



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:36 PM UTC

PDB ID : 8PV3 / pdb_00008pv3
EMDB ID : EMD-17952
Title : Chaetomium thermophilum pre-60S State 9 - pre-5S rotation - immature
H68/H69 - composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.80 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:

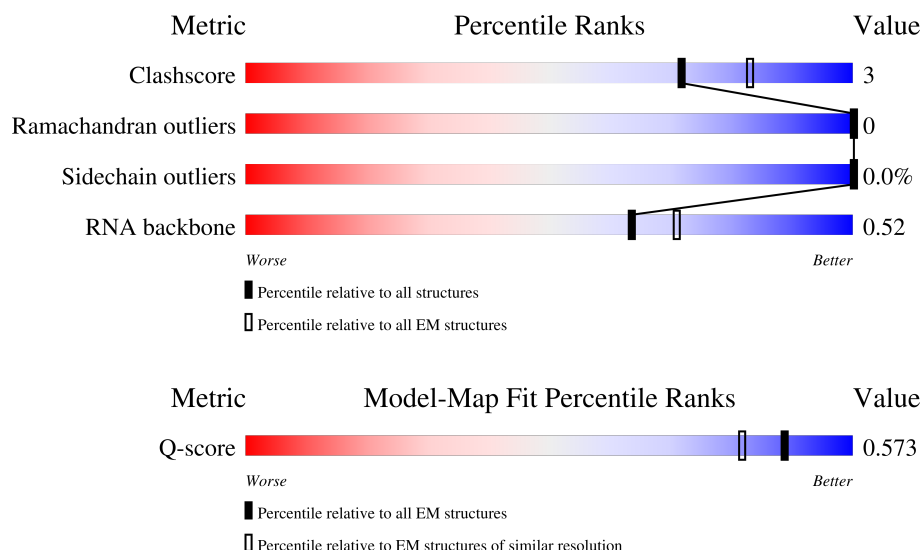
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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	11806 (2.30 - 3.30)

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	C1	3342	
2	C2	156	
3	C3	162	

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Mol	Chain	Length	Quality of chain
4	C4	119	
5	CB	391	
6	CF	270	
7	CH	661	
8	CI	414	
9	CJ	679	
10	CK	261	
11	CL	558	
12	CM	249	
12	LF	249	
13	CN	246	
14	CO	120	
15	CQ	225	
16	Cb	117	
17	Cd	627	
18	Ce	443	
19	Cf	350	
20	Cg	202	
21	Ch	517	
22	Cz	123	
23	LA	254	
24	LB	392	
25	LC	365	
26	LD	304	
27	LE	200	

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Mol	Chain	Length	Quality of chain
28	LG	262	
29	LH	229	
30	LJ	173	
31	LK	165	
32	LL	213	
33	LM	142	
34	LN	203	
35	LO	204	
36	LP	187	
37	LQ	213	
38	LR	2898	
39	LS	174	
40	LT	160	
41	LU	127	
42	LV	139	
43	LX	156	
44	LY	138	
45	LZ	135	
46	La	149	
47	Lc	108	
48	Ld	120	
49	Le	131	
50	Lf	109	
51	Lg	119	
52	Lh	935	

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Mol	Chain	Length	Quality of chain
53	Li	110	
54	Lj	95	
55	Lk	94	
56	Ll	51	
57	Lp	92	
58	Lq	147	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 155443 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	2998	Total	C	N	O	P	0	0
			64177	28664	11614	20901	2998		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	156	Total	C	N	O	P	0	0
			3319	1484	589	1090	156		

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C3	82	Total	C	N	O	P	0	0
			1754	780	316	576	82		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C4	119	Total	C	N	O	P	0	0
			2536	1131	453	833	119		

- Molecule 5 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CB	267	Total	C	N	O	S	0	0
			2119	1359	373	384	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CF	245	Total	C	N	O	S	0	0
			1934	1215	350	360	9		

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CH	627	Total	C	N	O	S	0	0
			5063	3181	924	939	19		

- Molecule 8 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CI	152	Total	C	N	O	S	0	0
			1234	791	230	208	5		

- Molecule 9 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CJ	382	Total	C	N	O	S	0	0
			3116	2008	548	550	10		

- Molecule 10 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CK	237	Total	C	N	O	S	0	0
			1903	1198	368	333	4		

- Molecule 11 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CL	79	Total	C	N	O	S	0	0
			622	389	125	108			

- Molecule 12 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CM	217	Total	C	N	O	S	0	0
			1773	1144	329	297	3		
12	LF	248	Total	C	N	O	S	0	0
			2023	1297	377	346	3		

- Molecule 13 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CN	246	Total	C	N	O	S	0	0
			1853	1156	322	368	7		

- Molecule 14 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 15 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CQ	183	Total	C	N	O	S	0	0
			1480	925	304	241	10		

- Molecule 16 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Cb	101	Total	C	N	O	S	0	0
			830	517	161	148	4		

- Molecule 17 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cd	462	Total	C	N	O	S	0	0
			3691	2350	671	659	11		

- Molecule 18 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ce	262	Total	C	N	O	S	0	0
			2148	1337	413	394	4		

- Molecule 19 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Cf	285	Total	C	N	O	S	0	0
			2282	1443	417	401	21		

- Molecule 20 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Cg	188	Total	C	N	O	S	0	0
			1478	924	283	270	1		

- Molecule 21 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ch	485	Total	C	N	O	S	1	0
			3812	2396	696	710	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	engineered mutation	UNP G0SC29

- Molecule 22 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Cz	101	Total	C	N	O	S	0	0
			869	541	180	144	4		

- Molecule 23 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LA	178	Total	C	N	O	S	0	0
			1365	863	260	240	2		

- Molecule 24 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LB	389	Total	C	N	O	S	0	0
			3104	1973	579	539	13		

- Molecule 25 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LC	363	Total	C	N	O	S	0	0
			2751	1737	527	478	9		

- Molecule 26 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LD	286	Total	C	N	O	S	0	0
			2266	1434	407	422	3		

- Molecule 27 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LE	191	Total	C	N	O	S	0	0
			1477	944	267	263	3		

- Molecule 28 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LG	235	Total	C	N	O	S	0	0
			1889	1210	350	324	5		

- Molecule 29 is a protein called 60S ribosomal protein L9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LH	190	Total	C	N	O	S	0	0
			1495	949	268	272	6		

- Molecule 30 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LJ	169	Total	C	N	O	S	0	0
			1357	850	266	235	6		

- Molecule 31 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LK	158	Total	C	N	O	S	0	0
			1184	743	215	224	2		

- Molecule 32 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 33 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 34 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 35 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 36 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 37 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LQ	150	Total	C	N	O	S	0	0
			1181	745	234	200	2		

- Molecule 38 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LR	155	Total	C	N	O	S	0	0
			1241	772	262	203	4		

- Molecule 39 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LS	174	Total	C	N	O	S	0	0
			1426	917	266	238	5		

- Molecule 40 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LT	129	Total	C	N	O	S	0	0
			1027	651	195	179	2		

- Molecule 41 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LU	105	Total	C	N	O	S	0	0
			846	548	146	151	1		

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LV	135	Total	C	N	O	S	0	0
			991	630	184	170	7		

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LX	145	Total	C	N	O	S	0	0
			1133	723	211	199			

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LY	133	Total	C	N	O	S	0	0
			1056	658	213	183	2		

- Molecule 45 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LZ	135	Total	C	N	O	S	0	0
			1112	713	207	188	4		

- Molecule 46 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	La	108	Total	C	N	O	S	0	0
			872	556	168	147	1		

- Molecule 47 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lc	95	Total	C	N	O	S	0	0
			705	449	122	129	5		

- Molecule 48 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ld	110	Total	C	N	O	S	0	0
			875	555	171	148	1		

- Molecule 49 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Le	126	Total	C	N	O	S	0	0
			1017	640	208	163	6		

- Molecule 50 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 51 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lg	118	Total	C	N	O	S	0	0
			914	567	186	157	4		

- Molecule 52 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Lh	122	Total	C	N	O	0	0
			1003	637	198	168		

- Molecule 53 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Li	101	Total	C	N	O	S	0	0
			827	509	181	136	1		

- Molecule 54 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Lj	88	Total	C	N	O	S	0	0
			698	427	154	112	5		

- Molecule 55 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

- Molecule 56 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Ll	50	Total	C	N	O	0	0
			436	275	97	64		

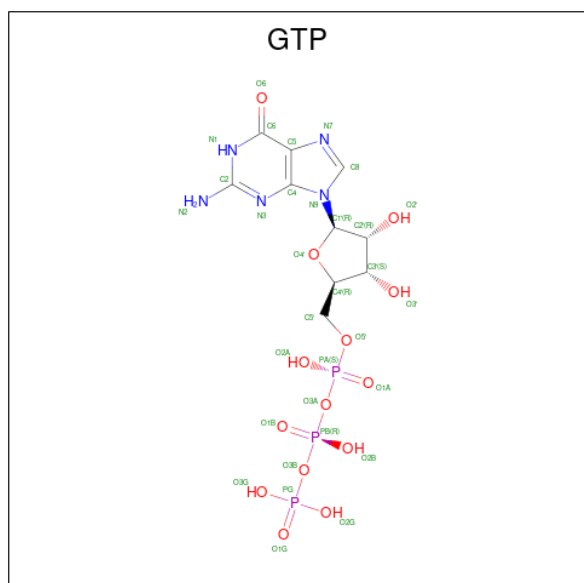
- Molecule 57 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lp	91	Total	C	N	O	S	0	0
			698	430	138	124	6		

- Molecule 58 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Lq	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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Mol	Chain	Residues	Atoms					AltConf
59	Cd	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	CH	1	Total	Mg	0
			1	1	
60	Cd	2	Total	Mg	0
			2	2	

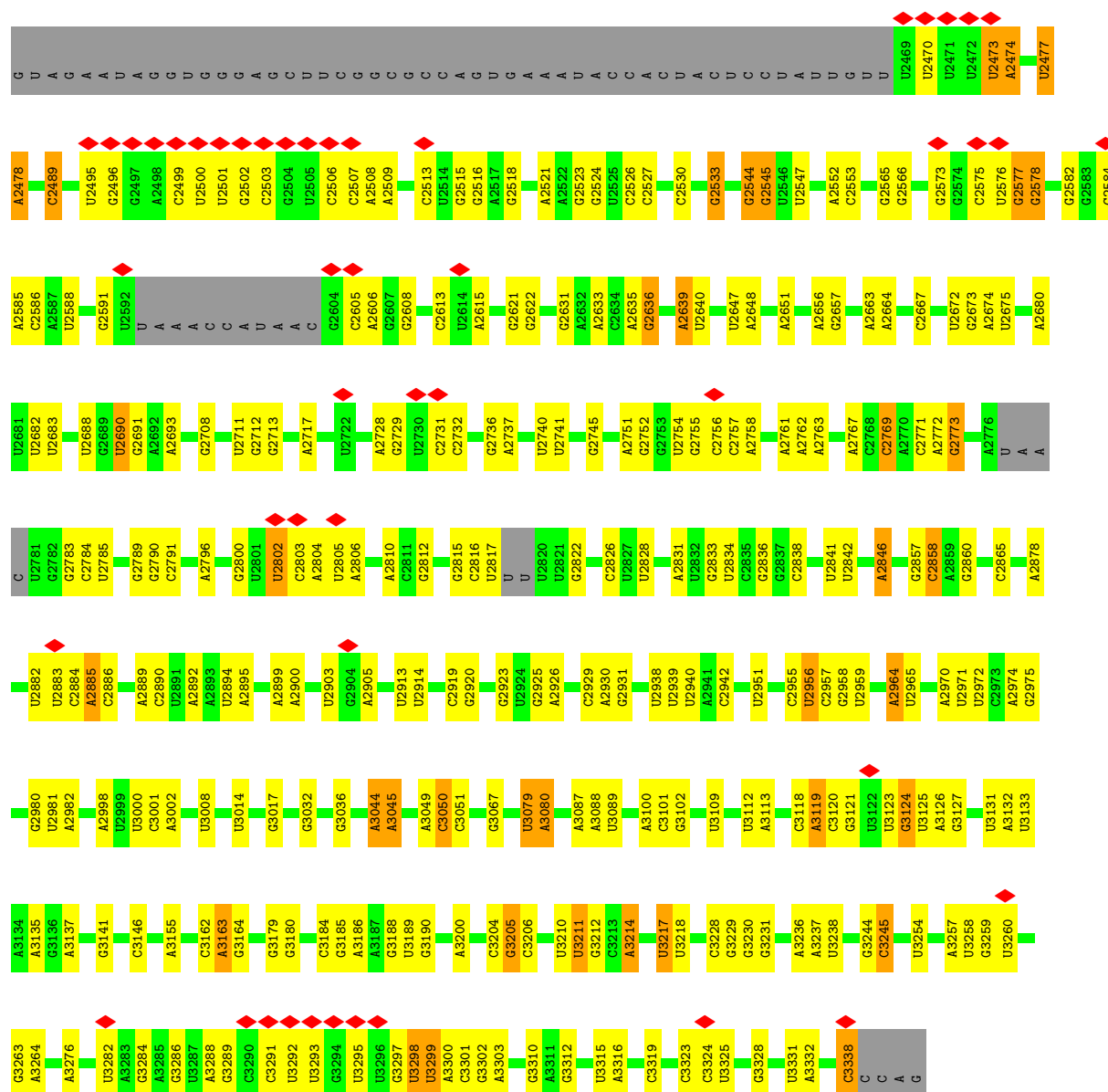
- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	CQ	1	Total	Zn	0
			1	1	
61	Cb	1	Total	Zn	0
			1	1	
61	Lg	1	Total	Zn	0
			1	1	
61	Lj	1	Total	Zn	0
			1	1	
61	Lp	1	Total	Zn	0
			1	1	

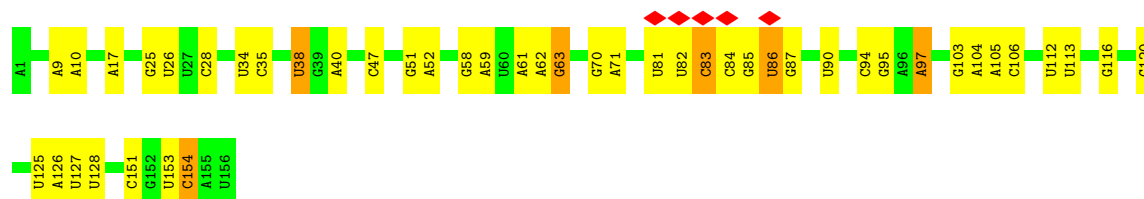
- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	CH	1	Total	O	0
			1	1	
62	Cd	2	Total	O	0
			2	2	

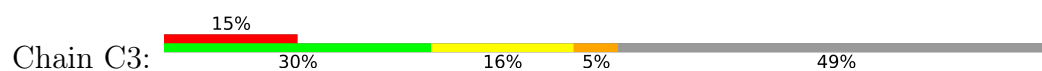
G2340	U2103	C	G1858	G1751	A1599	G1476	G1337	G1216	G1123	A1036
A2348	U2104	U	A1889	G1758	A1604	U1477	A1338	G1219	G1127	A1037
U2351	A2105	U	U1860	G1760	G1604	C1480	U1339	G1220	U1127	A1038
C2355	A2112	C	A1866	G1761	U1609	A1481	G1345	A1223	G1132	U1039
G2356	G2120	A	U1867	G1763	G1610	G1485	A1346	A1045	A1136	A1040
G2359	A2121	G	U1868	U1766	G1611	C1491	G1350	A1227	A1140	A1046
U2362	G2122	C	G1877	C1763	G1614	G1492	U1351	A1228	G1141	A1047
C2363	G2123	C	G1878	G1766	G1619	G1493	U1361	A1234	A1142	A1048
G2364	G2124	U	G1879	A1767	C1619	A1498	G1362	C1240	C1143	G1049
C2369	C2126	C	G1886	G1776	A1622	U1505	A1369	U1241	G1148	G1050
U2370	G2132	G	C1887	A1777	A1623	U1506	U1370	A1242	G1157	C1051
U2373	G2137	C	A1890	G1778	C1624	U1537	U1371	C1246	C1158	G1046
G2376	G2137	C	A1891	G1779	U1625	C1539	G1372	A1248	G1159	A1047
G2377	G2140	U	U1892	A1780	G1626	A1522	A1373	U1248	G1160	A1049
U2380	G2150	C	A1901	C1783	G1638	U1536	A1382	U1252	G1161	G1053
G2374	A2151	G	A1902	G1784	A1639	U1537	G1383	C1255	G1162	A1058
G2375	C2155	U	G1915	C1785	C1640	U1538	A1387	A1261	U1164	U1056
G2376	G2155	C	A1916	G1786	G1641	C1539	G1387	U1264	G1165	U1057
G2377	G2155	C	U1917	G1787	G1642	A1540	A1401	C1266	U1174	A1059
U2380	G2155	C	G1920	G1788	G1646	A1542	U1413	C1267	C1175	U1060
G2381	G2155	C	G1929	G1791	G1647	G1543	G1400	A1270	G1176	U1061
A2382	G2155	C	G1933	G1792	A1676	U1550	G1417	C1269	G1177	A1068
C2383	G2155	C	C1935	A1793	A1677	C1554	U1418	A1284	C1179	U1067
U2384	G2155	C	A1936	G1795	U1685	C1555	U1419	A1287	C1182	G1069
C2385	G2155	C	G1937	U1799	A1696	G1559	U1421	U1288	A1185	G1070
A2387	G2155	C	U1938	C1800	A1698	U1560	A1429	G1289	A1186	U1071
U2391	G2155	C	U1939	U1801	G1699	G1561	G1436	G1290	A1187	G1072
G2392	G2155	C	U1939	G1809	U1700	U1562	U1431	A1291	U1194	G1073
A2393	G2155	C	U1939	G1812	U1701	G1563	A1432	U1292	U1197	C1075
U2396	G2155	C	U1939	C1816	U1702	G1567	G1433	G1296	U1198	A1076
U2397	G2155	C	U1939	U1822	G1725	A1573	U1438	C1303	C1202	U1077
G2398	G2155	C	U1939	C1826	G1726	C1576	G1449	A1313	G1205	G1079
U2400	G2155	C	U1939	U1829	G1727	C1577	U1454	C1316	A1206	A1081
A2401	G2155	C	U1939	C1836	G1730	A1582	G1455	A1331	C1207	A1086
U2402	G2155	C	U1939	U1842	G1731	A1585	U1458	G1332	G1209	A1095
A2403	G2155	C	U1939	A1843	G1737	U1586	A1464	A1333	C1211	G1096
A2404	G2155	C	U1939	A1845	G1742	C1589	U1467	A1334	A1214	U1097
G	G	C	U1939	C1846	U1743	G1590	U1467	A1335	A1215	G1098
A	G	C	U1939	U1856	U1745	C1595	U1467	A1336	G1109	G1099
C	G	C	U1939	U1857	G1746	U1596	U1467	C1336	G1110	G1100
C	G	C	U1939	U1857	G1746	U1596	U1467	C1336	G1115	A1118

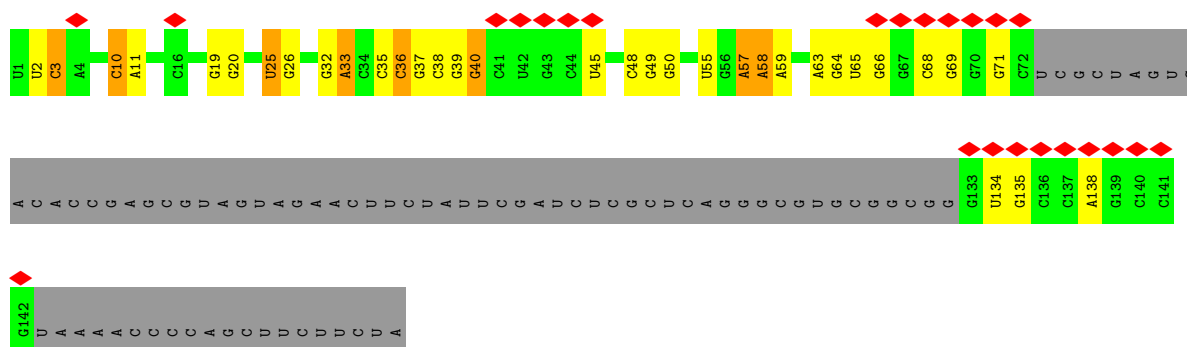


• Molecule 2: 5.8S rRNA

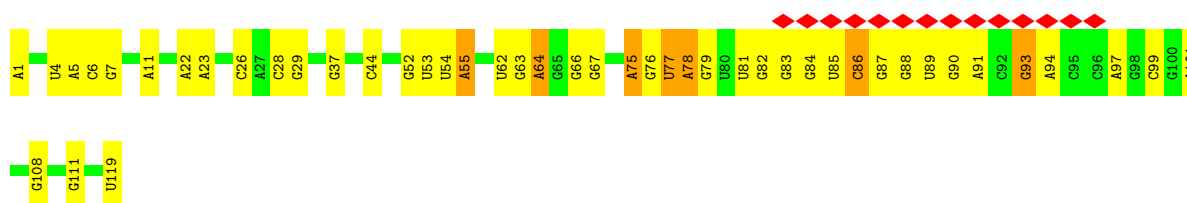


• Molecule 3: ITS2

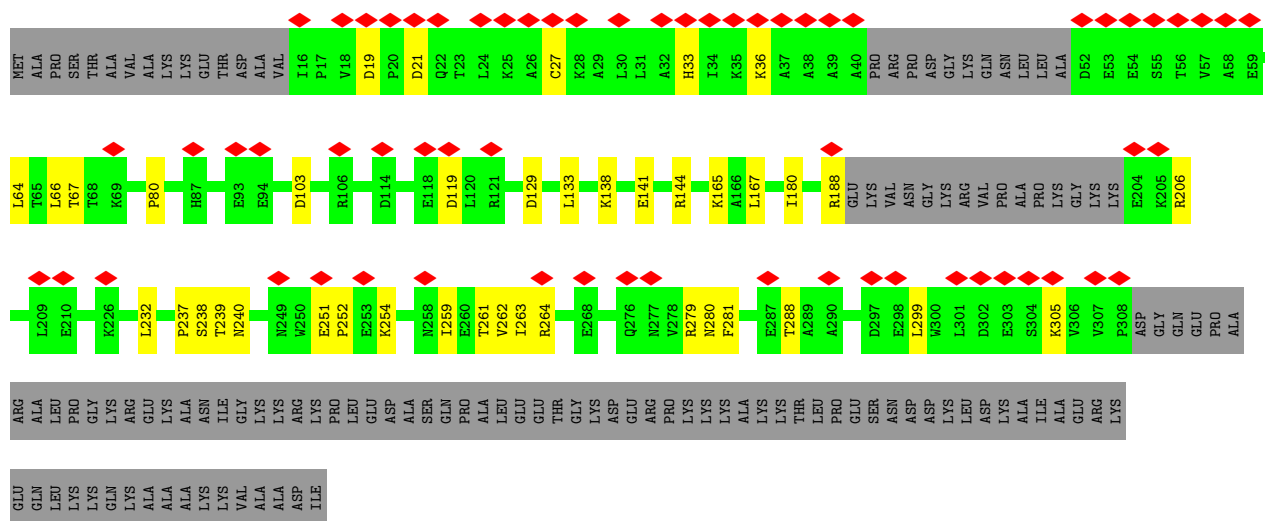




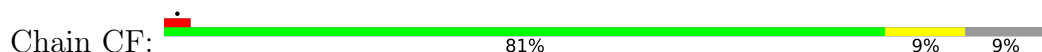
- Molecule 4: 5S rRNA

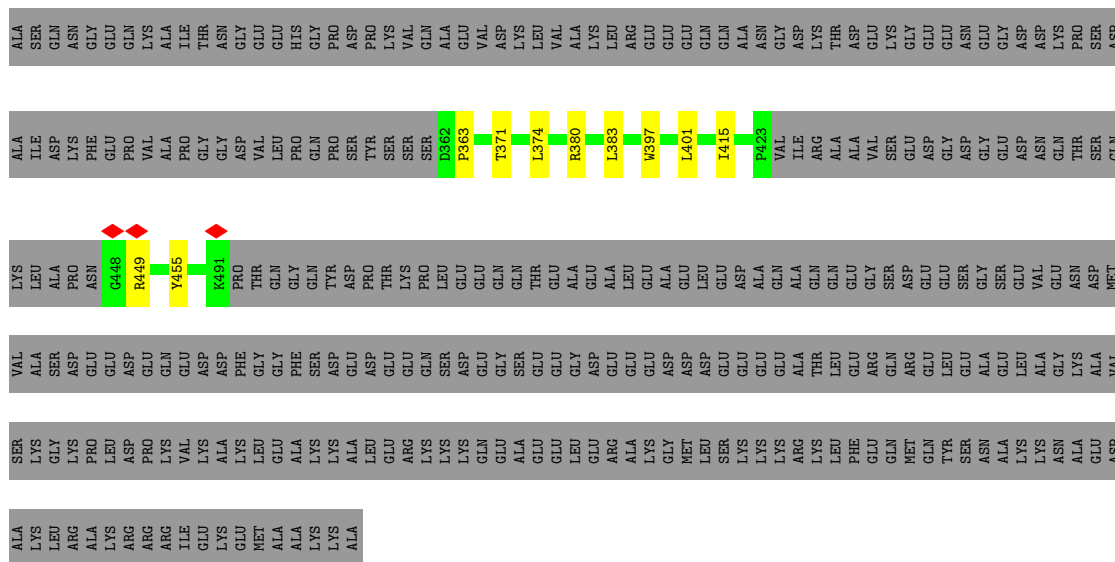


- Molecule 5: Utp30

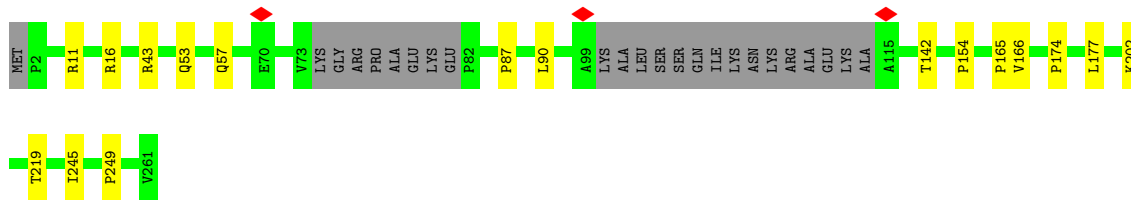
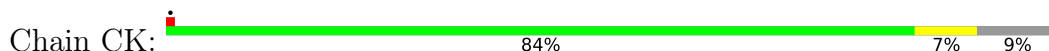


