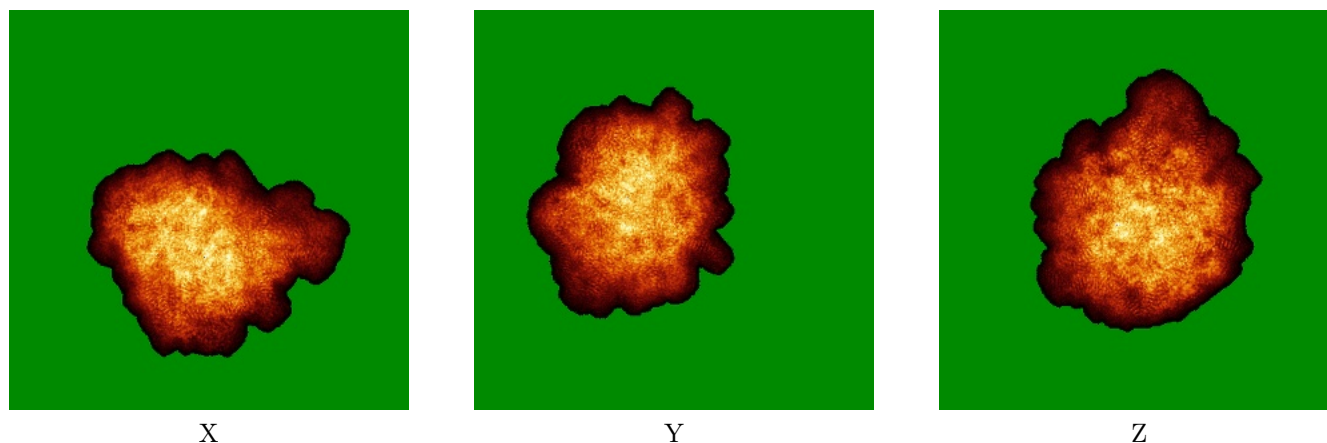


Z Index: 174

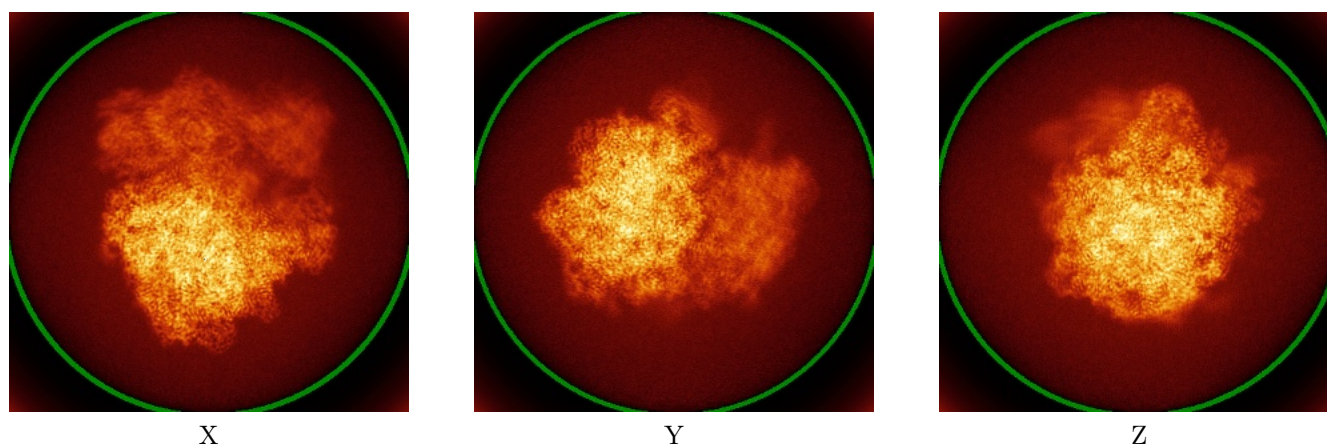
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

