



Full wwPDB EM Validation Report ⓘ

Mar 11, 2025 – 02:59 PM EDT

PDB ID : 6OST
EMDB ID : EMD-20188
Title : RF2 pre-accommodated state bound Release complex 70S at 24ms
Authors : Fu, Z.; Indrisiunaite, G.; Kaledhonkar, S.; Shah, B.; Sun, M.; Chen, B.; Grassucci, R.A.; Ehrenberg, M.; Frank, J.
Deposited on : 2019-05-02
Resolution : 4.20 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

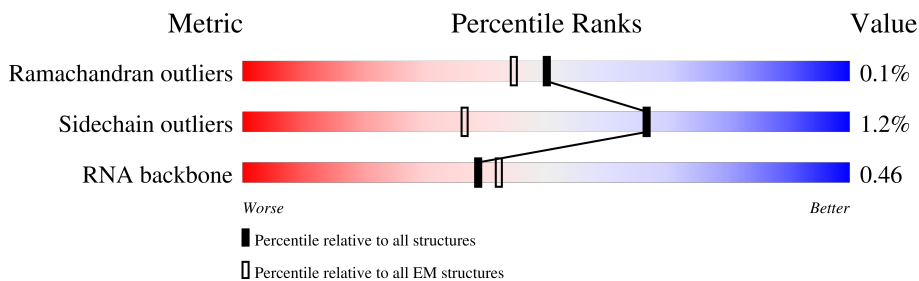
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



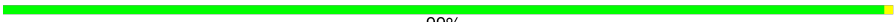
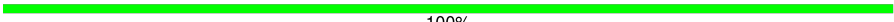
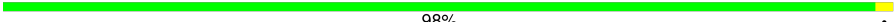
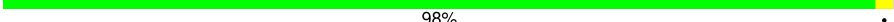


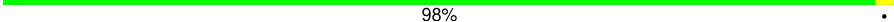
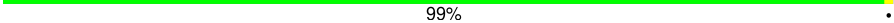
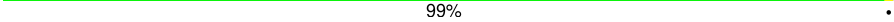
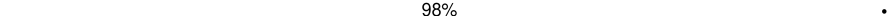
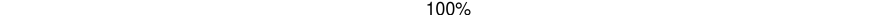
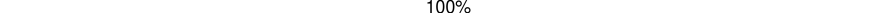
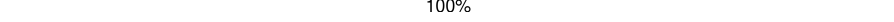
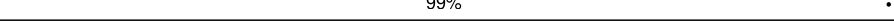
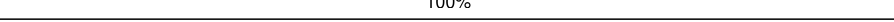
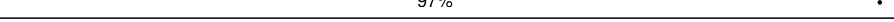
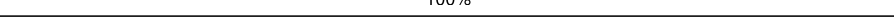
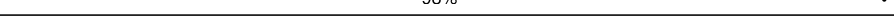
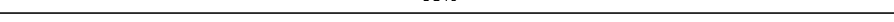






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	2903	
2	2	1534	
3	3	120	
4	B	271	
5	C	209	
6	D	201	
7	E	177	
8	F	175	

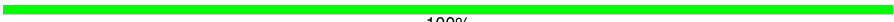













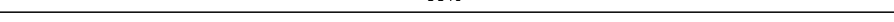
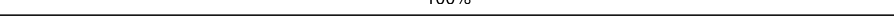
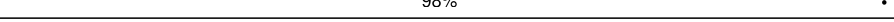
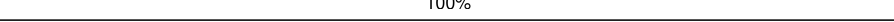
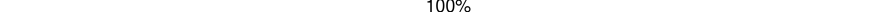

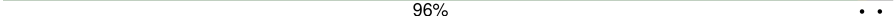

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Mol	Chain	Length	Quality of chain
9	G	149	 99% .
10	J	142	 100%
11	K	123	 98% .
12	L	144	 98% .
13	M	136	 100%
14	N	119	 100%
15	O	116	 98% .
16	P	114	 99% .
17	Q	117	 99% .
18	R	103	 98% .
19	S	110	 100%
20	T	94	 100%
21	U	103	 100%
22	V	94	 99% .
23	W	76	 100%
24	X	77	 97% .
25	Y	62	 100%
26	Z	58	 98% .
27	b	56	 98% .
28	c	52	 98% .
29	d	46	 100%
30	e	64	 98% .
31	f	38	 100%
32	g	225	 100%
33	h	208	 98% .