- Molecule 6: Large ribosomal subunit protein uL10

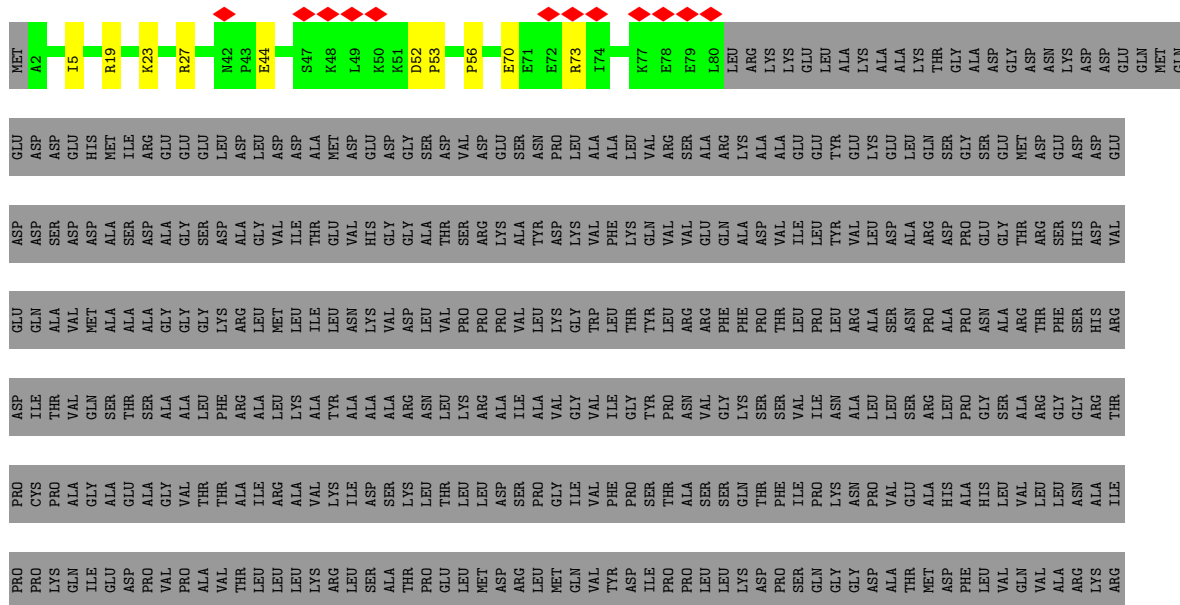


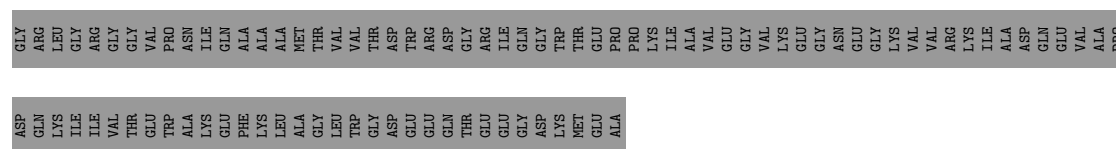


- Molecule 10: Ribosome biogenesis protein NSA2 homolog

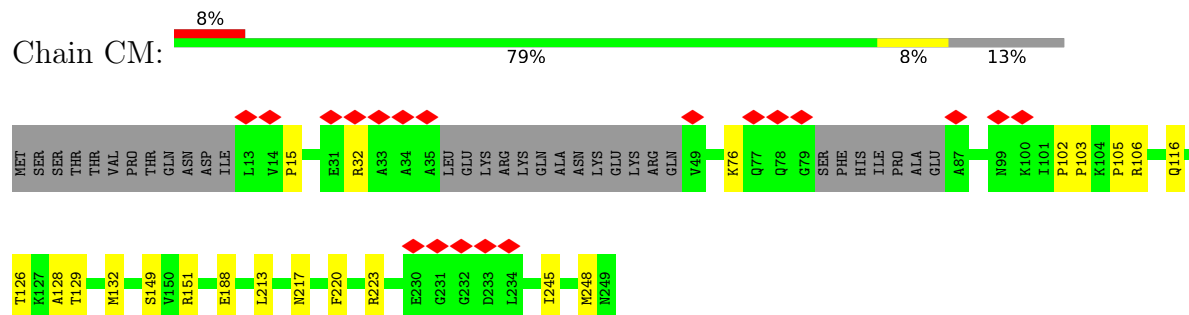


- Molecule 11: Putative GTP binding protein

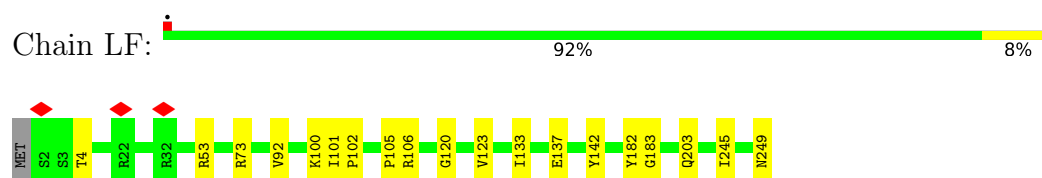




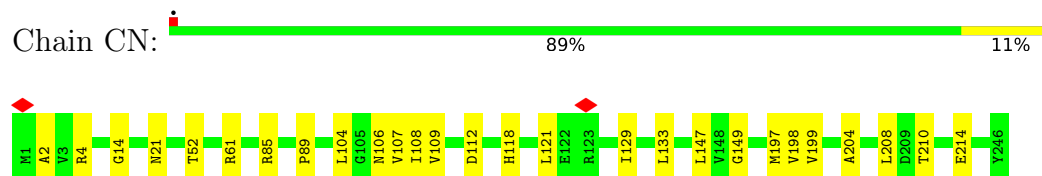
• Molecule 12: 60S ribosomal protein l7-like protein



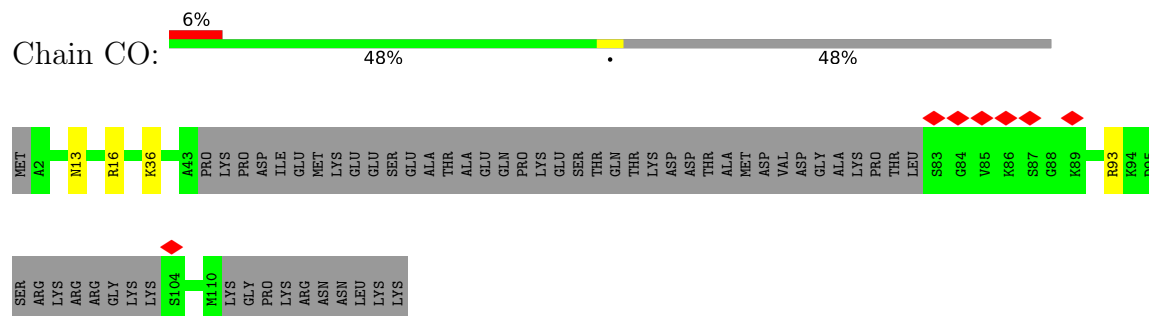
• Molecule 12: 60S ribosomal protein l7-like protein



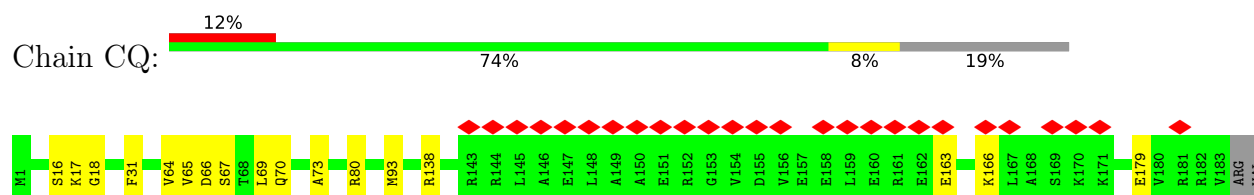
• Molecule 13: Eukaryotic translation initiation factor 6



• Molecule 14: DUF2423 domain-containing protein



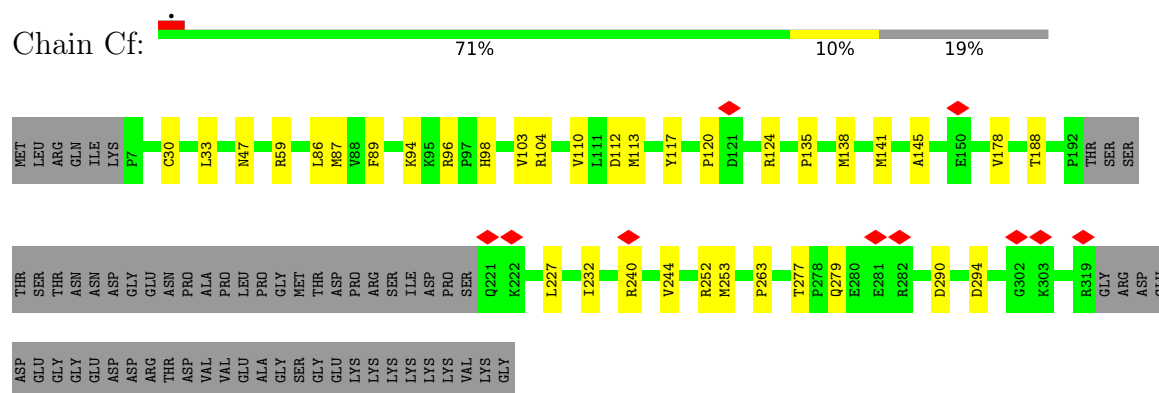
• Molecule 15: Ribosome biogenesis protein RLP24





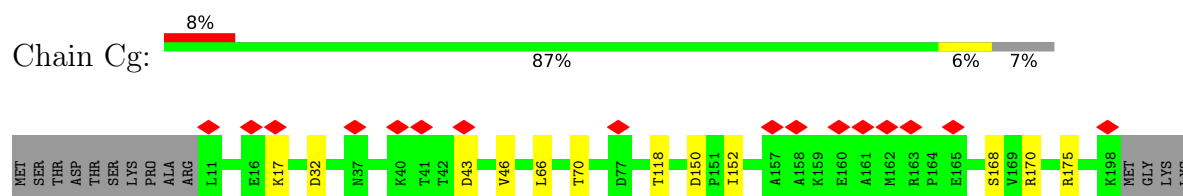
- Molecule 19: Ribosome production factor 2 homolog

Chain Cf:



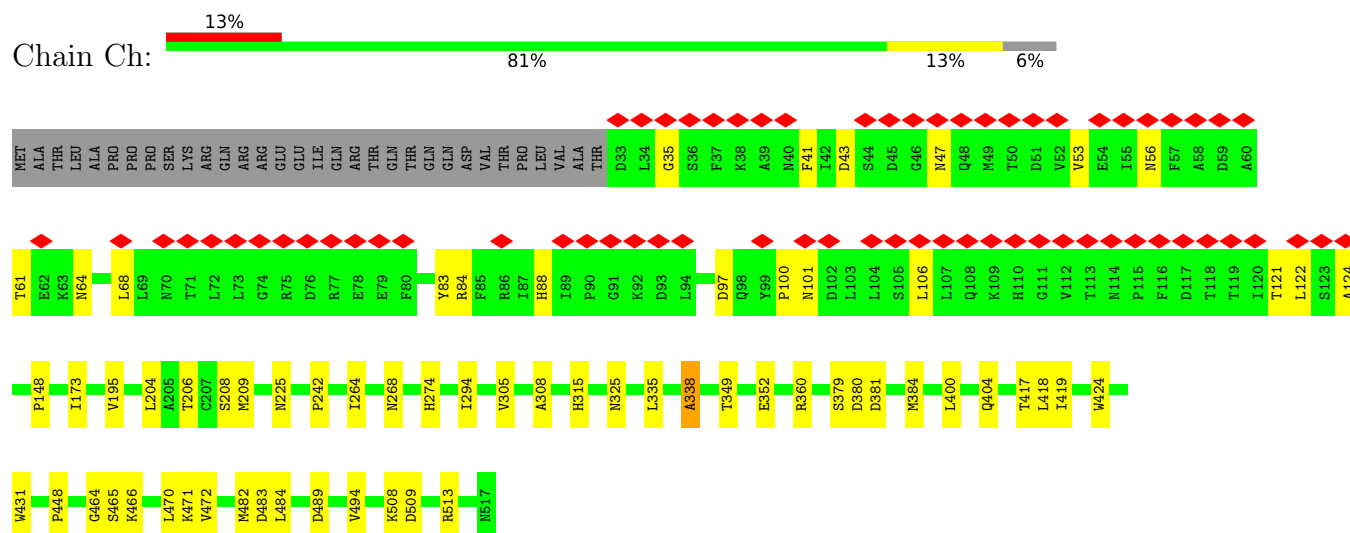
- Molecule 20: Ribosome biogenesis regulatory protein

Chain Cg:



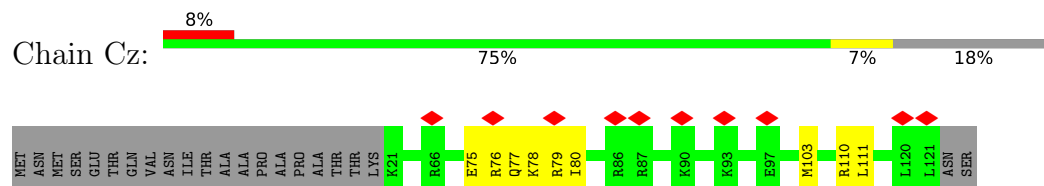
- Molecule 21: Ribosome assembly protein 4

Chain Ch:



- Molecule 22: rRNA-processing protein

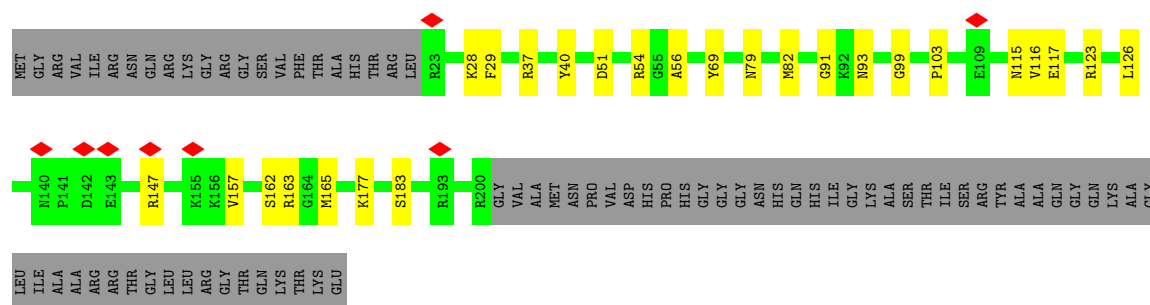
Chain Cz:



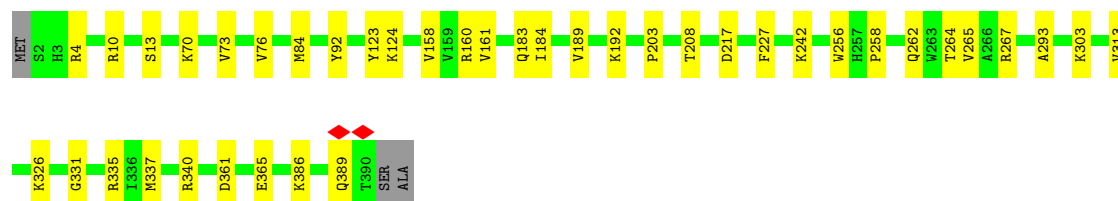
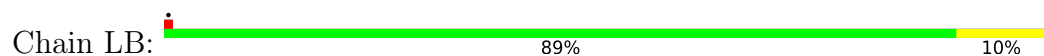
- Molecule 23: 60S ribosomal protein L2-like protein

Chain LA:





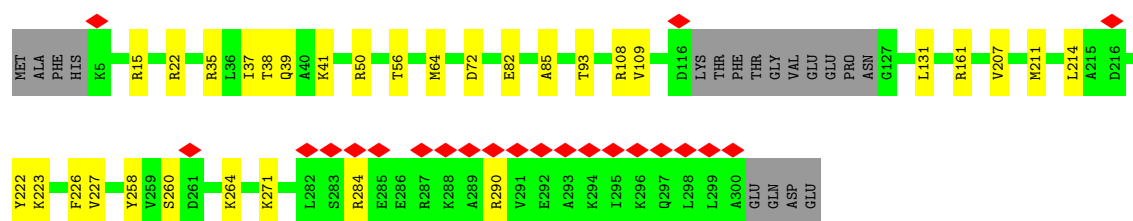
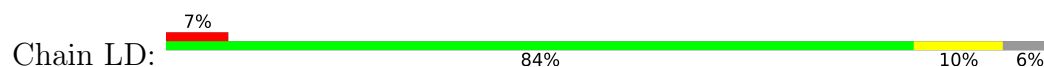
- Molecule 24: 60S ribosomal protein L3-like protein



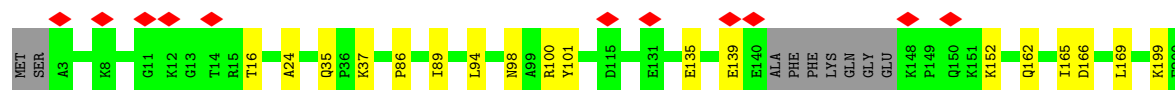
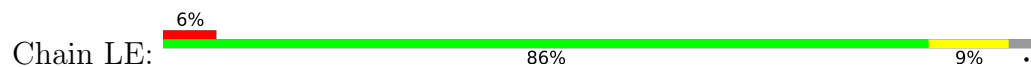
- Molecule 25: 60S ribosomal protein L4-like protein



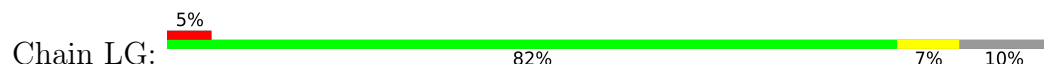
- Molecule 26: 60S ribosomal protein l5-like protein

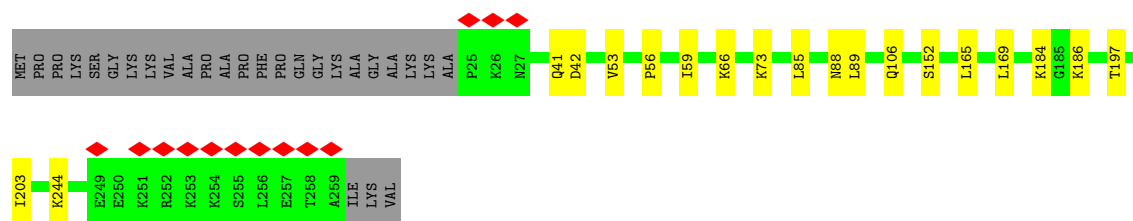


- Molecule 27: 60S ribosomal protein L6



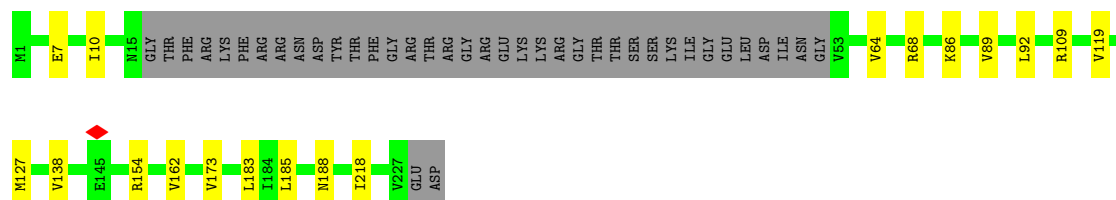
- Molecule 28: 60S ribosomal protein L8





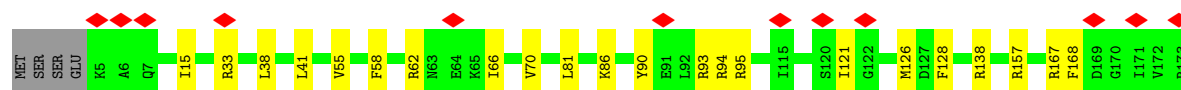
- Molecule 29: 60S ribosomal protein L9-like protein

Chain LH: 75% 8% 17%



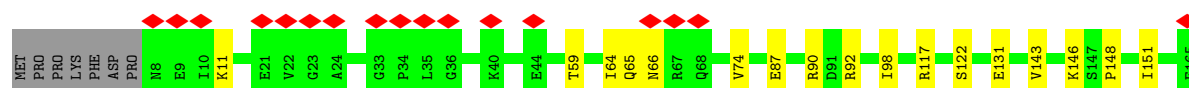
- Molecule 30: Putative ribosomal protein

Chain LJ: 7% 85% 13%



- Molecule 31: 60S ribosomal protein L12-like protein

Chain LK: 10% 85% 10%



- Molecule 32: 60S ribosomal protein L13

Chain LL: 7% 89% 6% 5%



- Molecule 33: 60S ribosomal protein L14-like protein

Chain LM: 7% 87% 12%



- Molecule 34: Ribosomal protein L15





GLN
ALA
ALA
LYS
ARG
ASN
ALA
LEU
LEU
GLY
GLY
GLU
GLU
GLU
SER
LYS

- Molecule 39: 60S ribosomal protein L20

Chain LS:  89% 11%

M1 Q8 L24 V59 E56 P69 L70 I77 R80 N89 R115 F118 V126 P138 Y139 I140 K141 R155 K158 R169 P170 S174

- Molecule 40: 60S ribosomal protein l21-like protein

Chain LT:  10% 72% 9% 19%

MET GLY HIS ALA ALA GLY LEU ARG SER GLY THR ARG TYR ALA PHE SER ARG GLY PHE ARG LYS HIS GLY GLN ILE PRO LEU SER THR TYR LEU R32 R35 V36 G37 D38 I39 I42 K43 G46 A47 V48 Q49 K50 G51 Y57 Y65 V74 K78 K87 R88 I89

E111 E114 K120 A121 E122 G123 V124 P125 R130 E157 I160

- Molecule 41: 60S ribosomal protein L22-like protein

Chain LU:  5% 78% 5% 17%

MET ALA PRO VAL GLN LYS LYS SER GLY ALA GLY LYS LYS PRO K16 V17 T18 K19 I33 D58 K61 T65 Q66 D67 D77 L78 R101 D120 GLU ALA GLU GLU ASP

- Molecule 42: 60S ribosomal protein l23-like protein

Chain LV:  88% 9% 3%

MET ALA LYS GLN K5 R6 P9 K14 L19 L36 R47 A62 N100 M106 E110 L127 S133 M139

- Molecule 43: 60S ribosomal protein L25-like protein

Chain LX:  85% 8% 7%

MET ALA PRO LYS ASP VAL LYS LYS GLY GLY ALA S12 K13 A14 K21 K36 T43 S63 H78 P79 L80 N81 T82 E83 K87 F97 Y116 D117 I118 K133 D142 V156

- Molecule 44: 60S ribosomal protein L26-like protein

Chain LY:  83% 13% 4%

M1 K2 R15 M30 S46 I47 E54 T85 R86 P95 I96 P100 K107 L108 H109 K112 D113 R114 R120 R125 K132 G133 LYS LYS THR ALA

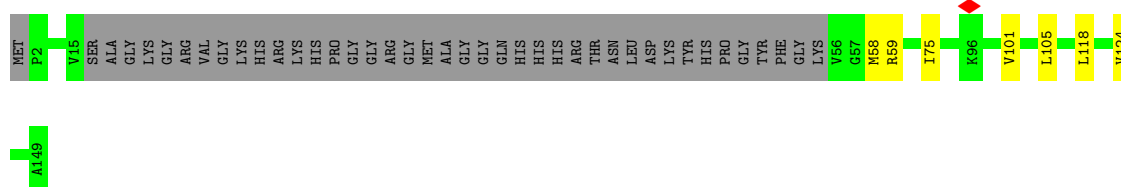
- Molecule 45: 60S ribosomal protein L27

Chain LZ:  82% 18%



- Molecule 46: 60S ribosomal protein L28-like protein

Chain La:  68% 5% 28%



- Molecule 47: 60S ribosomal protein l30-like protein

Chain Lc:  6% 80% 8% 12%



- Molecule 48: Putative 60S ribosomal protein

Chain Ld:  87% 5% 8%

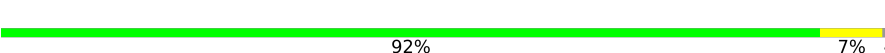


- Molecule 49: 60S ribosomal protein L32-like protein

Chain Le:  87% 9% 4%

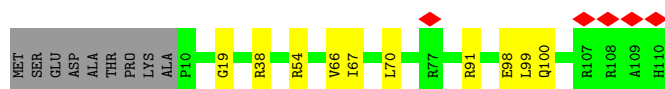
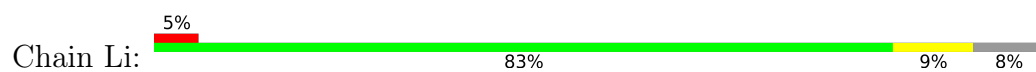


- Molecule 50: 60S ribosomal protein l33-like protein

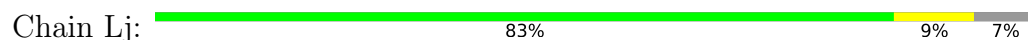
Chain Lf:  92% 7% 1%



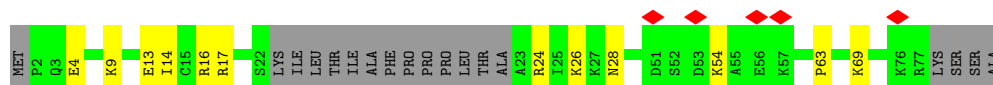
- Molecule 51: Ribosomal protein l34-like protein



- Molecule 54: Ribosomal protein L37



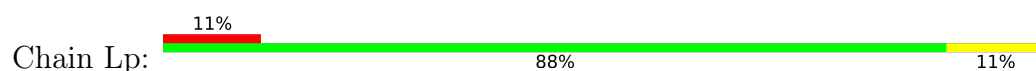
- Molecule 55: 60S ribosomal protein L38-like protein



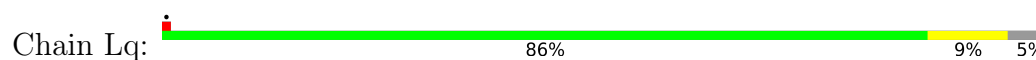
- Molecule 56: Ribosomal protein eL39



- Molecule 57: 60S ribosomal protein L43-like protein



- Molecule 58: Putative 60S ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35432	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.243	Depositor
Minimum map value	0.000	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.147	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A2M, GTP, OMC, OMG, MG, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C1	0.19	1/70966 (0.0%)	0.32	0/110644
2	C2	0.17	0/3710	0.30	0/5778
3	C3	0.13	0/1958	0.30	0/3050
4	C4	0.16	0/2833	0.32	0/4414
5	CB	0.18	0/2166	0.45	0/2945
6	CF	0.18	0/1972	0.43	0/2660
7	CH	0.18	0/5147	0.42	0/6926
8	CI	0.23	0/1265	0.63	0/1702
9	CJ	0.18	0/3196	0.40	1/4319 (0.0%)
10	CK	0.17	0/1939	0.38	0/2608
11	CL	0.18	0/631	0.42	0/843
12	CM	0.18	0/1805	0.42	0/2417
12	LF	0.20	0/2061	0.41	0/2765
13	CN	0.19	0/1878	0.48	0/2555
14	CO	0.21	0/470	0.44	0/619
15	CQ	0.20	0/1504	0.40	0/2000
16	Cb	0.20	0/845	0.53	0/1128
17	Cd	0.17	0/3770	0.38	0/5082
18	Ce	0.16	0/2173	0.39	0/2890
19	Cf	0.14	0/2326	0.35	0/3113
20	Cg	0.17	0/1508	0.38	0/2051
21	Ch	0.20	0/3914	0.47	1/5319 (0.0%)
22	Cz	0.25	0/877	0.65	2/1148 (0.2%)
23	LA	0.18	0/1395	0.47	0/1881
24	LB	0.20	0/3172	0.46	0/4260
25	LC	0.17	0/2808	0.39	0/3785
26	LD	0.16	0/2308	0.37	0/3105
27	LE	0.16	0/1504	0.41	0/2027
28	LG	0.18	0/1918	0.42	0/2565
29	LH	0.18	0/1515	0.44	0/2037
30	LJ	0.19	0/1379	0.50	0/1844
31	LK	0.20	0/1198	0.52	0/1611

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LL	0.16	0/1614	0.37	0/2168
33	LM	0.17	0/1145	0.37	0/1539
34	LN	0.18	0/1741	0.36	0/2332
35	LO	0.21	0/1645	0.41	0/2205
36	LP	0.17	0/1364	0.41	0/1835
37	LQ	0.16	0/1197	0.35	0/1612
38	LR	0.17	0/1260	0.38	0/1683
39	LS	0.19	0/1461	0.44	1/1966 (0.1%)
40	LT	0.20	0/1046	0.52	0/1409
41	LU	0.17	0/859	0.45	1/1151 (0.1%)
42	LV	0.21	0/1009	0.46	0/1357
43	LX	0.19	0/1151	0.45	0/1547
44	LY	0.17	0/1070	0.47	0/1432
45	LZ	0.19	0/1135	0.50	0/1519
46	La	0.15	0/892	0.33	0/1200
47	Lc	0.17	0/714	0.41	0/960
48	Ld	0.18	0/889	0.37	0/1192
49	Le	0.19	0/1035	0.43	0/1379
50	Lf	0.18	0/883	0.38	0/1187
51	Lg	0.20	0/927	0.47	0/1244
52	Lh	0.16	0/1014	0.35	0/1349
53	Li	0.16	0/834	0.38	0/1099
54	Lj	0.19	0/712	0.47	0/944
55	Lk	0.18	0/640	0.42	0/850
56	Ll	0.17	0/446	0.33	0/593
57	Lp	0.17	0/706	0.47	0/940
58	Lq	0.17	0/1091	0.36	0/1468
All	All	0.18	1/164591 (0.0%)	0.38	6/238251 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	O3'-P	5.07	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CJ	363	PRO	CA-N-CD	-7.64	101.31	112.00
22	Cz	79	ARG	CA-CB-CG	5.63	125.36	114.10
21	Ch	338	ALA	CB-CA-C	-5.34	109.97	117.23
41	LU	33	ILE	N-CA-C	-5.31	107.24	111.81
39	LS	140	ILE	N-CA-C	-5.31	107.65	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Cz	79	ARG	CB-CG-CD	5.10	123.03	111.30

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	C1	64177	0	32378	363	0
2	C2	3319	0	1678	24	0
3	C3	1754	0	890	22	0
4	C4	2536	0	1286	22	0
5	CB	2119	0	2170	34	0
6	CF	1934	0	1945	14	0
7	CH	5063	0	5157	39	0
8	CI	1234	0	1245	23	0
9	CJ	3116	0	3122	25	0
10	CK	1903	0	1990	12	0
11	CL	622	0	641	8	0
12	CM	1773	0	1879	13	0
12	LF	2023	0	2132	12	0
13	CN	1853	0	1852	15	0
14	CO	468	0	503	4	0
15	CQ	1480	0	1523	15	0
16	Cb	830	0	838	9	0
17	Cd	3691	0	3818	32	0
18	Ce	2148	0	2250	24	0
19	Cf	2282	0	2347	22	0
20	Cg	1478	0	1517	7	0
21	Ch	3812	0	3715	35	0
22	Cz	869	0	956	6	0
23	LA	1365	0	1411	17	0
24	LB	3104	0	3221	29	0
25	LC	2751	0	2875	18	0
26	LD	2266	0	2219	21	0
27	LE	1477	0	1567	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	LG	1889	0	2043	14	0
29	LH	1495	0	1573	9	0
30	LJ	1357	0	1385	16	0
31	LK	1184	0	1249	10	0
32	LL	1587	0	1655	10	0
33	LM	1126	0	1198	12	0
34	LN	1704	0	1767	16	0
35	LO	1611	0	1702	10	0
36	LP	1343	0	1369	6	0
37	LQ	1181	0	1266	10	0
38	LR	1241	0	1298	9	0
39	LS	1426	0	1481	16	0
40	LT	1027	0	1076	9	0
41	LU	846	0	883	3	0
42	LV	991	0	1044	8	0
43	LX	1133	0	1234	10	0
44	LY	1056	0	1143	12	0
45	LZ	1112	0	1181	17	0
46	La	872	0	903	5	0
47	Lc	705	0	751	6	0
48	Ld	875	0	918	5	0
49	Le	1017	0	1092	8	0
50	Lf	862	0	891	5	0
51	Lg	914	0	960	9	0
52	Lh	1003	0	1116	9	0
53	Li	827	0	906	7	0
54	Lj	698	0	726	9	0
55	Lk	632	0	693	7	0
56	Ll	436	0	473	4	0
57	Lp	698	0	737	7	0
58	Lq	1073	0	1130	9	0
59	CH	32	0	12	0	0
59	Cd	32	0	12	0	0
60	CH	1	0	0	0	0
60	Cd	2	0	0	0	0
61	CQ	1	0	0	0	0
61	Cb	1	0	0	0	0
61	Lg	1	0	0	0	0
61	Lj	1	0	0	0	0
61	Lp	1	0	0	0	0
62	CH	1	0	0	0	0
62	Cd	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	155443	0	122992	931	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 3.