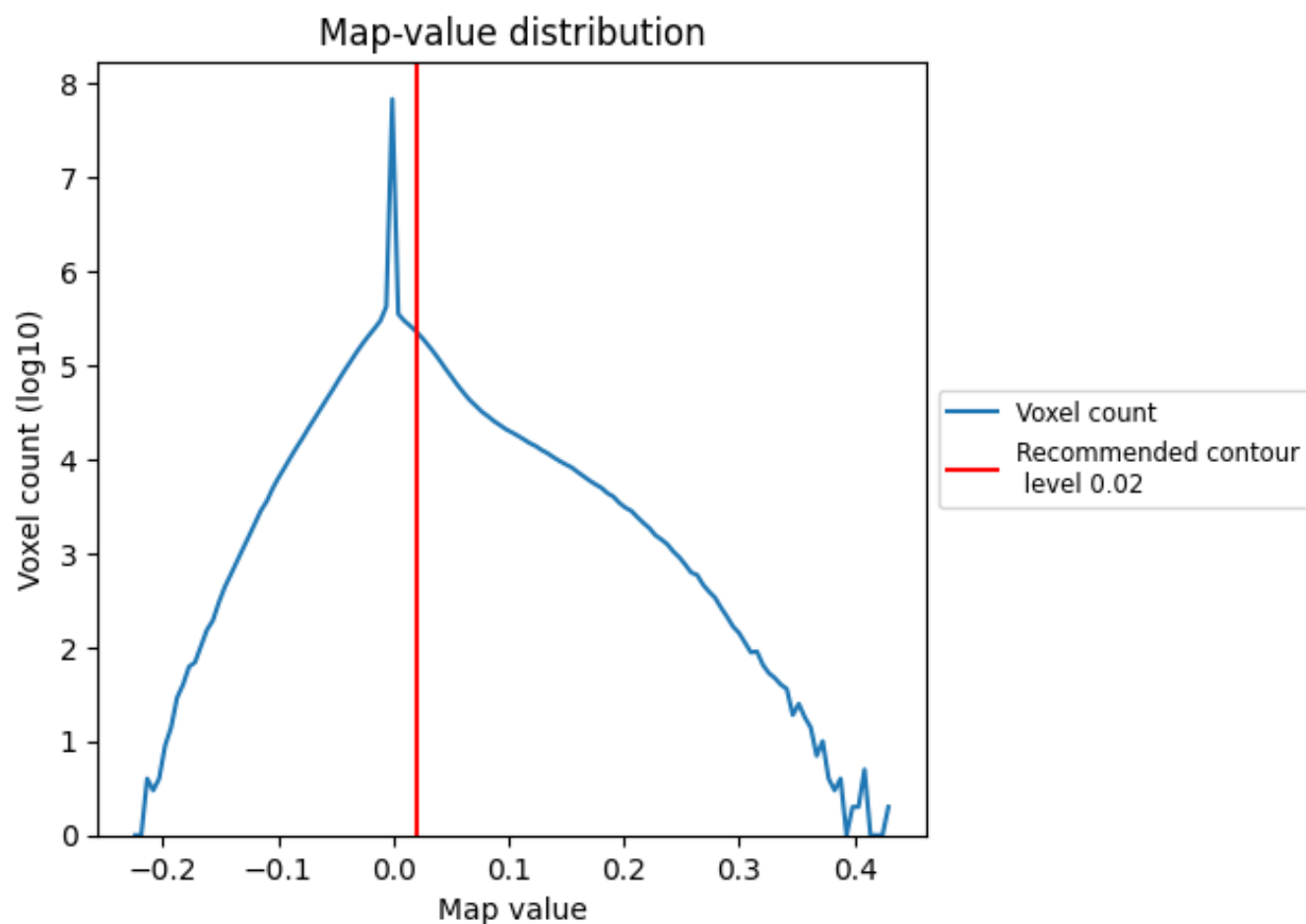
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