All (931) 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)
1:C1:1809:G:HO2'	9:CJ:2:GLY:N	1.61	0.97
1:C1:2400:G:H1	1:C1:2473:U:H3	1.13	0.96
1:C1:2101:A:HO2'	54:Lj:2:THR:N	1.72	0.88
3:C3:40:G:H1	3:C3:45:U:H3	1.26	0.80
1:C1:1054:U:H3	1:C1:1070:G:H1	0.85	0.73
1:C1:3001:C:OP1	42:LV:47:ARG:NH1	2.22	0.72
27:LE:162:GLN:NE2	27:LE:166:ASP:OD2	2.23	0.72
21:Ch:384:MET:HB2	21:Ch:400:LEU:HB2	1.74	0.70
21:Ch:35:GLY:O	21:Ch:56:ASN:ND2	2.26	0.68
58:Lq:31:ASP:HB3	58:Lq:34:ASN:HB2	1.76	0.67
1:C1:3289:G:H1	1:C1:3298:U:H3	1.41	0.65
1:C1:949:A:H62	1:C1:1098:G:H8	1.45	0.65
40:LT:78:LYS:HE3	40:LT:87:LYS:HG3	1.77	0.65
17:Cd:285:ILE:HD11	17:Cd:296:ALA:HB2	1.78	0.64
5:CB:279:ARG:NH2	8:CI:309:GLU:OE2	2.30	0.64
25:LC:148:GLU:HG3	58:Lq:73:LYS:HG2	1.80	0.63
26:LD:85:ALA:HB2	26:LD:258:TYR:HB2	1.80	0.63
1:C1:3204:C:H2'	1:C1:3205:G:H8	1.63	0.63
13:CN:129:ILE:HG23	13:CN:133:LEU:HD12	1.81	0.63
25:LC:185:VAL:HG11	25:LC:231:GLY:HA3	1.81	0.63
36:LP:125:GLN:HB3	36:LP:141:SER:HB2	1.81	0.63
3:C3:71:G:H1	3:C3:134:U:H3	1.47	0.62
1:C1:2327:G:H22	1:C1:2359:G:H1'	1.64	0.62
1:C1:2878:A:H61	1:C1:2886:C:H42	1.47	0.62
1:C1:1614:G:N7	45:LZ:16:ARG:NH1	2.47	0.62
45:LZ:49:PRO:HD3	45:LZ:67:ILE:HG12	1.81	0.62
21:Ch:470:LEU:HB2	21:Ch:484:LEU:HB2	1.80	0.62
7:CH:486:GLU:O	7:CH:490:GLN:NE2	2.33	0.61
11:CL:70:GLU:OE1	11:CL:73:ARG:NH2	2.33	0.61
24:LB:331:GLY:HA3	24:LB:337:MET:HE1	1.82	0.61
27:LE:139:GLU:HG2	27:LE:152:LYS:HE2	1.83	0.61
34:LN:28:TRP:O	34:LN:32:GLN:NE2	2.34	0.61
23:LA:82:MET:HE1	23:LA:165:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LB:84:MET:O	24:LB:203:PRO:HA	2.00	0.61
1:C1:2899:A:H2'	24:LB:256:TRP:HB3	1.81	0.61
36:LP:18:ARG:NH2	36:LP:147:GLU:OE2	2.33	0.61
1:C1:984:A:N1	1:C1:1033:U:O2'	2.34	0.61
14:CO:13:ASN:OD1	14:CO:16:ARG:NH2	2.34	0.60
27:LE:24:ALA:O	58:Lq:88:ARG:NH1	2.34	0.60
51:Lg:48:CYS:O	57:Lp:61:LYS:NZ	2.33	0.60
53:Li:67:ILE:HG13	53:Li:99:LEU:HD13	1.83	0.60
13:CN:21:ASN:ND2	13:CN:112:ASP:OD2	2.34	0.60
23:LA:147:ARG:HG2	23:LA:157:VAL:HG22	1.83	0.60
33:LM:54:ARG:NH2	33:LM:76:ALA:O	2.34	0.60
8:CI:246:ARG:NH2	18:Ce:443:ILE:OXT	2.34	0.60
1:C1:1929:G:OP2	38:LR:135:LYS:NZ	2.33	0.59
21:Ch:84:ARG:NH2	21:Ch:97:ASP:OD1	2.34	0.59
31:LK:117:ARG:NH2	31:LK:122:SER:O	2.35	0.59
1:C1:2362:A:OP1	25:LC:70:ARG:NH2	2.35	0.59
2:C2:71:A:O2'	2:C2:83:C:N4	2.35	0.59
1:C1:1619:C:OP2	51:Lg:75:ARG:NH1	2.35	0.59
19:Cf:227:LEU:HB3	19:Cf:253:MET:HB2	1.84	0.59
1:C1:69:C:OP2	1:C1:294:G:N2	2.36	0.59
1:C1:1431:U:H2'	1:C1:1432:A2M:H8	1.84	0.59
31:LK:65:GLN:NE2	31:LK:66:ASN:OD1	2.36	0.59
1:C1:2530:C:OP2	12:CM:32:ARG:NH1	2.36	0.59
15:CQ:179:GLU:OE1	48:Ld:86:ARG:NH1	2.36	0.59
26:LD:37:ILE:HG13	26:LD:38:THR:HG23	1.85	0.59
7:CH:426:ILE:O	15:CQ:80:ARG:NH1	2.35	0.58
13:CN:107:VAL:HG23	13:CN:108:ILE:HG13	1.84	0.58
19:Cf:145:ALA:HB3	19:Cf:188:THR:HG22	1.84	0.58
1:C1:1842:U:OP1	38:LR:70:ARG:NH2	2.37	0.58
1:C1:258:A:OP1	53:Li:38:ARG:NH1	2.37	0.58
31:LK:11:LYS:HD2	31:LK:64:ILE:HD11	1.85	0.58
7:CH:242:LEU:O	7:CH:280:LYS:NZ	2.34	0.58
23:LA:116:VAL:HB	23:LA:126:LEU:HB2	1.85	0.58
1:C1:2477:U:OP2	1:C1:2545:G:N2	2.35	0.58
7:CH:248:ALA:HB2	7:CH:338:LEU:HD21	1.86	0.58
44:LY:47:ILE:HD13	44:LY:114:ARG:HH21	1.67	0.58
8:CI:203:LEU:HD22	8:CI:233:ILE:HD11	1.86	0.58
1:C1:2842:U:OP1	24:LB:10:ARG:NH1	2.36	0.58
5:CB:80:PRO:HB2	5:CB:232:LEU:HD12	1.85	0.58
5:CB:279:ARG:NH1	5:CB:280:ASN:OD1	2.37	0.58
7:CH:527:LEU:HD13	7:CH:550:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Ch:195:VAL:HG12	21:Ch:206:THR:HG22	1.86	0.57
21:Ch:338:ALA:O	21:Ch:360:ARG:NH1	2.36	0.57
28:LG:165:LEU:HA	34:LN:7:LEU:HD11	1.85	0.57
41:LU:58:ASP:O	41:LU:61:LYS:NZ	2.36	0.57
17:Cd:47:ILE:HB	17:Cd:56:LYS:HB3	1.84	0.57
34:LN:96:ARG:NH2	34:LN:104:GLU:OE2	2.37	0.57
1:C1:706:G:OP2	1:C1:706:G:N2	2.33	0.57
21:Ch:419:ILE:HB	21:Ch:431:TRP:HB2	1.87	0.57
20:Cg:152:ILE:HD13	40:LT:57:TYR:HB2	1.87	0.57
1:C1:388:A:H2'	1:C1:389:A2M:H8	1.86	0.57
1:C1:1420:OMC:HM22	1:C1:1421:U:H5'	1.85	0.57
55:Lk:14:ILE:HA	55:Lk:17:ARG:HD3	1.86	0.57
7:CH:264:LYS:HE3	7:CH:301:MET:HE1	1.87	0.57
1:C1:2767:A:N6	1:C1:2913:U:O2'	2.36	0.57
23:LA:82:MET:HE2	23:LA:99:GLY:HA2	1.87	0.56
7:CH:186:VAL:HG23	7:CH:187:THR:HG23	1.86	0.56
21:Ch:509:ASP:OD1	21:Ch:513:ARG:NH1	2.39	0.56
1:C1:3189:U:OP2	14:CO:93:ARG:NH1	2.36	0.56
9:CJ:75:GLU:HG3	9:CJ:77:LEU:H	1.70	0.56
34:LN:87:GLN:NE2	34:LN:91:GLN:OE1	2.38	0.56
1:C1:1877:G:OP2	16:Cb:11:LYS:NZ	2.34	0.56
1:C1:2833:G:OP2	1:C1:2833:G:N2	2.38	0.56
6:CF:132:PRO:HD2	6:CF:216:LEU:HD23	1.87	0.56
17:Cd:427:TYR:O	17:Cd:445:LYS:NZ	2.38	0.56
1:C1:2478:A:N1	1:C1:2553:C:N4	2.53	0.56
5:CB:103:ASP:O	5:CB:206:ARG:NH1	2.38	0.56
1:C1:782:G:H22	25:LC:102:ALA:HA	1.69	0.56
21:Ch:53:VAL:HG21	21:Ch:68:LEU:HD21	1.88	0.56
21:Ch:417:THR:HG23	21:Ch:418:LEU:HG	1.88	0.56
1:C1:1685:U:O2	1:C1:1766:G:O2'	2.24	0.56
1:C1:3212:G:N1	27:LE:135:GLU:OE2	2.34	0.56
25:LC:136:LEU:HD23	25:LC:143:VAL:HG11	1.88	0.56
32:LL:115:ARG:NH2	32:LL:155:PHE:O	2.34	0.56
51:Lg:17:THR:HG22	51:Lg:38:LYS:HD3	1.88	0.56
1:C1:643:C:H2'	1:C1:644:A:H8	1.71	0.56
4:C4:53:U:O2'	4:C4:55:A:N7	2.37	0.56
9:CJ:46:GLU:OE2	18:Ce:367:ARG:NH2	2.36	0.56
10:CK:202:LYS:NZ	17:Cd:71:GLU:OE1	2.39	0.56
23:LA:79:ASN:HB2	23:LA:82:MET:HE3	1.89	0.56
1:C1:2509:A:OP1	23:LA:93:ASN:ND2	2.40	0.55
2:C2:120:G:H5'	18:Ce:182:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C4:88:G:N2	4:C4:91:A:OP2	2.37	0.55
24:LB:293:ALA:HB2	24:LB:303:LYS:HG3	1.88	0.55
1:C1:1095:A:H2'	1:C1:1096:G:C8	2.40	0.55
40:LT:42:ILE:HD11	40:LT:74:VAL:HG11	1.88	0.55
7:CH:86:ASP:HB3	7:CH:89:HIS:HB2	1.89	0.55
7:CH:535:ASP:OD2	15:CQ:138:ARG:NH1	2.37	0.55
18:Ce:443:ILE:O	43:LX:21:LYS:NZ	2.40	0.55
17:Cd:364:TRP:HA	17:Cd:377:ASP:O	2.07	0.55
1:C1:3:G:H1'	43:LX:36:LYS:HE3	1.87	0.55
1:C1:2087:G:O2'	17:Cd:448:ARG:NH1	2.40	0.55
17:Cd:358:PRO:HD2	17:Cd:400:ARG:HG2	1.89	0.55
1:C1:2400:G:O6	1:C1:2473:U:O4	2.24	0.55
1:C1:2789:G:H2'	1:C1:2790:G:C8	2.42	0.55
33:LM:44:PRO:HG3	33:LM:81:VAL:HG12	1.88	0.55
45:LZ:14:ARG:HE	51:Lg:87:ARG:HD3	1.71	0.55
17:Cd:121:PRO:HG2	21:Ch:404:GLN:HE21	1.70	0.55
31:LK:59:THR:HG23	31:LK:74:VAL:HB	1.87	0.55
1:C1:1174:U:OP2	35:LO:50:ARG:NH1	2.37	0.55
1:C1:2591:G:H21	1:C1:2605:C:H41	1.55	0.55
4:C4:108:G:OP1	26:LD:284:ARG:NH2	2.39	0.55
5:CB:64:LEU:HD13	5:CB:259:ILE:HD11	1.87	0.55
1:C1:1785:C:H2'	1:C1:1786:G:H8	1.72	0.54
2:C2:126:A:O2'	2:C2:128:U:OP2	2.25	0.54
21:Ch:264:ILE:HD12	21:Ch:274:HIS:HB2	1.88	0.54
1:C1:404:U:H2'	1:C1:405:G:H8	1.72	0.54
1:C1:2648:A:OP1	26:LD:15:ARG:NH1	2.40	0.54
1:C1:2769:C:OP2	1:C1:2914:U:O2'	2.25	0.54
1:C1:3109:U:H3	1:C1:3338:C:H42	1.56	0.54
7:CH:236:MET:HG3	17:Cd:154:PRO:HG3	1.88	0.54
28:LG:41:GLN:HG2	28:LG:42:ASP:H	1.73	0.54
1:C1:736:G:H2'	1:C1:737:A:H8	1.73	0.54
7:CH:446:VAL:HG22	15:CQ:93:MET:HE1	1.89	0.54
7:CH:591:ARG:HH21	43:LX:87:LYS:HE2	1.73	0.54
1:C1:64:A:H5''	34:LN:174:LEU:HD13	1.90	0.54
7:CH:303:GLN:NE2	7:CH:307:ASP:OD2	2.41	0.54
52:Lh:15:LYS:O	52:Lh:66:LYS:NZ	2.36	0.54
1:C1:1207:C:O2'	6:CF:8:ARG:NH2	2.34	0.54
17:Cd:336:ASN:ND2	17:Cd:356:PRO:O	2.40	0.54
44:LY:86:ARG:HB3	44:LY:96:ILE:HD11	1.89	0.54
4:C4:86:C:N4	4:C4:87:G:O6	2.41	0.54
1:C1:2518:G:OP1	23:LA:69:TYR:OH	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:59:GLU:OE1	6:CF:115:TYR:OH	2.24	0.54
7:CH:294:PHE:O	7:CH:302:GLN:NE2	2.41	0.54
17:Cd:273:ILE:HD13	17:Cd:296:ALA:HB1	1.90	0.54
29:LH:173:VAL:HG22	29:LH:185:LEU:HG	1.90	0.54
38:LR:28:GLU:HG3	38:LR:31:GLU:HB3	1.89	0.54
38:LR:44:LEU:HD22	38:LR:49:LEU:HD22	1.89	0.54
1:C1:2892:A:OP2	42:LV:6:ARG:NH1	2.41	0.54
13:CN:210:THR:HG23	13:CN:214:GLU:HG3	1.90	0.54
17:Cd:3:THR:O	17:Cd:9:ASN:ND2	2.36	0.54
1:C1:3184:C:O2	14:CO:93:ARG:NH2	2.39	0.53
4:C4:75:A:O2'	19:Cf:94:LYS:NZ	2.39	0.53
3:C3:36:C:H2'	3:C3:37:G:H8	1.73	0.53
18:Ce:300:THR:OG1	18:Ce:303:GLU:OE1	2.22	0.53
22:Cz:103:MET:HE1	22:Cz:111:LEU:HD13	1.90	0.53
43:LX:78:HIS:HB2	52:Lh:39:ILE:HD13	1.89	0.53
2:C2:94:C:H5''	54:Lj:76:ASN:HD21	1.73	0.53
14:CO:36:LYS:HE3	24:LB:208:THR:HG22	1.90	0.53
21:Ch:471:LYS:NZ	21:Ch:483:ASP:OD2	2.39	0.53
25:LC:36:VAL:HG21	25:LC:251:LEU:HD21	1.89	0.53
1:C1:1159:C:H4'	35:LO:91:PRO:HD3	1.90	0.53
1:C1:1264:U:H2'	1:C1:1265:G:H8	1.73	0.53
3:C3:49:G:H4'	5:CB:238:SER:HB2	1.91	0.53
12:CM:151:ARG:NH2	12:CM:188:GLU:OE2	2.41	0.53
26:LD:35:ARG:HA	26:LD:39:GLN:HG3	1.91	0.53
1:C1:1641:G:H2'	1:C1:1642:G:C8	2.43	0.53
1:C1:1826:C:OP1	1:C1:1829:C:N4	2.41	0.53
1:C1:1929:G:OP1	38:LR:104:ARG:NH1	2.40	0.53
12:CM:103:PRO:HA	12:CM:106:ARG:HG2	1.90	0.53
26:LD:93:THR:O	26:LD:161:ARG:NH1	2.37	0.53
32:LL:23:ARG:NH1	32:LL:24:CYS:O	2.41	0.53
45:LZ:16:ARG:NH2	45:LZ:17:TYR:OH	2.42	0.53
34:LN:44:ARG:NH1	34:LN:120:TRP:O	2.41	0.53
1:C1:1766:G:H2'	1:C1:1767:A:C8	2.43	0.53
1:C1:2355:C:O2'	24:LB:267:ARG:NH1	2.35	0.53
1:C1:2796:A:O2'	1:C1:2810:A:N6	2.42	0.53
31:LK:87:GLU:HB3	31:LK:90:ARG:HH21	1.72	0.53
12:LF:53:ARG:NH2	12:LF:183:GLY:O	2.41	0.53
1:C1:37:C:H4'	1:C1:790:A:H2	1.74	0.53
1:C1:1555:C:H5''	18:Ce:428:ALA:HB2	1.91	0.53
5:CB:251:GLU:HB2	5:CB:254:LYS:HE2	1.90	0.53
1:C1:1045:A:N3	40:LT:130:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1604:G:OP1	18:Ce:343:ARG:NH2	2.42	0.52
2:C2:83:C:OP1	2:C2:85:G:N2	2.42	0.52
21:Ch:489:ASP:HB3	21:Ch:508:LYS:HB3	1.90	0.52
33:LM:54:ARG:HG2	39:LS:70:LEU:HD22	1.91	0.52
4:C4:23:A:N3	4:C4:119:U:O2'	2.36	0.52
38:LR:105:LEU:HD23	38:LR:138:LEU:HD23	1.91	0.52
1:C1:2370:C:OP1	17:Cd:45:LYS:NZ	2.43	0.52
1:C1:2800:G:O2'	11:CL:44:GLU:OE2	2.24	0.52
1:C1:351:G:N2	1:C1:354:A:OP2	2.35	0.52
1:C1:2636:G:O6	1:C1:2639:A:N7	2.42	0.52
45:LZ:13:THR:HB	51:Lg:87:ARG:HG3	1.92	0.52
1:C1:1316:C:OP1	37:LQ:31:GLY:N	2.43	0.52
3:C3:40:G:O6	3:C3:45:U:O4	2.28	0.52
8:CI:284:PRO:HB2	8:CI:287:LYS:HB3	1.91	0.52
21:Ch:379:SER:OG	21:Ch:381:ASP:OD1	2.28	0.52
1:C1:967:U:H2'	1:C1:968:U:H6	1.75	0.52
1:C1:1211:A:H5''	6:CF:203:SER:HB3	1.91	0.52
1:C1:1599:A:OP2	9:CJ:52:LYS:NZ	2.38	0.52
6:CF:44:SER:HG	6:CF:222:SER:HG	1.58	0.52
13:CN:2:ALA:HA	13:CN:204:ALA:O	2.09	0.52
13:CN:118:HIS:HB3	13:CN:121:LEU:HD13	1.92	0.52
17:Cd:135:THR:HG22	17:Cd:138:ARG:HH12	1.75	0.52
24:LB:184:ILE:O	24:LB:192:LYS:NZ	2.42	0.52
1:C1:1337:G:N2	1:C1:1339:U:O2'	2.37	0.52
15:CQ:70:GLN:O	16:Cb:98:ARG:NH2	2.43	0.52
16:Cb:22:ILE:HD11	16:Cb:56:ALA:HB2	1.91	0.52
49:Le:61:ASN:HB3	49:Le:64:THR:HB	1.91	0.52
1:C1:626:C:OP2	49:Le:42:ARG:NH2	2.43	0.52
9:CJ:141:LEU:HD11	9:CJ:241:VAL:HG11	1.91	0.52
30:LJ:126:MET:HE3	30:LJ:128:PHE:HE1	1.75	0.52
1:C1:2925:G:O6	17:Cd:30:ARG:NH2	2.43	0.51
12:CM:102:PRO:HB2	12:CM:105:PRO:HD2	1.92	0.51
1:C1:259:C:OP1	34:LN:5:LYS:NZ	2.42	0.51
1:C1:210:G:OP1	44:LY:15:ARG:NH1	2.41	0.51
1:C1:2079:G:OP1	1:C1:2081:C:N4	2.43	0.51
11:CL:52:ASP:OD2	39:LS:80:ARG:NH2	2.43	0.51
31:LK:92:ARG:HH12	31:LK:98:ILE:HD13	1.74	0.51
44:LY:1:MET:HE3	44:LY:2:LYS:HG3	1.93	0.51
1:C1:643:C:H2'	1:C1:644:A:C8	2.45	0.51
1:C1:2100:U:OP2	1:C1:2105:A:N6	2.41	0.51
1:C1:2368:C:H4'	10:CK:142:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3000:U:OP2	1:C1:3050:C:N4	2.44	0.51
1:C1:1373:A:N6	1:C1:1401:A:O2'	2.43	0.51
1:C1:1758:G:O2'	1:C1:1760:G:OP2	2.28	0.51
1:C1:2523:G:H2'	1:C1:2524:G:H8	1.76	0.51
4:C4:99:C:H5'	19:Cf:96:ARG:HH22	1.74	0.51
13:CN:109:VAL:HB	13:CN:149:GLY:HA2	1.90	0.51
21:Ch:148:PRO:HB3	21:Ch:508:LYS:HA	1.92	0.51
24:LB:10:ARG:NH2	24:LB:264:THR:O	2.44	0.51
33:LM:20:LEU:HD21	33:LM:30:ILE:HD11	1.93	0.51
1:C1:219:C:OP1	44:LY:46:SER:OG	2.28	0.51
7:CH:156:LEU:HD23	7:CH:159:LEU:HD12	1.92	0.51
7:CH:365:MET:HA	7:CH:368:ILE:HG12	1.93	0.51
9:CJ:36:LEU:HD11	9:CJ:75:GLU:HG2	1.93	0.51
17:Cd:429:LEU:HD21	17:Cd:441:MET:HB2	1.91	0.51
1:C1:948:U:H2'	1:C1:949:A:H8	1.76	0.51
2:C2:154:C:H5'	28:LG:184:LYS:HD3	1.92	0.51
1:C1:877:A:O2'	1:C1:879:U:OP2	2.29	0.51
1:C1:2923:G:O2'	17:Cd:30:ARG:NH2	2.39	0.51
1:C1:1260:C:H2'	1:C1:1261:A:H8	1.76	0.51
33:LM:18:ARG:NH1	33:LM:65:THR:O	2.43	0.51
40:LT:111:GLU:HA	40:LT:114:GLU:HG3	1.93	0.51
43:LX:79:PRO:HA	43:LX:97:PHE:HA	1.93	0.51
1:C1:1737:G:OP1	41:LU:101:ARG:NH2	2.35	0.51
3:C3:48:C:OP2	8:CI:223:LYS:NZ	2.32	0.51
4:C4:44:C:OP2	30:LJ:138:ARG:NH2	2.43	0.51
1:C1:576:A:H5''	50:Lf:72:LYS:HD3	1.93	0.50
12:CM:220:PHE:HD2	12:CM:223:ARG:HG2	1.75	0.50
15:CQ:70:GLN:OE1	16:Cb:98:ARG:NH1	2.45	0.50
44:LY:54:GLU:HB3	44:LY:107:LYS:HB3	1.93	0.50
1:C1:639:G:O2'	1:C1:1418:A:OP1	2.29	0.50
1:C1:1866:A:O2'	24:LB:227:PHE:O	2.26	0.50
1:C1:1920:G:H21	1:C1:3303:A:H8	1.59	0.50
7:CH:174:PHE:HE2	7:CH:266:GLN:HA	1.74	0.50
15:CQ:16:SER:HB3	24:LB:73:VAL:HG11	1.91	0.50
28:LG:186:LYS:HB2	28:LG:197:THR:HG23	1.93	0.50
54:Lj:21:ARG:NH2	54:Lj:41:ALA:O	2.34	0.50
1:C1:341:C:O2	1:C1:345:A:O2'	2.29	0.50
2:C2:86:U:O2	54:Lj:87:ARG:NH1	2.43	0.50
10:CK:154:PRO:HG2	10:CK:249:PRO:HB2	1.94	0.50
1:C1:1582:A:N6	43:LX:83:GLU:OE2	2.33	0.50
9:CJ:131:TYR:OH	9:CJ:140:ASP:OD2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Cf:112:ASP:HB3	19:Cf:263:PRO:HG3	1.94	0.50
26:LD:50:ARG:NH2	26:LD:72:ASP:OD2	2.44	0.50
31:LK:143:VAL:HB	31:LK:151:ILE:HD13	1.94	0.50
6:CF:194:ILE:O	6:CF:205:GLN:NE2	2.37	0.50
21:Ch:465:SER:OG	21:Ch:466:LYS:N	2.45	0.50
26:LD:64:MET:HE3	26:LD:109:VAL:HG21	1.93	0.50
25:LC:29:ALA:O	58:Lq:3:ASN:ND2	2.45	0.50
1:C1:2318:G:OP1	36:LP:141:SER:OG	2.25	0.50
1:C1:3299:U:H2'	1:C1:3300:A:H8	1.77	0.50
4:C4:6:C:O2'	26:LD:50:ARG:NH2	2.45	0.50
6:CF:159:HIS:HB2	6:CF:174:MET:HE1	1.94	0.50
15:CQ:163:GLU:HA	15:CQ:166:LYS:HD2	1.93	0.50
18:Ce:248:ARG:NH2	18:Ce:252:GLU:OE2	2.45	0.50
11:CL:5:ILE:HD13	35:LO:49:PHE:HB2	1.93	0.49
23:LA:117:GLU:HB2	23:LA:162:SER:HB3	1.93	0.49
24:LB:92:TYR:HB2	24:LB:158:VAL:HB	1.93	0.49
1:C1:1879:G:O2'	1:C1:2297:U:O4	2.25	0.49
1:C1:2092:U:H2'	1:C1:2093:G:C8	2.47	0.49
1:C1:2588:U:H3	1:C1:2608:G:H1	1.60	0.49
8:CI:191:ILE:HA	8:CI:259:THR:O	2.11	0.49
20:Cg:43:ASP:HB3	20:Cg:46:VAL:HG12	1.93	0.49
24:LB:262:GLN:HB2	24:LB:265:VAL:HG23	1.94	0.49
27:LE:199:LYS:O	33:LM:117:ARG:NH2	2.45	0.49
29:LH:10:ILE:HD11	29:LH:109:ARG:HA	1.93	0.49
1:C1:450:U:O4	1:C1:468:G:N2	2.45	0.49
1:C1:1395:G:H5''	49:Le:125:ALA:HB2	1.93	0.49
13:CN:61:ARG:HD3	42:LV:133:SER:HA	1.94	0.49
1:C1:1214:A:H5''	1:C1:1215:C:H5'	1.95	0.49
2:C2:103:G:OP2	2:C2:105:A:O2'	2.26	0.49
9:CJ:164:MET:HG3	9:CJ:235:MET:HE1	1.93	0.49
25:LC:42:GLY:HA3	25:LC:114:ILE:HD11	1.93	0.49
1:C1:2981:U:H2'	1:C1:2982:A:H8	1.78	0.49
15:CQ:73:ALA:HB2	16:Cb:98:ARG:HE	1.77	0.49
32:LL:192:ALA:HB2	53:Li:19:GLY:HA2	1.95	0.49
1:C1:563:U:H2'	1:C1:564:A:H8	1.77	0.49
6:CF:30:ILE:O	6:CF:34:ILE:HD12	2.12	0.49
1:C1:2919:C:H2'	1:C1:2920:G:H8	1.78	0.49
10:CK:165:PRO:HG2	17:Cd:326:GLN:NE2	2.27	0.49
1:C1:151:G:H5''	1:C1:152:G:H2'	1.94	0.49
1:C1:3315:U:OP1	48:Ld:23:HIS:NE2	2.36	0.49
7:CH:183:VAL:HG21	7:CH:219:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:410:A:H2'	1:C1:411:A:C8	2.48	0.49
1:C1:1480:C:H2'	1:C1:1481:A:H8	1.78	0.49
1:C1:2920:G:O2'	17:Cd:366:TYR:O	2.31	0.49
10:CK:165:PRO:HG2	17:Cd:326:GLN:HE21	1.77	0.49
19:Cf:87:MET:HB2	19:Cf:103:VAL:HB	1.95	0.49
25:LC:4:ARG:NH2	25:LC:23:LEU:O	2.45	0.49
29:LH:138:VAL:HG11	29:LH:183:LEU:HD21	1.95	0.49
34:LN:36:ILE:HG12	34:LN:64:VAL:HG23	1.95	0.49
41:LU:19:LYS:NZ	41:LU:78:LEU:O	2.44	0.49
42:LV:36:LEU:HB3	42:LV:62:ALA:HB1	1.94	0.49
55:Lk:26:LYS:NZ	55:Lk:28:ASN:OD1	2.42	0.49
1:C1:464:C:H2'	1:C1:465:G:H8	1.77	0.49
1:C1:2586:C:OP1	30:LJ:62:ARG:NH2	2.46	0.49
3:C3:25:U:OP1	12:CM:76:LYS:NZ	2.34	0.49
7:CH:508:MET:HE1	48:Ld:66:LYS:HB2	1.94	0.49
9:CJ:397:TRP:HB2	9:CJ:401:LEU:HD12	1.95	0.49
34:LN:159:ARG:HB3	34:LN:164:LEU:HB2	1.95	0.49
2:C2:112:U:OP2	56:Ll:8:ARG:NH1	2.46	0.48
42:LV:19:LEU:HD11	42:LV:100:ASN:HB3	1.95	0.48
58:Lq:9:ILE:HG22	58:Lq:47:VAL:HG22	1.94	0.48
1:C1:20:U:H2'	1:C1:21:A:C8	2.49	0.48
2:C2:63:G:H22	2:C2:97:A:H2	1.61	0.48
6:CF:236:GLU:HG2	6:CF:241:LYS:HD3	1.95	0.48
7:CH:264:LYS:NZ	7:CH:304:GLU:OE1	2.41	0.48
50:Lf:16:LEU:HD11	50:Lf:33:LYS:HB2	1.95	0.48
1:C1:2923:G:H5''	17:Cd:34:LYS:HE3	1.94	0.48
9:CJ:189:PHE:HB3	9:CJ:196:TYR:HB2	1.95	0.48
19:Cf:277:THR:HG22	19:Cf:279:GLN:H	1.79	0.48
1:C1:1077:U:O2'	1:C1:1078:U:O2	2.28	0.48
1:C1:1890:A:O2'	16:Cb:7:ARG:NH2	2.46	0.48
1:C1:3002:A:H4'	24:LB:13:SER:HB2	1.96	0.48
1:C1:1611:C:OP2	45:LZ:47:ARG:NH2	2.46	0.48
1:C1:1624:C:H5'	1:C1:1625:U:H5''	1.94	0.48
9:CJ:42:ILE:HD13	18:Ce:189:LEU:HD21	1.95	0.48
19:Cf:135:PRO:HD2	19:Cf:138:MET:HE2	1.94	0.48
3:C3:55:U:O2'	3:C3:58:A:N7	2.43	0.48
8:Cl:297:LEU:HB3	8:Cl:301:GLN:HE21	1.78	0.48
9:CJ:17:MET:HE3	9:CJ:66:THR:HA	1.94	0.48
1:C1:230:G:H2'	1:C1:231:A:H8	1.79	0.48
1:C1:696:G:N2	1:C1:699:A:OP2	2.36	0.48
1:C1:976:G:H4'	1:C1:977:U:H5'	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3284:G:H21	1:C1:3303:A:H2	1.61	0.48
5:CB:133:LEU:HD21	5:CB:167:LEU:HD21	1.96	0.48
7:CH:361:LEU:O	7:CH:365:MET:HG2	2.13	0.48
12:CM:217:ASN:OD1	12:CM:223:ARG:NH1	2.46	0.48
38:LR:98:ARG:NH1	38:LR:130:ASN:OD1	2.42	0.48
45:LZ:8:ARG:HB3	45:LZ:24:ILE:HD12	1.95	0.48
45:LZ:69:PRO:HG3	45:LZ:114:LYS:HB2	1.96	0.48
15:CQ:18:GLY:HA3	15:CQ:31:PHE:O	2.14	0.48
1:C1:21:A:H2'	1:C1:22:G:C8	2.49	0.48
1:C1:464:C:H2'	1:C1:465:G:C8	2.49	0.48
1:C1:2751:A:H2'	1:C1:2752:G:H8	1.79	0.48
1:C1:3079:U:H1'	1:C1:3080:A:H5''	1.96	0.48
13:CN:104:LEU:HA	13:CN:107:VAL:HG22	1.96	0.48
23:LA:177:LYS:HB2	57:Lp:29:GLN:HG2	1.96	0.48
29:LH:68:ARG:NH1	29:LH:188:ASN:OD1	2.47	0.48
30:LJ:167:ARG:HG3	30:LJ:168:PHE:CD1	2.49	0.48
12:CM:128:ALA:O	12:CM:132:MET:HG3	2.14	0.48
21:Ch:472:VAL:HB	21:Ch:482:MET:HB2	1.95	0.48
32:LL:141:ASP:N	32:LL:141:ASP:OD1	2.46	0.48
1:C1:1476:G:H2'	56:Ll:13:LEU:HD22	1.96	0.47
7:CH:520:ARG:O	7:CH:525:LYS:NZ	2.46	0.47
1:C1:974:A:H5''	40:LT:43:LYS:HD2	1.95	0.47
1:C1:1779:A:H2'	1:C1:1780:A:H8	1.79	0.47
40:LT:36:VAL:HG13	40:LT:65:TYR:HA	1.95	0.47
47:Lc:47:ILE:HG21	47:Lc:56:LYS:HG3	1.95	0.47
1:C1:404:U:H2'	1:C1:405:G:C8	2.50	0.47
1:C1:2841:U:H5	24:LB:4:ARG:HH21	1.61	0.47
9:CJ:200:ASN:ND2	9:CJ:205:ASP:OD1	2.43	0.47
12:CM:213:LEU:HB3	12:CM:248:MET:HB3	1.96	0.47
1:C1:269:A:H2'	1:C1:270:G:C8	2.49	0.47
1:C1:679:A:N1	2:C2:28:C:O2'	2.44	0.47
1:C1:1698:A:H2'	1:C1:1699:G:C8	2.50	0.47
1:C1:2495:U:H2'	1:C1:2496:G:C8	2.49	0.47
1:C1:1559:G:OP2	1:C1:1559:G:N2	2.36	0.47
19:Cf:96:ARG:HG2	19:Cf:117:TYR:CE2	2.50	0.47
47:Lc:17:LEU:O	47:Lc:21:ILE:HG12	2.14	0.47
1:C1:716:G:H5''	37:LQ:71:PRO:HB2	1.96	0.47
1:C1:2069:A:H2'	1:C1:2070:A:C8	2.49	0.47
1:C1:2745:G:H21	46:La:58:MET:HE2	1.79	0.47
8:CI:225:GLY:HA3	8:CI:282:VAL:HG12	1.95	0.47
21:Ch:294:ILE:HG13	21:Ch:308:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1054:U:O2	1:C1:1070:G:N2	2.37	0.47
1:C1:1202:C:O2'	1:C1:1269:A:N1	2.45	0.47
1:C1:2802:U:H3'	22:Cz:76:ARG:HH22	1.79	0.47
1:C1:3179:G:H2'	1:C1:3180:G:C8	2.50	0.47
3:C3:64:G:OP2	8:CI:274:LYS:NZ	2.48	0.47
5:CB:64:LEU:HD11	5:CB:281:PHE:HD1	1.80	0.47
7:CH:466:GLU:HG3	7:CH:470:LYS:HE3	1.96	0.47
9:CJ:42:ILE:HG13	9:CJ:72:LEU:HD11	1.95	0.47
9:CJ:266:ALA:O	9:CJ:380:ARG:NH2	2.45	0.47
23:LA:28:LYS:HB3	23:LA:123:ARG:HB3	1.97	0.47
23:LA:103:PRO:HA	23:LA:163:ARG:HA	1.96	0.47
24:LB:76:VAL:HG12	24:LB:326:LYS:HA	1.97	0.47
24:LB:161:VAL:HG13	24:LB:184:ILE:HD11	1.96	0.47
31:LK:146:LYS:HB2	31:LK:151:ILE:HD11	1.95	0.47
35:LO:13:LYS:O	39:LS:169:ARG:NH2	2.43	0.47
37:LQ:110:VAL:HG12	37:LQ:112:ALA:H	1.80	0.47
55:Lk:24:ARG:HA	55:Lk:69:LYS:O	2.15	0.47
1:C1:230:G:H2'	1:C1:231:A:C8	2.50	0.47
1:C1:575:G:H2'	1:C1:576:A:H8	1.79	0.47
1:C1:967:U:H2'	1:C1:968:U:C6	2.50	0.47
1:C1:979:A:N6	1:C1:1033:U:O4	2.48	0.47
1:C1:1067:A:H2'	1:C1:1068:A:C8	2.50	0.47
1:C1:1939:U:O2'	1:C1:2045:G:N2	2.48	0.47
1:C1:2544:G:H5'	18:Ce:436:TRP:HE1	1.79	0.47
1:C1:2640:U:H5'	30:LJ:66:ILE:HD11	1.97	0.47
12:LF:102:PRO:HB2	12:LF:105:PRO:HD2	1.95	0.47
45:LZ:50:SER:HB2	45:LZ:64:ARG:HB3	1.96	0.47
25:LC:114:ILE:HB	25:LC:119:LYS:HE3	1.96	0.47
30:LJ:15:ILE:HD13	30:LJ:81:LEU:HD21	1.97	0.47
1:C1:2974:A:H2'	1:C1:2975:G:H8	1.79	0.47
30:LJ:86:LYS:HD3	30:LJ:90:TYR:HE1	1.80	0.47
30:LJ:94:ARG:O	30:LJ:157:ARG:NH2	2.47	0.47
32:LL:14:PHE:HB3	32:LL:18:TRP:CD1	2.50	0.47
1:C1:523:G:H2'	1:C1:524:A:C8	2.50	0.46
1:C1:2335:A:OP1	11:CL:19:ARG:NH1	2.49	0.46
1:C1:2396:U:H1'	34:LN:125:SER:HB3	1.97	0.46
2:C2:26:U:O2'	25:LC:52:ALA:O	2.34	0.46
8:CI:303:GLN:HA	8:CI:306:VAL:HG22	1.97	0.46
1:C1:1303:C:O2	39:LS:115:ARG:NH2	2.49	0.46
1:C1:1779:A:H2'	1:C1:1780:A:C8	2.50	0.46
1:C1:2400:G:OP1	28:LG:73:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Cg:168:SER:O	20:Cg:175:ARG:NH2	2.48	0.46
50:Lf:17:SER:OG	50:Lf:18:TYR:N	2.48	0.46
1:C1:64:A:N3	1:C1:79:U:O2'	2.40	0.46
1:C1:92:G:N2	1:C1:95:G:O2'	2.48	0.46
1:C1:582:G:H1'	27:LE:37:LYS:HG3	1.97	0.46
1:C1:2330:A:H2'	1:C1:2331:A:C8	2.50	0.46
3:C3:57:A:OP2	5:CB:144:ARG:NH2	2.48	0.46
15:CQ:66:ASP:HB3	15:CQ:69:LEU:HG	1.97	0.46
18:Ce:331:GLU:HG3	55:Lk:54:LYS:HE2	1.98	0.46
22:Cz:75:GLU:O	22:Cz:78:LYS:HG3	2.15	0.46
48:Ld:28:LEU:HD11	48:Ld:40:ALA:HB2	1.96	0.46
1:C1:231:A:H2'	1:C1:232:A:C8	2.50	0.46
1:C1:3179:G:H2'	1:C1:3180:G:H8	1.81	0.46
1:C1:604:G:H2'	1:C1:605:G:C8	2.50	0.46
1:C1:2846:A:N7	7:CH:30:THR:OG1	2.41	0.46
15:CQ:17:LYS:NZ	24:LB:361:ASP:OD2	2.48	0.46
19:Cf:47:ASN:HA	19:Cf:59:ARG:HH22	1.81	0.46
24:LB:386:LYS:HA	24:LB:389:GLN:HB2	1.98	0.46
1:C1:430:G:O6	58:Lq:134:ARG:NH1	2.45	0.46
1:C1:1177:G:H2'	1:C1:1178:A:C8	2.51	0.46
1:C1:1901:A:H2'	1:C1:1902:A:C8	2.51	0.46
2:C2:70:G:OP1	44:LY:120:ARG:NH2	2.39	0.46
13:CN:4:ARG:HB3	13:CN:208:LEU:HA	1.98	0.46
1:C1:101:A:H3'	1:C1:102:G:H21	1.80	0.46
1:C1:300:A:H2'	1:C1:301:A:H8	1.81	0.46
1:C1:644:A:H2'	1:C1:645:A:C8	2.51	0.46
1:C1:1701:U:O2'	1:C1:1703:G:N7	2.41	0.46
8:CI:220:ARG:HD2	8:CI:280:PHE:HB3	1.97	0.46
10:CK:87:PRO:HD2	10:CK:90:LEU:HD12	1.97	0.46
28:LG:85:LEU:HD22	28:LG:89:LEU:HD23	1.97	0.46
39:LS:24:LEU:HD22	39:LS:59:VAL:HG21	1.98	0.46
45:LZ:21:LYS:NZ	45:LZ:128:TRP:O	2.43	0.46
45:LZ:52:ILE:HD12	45:LZ:61:ILE:HG12	1.97	0.46
1:C1:1350:G:N2	1:C1:1351:U:O4	2.49	0.46
1:C1:1626:G:O2'	1:C1:1788:G:N2	2.41	0.46
7:CH:635:GLU:OE2	56:Ll:41:ARG:NH1	2.43	0.46
21:Ch:83:TYR:HD2	21:Ch:124:ALA:HB1	1.81	0.46
56:Ll:20:ASN:ND2	56:Ll:42:ARG:O	2.48	0.46
1:C1:264:C:O2	53:Li:91:ARG:NH2	2.39	0.46
1:C1:1216:G:N2	31:LK:131:GLU:OE2	2.36	0.46
1:C1:1698:A:H2'	1:C1:1699:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CB:299:LEU:HD12	8:CI:306:VAL:HG12	1.98	0.46
17:Cd:213:ILE:HD12	17:Cd:403:ASN:HB2	1.97	0.46
17:Cd:418:VAL:HG22	17:Cd:475:TRP:HB3	1.98	0.46
24:LB:313:VAL:HG23	24:LB:365:GLU:HG3	1.98	0.46
1:C1:243:U:O2'	1:C1:244:G:O5'	2.29	0.46
1:C1:2925:G:H2'	1:C1:2926:A:C8	2.51	0.46
1:C1:2998:A:H5''	42:LV:14:LYS:HB2	1.98	0.46
13:CN:85:ARG:NH2	13:CN:89:PRO:O	2.49	0.46
19:Cf:240:ARG:NH1	21:Ch:101:ASN:OD1	2.49	0.46
26:LD:214:LEU:HB3	26:LD:222:TYR:HB2	1.98	0.46
1:C1:243:U:O4	32:LL:132:LYS:NZ	2.43	0.45
1:C1:1449:G:N2	1:C1:1493:G:H5''	2.31	0.45
1:C1:2516:G:O2'	45:LZ:135:PHE:OXT	2.32	0.45
7:CH:168:THR:HA	7:CH:216:GLN:O	2.15	0.45
12:CM:126:THR:H	12:CM:129:THR:HG1	1.63	0.45
1:C1:1240:C:O2	6:CF:54:LYS:NZ	2.49	0.45
2:C2:38:U:H5'	52:Lh:83:LEU:HD13	1.98	0.45
3:C3:35:C:O2'	5:CB:288:THR:O	2.33	0.45
11:CL:23:LYS:HE2	11:CL:27:ARG:HH21	1.79	0.45
18:Ce:386:PRO:HA	18:Ce:389:LEU:HD13	1.98	0.45
19:Cf:232:ILE:HG23	19:Cf:244:VAL:HG13	1.98	0.45
21:Ch:325:ASN:ND2	21:Ch:380:ASP:OD2	2.45	0.45
25:LC:100:MET:HE3	25:LC:103:PRO:HA	1.99	0.45
28:LG:152:SER:N	28:LG:203:ILE:O	2.48	0.45
37:LQ:126:MET:O	37:LQ:146:GLY:HA3	2.16	0.45
52:Lh:36:ILE:HA	52:Lh:39:ILE:HG12	1.98	0.45
1:C1:1252:U:H1'	1:C1:1255:C:H5	1.80	0.45
1:C1:2123:G:H2'	1:C1:2124:G:H8	1.81	0.45
19:Cf:33:LEU:HG	19:Cf:89:PHE:HD1	1.82	0.45
25:LC:236:PRO:HG2	25:LC:239:ALA:HB3	1.99	0.45
12:LF:245:ILE:O	12:LF:249:ASN:HB3	2.17	0.45
42:LV:106:ASN:OD1	42:LV:110:GLU:N	2.48	0.45
46:La:75:ILE:HD12	46:La:118:LEU:HG	1.97	0.45
1:C1:1576:C:H2'	1:C1:1577:C:C6	2.51	0.45
1:C1:3288:A:H2'	1:C1:3289:G:H8	1.81	0.45
1:C1:3289:G:O6	1:C1:3298:U:O4	2.34	0.45
16:Cb:18:ASP:OD1	16:Cb:19:LEU:N	2.47	0.45
23:LA:54:ARG:HG2	23:LA:56:ALA:H	1.80	0.45
1:C1:88:U:H2'	1:C1:89:A:H8	1.81	0.45
1:C1:420:C:OP2	49:Le:16:LYS:NZ	2.40	0.45
1:C1:1361:U:H2'	1:C1:1362:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CB:305:LYS:NZ	8:CI:294:GLU:O	2.48	0.45
30:LJ:41:LEU:HD22	30:LJ:126:MET:HE1	1.98	0.45
1:C1:2971:U:H2'	1:C1:2972:U:C6	2.52	0.45
12:LF:92:VAL:O	12:LF:120:GLY:HA2	2.16	0.45
31:LK:143:VAL:HG23	31:LK:148:PRO:HG3	1.99	0.45
1:C1:582:G:O2'	27:LE:35:GLN:O	2.33	0.45
1:C1:820:G:O6	57:Lp:4:ARG:NH1	2.50	0.45
1:C1:3044:A:H3'	1:C1:3045:A:H8	1.82	0.45
5:CB:19:ASP:OD1	5:CB:19:ASP:N	2.45	0.45
8:CI:194:LEU:HD22	8:CI:198:PHE:HD2	1.82	0.45
58:Lq:11:GLU:HA	58:Lq:14:ARG:HD2	1.99	0.45
1:C1:282:U:H2'	1:C1:283:G:H8	1.81	0.45
1:C1:1054:U:O4	1:C1:1070:G:O6	2.35	0.45
1:C1:2386:U:H2'	1:C1:2387:A:H8	1.81	0.45
7:CH:542:GLU:OE1	7:CH:547:ARG:NH2	2.50	0.45
21:Ch:242:PRO:HB3	21:Ch:335:LEU:HD22	1.99	0.45
1:C1:1186:A:H62	1:C1:1283:G:H21	1.62	0.45
18:Ce:237:GLU:HA	18:Ce:240:ARG:HG2	1.99	0.45
20:Cg:150:ASP:O	20:Cg:170:ARG:NH1	2.37	0.45
30:LJ:55:VAL:HG12	30:LJ:58:PHE:H	1.82	0.45
55:Lk:16:ARG:HG2	55:Lk:63:PRO:HG3	1.98	0.45
1:C1:159:U:H2'	1:C1:160:G:C8	2.52	0.45
1:C1:842:G:H8	23:LA:183:SER:HB3	1.82	0.45
1:C1:848:A2M:HM'2	1:C1:849:G:H5'	1.99	0.45
1:C1:2120:G:N2	1:C1:2140:G:O2'	2.50	0.45
11:CL:56:PRO:HG3	39:LS:89:ASN:HB3	1.99	0.45
18:Ce:222:TYR:OH	18:Ce:384:VAL:O	2.34	0.45
20:Cg:17:LYS:NZ	20:Cg:32:ASP:OD2	2.48	0.45
25:LC:287:LEU:HD11	37:LQ:60:LEU:HB2	1.98	0.45
28:LG:53:VAL:HG22	43:LX:43:THR:HA	1.99	0.45
32:LL:86:PRO:HG2	32:LL:89:LEU:HB3	1.99	0.45
34:LN:177:GLY:O	34:LN:184:ARG:NH1	2.50	0.45
39:LS:77:ILE:HG12	39:LS:126:VAL:HG22	1.99	0.45
1:C1:400:A:C2	2:C2:17:A:H1'	2.52	0.44
3:C3:10:C:H2'	3:C3:11:A:H8	1.81	0.44
7:CH:231:MET:HB2	7:CH:236:MET:HE3	1.98	0.44
8:CI:298:SER:H	8:CI:301:GLN:NE2	2.14	0.44
1:C1:768:A:H4'	1:C1:769:G:H5'	1.99	0.44
1:C1:1480:C:H2'	1:C1:1481:A:C8	2.52	0.44
1:C1:3120:C:H2'	1:C1:3121:G:H8	1.83	0.44
9:CJ:374:LEU:HD22	9:CJ:383:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Ch:464:GLY:HA3	21:Ch:494:VAL:HG21	1.99	0.44
1:C1:1816:C:O2'	1:C1:1822:A:N1	2.42	0.44
1:C1:2314:U:H2'	1:C1:2315:A:H8	1.83	0.44
2:C2:58:G:O6	54:Lj:63:ARG:NH1	2.41	0.44
6:CF:64:ARG:NH1	6:CF:65:ILE:O	2.50	0.44
9:CJ:143:ASP:OD2	18:Ce:413:ARG:NH2	2.37	0.44
15:CQ:66:ASP:OD1	15:CQ:67:SER:N	2.50	0.44
1:C1:813:G:O2'	1:C1:1844:A:N3	2.41	0.44
1:C1:866:A:OP1	54:Lj:5:THR:OG1	2.32	0.44
1:C1:980:A:H2'	1:C1:981:G:C8	2.52	0.44
21:Ch:173:ILE:HD11	21:Ch:204:LEU:HD22	2.00	0.44
1:C1:652:A:H2'	1:C1:653:A:C8	2.53	0.44
1:C1:1638:G:H2'	1:C1:1639:A:C8	2.53	0.44
1:C1:2741:U:H5'	32:LL:200:LYS:HZ3	1.82	0.44
1:C1:2790:G:H2'	1:C1:2791:C:C6	2.52	0.44
5:CB:33:HIS:HA	5:CB:36:LYS:HG2	2.00	0.44
5:CB:259:ILE:HA	5:CB:262:VAL:HG12	1.98	0.44
21:Ch:41:PHE:HE2	21:Ch:122:LEU:HD12	1.83	0.44
26:LD:223:LYS:O	26:LD:227:VAL:HB	2.17	0.44
51:Lg:93:ALA:O	51:Lg:97:GLU:HG3	2.18	0.44
1:C1:2074:G:C6	16:Cb:76:ARG:HD3	2.52	0.44
1:C1:2577:G:H21	1:C1:2578:OMG:HM23	1.81	0.44
5:CB:67:THR:HA	5:CB:239:THR:O	2.18	0.44
6:CF:78:GLY:HA3	6:CF:84:GLU:HA	1.98	0.44
17:Cd:328:SER:HB3	17:Cd:376:ILE:HD11	2.00	0.44
47:Lc:17:LEU:HD11	47:Lc:93:MET:HE1	1.99	0.44
50:Lf:55:TYR:CZ	50:Lf:67:ARG:HB2	2.52	0.44
54:Lj:43:LYS:HE3	54:Lj:43:LYS:HB2	1.73	0.44
1:C1:2802:U:H3'	22:Cz:76:ARG:NH2	2.33	0.44
27:LE:86:PRO:HD2	27:LE:89:ILE:HD12	2.00	0.44
1:C1:638:C:H2'	1:C1:639:G:C8	2.53	0.44
2:C2:85:G:C8	44:LY:112:LYS:HE3	2.53	0.44
4:C4:77:U:H2'	4:C4:78:A:H8	1.82	0.44
5:CB:237:PRO:HB2	8:CI:286:ASN:ND2	2.32	0.44
29:LH:154:ARG:HG2	29:LH:162:VAL:HG22	2.00	0.44
43:LX:116:TYR:HB2	43:LX:118:ILE:HG12	1.99	0.44
55:Lk:9:LYS:O	55:Lk:13:GLU:HG3	2.18	0.44
1:C1:530:G:H1	1:C1:543:U:H3	1.66	0.44
1:C1:651:C:H2'	1:C1:652:A:H8	1.82	0.44
13:CN:106:ASN:HB3	13:CN:147:LEU:HD22	2.00	0.44
49:Le:30:ASP:OD1	49:Le:31:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:489:A:O2'	1:C1:3214:A:N1	2.47	0.43
12:CM:15:PRO:HG3	18:Ce:234:ILE:HD11	1.99	0.43
35:LO:23:ILE:HD13	35:LO:122:VAL:HG11	1.99	0.43
43:LX:63:SER:HB2	52:Lh:71:LEU:HD13	2.00	0.43
1:C1:203:A:N3	25:LC:228:ASN:ND2	2.62	0.43
1:C1:638:C:H2'	1:C1:639:G:H8	1.83	0.43
1:C1:1197:U:H2'	1:C1:1198:A:C8	2.53	0.43
3:C3:11:A:OP1	5:CB:188:ARG:NH2	2.51	0.43
3:C3:36:C:H2'	3:C3:37:G:C8	2.53	0.43
3:C3:57:A:N6	5:CB:138:LYS:O	2.46	0.43
10:CK:219:THR:HB	10:CK:245:ILE:HD12	2.01	0.43
13:CN:14:GLY:HA2	13:CN:198:VAL:HG13	2.00	0.43
18:Ce:258:ALA:HB2	45:LZ:123:SER:HB2	1.99	0.43
18:Ce:307:ILE:HG12	18:Ce:310:ARG:HH21	1.82	0.43
19:Cf:98:HIS:CD2	19:Cf:120:PRO:HG3	2.53	0.43
1:C1:2860:G:O2'	1:C1:2982:A:N1	2.50	0.43
4:C4:93:G:H2'	4:C4:94:A:C8	2.53	0.43
5:CB:180:ILE:HG23	5:CB:232:LEU:HD11	2.00	0.43
5:CB:263:ILE:HG12	5:CB:281:PHE:CE1	2.53	0.43
26:LD:214:LEU:HD12	26:LD:226:PHE:HE2	1.84	0.43
27:LE:16:THR:HG23	12:LF:4:THR:HA	1.99	0.43
29:LH:86:LYS:HB3	29:LH:89:VAL:HB	2.00	0.43
29:LH:127:MET:HE2	29:LH:218:ILE:HG22	2.00	0.43
32:LL:67:ARG:NE	46:La:105:LEU:O	2.51	0.43
34:LN:183:THR:HG22	34:LN:187:ARG:HB2	1.99	0.43
46:La:101:VAL:HG22	46:La:124:VAL:HB	2.00	0.43
1:C1:1595:C:H2'	1:C1:1596:U:C6	2.53	0.43
1:C1:2069:A:H2'	1:C1:2070:A:H8	1.83	0.43
1:C1:2489:C:OP1	23:LA:37:ARG:NH1	2.48	0.43
1:C1:2974:A:H2'	1:C1:2975:G:C8	2.52	0.43
1:C1:3008:U:O2'	15:CQ:16:SER:O	2.28	0.43
10:CK:11:ARG:HD3	10:CK:16:ARG:HH12	1.84	0.43
17:Cd:238:HIS:HD2	17:Cd:268:PHE:HE1	1.66	0.43
1:C1:88:U:H2'	1:C1:89:A:C8	2.53	0.43
1:C1:651:C:H2'	1:C1:652:A:C8	2.53	0.43
1:C1:663:C:O2'	1:C1:667:U:OP1	2.30	0.43
1:C1:2547:U:OP1	28:LG:244:LYS:NZ	2.47	0.43
7:CH:77:HIS:O	7:CH:81:MET:HG3	2.19	0.43
10:CK:174:PRO:HG2	10:CK:177:LEU:HD12	2.00	0.43
17:Cd:347:ARG:HD3	17:Cd:369:LEU:HA	1.99	0.43
1:C1:619:A:H2'	1:C1:620:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1345:G:H2'	1:C1:1346:A:C8	2.54	0.43
17:Cd:226:LEU:HD22	17:Cd:381:ILE:HD13	2.00	0.43
30:LJ:38:LEU:HD13	30:LJ:70:VAL:HG23	2.01	0.43
54:Lj:64:MET:HE3	54:Lj:64:MET:HB3	1.88	0.43
58:Lq:10:TRP:HB2	58:Lq:47:VAL:HG11	2.01	0.43
1:C1:575:G:H2'	1:C1:576:A:C8	2.53	0.43
1:C1:1454:U:H2'	1:C1:1455:G:C8	2.54	0.43
5:CB:27:CYS:HB2	5:CB:252:PRO:HB3	2.00	0.43
13:CN:52:THR:HG21	24:LB:70:LYS:HE2	2.00	0.43
22:Cz:77:GLN:HA	22:Cz:80:ILE:HG12	2.00	0.43
35:LO:157:ARG:O	35:LO:161:ARG:HG3	2.18	0.43
40:LT:74:VAL:HB	40:LT:89:ILE:HG13	2.00	0.43
45:LZ:24:ILE:HA	45:LZ:42:VAL:HG12	2.00	0.43
1:C1:91:C:OP1	46:La:59:ARG:NH1	2.52	0.43
1:C1:656:U:H2'	1:C1:657:U:C6	2.54	0.43
1:C1:1677:A:OP1	51:Lg:22:ARG:NH2	2.52	0.43
3:C3:65:U:H3	8:CI:281:LYS:HD3	1.82	0.43
36:LP:122:ALA:HB3	36:LP:143:PRO:HG2	2.00	0.43
49:Le:80:VAL:HA	49:Le:83:VAL:HG12	2.01	0.43
1:C1:405:G:OP1	36:LP:62:ARG:NH1	2.51	0.43
1:C1:1282:U:H5''	10:CK:43:ARG:HE	1.84	0.43
1:C1:1778:A:H2'	1:C1:1779:A:C8	2.54	0.43
1:C1:1785:C:OP2	51:Lg:68:LYS:NZ	2.43	0.43
1:C1:2320:A:H2'	1:C1:2321:A:H8	1.83	0.43
1:C1:2885:A:H2'	1:C1:2886:C:C6	2.54	0.43
17:Cd:411:ILE:HG13	17:Cd:439:LEU:HD11	2.00	0.43
21:Ch:349:THR:HG23	21:Ch:352:GLU:H	1.84	0.43
29:LH:7:GLU:HA	29:LH:92:LEU:O	2.18	0.43
47:Lc:77:ASN:OD1	47:Lc:77:ASN:N	2.52	0.43
4:C4:1:A:C8	26:LD:271:LYS:HG2	2.54	0.43
8:CI:317:ALA:HA	8:CI:320:LEU:HG	2.01	0.43
10:CK:53:GLN:O	10:CK:57:GLN:HG3	2.19	0.43
1:C1:1157:G:N2	35:LO:89:MET:HE2	2.34	0.42
1:C1:2956:U:H2'	1:C1:2957:C:C6	2.53	0.42
24:LB:189:VAL:HA	24:LB:192:LYS:HD2	2.01	0.42
1:C1:2376:A:H2'	1:C1:2377:G:H8	1.84	0.42
1:C1:2392:G:H2'	1:C1:2393:A:H8	1.84	0.42
5:CB:261:THR:HA	5:CB:264:ARG:HG2	2.01	0.42
1:C1:129:G:OP2	52:Lh:79:LYS:NZ	2.49	0.42
7:CH:331:LYS:HE2	7:CH:331:LYS:HB3	1.91	0.42
52:Lh:100:GLU:O	52:Lh:104:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:268:U:H2'	1:C1:269:A:C8	2.54	0.42
1:C1:1723:G:H2'	1:C1:1724:G:H8	1.84	0.42
4:C4:78:A:H3'	4:C4:79:G:H8	1.83	0.42
5:CB:21:ASP:OD1	5:CB:21:ASP:N	2.52	0.42
19:Cf:290:ASP:OD1	19:Cf:294:ASP:N	2.52	0.42
25:LC:211:ILE:HG13	25:LC:256:VAL:HB	2.01	0.42
35:LO:129:LEU:HD11	39:LS:170:PRO:HG2	2.01	0.42
37:LQ:174:ARG:HB2	37:LQ:177:VAL:HG23	2.01	0.42
39:LS:138:PRO:HA	39:LS:141:LYS:HB2	2.02	0.42
1:C1:338:G:O2'	2:C2:25:G:N3	2.53	0.42
1:C1:551:C:H2'	1:C1:552:C:H6	1.83	0.42
1:C1:1148:G:OP1	50:Lf:86:LYS:NZ	2.50	0.42
1:C1:1892:U:N3	1:C1:2085:G:OP2	2.44	0.42
1:C1:2728:A:H2'	1:C1:2729:G:C8	2.55	0.42
1:C1:3137:A:OP1	35:LO:38:ARG:NH2	2.45	0.42
2:C2:94:C:H5''	54:Lj:76:ASN:ND2	2.34	0.42
15:CQ:64:VAL:HG13	15:CQ:65:VAL:HG23	2.02	0.42
19:Cf:30:CYS:HA	19:Cf:86:LEU:O	2.18	0.42
38:LR:105:LEU:HD22	38:LR:135:LYS:HG3	2.00	0.42
57:Lp:25:LEU:O	57:Lp:29:GLN:NE2	2.53	0.42
1:C1:508:G:OP1	12:LF:73:ARG:NH2	2.50	0.42
1:C1:3163:A:N6	1:C1:3217:U:O2	2.38	0.42
2:C2:47:C:H1'	2:C2:61:A:H2'	2.02	0.42
5:CB:129:ASP:N	5:CB:129:ASP:OD1	2.48	0.42
18:Ce:303:GLU:HG3	18:Ce:306:ARG:NH2	2.35	0.42
25:LC:361:LEU:HG	39:LS:8:GLN:HE22	1.85	0.42
34:LN:99:ARG:O	34:LN:103:GLU:HG3	2.18	0.42
45:LZ:14:ARG:NE	51:Lg:87:ARG:HD3	2.35	0.42
53:Li:66:VAL:O	53:Li:70:LEU:HG	2.19	0.42
1:C1:498:U:H2'	1:C1:499:C:C6	2.54	0.42
1:C1:1901:A:H2'	1:C1:1902:A:H8	1.84	0.42
1:C1:2621:G:H2'	1:C1:2622:G:H8	1.84	0.42
19:Cf:103:VAL:HG22	19:Cf:113:MET:HG2	2.01	0.42
21:Ch:208:SER:OG	21:Ch:209:MET:N	2.53	0.42
1:C1:494:C:H2'	1:C1:495:G:H8	1.84	0.42
1:C1:1371:U:O2'	49:Le:100:ASN:O	2.37	0.42
1:C1:2473:U:O2'	1:C1:2474:A:O5'	2.32	0.42
1:C1:2958:G:H2'	1:C1:2959:U:C6	2.55	0.42
4:C4:62:U:H4'	26:LD:290:ARG:HH12	1.84	0.42
19:Cf:110:VAL:HG11	19:Cf:113:MET:HE2	2.02	0.42
23:LA:29:PHE:CZ	23:LA:115:ASN:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LE:166:ASP:HA	27:LE:169:LEU:HB2	2.02	0.42
36:LP:174:ARG:O	36:LP:178:VAL:HG23	2.20	0.42
39:LS:66:GLU:HB3	39:LS:69:PRO:HG3	2.00	0.42
45:LZ:28:VAL:HG12	45:LZ:31:GLY:H	1.84	0.42
1:C1:1100:G:H2'	1:C1:1101:C:C6	2.55	0.42
1:C1:1123:G:H5'	12:LF:100:LYS:HG2	2.02	0.42
1:C1:1140:G:O2'	1:C1:1152:A:N3	2.49	0.42
1:C1:1387:G:N2	1:C1:1390:A:OP2	2.36	0.42
1:C1:2103:U:OP2	7:CH:657:LYS:NZ	2.49	0.42
1:C1:2495:U:H2'	1:C1:2496:G:H8	1.85	0.42
4:C4:26:C:H5'	26:LD:56:THR:HB	2.02	0.42
17:Cd:448:ARG:HB3	17:Cd:456:ASP:HB3	2.00	0.42
33:LM:59:LEU:O	39:LS:155:ARG:NH2	2.52	0.42
1:C1:287:A:P	34:LN:15:GLN:HE22	2.43	0.42
1:C1:1702:U:O4'	38:LR:96:MET:HG3	2.20	0.42
1:C1:2367:A:H4'	7:CH:655:ILE:HD13	2.02	0.42
2:C2:153:U:OP1	28:LG:66:LYS:NZ	2.48	0.42
6:CF:227:TRP:HB2	6:CF:234:VAL:HG22	2.02	0.42
44:LY:30:MET:HB3	44:LY:100:PRO:HG2	2.02	0.42
1:C1:300:A:H2'	1:C1:301:A:C8	2.55	0.41
1:C1:703:A:N1	1:C1:763:G:O2'	2.50	0.41
1:C1:942:U:OP1	1:C1:945:G:N1	2.53	0.41
1:C1:1697:C:H2'	1:C1:1698:A:C8	2.55	0.41
1:C1:1783:C:H2'	1:C1:1784:G:C8	2.55	0.41
9:CJ:223:ASP:HB3	9:CJ:226:ILE:HG22	2.02	0.41
9:CJ:266:ALA:HB3	9:CJ:270:ALA:HB2	2.02	0.41
33:LM:61:ARG:HH11	39:LS:158:LYS:NZ	2.17	0.41
1:C1:106:C:H2'	1:C1:107:A:H8	1.84	0.41
1:C1:116:A:H2'	1:C1:258:A:H2'	2.02	0.41
1:C1:117:A:C4	18:Ce:104:ARG:HD3	2.55	0.41
1:C1:282:U:H2'	1:C1:283:G:C8	2.55	0.41
1:C1:869:G:H2'	1:C1:870:A:C8	2.55	0.41
1:C1:957:C:H2'	1:C1:958:G:C8	2.54	0.41
1:C1:1646:G:H2'	1:C1:1647:G:H8	1.84	0.41
1:C1:2277:OMU:O5'	1:C1:2277:OMU:H6	2.21	0.41
1:C1:2889:A:H2'	1:C1:2890:C:C6	2.55	0.41
2:C2:83:C:O2	44:LY:109:HIS:NE2	2.37	0.41
3:C3:3:C:N4	28:LG:88:ASN:OD1	2.50	0.41
7:CH:250:LEU:HD11	7:CH:334:VAL:HG11	2.01	0.41
8:CI:302:TRP:HA	8:CI:305:LYS:HG2	2.02	0.41
26:LD:82:GLU:OE1	26:LD:108:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LJ:167:ARG:HG3	30:LJ:168:PHE:HD1	1.85	0.41
1:C1:224:U:H2'	1:C1:225:A:C8	2.55	0.41
1:C1:2964:A:H2'	1:C1:2965:U:O4'	2.20	0.41
4:C4:37:G:O6	22:Cz:110:ARG:NH2	2.53	0.41
6:CF:141:ILE:HD11	6:CF:184:GLU:HG3	2.01	0.41
11:CL:53:PRO:HB2	39:LS:89:ASN:ND2	2.35	0.41
19:Cf:124:ARG:HB2	19:Cf:252:ARG:HB3	2.01	0.41
20:Cg:66:LEU:O	20:Cg:70:THR:OG1	2.32	0.41
21:Ch:88:HIS:HB2	21:Ch:121:THR:HB	2.02	0.41
12:LF:101:ILE:HG23	12:LF:106:ARG:HG3	2.02	0.41
28:LG:106:GLN:OE1	28:LG:106:GLN:N	2.53	0.41
30:LJ:126:MET:HE3	30:LJ:128:PHE:CE1	2.54	0.41
33:LM:69:ILE:HA	33:LM:70:PRO:HD3	1.95	0.41
39:LS:1:MET:HG3	39:LS:118:PHE:HB2	2.03	0.41
1:C1:767:G:OP2	37:LQ:91:SER:OG	2.25	0.41
1:C1:1762:U:H2'	1:C1:1763:C:C6	2.54	0.41
1:C1:3211:U:OP2	27:LE:152:LYS:NZ	2.46	0.41
3:C3:38:C:H5'	5:CB:67:THR:HG21	2.03	0.41
3:C3:49:G:H21	5:CB:240:ASN:HD22	1.67	0.41
8:CI:297:LEU:HB2	8:CI:302:TRP:HE1	1.85	0.41
9:CJ:119:PRO:HD3	9:CJ:235:MET:HE3	2.03	0.41
12:CM:116:GLN:N	12:CM:116:GLN:OE1	2.52	0.41
21:Ch:100:PRO:HG3	21:Ch:106:LEU:HD22	2.01	0.41
24:LB:217:ASP:OD2	24:LB:340:ARG:NH2	2.37	0.41
26:LD:260:SER:HB3	26:LD:264:LYS:HZ1	1.85	0.41
34:LN:103:GLU:OE1	34:LN:118:SER:OG	2.35	0.41
37:LQ:150:THR:OG1	37:LQ:152:ASP:OD1	2.34	0.41
52:Lh:107:GLU:HG2	52:Lh:111:LYS:HE3	2.02	0.41
1:C1:405:G:H2'	1:C1:406:U:C6	2.56	0.41
1:C1:1220:G:H22	1:C1:1234:A:H2	1.67	0.41
1:C1:1577:C:H5'	1:C1:1676:A:H1'	2.02	0.41
1:C1:1809:G:O2'	9:CJ:2:GLY:N	2.39	0.41
1:C1:2740:U:O3'	32:LL:200:LYS:NZ	2.49	0.41
1:C1:2771:C:H2'	1:C1:2772:A:C8	2.56	0.41
1:C1:2773:G:OP1	25:LC:74:ARG:NH1	2.40	0.41
1:C1:3204:C:H2'	1:C1:3205:G:C8	2.49	0.41
4:C4:63:G:H2'	4:C4:64:A:C8	2.56	0.41
4:C4:88:G:O2'	4:C4:91:A:N6	2.54	0.41
9:CJ:228:GLY:O	9:CJ:232:GLU:HG3	2.21	0.41
18:Ce:189:LEU:HD23	18:Ce:189:LEU:HA	1.94	0.41
27:LE:98:ASN:HB3	27:LE:101:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:Lp:79:MET:O	57:Lp:83:LEU:HB2	2.20	0.41
1:C1:262:G:H5''	34:LN:14:LYS:HE2	2.01	0.41
1:C1:2822:G:C2	7:CH:94:LEU:HD13	2.56	0.41
1:C1:2858:C:O2'	1:C1:2860:G:OP2	2.30	0.41
3:C3:64:G:O6	8:CI:278:ARG:NH1	2.54	0.41
26:LD:207:VAL:O	26:LD:211:MET:HG3	2.20	0.41
37:LQ:87:ARG:HB3	37:LQ:112:ALA:HB2	2.00	0.41
49:Le:112:ARG:NH1	49:Le:115:GLN:OE1	2.53	0.41
53:Li:54:ARG:NH2	53:Li:98:GLU:OE2	2.53	0.41
58:Lq:54:ILE:HG12	58:Lq:63:VAL:HG22	2.02	0.41
1:C1:213:A:O2'	1:C1:214:G:N2	2.44	0.41
1:C1:742:G:O2'	1:C1:752:G:N2	2.37	0.41
1:C1:1219:G:N2	1:C1:1227:A:OP1	2.54	0.41
1:C1:1589:C:H2'	1:C1:1590:G:C8	2.55	0.41
1:C1:1812:OMC:OP1	43:LX:133:LYS:NZ	2.47	0.41
1:C1:2708:G:H5''	26:LD:41:LYS:HE3	2.02	0.41
5:CB:165:LYS:HE2	5:CB:165:LYS:HB2	1.89	0.41
9:CJ:449:ARG:HG3	9:CJ:455:TYR:CE2	2.55	0.41
24:LB:160:ARG:HG2	24:LB:183:GLN:HA	2.02	0.41
24:LB:242:LYS:HD2	24:LB:242:LYS:HA	1.94	0.41
27:LE:94:LEU:HD11	27:LE:165:ILE:HD12	2.03	0.41
12:LF:137:GLU:HG2	12:LF:142:TYR:HE1	1.86	0.41
12:LF:182:TYR:CZ	12:LF:203:GLN:HG2	2.55	0.41
57:Lp:51:ALA:HB3	57:Lp:54:ILE:HD12	2.03	0.41
1:C1:650:U:H2'	1:C1:651:C:C6	2.56	0.41
1:C1:777:C:H2'	1:C1:778:OMC:H6	1.85	0.41
1:C1:2069:A:OP2	16:Cb:70:LYS:NZ	2.52	0.41
21:Ch:225:ASN:ND2	21:Ch:268:ASN:O	2.54	0.41
23:LA:40:TYR:HA	23:LA:91:GLY:HA3	2.02	0.41
42:LV:9:PRO:HB2	42:LV:127:LEU:HD22	2.01	0.41
1:C1:163:U:H2'	1:C1:164:U:C6	2.56	0.41
1:C1:425:G:H2'	1:C1:426:A:C8	2.56	0.41
1:C1:735:C:H2'	1:C1:736:G:H8	1.85	0.41
1:C1:804:G:H2'	1:C1:805:C:H6	1.86	0.41
1:C1:2308:A:H5''	48:Ld:32:THR:HG23	2.02	0.41
1:C1:2533:G:O2'	18:Ce:424:PHE:O	2.32	0.41
2:C2:9:A:H2'	2:C2:10:A:C8	2.56	0.41
4:C4:4:U:H2'	4:C4:5:A:C8	2.56	0.41
5:CB:141:GLU:HA	5:CB:144:ARG:HE	1.86	0.41
7:CH:191:THR:HA	7:CH:192:PRO:HD3	1.97	0.41
9:CJ:371:THR:HB	9:CJ:415:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CM:149:SER:HB2	12:CM:245:ILE:HG21	2.03	0.41
18:Ce:376:LEU:HD23	18:Ce:376:LEU:HA	1.97	0.41
19:Cf:178:VAL:HB	26:LD:131:LEU:HB3	2.02	0.41
23:LA:51:ASP:HB3	23:LA:54:ARG:HB3	2.03	0.41
28:LG:56:PRO:HD2	28:LG:59:ILE:HD12	2.03	0.41
29:LH:64:VAL:HG12	29:LH:119:VAL:HG21	2.02	0.41
44:LY:85:THR:HG22	44:LY:95:PRO:HA	2.02	0.41
1:C1:684:C:H2'	1:C1:685:G:C8	2.56	0.41
1:C1:927:C:H2'	1:C1:928:C:C6	2.56	0.41
1:C1:957:C:H2'	1:C1:958:G:H8	1.86	0.41
1:C1:1142:A:OP1	37:LQ:31:GLY:N	2.54	0.41
1:C1:1159:C:H2'	1:C1:1160:G:N2	2.36	0.41
1:C1:3245:C:O3'	24:LB:335:ARG:NH2	2.55	0.41
4:C4:11:A:N1	4:C4:67:G:O2'	2.38	0.41
4:C4:28:C:H5''	30:LJ:138:ARG:HB3	2.03	0.41
5:CB:138:LYS:H	5:CB:138:LYS:HG2	1.73	0.41
7:CH:524:LYS:NZ	7:CH:551:GLN:OE1	2.54	0.41
17:Cd:248:THR:HA	17:Cd:334:TYR:CE2	2.56	0.41
21:Ch:43:ASP:OD1	21:Ch:47:ASN:N	2.42	0.41
21:Ch:424:TRP:HA	21:Ch:448:PRO:HB3	2.03	0.41
30:LJ:33:ARG:HD3	30:LJ:121:ILE:HA	2.03	0.41
30:LJ:93:ARG:HH12	30:LJ:95:ARG:CZ	2.34	0.41
33:LM:94:TRP:O	33:LM:97:THR:OG1	2.34	0.41
47:Lc:21:ILE:HD13	47:Lc:26:VAL:HG21	2.02	0.41
1:C1:1917:OMU:H1'	1:C1:1917:OMU:HM23	1.57	0.40
1:C1:2386:U:H2'	1:C1:2387:A:C8	2.56	0.40
1:C1:3123:U:H2'	1:C1:3124:G:C8	2.56	0.40
5:CB:66:LEU:O	5:CB:240:ASN:HA	2.21	0.40
10:CK:166:VAL:HG21	17:Cd:364:TRP:HH2	1.86	0.40
13:CN:197:MET:HE2	13:CN:199:VAL:HB	2.03	0.40
18:Ce:417:GLU:OE2	18:Ce:419:ARG:NH1	2.48	0.40
21:Ch:61:THR:OG1	21:Ch:64:ASN:OD1	2.33	0.40
21:Ch:305:VAL:HB	21:Ch:315:HIS:HB2	2.02	0.40
12:LF:101:ILE:HA	12:LF:102:PRO:HD3	1.97	0.40
28:LG:169:LEU:HD23	28:LG:169:LEU:HA	1.96	0.40
39:LS:1:MET:HE2	39:LS:118:PHE:HB2	2.02	0.40
1:C1:491:C:H5''	27:LE:100:ARG:HG3	2.01	0.40
1:C1:1676:A:H2'	1:C1:1677:A:C8	2.56	0.40
1:C1:2236:G:N2	1:C1:2238:A:N3	2.68	0.40
1:C1:2307:U:H2'	1:C1:2308:A:C8	2.56	0.40
1:C1:3236:A:H2'	1:C1:3237:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:40:A:OP2	2:C2:103:G:N1	2.49	0.40
3:C3:10:C:H2'	3:C3:11:A:C8	2.56	0.40
4:C4:6:C:OP2	26:LD:22:ARG:NH2	2.54	0.40
5:CB:305:LYS:HA	8:CI:296:PRO:HB3	2.02	0.40
19:Cf:141:MET:HE2	19:Cf:141:MET:HB3	2.01	0.40
40:LT:38:ASP:OD2	40:LT:39:ILE:N	2.53	0.40
1:C1:181:G:OP1	44:LY:125:ARG:NE	2.54	0.40
1:C1:629:C:H2'	1:C1:630:U:C6	2.56	0.40
1:C1:757:A:H2'	1:C1:758:U:C6	2.57	0.40
1:C1:1915:G:OP1	17:Cd:452:GLY:N	2.41	0.40
1:C1:2112:A:N6	1:C1:2150:G:O2'	2.40	0.40
1:C1:2693:A:H5'	20:Cg:118:THR:HA	2.03	0.40
1:C1:3238:U:O4	24:LB:124:LYS:NZ	2.55	0.40
24:LB:123:TYR:CZ	24:LB:124:LYS:HG3	2.57	0.40
33:LM:27:LEU:HD11	33:LM:94:TRP:CG	2.57	0.40
47:Lc:37:LEU:HD13	47:Lc:62:TYR:HB3	2.03	0.40
52:Lh:46:LEU:HA	52:Lh:49:ILE:HG12	2.03	0.40
57:Lp:82:THR:HA	57:Lp:85:ARG:HG2	2.04	0.40
1:C1:743:A:C2	1:C1:753:A:H1'	2.56	0.40
1:C1:2865:C:OP1	7:CH:23:ARG:NH2	2.55	0.40
1:C1:3118:C:O2'	1:C1:3119:A:H8	2.04	0.40
7:CH:19:ILE:O	7:CH:23:ARG:HG2	2.22	0.40
8:CI:207:PHE:HB2	8:CI:213:ILE:HD11	2.02	0.40
19:Cf:104:ARG:HB3	19:Cf:112:ASP:OD1	2.21	0.40
33:LM:127:ARG:HG3	35:LO:191:VAL:HG21	2.03	0.40
45:LZ:22:VAL:HG12	45:LZ:44:GLY:HA3	2.03	0.40
1:C1:364:G:O2'	1:C1:389:A2M:N6	2.55	0.40
1:C1:1288:U:C2	24:LB:258:PRO:HG3	2.57	0.40
1:C1:1726:C:O2'	55:Lk:4:GLU:OE1	2.38	0.40
1:C1:1791:G:H5''	9:CJ:59:ALA:HB2	2.03	0.40
1:C1:2711:U:H2'	1:C1:2712:G:C8	2.57	0.40
1:C1:3263:G:H2'	1:C1:3264:A:C8	2.57	0.40
3:C3:32:G:H2'	3:C3:33:A:C8	2.56	0.40
5:CB:119:ASP:OD1	5:CB:119:ASP:N	2.53	0.40
7:CH:307:ASP:HA	7:CH:310:LYS:HG3	2.03	0.40
12:LF:123:VAL:HG11	12:LF:133:ILE:HD11	2.03	0.40
53:Li:70:LEU:HD13	53:Li:100:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CB	261/391 (67%)	256 (98%)	5 (2%)	0	100	100
6	CF	243/270 (90%)	241 (99%)	2 (1%)	0	100	100
7	CH	621/661 (94%)	614 (99%)	7 (1%)	0	100	100
8	CI	150/414 (36%)	149 (99%)	1 (1%)	0	100	100
9	CJ	376/679 (55%)	372 (99%)	4 (1%)	0	100	100
10	CK	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
11	CL	77/558 (14%)	76 (99%)	1 (1%)	0	100	100
12	CM	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
12	LF	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
13	CN	244/246 (99%)	239 (98%)	5 (2%)	0	100	100
14	CO	56/120 (47%)	56 (100%)	0	0	100	100
15	CQ	181/225 (80%)	179 (99%)	2 (1%)	0	100	100
16	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
17	Cd	458/627 (73%)	451 (98%)	7 (2%)	0	100	100
18	Ce	252/443 (57%)	251 (100%)	1 (0%)	0	100	100
19	Cf	281/350 (80%)	277 (99%)	4 (1%)	0	100	100
20	Cg	186/202 (92%)	183 (98%)	3 (2%)	0	100	100
21	Ch	484/517 (94%)	471 (97%)	13 (3%)	0	100	100
22	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
23	LA	176/254 (69%)	172 (98%)	4 (2%)	0	100	100
24	LB	387/392 (99%)	380 (98%)	7 (2%)	0	100	100
25	LC	361/365 (99%)	356 (99%)	5 (1%)	0	100	100
26	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
27	LE	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
28	LG	233/262 (89%)	228 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LH	188/229 (82%)	186 (99%)	2 (1%)	0	100	100
30	LJ	167/173 (96%)	167 (100%)	0	0	100	100
31	LK	156/165 (94%)	156 (100%)	0	0	100	100
32	LL	201/213 (94%)	198 (98%)	3 (2%)	0	100	100
33	LM	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
34	LN	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
35	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
36	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
37	LQ	148/213 (70%)	147 (99%)	1 (1%)	0	100	100
38	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
39	LS	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
40	LT	127/160 (79%)	126 (99%)	1 (1%)	0	100	100
41	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
42	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
43	LX	143/156 (92%)	139 (97%)	4 (3%)	0	100	100
44	LY	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
45	LZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
46	La	104/149 (70%)	102 (98%)	2 (2%)	0	100	100
47	Lc	93/108 (86%)	93 (100%)	0	0	100	100
48	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
49	Le	124/131 (95%)	124 (100%)	0	0	100	100
50	Lf	106/109 (97%)	106 (100%)	0	0	100	100
51	Lg	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
52	Lh	120/935 (13%)	117 (98%)	3 (2%)	0	100	100
53	Li	99/110 (90%)	99 (100%)	0	0	100	100
54	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
55	Lk	74/94 (79%)	74 (100%)	0	0	100	100
56	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
57	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
58	Lq	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
All	All	10348/16395 (63%)	10194 (98%)	154 (2%)	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	
5	CB	228/329 (69%)	228 (100%)	0	100	100
6	CF	212/236 (90%)	212 (100%)	0	100	100
7	CH	549/575 (96%)	549 (100%)	0	100	100
8	CI	124/336 (37%)	124 (100%)	0	100	100
9	CJ	331/579 (57%)	331 (100%)	0	100	100
10	CK	206/225 (92%)	206 (100%)	0	100	100
11	CL	61/458 (13%)	61 (100%)	0	100	100
12	CM	185/215 (86%)	185 (100%)	0	100	100
12	LF	213/215 (99%)	213 (100%)	0	100	100
13	CN	205/206 (100%)	205 (100%)	0	100	100
14	CO	48/99 (48%)	48 (100%)	0	100	100
15	CQ	144/192 (75%)	144 (100%)	0	100	100
16	Cb	85/101 (84%)	85 (100%)	0	100	100
17	Cd	403/541 (74%)	403 (100%)	0	100	100
18	Ce	223/383 (58%)	223 (100%)	0	100	100
19	Cf	250/310 (81%)	250 (100%)	0	100	100
20	Cg	158/176 (90%)	158 (100%)	0	100	100
21	Ch	408/436 (94%)	408 (100%)	0	100	100
22	Cz	89/107 (83%)	89 (100%)	0	100	100
23	LA	141/198 (71%)	141 (100%)	0	100	100
24	LB	329/331 (99%)	329 (100%)	0	100	100
25	LC	282/285 (99%)	282 (100%)	0	100	100
26	LD	221/253 (87%)	221 (100%)	0	100	100
27	LE	157/166 (95%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LG	200/222 (90%)	200 (100%)	0	100	100
29	LH	167/200 (84%)	167 (100%)	0	100	100
30	LJ	140/150 (93%)	140 (100%)	0	100	100
31	LK	127/136 (93%)	127 (100%)	0	100	100
32	LL	158/176 (90%)	158 (100%)	0	100	100
33	LM	116/117 (99%)	116 (100%)	0	100	100
34	LN	179/180 (99%)	179 (100%)	0	100	100
35	LO	162/163 (99%)	162 (100%)	0	100	100
36	LP	133/152 (88%)	133 (100%)	0	100	100
37	LQ	125/178 (70%)	125 (100%)	0	100	100
38	LR	125/2396 (5%)	125 (100%)	0	100	100
39	LS	152/154 (99%)	152 (100%)	0	100	100
40	LT	110/135 (82%)	110 (100%)	0	100	100
41	LU	92/108 (85%)	92 (100%)	0	100	100
42	LV	98/102 (96%)	98 (100%)	0	100	100
43	LX	122/129 (95%)	121 (99%)	1 (1%)	73	90
44	LY	116/119 (98%)	116 (100%)	0	100	100
45	LZ	121/121 (100%)	121 (100%)	0	100	100
46	La	93/122 (76%)	93 (100%)	0	100	100
47	Lc	76/88 (86%)	76 (100%)	0	100	100
48	Ld	90/105 (86%)	90 (100%)	0	100	100
49	Le	109/114 (96%)	109 (100%)	0	100	100
50	Lf	89/90 (99%)	89 (100%)	0	100	100
51	Lg	95/102 (93%)	95 (100%)	0	100	100
52	Lh	109/781 (14%)	109 (100%)	0	100	100
53	Li	85/93 (91%)	85 (100%)	0	100	100
54	Lj	72/78 (92%)	72 (100%)	0	100	100
55	Lk	73/88 (83%)	73 (100%)	0	100	100
56	Ll	45/46 (98%)	45 (100%)	0	100	100
57	Lp	73/74 (99%)	73 (100%)	0	100	100
58	Lq	109/112 (97%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8813/13783 (64%)	8812 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	LX	81	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
5	CB	79	GLN
5	CB	150	HIS
5	CB	277	ASN
7	CH	226	HIS
7	CH	244	HIS
7	CH	490	GLN
7	CH	619	GLN
8	CI	301	GLN
9	CJ	176	GLN
10	CK	60	GLN
10	CK	72	ASN
10	CK	95	ASN
10	CK	248	ASN
12	CM	64	GLN
12	CM	119	ASN
12	CM	163	ASN
12	CM	178	ASN
14	CO	20	ASN
15	CQ	130	ASN
16	Cb	68	HIS
17	Cd	271	ASN
17	Cd	387	HIS
18	Ce	216	ASN
18	Ce	370	GLN
20	Cg	65	GLN
21	Ch	47	ASN
21	Ch	114	ASN
21	Ch	133	HIS
21	Ch	408	ASN
24	LB	121	ASN
24	LB	319	ASN