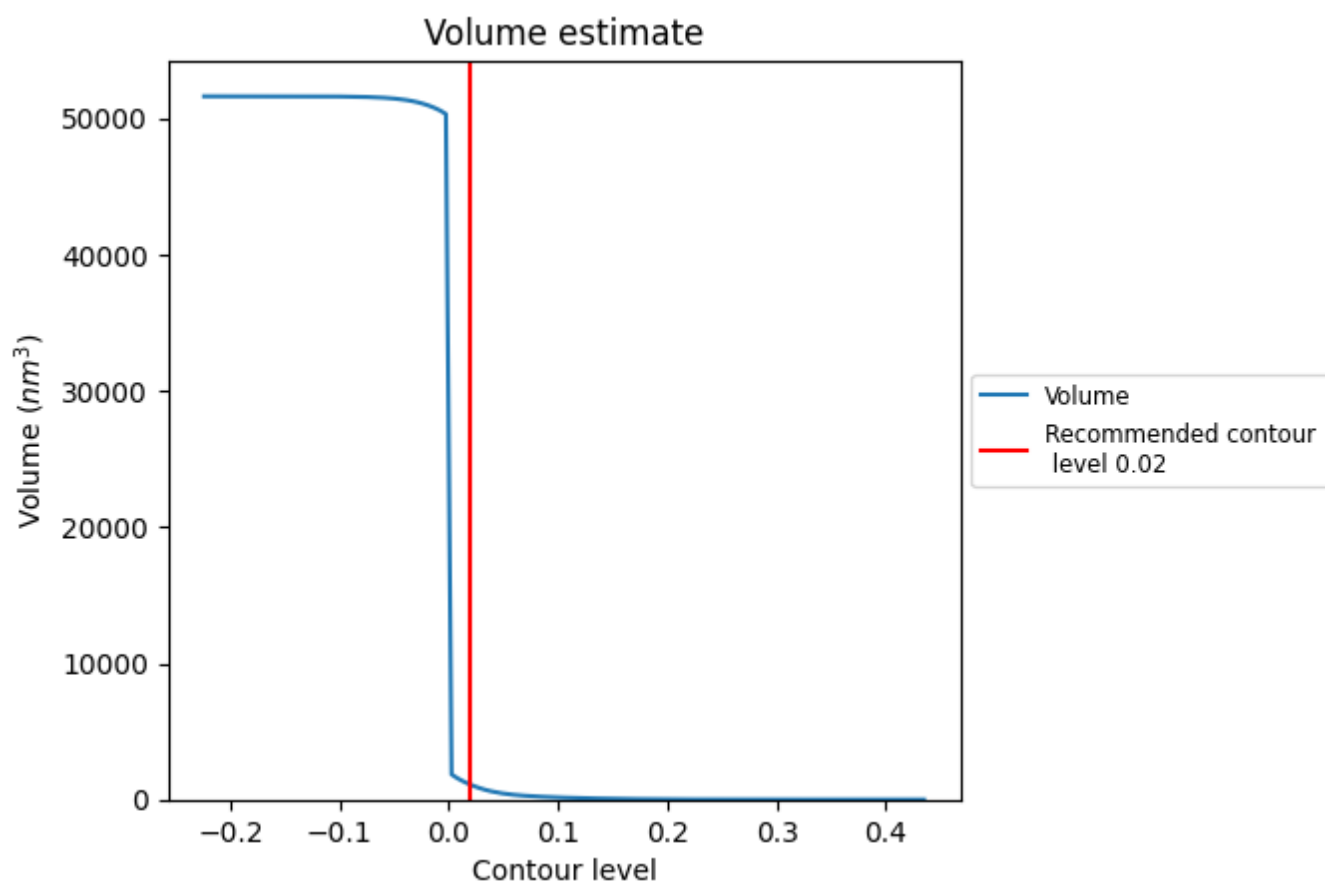
This section contains the results of statistical analysis of the map.

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.