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Mol	Chain	Res	Type
24	LB	346	HIS
25	LC	38	HIS
25	LC	118	GLN
25	LC	217	HIS
25	LC	292	ASN
25	LC	324	GLN
25	LC	330	ASN
12	LF	82	HIS
12	LF	200	ASN
12	LF	249	ASN
28	LG	141	HIS
28	LG	148	ASN
28	LG	194	HIS
29	LH	95	HIS
31	LK	65	GLN
31	LK	66	ASN
34	LN	32	GLN
34	LN	87	GLN
34	LN	95	GLN
36	LP	116	HIS
38	LR	91	GLN
39	LS	8	GLN
39	LS	147	ASN
45	LZ	30	GLN
46	La	62	HIS
52	Lh	33	GLN
52	Lh	64	ASN
53	Li	21	ASN
53	Li	42	GLN
56	Ll	11	GLN
58	Lq	43	HIS
58	Lq	101	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2989/3342 (89%)	553 (18%)	20 (0%)
2	C2	155/156 (99%)	25 (16%)	0
3	C3	80/162 (49%)	21 (26%)	0
4	C4	118/119 (99%)	24 (20%)	0
All	All	3342/3779 (88%)	623 (18%)	20 (0%)

All (623) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	4	U
1	C1	6	G
1	C1	27	A
1	C1	44	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	68	A
1	C1	94	C
1	C1	95	G
1	C1	96	A
1	C1	110	A
1	C1	111	G
1	C1	116	A
1	C1	117	A
1	C1	123	A
1	C1	132	U
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	146	A
1	C1	152	G
1	C1	153	A
1	C1	157	G
1	C1	181	G
1	C1	184	U
1	C1	185	U
1	C1	193	A
1	C1	194	C
1	C1	200	G
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	225	A
1	C1	240	C
1	C1	241	U
1	C1	242	G
1	C1	244	G
1	C1	247	A
1	C1	258	A

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Mol	Chain	Res	Type
1	C1	259	C
1	C1	262	G
1	C1	276	G
1	C1	277	A
1	C1	288	A
1	C1	291	U
1	C1	298	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	332	C
1	C1	342	A
1	C1	343	C
1	C1	369	G
1	C1	388	A
1	C1	389	A2M
1	C1	391	U
1	C1	392	A
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	430	G
1	C1	434	U
1	C1	435	G
1	C1	443	C
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	512	A
1	C1	514	A
1	C1	527	G

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Mol	Chain	Res	Type
1	C1	535	U
1	C1	536	C
1	C1	537	C
1	C1	545	U
1	C1	547	A
1	C1	549	A
1	C1	550	G
1	C1	559	G
1	C1	561	A
1	C1	570	G
1	C1	583	A
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	632	G
1	C1	634	A
1	C1	648	A
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	743	A
1	C1	747	A
1	C1	748	U
1	C1	756	G
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A

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Mol	Chain	Res	Type
1	C1	763	G
1	C1	766	G
1	C1	767	G
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	830	A
1	C1	843	C
1	C1	856	U
1	C1	857	G
1	C1	862	G
1	C1	877	A
1	C1	889	G
1	C1	890	G
1	C1	891	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	905	C
1	C1	906	G
1	C1	915	A
1	C1	919	G
1	C1	926	A
1	C1	931	C
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	937	U
1	C1	940	C
1	C1	941	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	964	C
1	C1	976	G
1	C1	977	U
1	C1	983	G
1	C1	984	A

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Mol	Chain	Res	Type
1	C1	1032	C
1	C1	1034	U
1	C1	1040	A
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1051	C
1	C1	1055	G
1	C1	1058	A
1	C1	1059	C
1	C1	1064	C
1	C1	1065	U
1	C1	1066	G
1	C1	1070	G
1	C1	1075	C
1	C1	1076	A
1	C1	1077	U
1	C1	1078	U
1	C1	1079	C
1	C1	1080	G
1	C1	1081	A
1	C1	1086	A
1	C1	1099	G
1	C1	1109	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A
1	C1	1127	U
1	C1	1132	G
1	C1	1136	A
1	C1	1143	C
1	C1	1161	G
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1169	G
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1182	C
1	C1	1185	A
1	C1	1187	A

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Mol	Chain	Res	Type
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1241	U
1	C1	1242	A
1	C1	1246	A
1	C1	1248	U
1	C1	1255	C
1	C1	1268	G
1	C1	1269	A
1	C1	1270	A
1	C1	1284	A
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C
1	C1	1337	G
1	C1	1369	A
1	C1	1370	G
1	C1	1375	G
1	C1	1382	A
1	C1	1383	G
1	C1	1400	G
1	C1	1401	A
1	C1	1413	U
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1458	G
1	C1	1464	A
1	C1	1467	U

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Mol	Chain	Res	Type
1	C1	1477	U
1	C1	1485	G
1	C1	1491	OMC
1	C1	1498	A
1	C1	1505	U
1	C1	1506	U
1	C1	1522	A
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1542	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U
1	C1	1554	G
1	C1	1560	U
1	C1	1561	G
1	C1	1563	G
1	C1	1567	A
1	C1	1568	A
1	C1	1569	A
1	C1	1570	G
1	C1	1573	A
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1638	G
1	C1	1685	U
1	C1	1696	A
1	C1	1697	C
1	C1	1704	U
1	C1	1721	A
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1745	U
1	C1	1746	G

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Mol	Chain	Res	Type
1	C1	1751	G
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1788	G
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1799	U
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A
1	C1	1886	G
1	C1	1887	C
1	C1	1933	G
1	C1	1934	G
1	C1	1935	C
1	C1	1937	C
1	C1	2046	C
1	C1	2048	U
1	C1	2050	C
1	C1	2052	G
1	C1	2054	U
1	C1	2056	A
1	C1	2076	A
1	C1	2084	G
1	C1	2085	G
1	C1	2089	A
1	C1	2094	A
1	C1	2103	U
1	C1	2121	A
1	C1	2126	C

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Mol	Chain	Res	Type
1	C1	2132	G
1	C1	2137	G
1	C1	2151	A
1	C1	2237	U
1	C1	2279	G
1	C1	2281	U
1	C1	2282	U
1	C1	2284	A
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2310	U
1	C1	2326	A
1	C1	2328	C
1	C1	2340	G
1	C1	2348	A
1	C1	2351	U
1	C1	2355	C
1	C1	2356	G
1	C1	2362	A
1	C1	2364	A
1	C1	2373	U
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2398	G
1	C1	2401	A
1	C1	2403	A
1	C1	2470	U
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2478	A
1	C1	2489	C
1	C1	2499	C
1	C1	2500	U
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A

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Mol	Chain	Res	Type
1	C1	2513	C
1	C1	2515	G
1	C1	2521	A
1	C1	2526	C
1	C1	2527	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2575	C
1	C1	2576	U
1	C1	2577	G
1	C1	2578	OMG
1	C1	2582	G
1	C1	2584	C
1	C1	2585	A
1	C1	2606	A
1	C1	2613	C
1	C1	2615	A
1	C1	2631	G
1	C1	2633	A
1	C1	2635	A
1	C1	2636	G
1	C1	2639	A
1	C1	2647	U
1	C1	2651	A
1	C1	2656	A
1	C1	2657	G
1	C1	2663	A
1	C1	2664	A
1	C1	2667	C
1	C1	2672	U
1	C1	2673	G
1	C1	2674	A
1	C1	2675	U
1	C1	2680	A
1	C1	2682	U
1	C1	2690	OMU
1	C1	2691	G

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Mol	Chain	Res	Type
1	C1	2713	G
1	C1	2717	A
1	C1	2731	C
1	C1	2732	C
1	C1	2736	G
1	C1	2737	A
1	C1	2754	U
1	C1	2755	G
1	C1	2756	C
1	C1	2757	C
1	C1	2758	A
1	C1	2761	A
1	C1	2762	A
1	C1	2763	A
1	C1	2769	C
1	C1	2773	G
1	C1	2783	G
1	C1	2784	C
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C
1	C1	2804	A
1	C1	2805	U
1	C1	2806	A
1	C1	2812	G
1	C1	2815	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2831	A
1	C1	2834	U
1	C1	2836	G
1	C1	2846	A
1	C1	2857	G
1	C1	2858	C
1	C1	2882	U
1	C1	2883	U
1	C1	2884	C
1	C1	2885	A
1	C1	2894	U
1	C1	2895	A

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Mol	Chain	Res	Type
1	C1	2900	A
1	C1	2903	U
1	C1	2905	A
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2951	U
1	C1	2955	C
1	C1	2956	U
1	C1	2964	A
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3032	G
1	C1	3036	G
1	C1	3044	A
1	C1	3045	A
1	C1	3049	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3080	A
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3119	A
1	C1	3124	G
1	C1	3125	U
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U
1	C1	3133	U

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Mol	Chain	Res	Type
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U
1	C1	3214	A
1	C1	3217	U
1	C1	3218	U
1	C1	3228	C
1	C1	3229	G
1	C1	3231	G
1	C1	3244	G
1	C1	3245	C
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3276	A
1	C1	3282	U
1	C1	3286	G
1	C1	3291	C
1	C1	3292	U
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3312	G
1	C1	3316	A
1	C1	3319	C

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Mol	Chain	Res	Type
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U
1	C1	3328	G
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	38	U
2	C2	51	G
2	C2	52	A
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	97	A
2	C2	104	A
2	C2	106	C
2	C2	113	U
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
2	C2	154	C
3	C3	2	U
3	C3	3	C
3	C3	10	C
3	C3	19	G
3	C3	20	G
3	C3	25	U
3	C3	26	G
3	C3	33	A
3	C3	36	C
3	C3	39	G

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Mol	Chain	Res	Type
3	C3	40	G
3	C3	50	G
3	C3	57	A
3	C3	58	A
3	C3	59	A
3	C3	63	A
3	C3	66	G
3	C3	68	C
3	C3	69	G
3	C3	135	G
3	C3	138	A
4	C4	7	G
4	C4	22	A
4	C4	29	G
4	C4	52	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	66	G
4	C4	75	A
4	C4	76	G
4	C4	77	U
4	C4	78	A
4	C4	81	U
4	C4	82	G
4	C4	83	G
4	C4	84	G
4	C4	85	U
4	C4	86	C
4	C4	89	U
4	C4	90	G
4	C4	93	G
4	C4	97	A
4	C4	101	A
4	C4	111	G

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	243	U
1	C1	898	G

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Mol	Chain	Res	Type
1	C1	1047	A
1	C1	1064	C
1	C1	1077	U
1	C1	1267	C
1	C1	1537	U
1	C1	2280	A
1	C1	2575	C
1	C1	2883	U
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C
1	C1	3324	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMC	C1	1420	1	19,22,23	0.62	0	25,31,34	1.43	4 (16%)
1	OMG	C1	1433	1	23,26,27	0.50	0	32,38,41	0.51	0
1	OMG	C1	2876	1	23,26,27	0.47	0	32,38,41	0.50	0
1	OMC	C1	778	1	19,22,23	0.58	0	25,31,34	0.91	1 (4%)
1	OMG	C1	385	1	23,26,27	0.48	0	32,38,41	0.55	0
1	OMU	C1	2690	1	19,22,23	3.09	6 (31%)	25,31,34	1.81	5 (20%)
1	OMU	C1	1868	1	19,22,23	3.10	6 (31%)	25,31,34	1.85	4 (16%)
1	A2M	C1	1223	1	22,25,26	3.97	11 (50%)	30,36,39	3.34	13 (43%)
1	OMG	C1	2358	1	23,26,27	0.49	0	32,38,41	0.54	0
1	OMU	C1	2277	1	19,22,23	3.12	6 (31%)	25,31,34	1.73	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	C1	1432	1	22,25,26	3.98	12 (54%)	30,36,39	3.40	13 (43%)
1	OMG	C1	2774	1	23,26,27	0.47	0	32,38,41	0.52	0
1	A2M	C1	637	1	22,25,26	3.99	11 (50%)	30,36,39	3.36	13 (43%)
1	OMG	C1	627	1	23,26,27	0.49	0	32,38,41	0.56	0
1	OMC	C1	1812	1	19,22,23	0.60	0	25,31,34	0.74	0
1	A2M	C1	2289	1	22,25,26	4.01	11 (50%)	30,36,39	3.35	14 (46%)
1	OMU	C1	2683	1	19,22,23	3.11	6 (31%)	25,31,34	1.79	5 (20%)
1	OMU	C1	2384	1	19,22,23	3.15	6 (31%)	25,31,34	1.79	5 (20%)
1	OMC	C1	1836	1	19,22,23	0.58	0	25,31,34	0.84	1 (4%)
1	OMC	C1	1491	1	19,22,23	0.57	0	25,31,34	0.73	0
1	A2M	C1	848	1	22,25,26	4.01	12 (54%)	30,36,39	3.45	15 (50%)
1	A2M	C1	858	1	22,25,26	4.00	12 (54%)	30,36,39	3.38	13 (43%)
1	OMC	C1	2300	1	19,22,23	0.57	0	25,31,34	0.81	1 (4%)
1	A2M	C1	389	1	22,25,26	4.02	11 (50%)	30,36,39	3.43	14 (46%)
1	OMG	C1	2881	1	23,26,27	0.47	0	32,38,41	0.46	0
1	OMU	C1	2688	1	19,22,23	3.11	6 (31%)	25,31,34	1.80	5 (20%)
1	OMC	C1	2838	1	19,22,23	0.66	0	25,31,34	1.58	4 (16%)
1	A2M	C1	1847	1	22,25,26	3.99	12 (54%)	30,36,39	3.48	14 (46%)
1	OMG	C1	787	1	23,26,27	0.49	0	32,38,41	0.55	0
1	OMU	C1	2380	1	19,22,23	3.12	6 (31%)	25,31,34	1.80	5 (20%)
1	OMG	C1	646	1	23,26,27	0.53	0	32,38,41	0.51	0
1	OMU	C1	1917	1	19,22,23	3.10	6 (31%)	25,31,34	1.82	5 (20%)
1	OMC	C1	2918	1	19,22,23	0.55	0	25,31,34	0.77	0
1	OMG	C1	2578	1	23,26,27	0.47	0	32,38,41	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	C1	1420	1	-	3/9/27/28	0/2/2/2
1	OMG	C1	1433	1	-	2/9/27/28	0/3/3/3
1	OMG	C1	2876	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	2/9/27/28	0/3/3/3
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	C1	1223	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	2358	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2277	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	2774	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	637	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	627	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	1812	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2384	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	848	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	858	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	389	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	787	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	646	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	2918	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	2578	1	-	3/9/27/28	0/3/3/3

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-13.15	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-13.02	1.24	1.53
1	C1	858	A2M	C3'-C2'	-13.01	1.24	1.53
1	C1	389	A2M	C3'-C2'	-12.99	1.24	1.53
1	C1	848	A2M	C3'-C2'	-12.98	1.24	1.53
1	C1	1847	A2M	C3'-C2'	-12.96	1.24	1.53
1	C1	637	A2M	C3'-C2'	-12.94	1.24	1.53
1	C1	1223	A2M	C3'-C2'	-12.92	1.24	1.53
1	C1	2384	OMU	C2-N1	7.63	1.50	1.38
1	C1	2277	OMU	C2-N1	7.52	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1917	OMU	C2-N1	7.51	1.50	1.38
1	C1	1868	OMU	C2-N1	7.47	1.50	1.38
1	C1	2380	OMU	C2-N1	7.45	1.50	1.38
1	C1	2683	OMU	C2-N1	7.42	1.50	1.38
1	C1	2688	OMU	C2-N1	7.39	1.50	1.38
1	C1	2690	OMU	C2-N1	7.33	1.49	1.38
1	C1	2384	OMU	C2-N3	7.31	1.50	1.38
1	C1	2380	OMU	C2-N3	7.29	1.50	1.38
1	C1	2277	OMU	C2-N3	7.28	1.50	1.38
1	C1	1868	OMU	C2-N3	7.25	1.50	1.38
1	C1	2688	OMU	C2-N3	7.25	1.50	1.38
1	C1	2683	OMU	C2-N3	7.24	1.50	1.38
1	C1	2690	OMU	C2-N3	7.17	1.50	1.38
1	C1	1917	OMU	C2-N3	7.14	1.50	1.38
1	C1	389	A2M	O4'-C4'	-6.76	1.30	1.45
1	C1	637	A2M	O4'-C4'	-6.63	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.58	1.30	1.45
1	C1	1847	A2M	O4'-C4'	-6.52	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.51	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.49	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.44	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.42	1.30	1.45
1	C1	2688	OMU	C6-C5	6.23	1.49	1.35
1	C1	2683	OMU	C6-C5	6.21	1.49	1.35
1	C1	2277	OMU	C6-C5	6.20	1.49	1.35
1	C1	2384	OMU	C6-C5	6.19	1.49	1.35
1	C1	2380	OMU	C6-C5	6.18	1.49	1.35
1	C1	2690	OMU	C6-C5	6.17	1.49	1.35
1	C1	1917	OMU	C6-C5	6.15	1.49	1.35
1	C1	1868	OMU	C6-C5	6.12	1.49	1.35
1	C1	858	A2M	C3'-C4'	5.37	1.66	1.53
1	C1	2289	A2M	C3'-C4'	5.29	1.66	1.53
1	C1	848	A2M	C3'-C4'	5.24	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.20	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.15	1.66	1.53
1	C1	637	A2M	C3'-C4'	5.11	1.65	1.53
1	C1	1847	A2M	C3'-C4'	5.08	1.65	1.53
1	C1	389	A2M	C3'-C4'	4.97	1.65	1.53
1	C1	1847	A2M	O4'-C1'	4.51	1.52	1.42
1	C1	2289	A2M	O4'-C1'	4.47	1.52	1.42
1	C1	2384	OMU	C4-N3	4.46	1.46	1.38
1	C1	848	A2M	C1'-N9	-4.45	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2688	OMU	C4-N3	4.43	1.46	1.38
1	C1	848	A2M	O4'-C1'	4.42	1.52	1.42
1	C1	858	A2M	O4'-C1'	4.42	1.52	1.42
1	C1	637	A2M	C1'-N9	-4.42	1.34	1.46
1	C1	848	A2M	C6-N6	4.42	1.45	1.34
1	C1	2289	A2M	C6-N6	4.41	1.45	1.34
1	C1	2380	OMU	C4-N3	4.41	1.46	1.38
1	C1	1847	A2M	C1'-N9	-4.40	1.34	1.46
1	C1	389	A2M	C6-N6	4.40	1.45	1.34
1	C1	389	A2M	O4'-C1'	4.40	1.52	1.42
1	C1	2289	A2M	C1'-N9	-4.39	1.34	1.46
1	C1	1223	A2M	C6-N6	4.39	1.45	1.34
1	C1	2690	OMU	C4-N3	4.37	1.46	1.38
1	C1	2683	OMU	C4-N3	4.37	1.46	1.38
1	C1	858	A2M	C6-N6	4.36	1.45	1.34
1	C1	637	A2M	C6-N6	4.36	1.45	1.34
1	C1	1847	A2M	C6-N6	4.35	1.45	1.34
1	C1	1432	A2M	C6-N6	4.34	1.45	1.34
1	C1	2277	OMU	C4-N3	4.33	1.46	1.38
1	C1	1432	A2M	O4'-C1'	4.32	1.52	1.42
1	C1	1223	A2M	C1'-N9	-4.32	1.34	1.46
1	C1	858	A2M	C1'-N9	-4.32	1.34	1.46
1	C1	1917	OMU	C4-N3	4.32	1.46	1.38
1	C1	637	A2M	O4'-C1'	4.32	1.52	1.42
1	C1	1868	OMU	C4-N3	4.31	1.46	1.38
1	C1	1223	A2M	O4'-C1'	4.27	1.51	1.42
1	C1	389	A2M	C1'-N9	-4.22	1.34	1.46
1	C1	1432	A2M	C1'-N9	-4.18	1.34	1.46
1	C1	389	A2M	O2'-C2'	3.91	1.52	1.42
1	C1	637	A2M	O2'-C2'	3.61	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.58	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.58	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.58	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.49	1.51	1.42
1	C1	389	A2M	C2'-C1'	3.19	1.61	1.53
1	C1	848	A2M	C5-C4	-3.14	1.33	1.39
1	C1	848	A2M	C2'-C1'	3.11	1.60	1.53
1	C1	1432	A2M	C5-C4	-3.09	1.33	1.39
1	C1	2289	A2M	C5-C4	-3.07	1.33	1.39
1	C1	1847	A2M	C2'-C1'	3.06	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1223	A2M	C5-C4	-3.04	1.33	1.39
1	C1	389	A2M	C5-C4	-3.03	1.33	1.39
1	C1	858	A2M	C5-C4	-3.02	1.33	1.39
1	C1	637	A2M	C2'-C1'	2.97	1.60	1.53
1	C1	637	A2M	C5-C4	-2.96	1.33	1.39
1	C1	1847	A2M	C5-C4	-2.93	1.33	1.39
1	C1	1432	A2M	C2'-C1'	2.92	1.60	1.53
1	C1	2289	A2M	C2'-C1'	2.87	1.60	1.53
1	C1	858	A2M	C2'-C1'	2.87	1.60	1.53
1	C1	389	A2M	C5-N7	-2.77	1.34	1.39
1	C1	1223	A2M	C2'-C1'	2.77	1.60	1.53
1	C1	2690	OMU	C6-N1	2.75	1.44	1.38
1	C1	2277	OMU	C6-N1	2.72	1.44	1.38
1	C1	2380	OMU	C6-N1	2.72	1.44	1.38
1	C1	2384	OMU	C6-N1	2.70	1.44	1.38
1	C1	1223	A2M	C5-N7	-2.70	1.34	1.39
1	C1	1917	OMU	C6-N1	2.69	1.44	1.38
1	C1	1432	A2M	C5-N7	-2.68	1.34	1.39
1	C1	2683	OMU	C6-N1	2.68	1.44	1.38
1	C1	2688	OMU	C6-N1	2.67	1.44	1.38
1	C1	637	A2M	C5-N7	-2.66	1.34	1.39
1	C1	858	A2M	C5-N7	-2.62	1.34	1.39
1	C1	1847	A2M	C5-N7	-2.61	1.34	1.39
1	C1	1868	OMU	C6-N1	2.60	1.44	1.38
1	C1	848	A2M	C5-N7	-2.55	1.34	1.39
1	C1	2289	A2M	C5-N7	-2.53	1.34	1.39
1	C1	2688	OMU	C5-C4	2.32	1.48	1.43
1	C1	2380	OMU	C5-C4	2.30	1.48	1.43
1	C1	2277	OMU	C5-C4	2.28	1.48	1.43
1	C1	1868	OMU	C5-C4	2.27	1.48	1.43
1	C1	1432	A2M	C8-N9	-2.25	1.33	1.37
1	C1	2690	OMU	C5-C4	2.24	1.48	1.43
1	C1	1847	A2M	C8-N9	-2.24	1.33	1.37
1	C1	389	A2M	C8-N9	-2.23	1.33	1.37
1	C1	2384	OMU	C5-C4	2.23	1.48	1.43
1	C1	2683	OMU	C5-C4	2.22	1.48	1.43
1	C1	848	A2M	C8-N9	-2.20	1.33	1.37
1	C1	1917	OMU	C5-C4	2.15	1.48	1.43
1	C1	637	A2M	C8-N9	-2.14	1.33	1.37
1	C1	1847	A2M	O3'-C3'	2.14	1.48	1.43
1	C1	1223	A2M	C8-N9	-2.14	1.33	1.37
1	C1	858	A2M	C8-N9	-2.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	O3'-C3'	2.10	1.48	1.43
1	C1	1432	A2M	O3'-C3'	2.06	1.48	1.43
1	C1	2289	A2M	O3'-C3'	2.04	1.48	1.43
1	C1	858	A2M	O3'-C3'	2.03	1.48	1.43