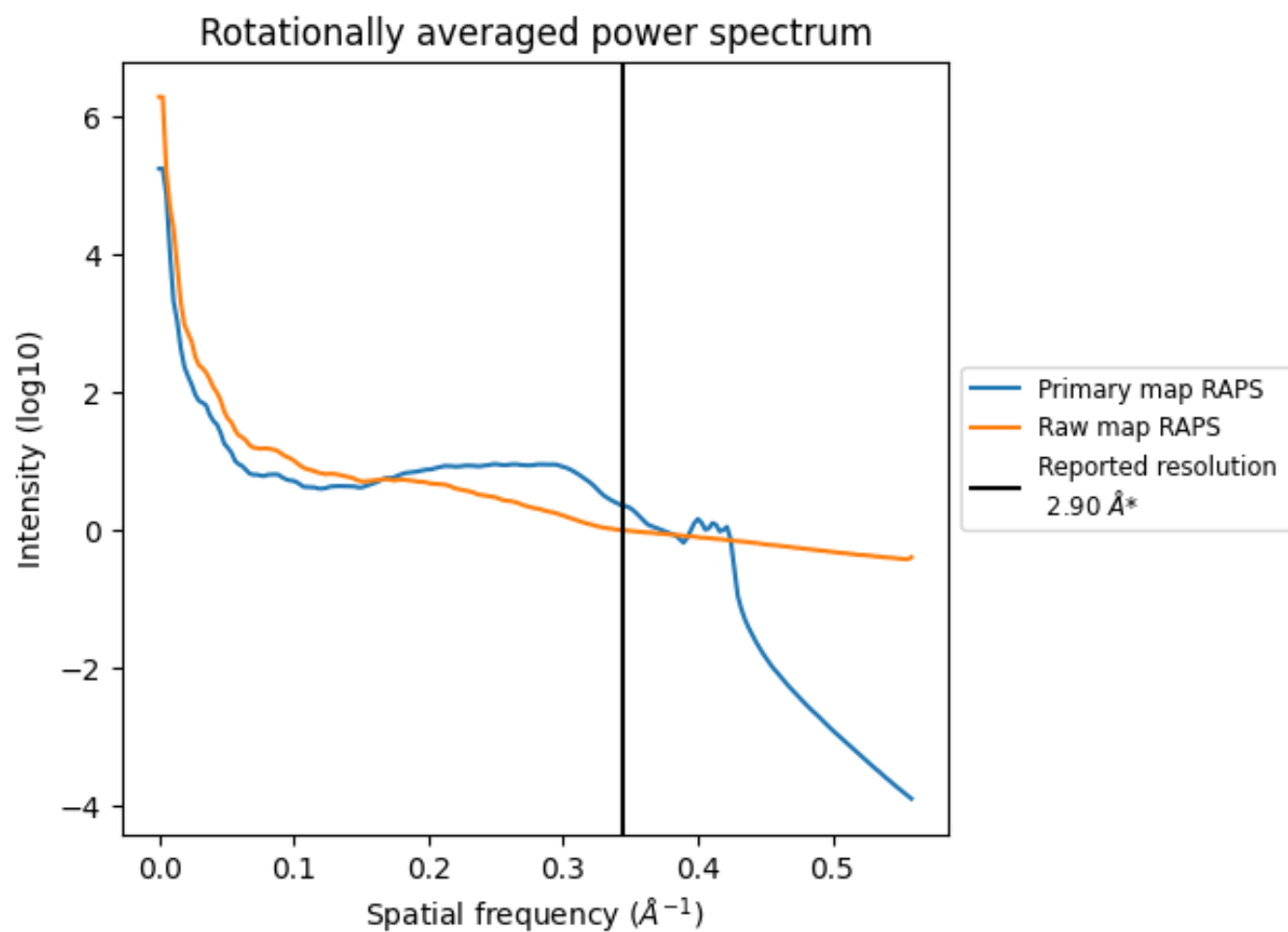
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1087 nm³; this corresponds to an approximate mass of 982 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 ⓘ

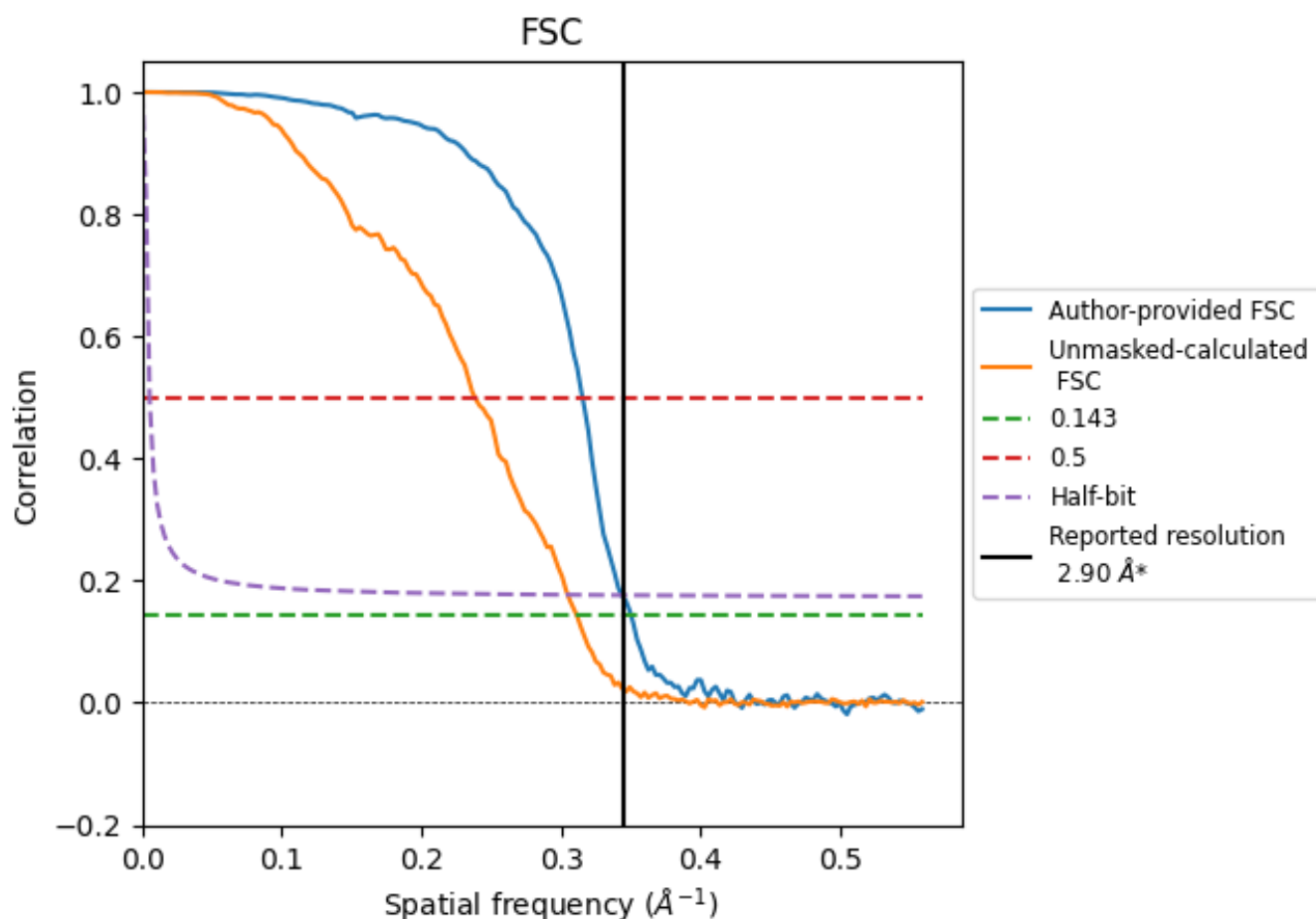


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.17	2.91
Unmasked-calculated*	3.21	4.19	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.9 by more than 10 %

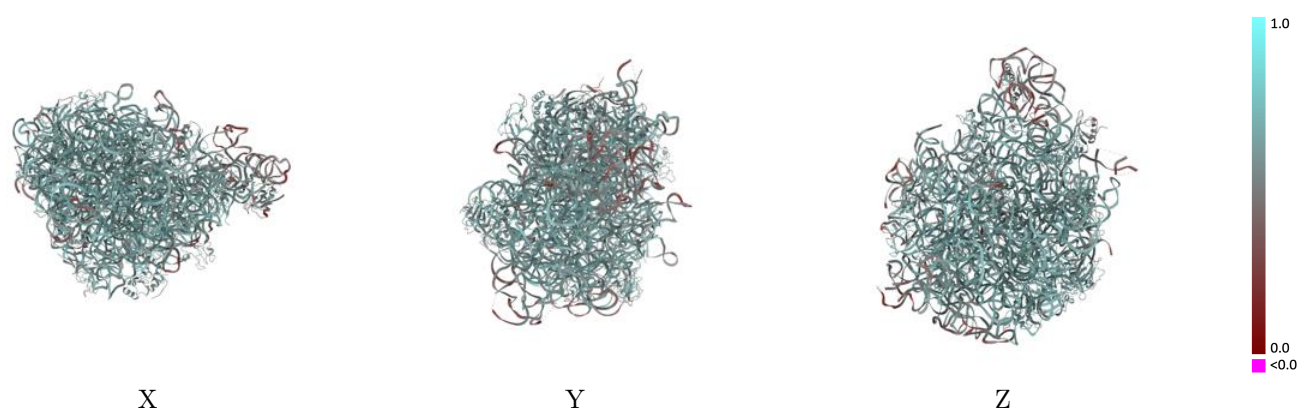
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21872 and PDB model 6WQN. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

This section was not generated.