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.49	106.04	127.09
1	C1	389	A2M	C1'-N9-C8	-9.48	106.06	127.09
1	C1	637	A2M	C1'-N9-C8	-9.25	106.57	127.09
1	C1	1432	A2M	C1'-N9-C8	-9.18	106.72	127.09
1	C1	848	A2M	C1'-N9-C8	-9.09	106.92	127.09
1	C1	858	A2M	C1'-N9-C8	-8.98	107.17	127.09
1	C1	1223	A2M	C1'-N9-C8	-8.91	107.32	127.09
1	C1	2289	A2M	C1'-N9-C8	-8.76	107.66	127.09
1	C1	389	A2M	C4-N9-C1'	8.25	145.92	126.63
1	C1	1847	A2M	C4-N9-C1'	8.14	145.67	126.63
1	C1	637	A2M	C4-N9-C1'	7.96	145.26	126.63
1	C1	1432	A2M	C4-N9-C1'	7.95	145.22	126.63
1	C1	1223	A2M	C4-N9-C1'	7.68	144.58	126.63
1	C1	848	A2M	C4-N9-C1'	7.64	144.50	126.63
1	C1	858	A2M	C4-N9-C1'	7.64	144.50	126.63
1	C1	2289	A2M	C4-N9-C1'	7.39	143.91	126.63
1	C1	858	A2M	N3-C2-N1	-6.00	119.50	128.58
1	C1	1847	A2M	N3-C2-N1	-5.92	119.62	128.58
1	C1	2289	A2M	N3-C2-N1	-5.84	119.74	128.58
1	C1	848	A2M	N3-C2-N1	-5.84	119.75	128.58
1	C1	1432	A2M	N3-C2-N1	-5.78	119.83	128.58
1	C1	637	A2M	N3-C2-N1	-5.77	119.86	128.58
1	C1	1223	A2M	N3-C2-N1	-5.74	119.90	128.58
1	C1	1432	A2M	N6-C6-N1	-5.72	105.65	118.38
1	C1	1868	OMU	C4-N3-C2	-5.71	119.53	126.61
1	C1	858	A2M	N6-C6-N1	-5.70	105.69	118.38
1	C1	1847	A2M	N6-C6-N1	-5.70	105.69	118.38
1	C1	389	A2M	N3-C2-N1	-5.68	119.99	128.58
1	C1	2688	OMU	C4-N3-C2	-5.66	119.59	126.61
1	C1	848	A2M	N6-C6-N1	-5.64	105.81	118.38
1	C1	2690	OMU	C4-N3-C2	-5.61	119.65	126.61
1	C1	1223	A2M	N6-C6-N1	-5.58	105.96	118.38
1	C1	2289	A2M	N6-C6-N1	-5.55	106.01	118.38
1	C1	2683	OMU	C4-N3-C2	-5.53	119.75	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2380	OMU	C4-N3-C2	-5.52	119.76	126.61
1	C1	389	A2M	N6-C6-N1	-5.45	106.23	118.38
1	C1	1917	OMU	C4-N3-C2	-5.44	119.86	126.61
1	C1	637	A2M	N6-C6-N1	-5.42	106.30	118.38
1	C1	2384	OMU	C4-N3-C2	-5.32	120.01	126.61
1	C1	2277	OMU	C4-N3-C2	-5.25	120.10	126.61
1	C1	1432	A2M	C5-C4-N3	-4.94	119.92	126.72
1	C1	389	A2M	C5-C4-N3	-4.90	119.97	126.72
1	C1	2838	OMC	C1'-N1-C2	4.86	129.17	118.44
1	C1	1847	A2M	C5-C4-N3	-4.85	120.04	126.72
1	C1	637	A2M	C5-C4-N3	-4.82	120.08	126.72
1	C1	848	A2M	C5-C4-N3	-4.76	120.17	126.72
1	C1	1223	A2M	C5-C4-N3	-4.74	120.18	126.72
1	C1	848	A2M	N9-C8-N7	-4.58	107.44	113.94
1	C1	2289	A2M	C5-C4-N3	-4.57	120.42	126.72
1	C1	858	A2M	C5-C4-N3	-4.56	120.44	126.72
1	C1	858	A2M	C5-C6-N6	4.50	134.44	123.29
1	C1	2289	A2M	N9-C8-N7	-4.47	107.59	113.94
1	C1	1432	A2M	C5-C6-N6	4.43	134.25	123.29
1	C1	1847	A2M	C5-C6-N6	4.41	134.21	123.29
1	C1	1223	A2M	C5-C6-N6	4.38	134.14	123.29
1	C1	2289	A2M	C5-C6-N6	4.35	134.05	123.29
1	C1	858	A2M	N9-C8-N7	-4.32	107.80	113.94
1	C1	848	A2M	C5-C6-N6	4.32	133.99	123.29
1	C1	1847	A2M	N9-C8-N7	-4.31	107.82	113.94
1	C1	389	A2M	C5-C6-N6	4.27	133.86	123.29
1	C1	2289	A2M	O4'-C1'-N9	4.25	116.25	108.09
1	C1	637	A2M	C5-C6-N6	4.24	133.79	123.29
1	C1	1420	OMC	C1'-N1-C2	4.20	127.71	118.44
1	C1	1223	A2M	N9-C8-N7	-4.15	108.05	113.94
1	C1	1432	A2M	N9-C8-N7	-4.14	108.06	113.94
1	C1	637	A2M	N9-C8-N7	-4.14	108.07	113.94
1	C1	389	A2M	N9-C8-N7	-4.08	108.15	113.94
1	C1	1223	A2M	O4'-C1'-N9	4.06	115.90	108.09
1	C1	858	A2M	O4'-C1'-N9	4.01	115.79	108.09
1	C1	1868	OMU	N3-C2-N1	4.01	120.11	114.89
1	C1	848	A2M	O4'-C1'-N9	3.96	115.70	108.09
1	C1	1917	OMU	N3-C2-N1	3.96	120.05	114.89
1	C1	2688	OMU	N3-C2-N1	3.93	120.00	114.89
1	C1	2384	OMU	N3-C2-N1	3.91	119.98	114.89
1	C1	2690	OMU	N3-C2-N1	3.88	119.94	114.89
1	C1	2380	OMU	N3-C2-N1	3.84	119.89	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2683	OMU	N3-C2-N1	3.80	119.84	114.89
1	C1	1432	A2M	O4'-C1'-N9	3.80	115.38	108.09
1	C1	2277	OMU	N3-C2-N1	3.70	119.71	114.89
1	C1	2683	OMU	C5-C4-N3	3.68	119.95	114.80
1	C1	2690	OMU	C5-C4-N3	3.64	119.90	114.80
1	C1	2380	OMU	C5-C4-N3	3.59	119.82	114.80
1	C1	2838	OMC	C1'-N1-C6	-3.58	113.12	120.78
1	C1	2688	OMU	C5-C4-N3	3.57	119.81	114.80
1	C1	637	A2M	O4'-C1'-N9	3.55	114.90	108.09
1	C1	1868	OMU	C5-C4-N3	3.52	119.73	114.80
1	C1	389	A2M	O4'-C1'-N9	3.52	114.85	108.09
1	C1	1847	A2M	C2-N3-C4	3.51	120.39	111.83
1	C1	1432	A2M	C2-N3-C4	3.48	120.33	111.83
1	C1	1917	OMU	C5-C4-N3	3.48	119.67	114.80
1	C1	2277	OMU	C5-C4-N3	3.45	119.64	114.80
1	C1	848	A2M	C2-N3-C4	3.44	120.23	111.83
1	C1	2384	OMU	C5-C4-N3	3.40	119.56	114.80
1	C1	1847	A2M	O4'-C1'-N9	3.37	114.56	108.09
1	C1	858	A2M	C2-N3-C4	3.37	120.06	111.83
1	C1	637	A2M	C2-N3-C4	3.36	120.05	111.83
1	C1	389	A2M	C2-N3-C4	3.34	119.99	111.83
1	C1	2289	A2M	C2-N3-C4	3.32	119.94	111.83
1	C1	848	A2M	C2'-C1'-N9	-3.32	108.29	113.75
1	C1	1223	A2M	C2-N3-C4	3.31	119.92	111.83
1	C1	389	A2M	N3-C4-N9	3.05	132.35	127.17
1	C1	848	A2M	C5-N7-C8	3.03	108.22	103.45
1	C1	1847	A2M	N3-C4-N9	3.00	132.28	127.17
1	C1	1847	A2M	C5-N7-C8	3.00	108.17	103.45
1	C1	1420	OMC	C1'-N1-C6	-3.00	114.37	120.78
1	C1	1432	A2M	N3-C4-N9	2.98	132.24	127.17
1	C1	637	A2M	N3-C4-N9	2.97	132.22	127.17
1	C1	2380	OMU	O4-C4-C5	-2.96	120.05	125.16
1	C1	2683	OMU	O4-C4-C5	-2.94	120.08	125.16
1	C1	2289	A2M	C5-N7-C8	2.93	108.05	103.45
1	C1	1868	OMU	O4-C4-C5	-2.91	120.15	125.16
1	C1	2384	OMU	O4-C4-C5	-2.91	120.15	125.16
1	C1	848	A2M	N3-C4-N9	2.90	132.10	127.17
1	C1	1223	A2M	N3-C4-N9	2.88	132.07	127.17
1	C1	1917	OMU	O4-C4-C5	-2.87	120.20	125.16
1	C1	2690	OMU	O4-C4-C5	-2.86	120.22	125.16
1	C1	389	A2M	C5-N7-C8	2.84	107.91	103.45
1	C1	858	A2M	C5-N7-C8	2.84	107.91	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2688	OMU	O4-C4-C5	-2.83	120.28	125.16
1	C1	1432	A2M	C5-N7-C8	2.83	107.90	103.45
1	C1	2277	OMU	O4-C4-C5	-2.83	120.28	125.16
1	C1	1223	A2M	C5-N7-C8	2.80	107.85	103.45
1	C1	637	A2M	C5-N7-C8	2.76	107.79	103.45
1	C1	858	A2M	N3-C4-N9	2.75	131.84	127.17
1	C1	2838	OMC	O2-C2-N3	-2.74	118.01	122.33
1	C1	2289	A2M	N3-C4-N9	2.74	131.83	127.17
1	C1	848	A2M	C4-N9-C8	2.70	108.58	105.74
1	C1	2289	A2M	C4-N9-C8	2.56	108.42	105.74
1	C1	1847	A2M	C2'-C1'-N9	-2.54	109.56	113.75
1	C1	2289	A2M	C2'-C1'-N9	-2.54	109.57	113.75
1	C1	778	OMC	C1'-N1-C2	2.49	123.94	118.44
1	C1	858	A2M	C4-N9-C8	2.48	108.34	105.74
1	C1	1420	OMC	O2-C2-N1	2.46	123.72	118.90
1	C1	1847	A2M	C4-N9-C8	2.43	108.29	105.74
1	C1	2384	OMU	C1'-N1-C2	2.34	121.80	117.59
1	C1	2300	OMC	C1'-N1-C2	2.34	123.60	118.44
1	C1	1836	OMC	C1'-N1-C2	2.33	123.58	118.44
1	C1	2838	OMC	O2-C2-N1	2.31	123.42	118.90
1	C1	637	A2M	C4-N9-C8	2.30	108.16	105.74
1	C1	1420	OMC	O2-C2-N3	-2.26	118.77	122.33
1	C1	1223	A2M	C4-N9-C8	2.25	108.10	105.74
1	C1	1847	A2M	C4-C5-N7	-2.23	108.03	110.58
1	C1	1917	OMU	C1'-N1-C2	2.23	121.60	117.59
1	C1	848	A2M	C4-C5-N7	-2.22	108.04	110.58
1	C1	1432	A2M	C4-N9-C8	2.20	108.05	105.74
1	C1	848	A2M	C4'-O4'-C1'	-2.16	104.69	109.47
1	C1	389	A2M	C4-N9-C8	2.15	108.00	105.74
1	C1	1432	A2M	C4-C5-N7	-2.13	108.15	110.58
1	C1	2688	OMU	O2-C2-N1	-2.11	120.05	122.80
1	C1	2380	OMU	O2-C2-N1	-2.10	120.06	122.80
1	C1	2289	A2M	C4-C5-N7	-2.09	108.19	110.58
1	C1	2690	OMU	O2-C2-N1	-2.08	120.09	122.80
1	C1	858	A2M	C4-C5-N7	-2.05	108.23	110.58
1	C1	1223	A2M	C4-C5-N7	-2.03	108.26	110.58
1	C1	389	A2M	C4-C5-N7	-2.03	108.26	110.58
1	C1	2683	OMU	O2-C2-N1	-2.02	120.17	122.80
1	C1	389	A2M	C6-C5-C4	2.01	119.92	117.18
1	C1	637	A2M	C4-C5-N7	-2.00	108.29	110.58

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1917	OMU	C1'-C2'-O2'-CM2
1	C1	2277	OMU	C1'-C2'-O2'-CM2
1	C1	2578	OMG	O4'-C4'-C5'-O5'
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2690	OMU	O4'-C4'-C5'-O5'
1	C1	2838	OMC	O4'-C1'-N1-C2
1	C1	2838	OMC	O4'-C1'-N1-C6
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	2578	OMG	C3'-C4'-C5'-O5'
1	C1	2690	OMU	C3'-C4'-C5'-O5'
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	1491	OMC	O4'-C4'-C5'-O5'
1	C1	1917	OMU	O4'-C4'-C5'-O5'
1	C1	2578	OMG	C4'-C5'-O5'-P
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	1420	OMC	C2'-C1'-N1-C6
1	C1	2918	OMC	C1'-C2'-O2'-CM2
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	1420	OMC	O4'-C4'-C5'-O5'
1	C1	1420	OMC	C2'-C1'-N1-C2

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	1420	OMC	1	0
1	C1	778	OMC	1	0
1	C1	2277	OMU	1	0
1	C1	1432	A2M	1	0
1	C1	1812	OMC	1	0
1	C1	848	A2M	1	0
1	C1	389	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	1917	OMU	1	0
1	C1	2578	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	GTP	Cd	1003	60	33,34,34	0.97	1 (3%)	50,54,54	1.60	8 (16%)
59	GTP	CH	701	60	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)

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
59	GTP	Cd	1003	60	-	7/22/38/38	0/3/3/3
59	GTP	CH	701	60	-	5/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CH	701	GTP	C2-N3	2.13	1.38	1.33
59	Cd	1003	GTP	C2-N3	2.11	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CH	701	GTP	C5-C4-N3	-5.04	120.36	128.39
59	Cd	1003	GTP	C5-C4-N3	-4.99	120.45	128.39
59	CH	701	GTP	C2-N3-C4	4.65	120.31	112.30
59	Cd	1003	GTP	C2-N3-C4	4.49	120.04	112.30
59	Cd	1003	GTP	N9-C4-N3	3.29	132.53	125.95
59	CH	701	GTP	N9-C4-N3	3.23	132.42	125.95
59	Cd	1003	GTP	C2-N1-C6	-2.97	119.72	125.11
59	CH	701	GTP	C2-N1-C6	-2.93	119.80	125.11
59	Cd	1003	GTP	N9-C8-N7	-2.64	108.51	113.40
59	CH	701	GTP	N9-C8-N7	-2.63	108.53	113.40
59	Cd	1003	GTP	C5-C6-N1	2.55	119.75	113.25
59	CH	701	GTP	C5-C6-N1	2.54	119.73	113.25
59	Cd	1003	GTP	O6-C6-C5	-2.50	119.93	126.53
59	CH	701	GTP	C8-N7-C5	2.48	108.67	104.26
59	Cd	1003	GTP	C8-N7-C5	2.43	108.59	104.26
59	CH	701	GTP	O6-C6-C5	-2.42	120.16	126.53
59	CH	701	GTP	C3'-C2'-C1'	2.16	105.54	101.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

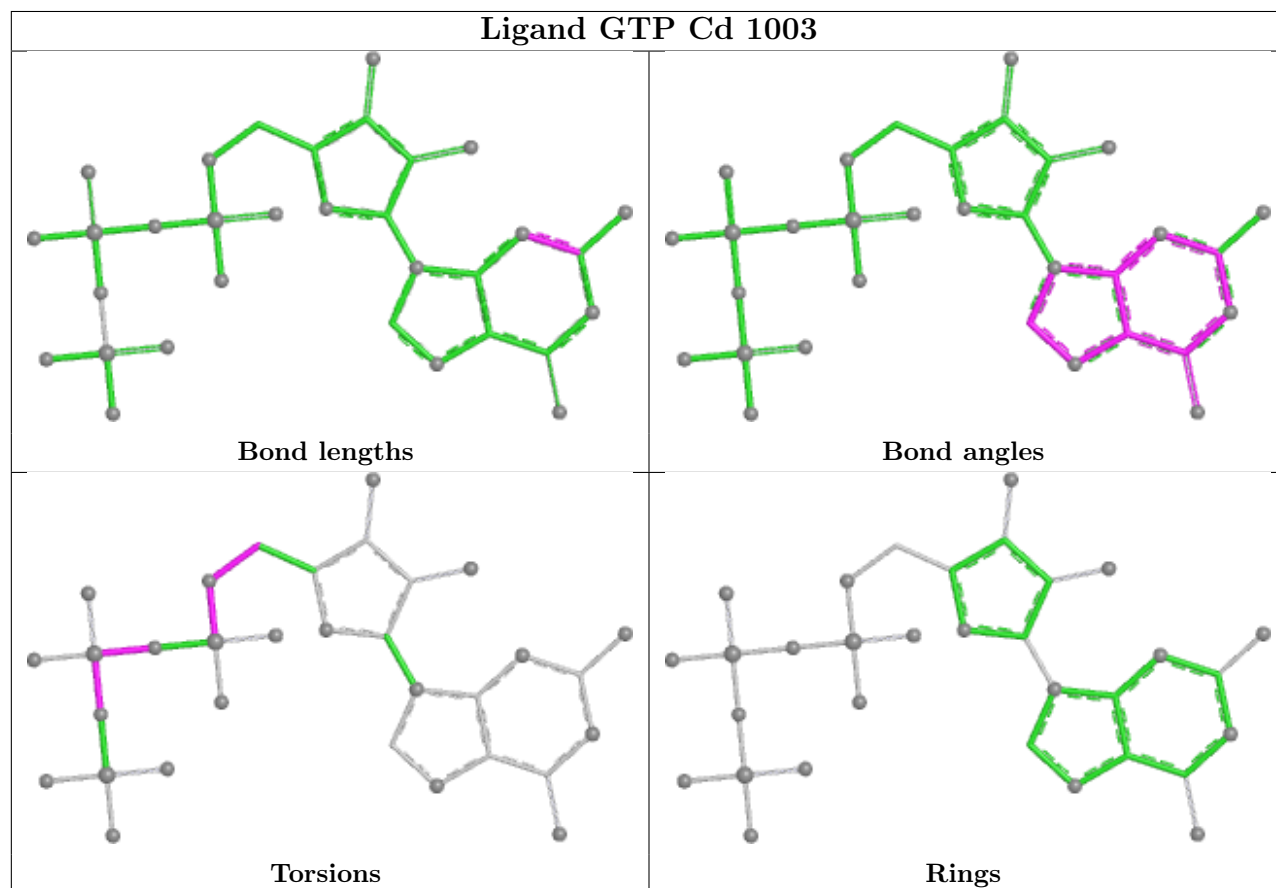
Mol	Chain	Res	Type	Atoms
59	Cd	1003	GTP	C5'-O5'-PA-O3A
59	Cd	1003	GTP	C5'-O5'-PA-O1A
59	Cd	1003	GTP	C5'-O5'-PA-O2A
59	CH	701	GTP	PB-O3B-PG-O2G
59	Cd	1003	GTP	PG-O3B-PB-O1B
59	CH	701	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3A-PA-O2A
59	Cd	1003	GTP	PA-O3A-PB-O1B
59	Cd	1003	GTP	C4'-C5'-O5'-PA
59	CH	701	GTP	O4'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3B-PG-O3G
59	Cd	1003	GTP	PG-O3B-PB-O2B

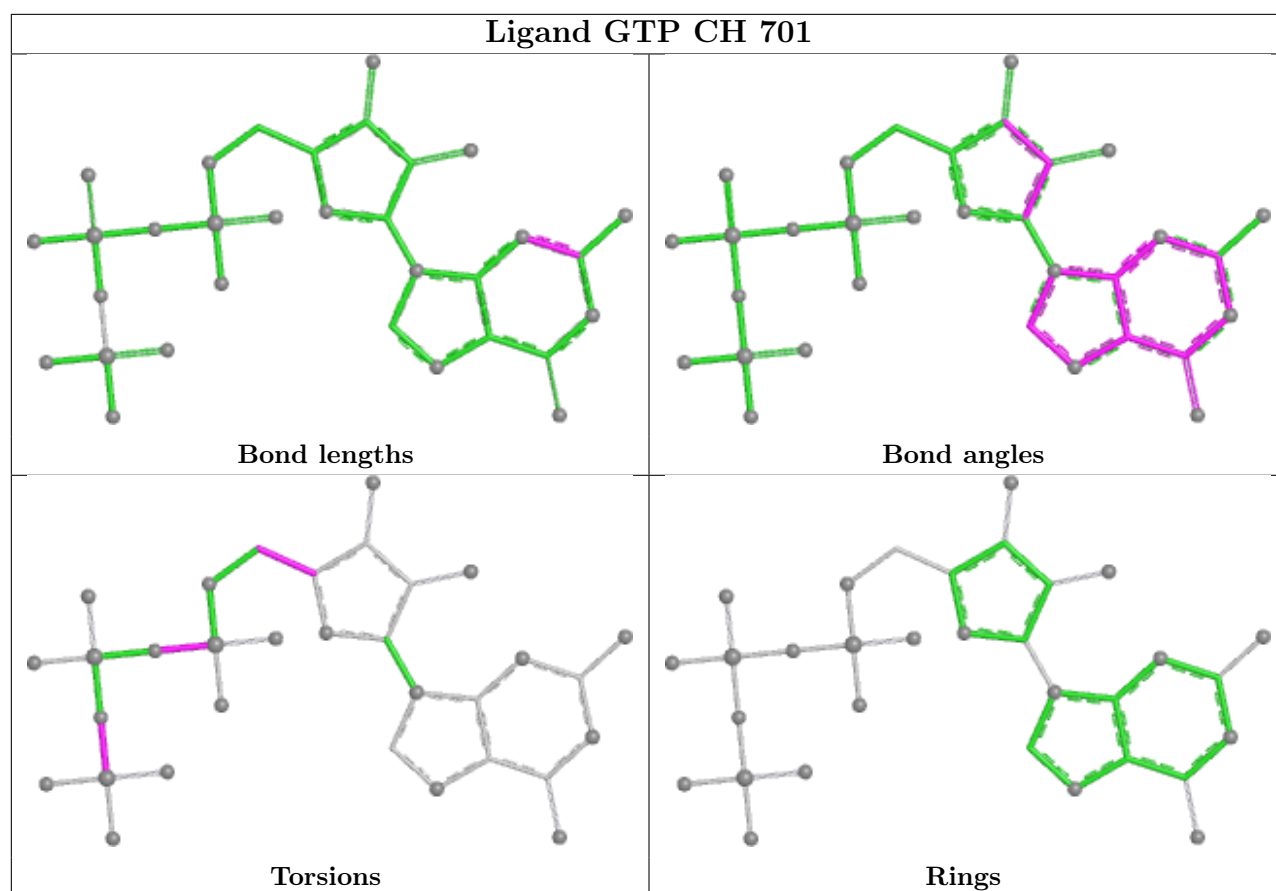
There are no ring outliers.

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.

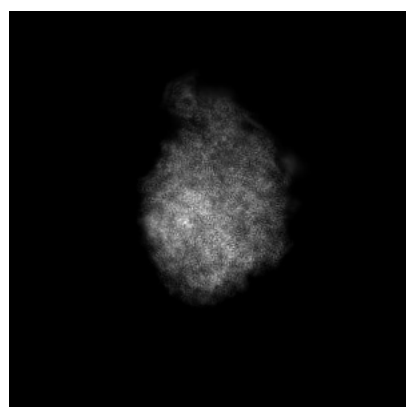
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17952. These allow visual inspection of the internal detail of the map and identification of artifacts.