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

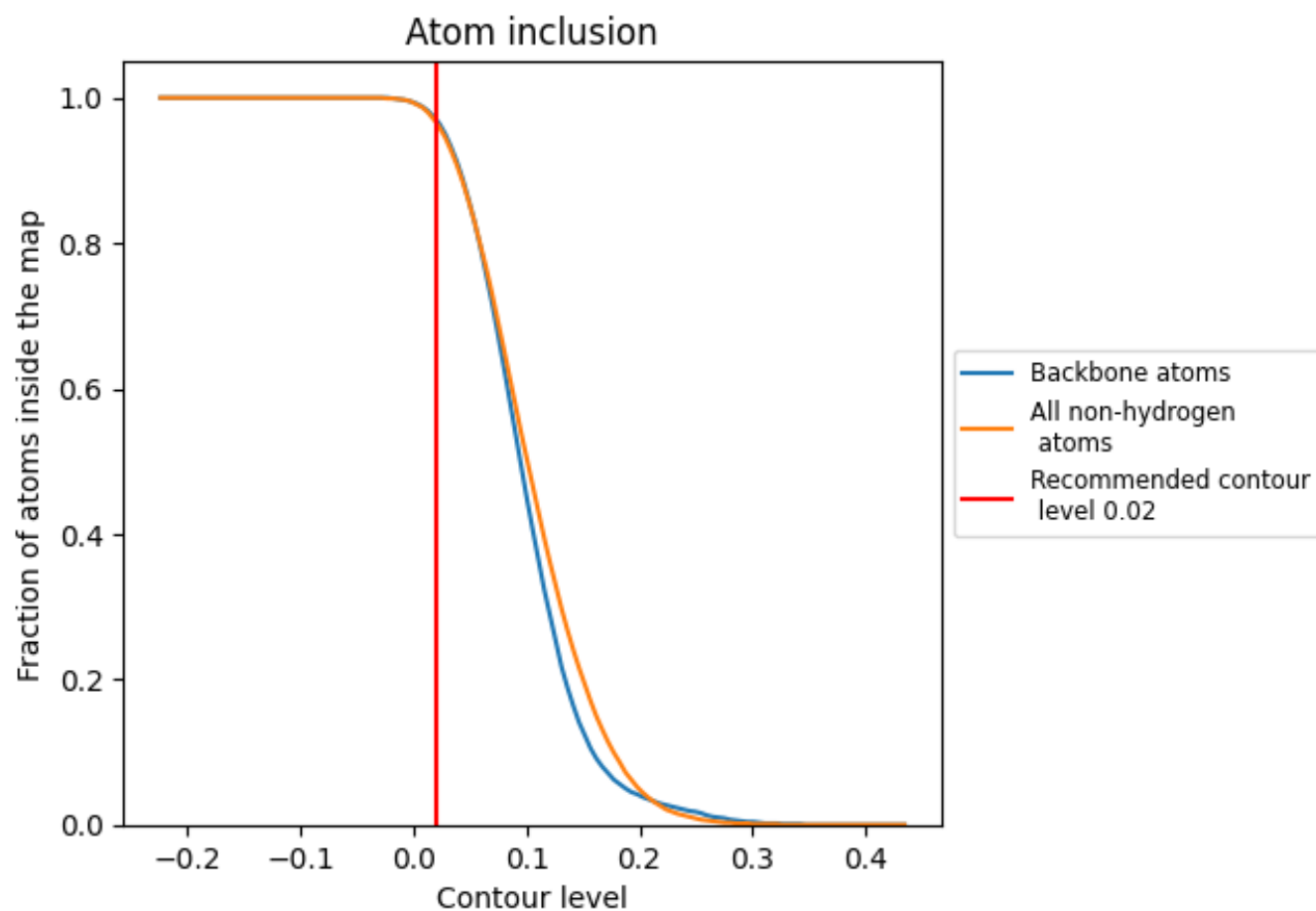


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.6010
1	 0.9680	 0.6040
2	 0.9400	 0.4950
A	 0.9660	 0.5960
B	 0.9690	 0.6230
C	 0.9920	 0.6480
D	 0.9530	 0.6090
E	 0.9830	 0.6390
F	 0.9560	 0.5870
G	 0.9290	 0.5440
H	 0.9030	 0.5040
I	 0.9900	 0.6410
J	 0.9460	 0.5890
K	 0.9340	 0.5600
L	 0.9750	 0.6200
M	 0.9650	 0.6180
N	 0.9690	 0.6140
O	 0.9440	 0.5800
P	 0.9890	 0.6630
Q	 0.9960	 0.6600
R	 0.9790	 0.6000
S	 0.9700	 0.6090
V	 0.9860	 0.6340
W	 0.9710	 0.6150
X	 0.9620	 0.6010
Y	 0.9740	 0.6160
Z	 0.9640	 0.6190
a	 0.9340	 0.5200