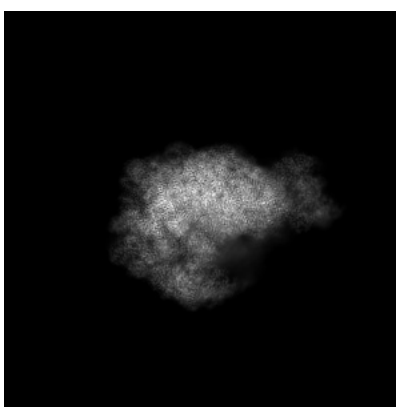
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

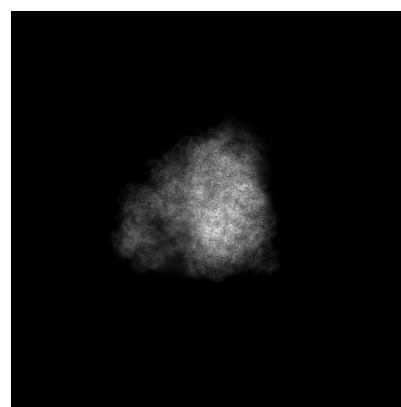
6.1.1 Primary map



X



Y



Z

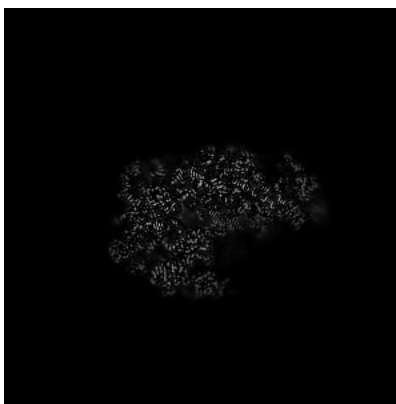
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

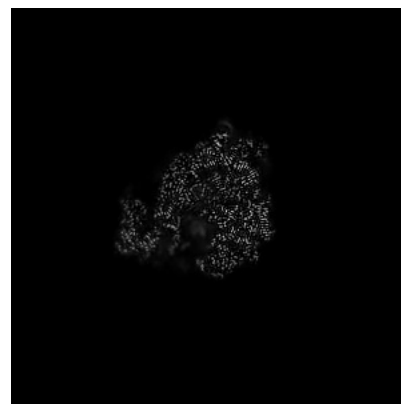
6.2.1 Primary map



X Index: 250



Y Index: 250

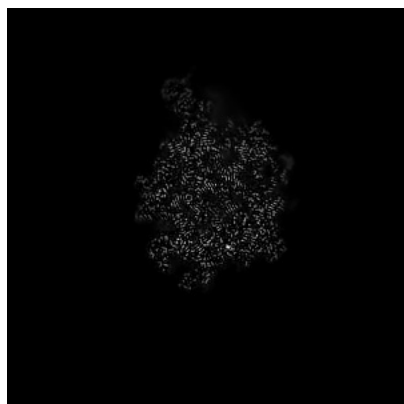


Z Index: 250

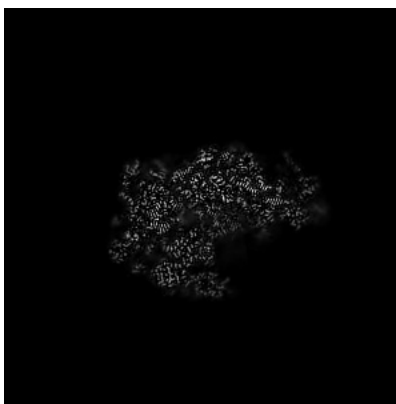
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

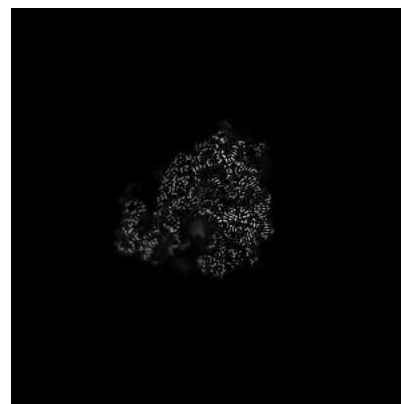
6.3.1 Primary map



X Index: 259



Y Index: 248

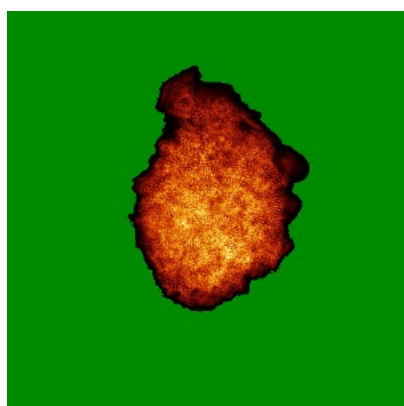


Z Index: 248

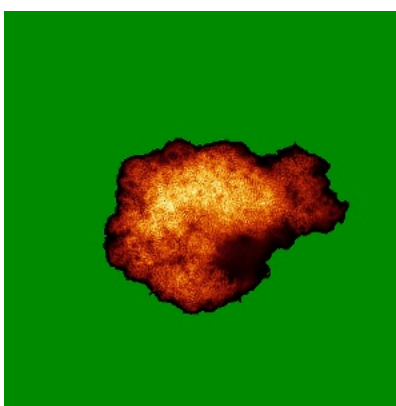
The images above show the largest variance slices of the map in three orthogonal directions.

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

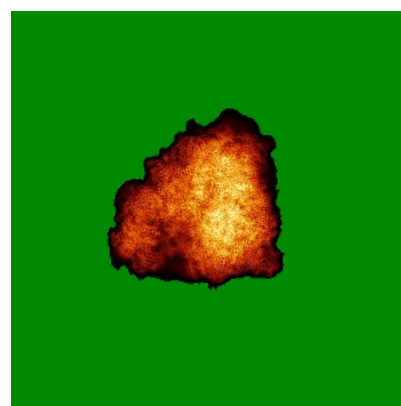
6.4.1 Primary map



X



Y

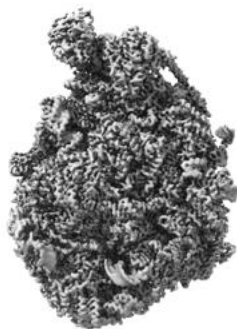


Z

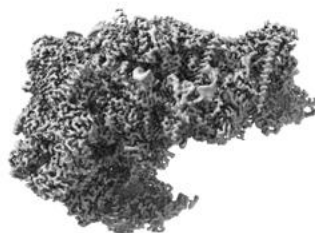
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

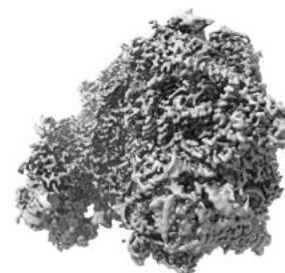
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

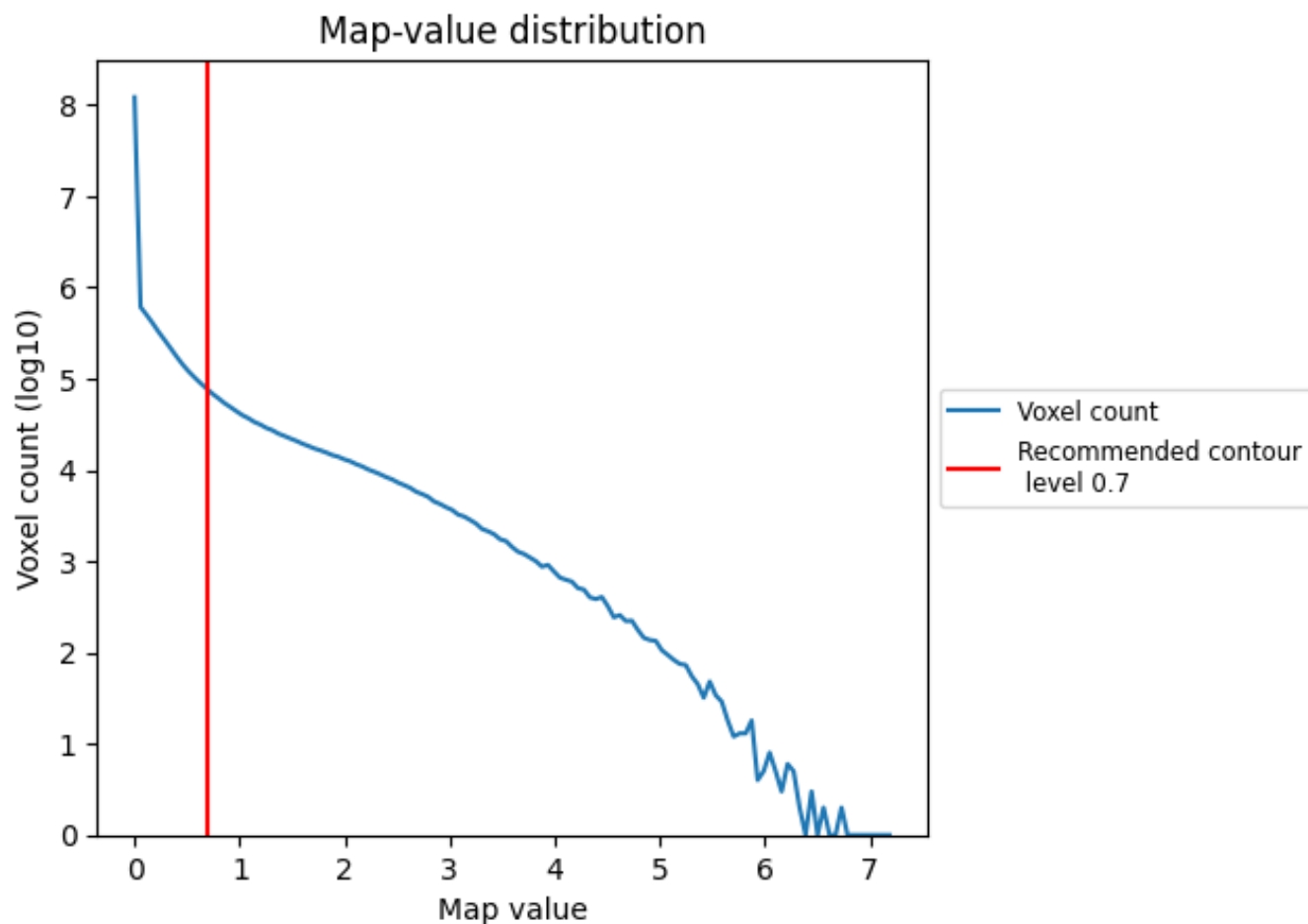
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

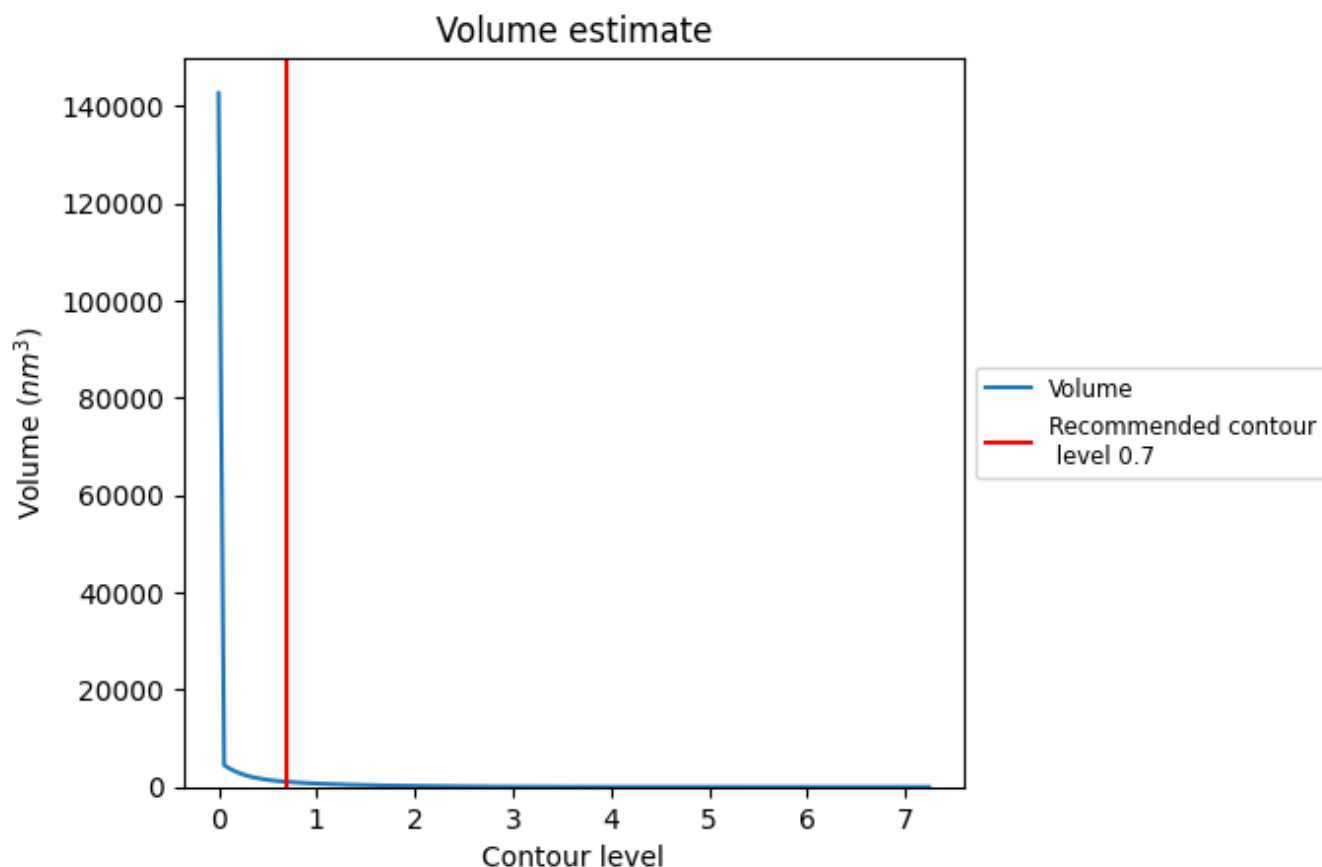
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

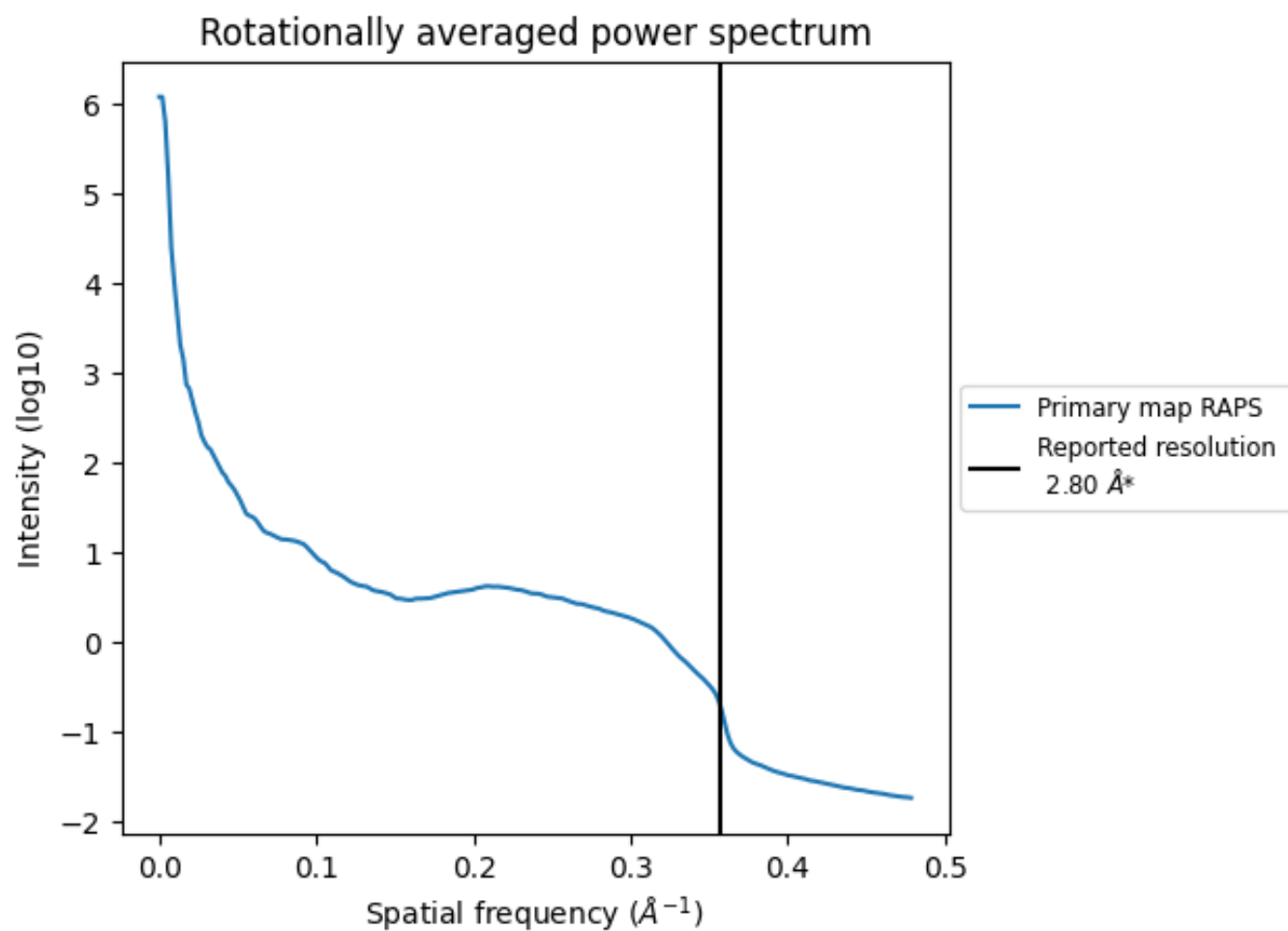
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1050 nm^3 ; this corresponds to an approximate mass of 949 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 0.357 Å⁻¹

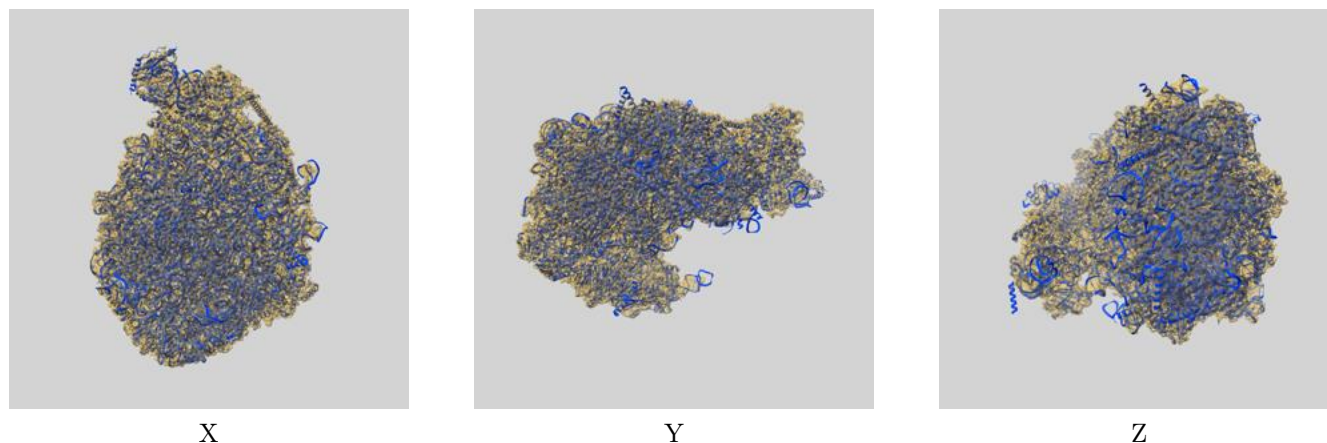
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

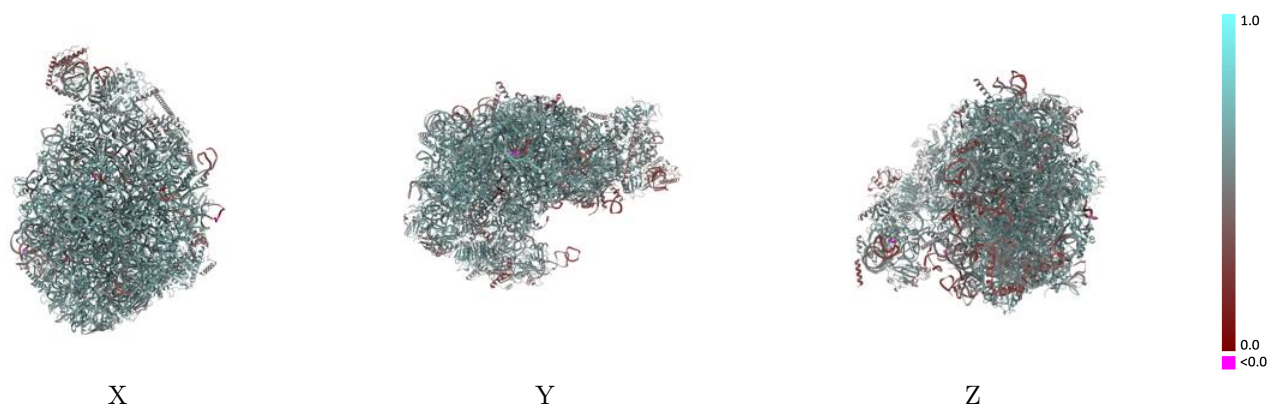
This section contains information regarding the fit between EMDB map EMD-17952 and PDB model 8PV3. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



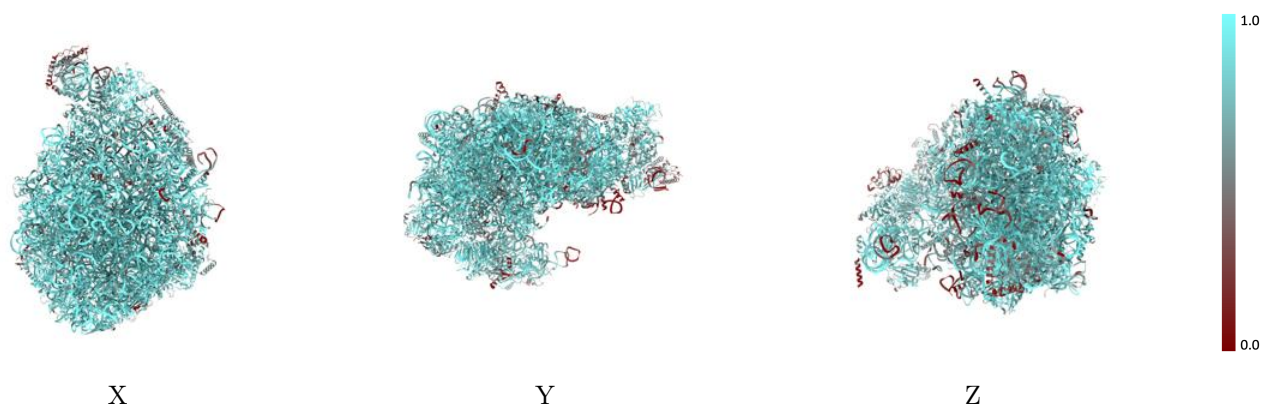
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



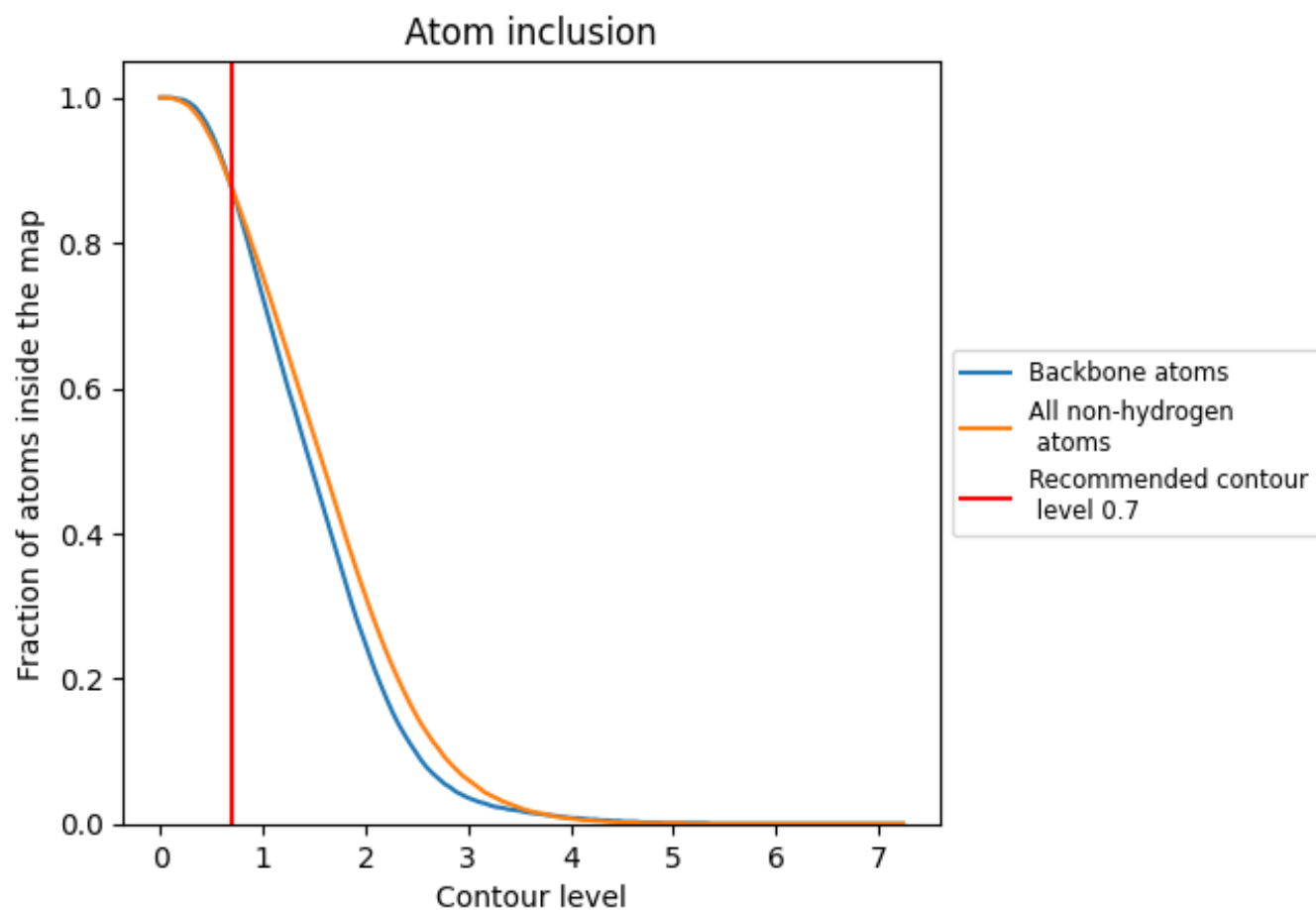
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 88% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.5730
C1	 0.9270	 0.5820
C2	 0.9590	 0.6120
C3	 0.6240	 0.4030
C4	 0.8460	 0.4860
CB	 0.5740	 0.4370
CF	 0.8050	 0.5430
CH	 0.8330	 0.5680
CI	 0.6530	 0.4580
CJ	 0.8820	 0.5720
CK	 0.9310	 0.6070
CL	 0.7820	 0.5390
CM	 0.7680	 0.5180
CN	 0.9000	 0.6070
CO	 0.8290	 0.5790
CQ	 0.8070	 0.5700
Cb	 0.7230	 0.5420
Cd	 0.8620	 0.5720
Ce	 0.6850	 0.4980
Cf	 0.8270	 0.5480
Cg	 0.7790	 0.5240
Ch	 0.7990	 0.5400
Cz	 0.6970	 0.4720
LA	 0.8420	 0.5570
LB	 0.9450	 0.6360
LC	 0.9300	 0.6260
LD	 0.8350	 0.5410
LE	 0.8160	 0.5700
LF	 0.8990	 0.6040
LG	 0.8470	 0.5670
LH	 0.9040	 0.6050
LJ	 0.7350	 0.4590
LK	 0.7190	 0.5000
LL	 0.8470	 0.5830
LM	 0.9040	 0.6040



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Chain	Atom inclusion	Q-score
LN	 0.9370	 0.6270
LO	 0.9570	 0.6400
LP	 0.9490	 0.6350
LQ	 0.8960	 0.6000
LR	 0.9140	 0.6070
LS	 0.9110	 0.6070
LT	 0.7060	 0.4770
LU	 0.8050	 0.5540
LV	 0.9560	 0.6350
LX	 0.8660	 0.5810
LY	 0.9040	 0.6040
LZ	 0.8510	 0.5560
La	 0.9120	 0.5990
Lc	 0.7910	 0.5520
Ld	 0.9010	 0.6240
Le	 0.9460	 0.6340
Lf	 0.9780	 0.6520
Lg	 0.8510	 0.5800
Lh	 0.8380	 0.5610
Li	 0.7950	 0.5330
Lj	 0.9730	 0.6510
Lk	 0.7710	 0.5510
Ll	 0.9860	 0.6570
Lp	 0.7860	 0.5470
Lq	 0.8990	 0.5900