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Mol	Chain	Length	Quality of chain
34	i	205	 100%
35	j	156	 99%
36	k	104	 100%
37	l	151	 99%
38	m	129	 100%
39	n	127	 98%
40	o	99	 98%
41	p	117	 98%
42	q	123	 98%
43	r	116	 100%
44	s	100	 99%
45	t	88	 99%
46	u	82	 99%
47	v	80	 99%
48	w	66	 100%
49	x	83	 98%
50	y	86	 100%
51	z	70	 100%
52	4	9	 78% 22%
53	7	362	 9% 96%
54	5	76	 66% 30%
55	6	3	 33% 100%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146620 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	103	Total	C	N	O		
			788	498	148	142	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	76	Total	C	N	O	S	
			582	360	117	104	1	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	58	Total	C	N	O	S	
			448	281	87	78	2	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 52 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	9	Total	C	N	O	P	0	0
			184	83	26	66	9		

- Molecule 53 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	7	352	Total	C	N	O	S	0	0
			2793	1722	484	577	10		

- Molecule 54 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	5	76	Total	C	N	O	P	S	0	0
			1627	727	296	527	76	1		

- Molecule 55 is a protein called FME-PHE-PHE.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	3	Total	C	N	O	S	0	0
			32	24	3	4	1		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	1	Total 1	Mg 1	0
56	2	1	Total 1	Mg 1	0
56	3	8	Total 8	Mg 8	0
56	b	1	Total 1	Mg 1	0
56	i	1	Total 1	Mg 1	0

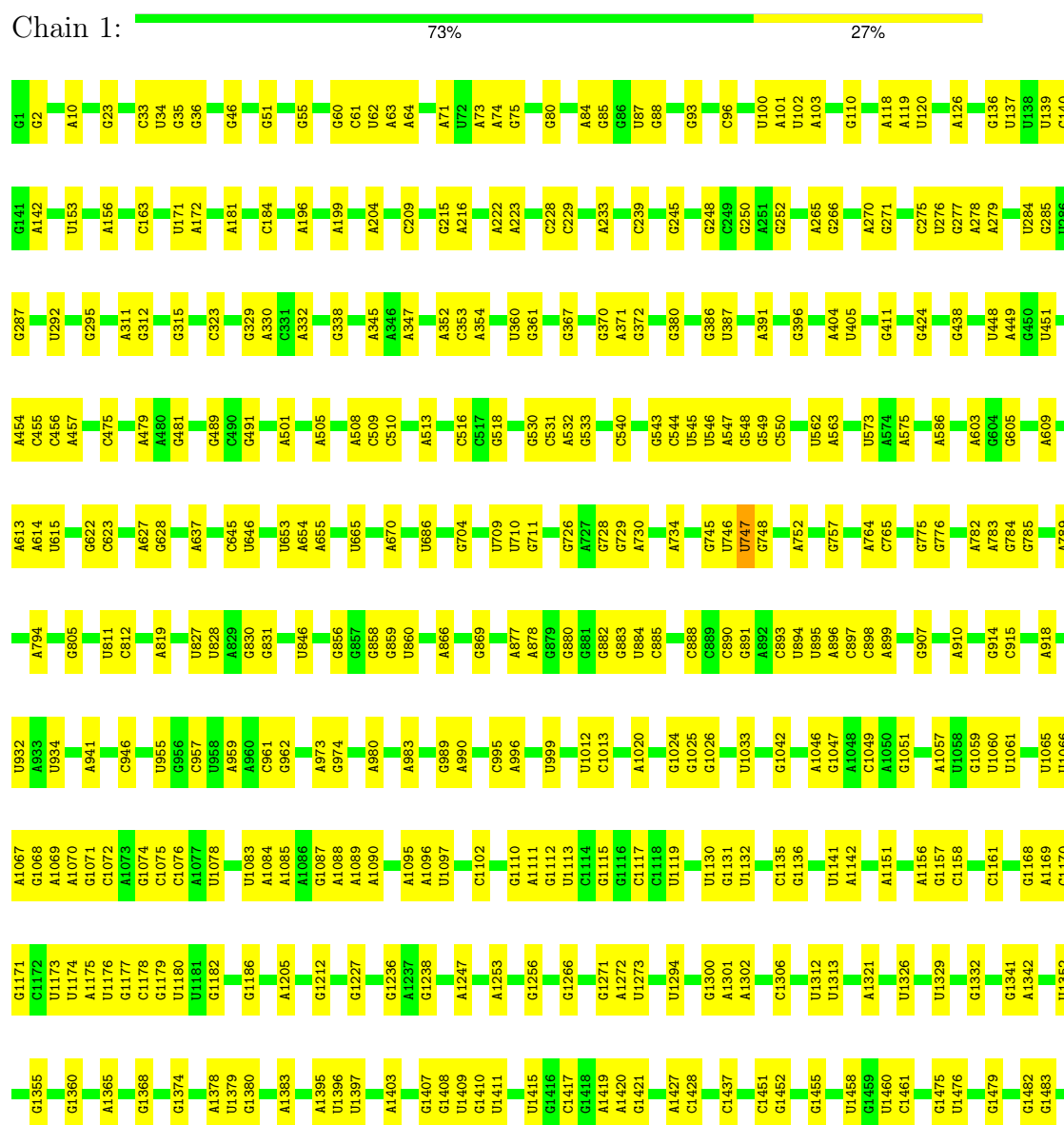
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	f	1	Total 1	Zn 1	0

3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA

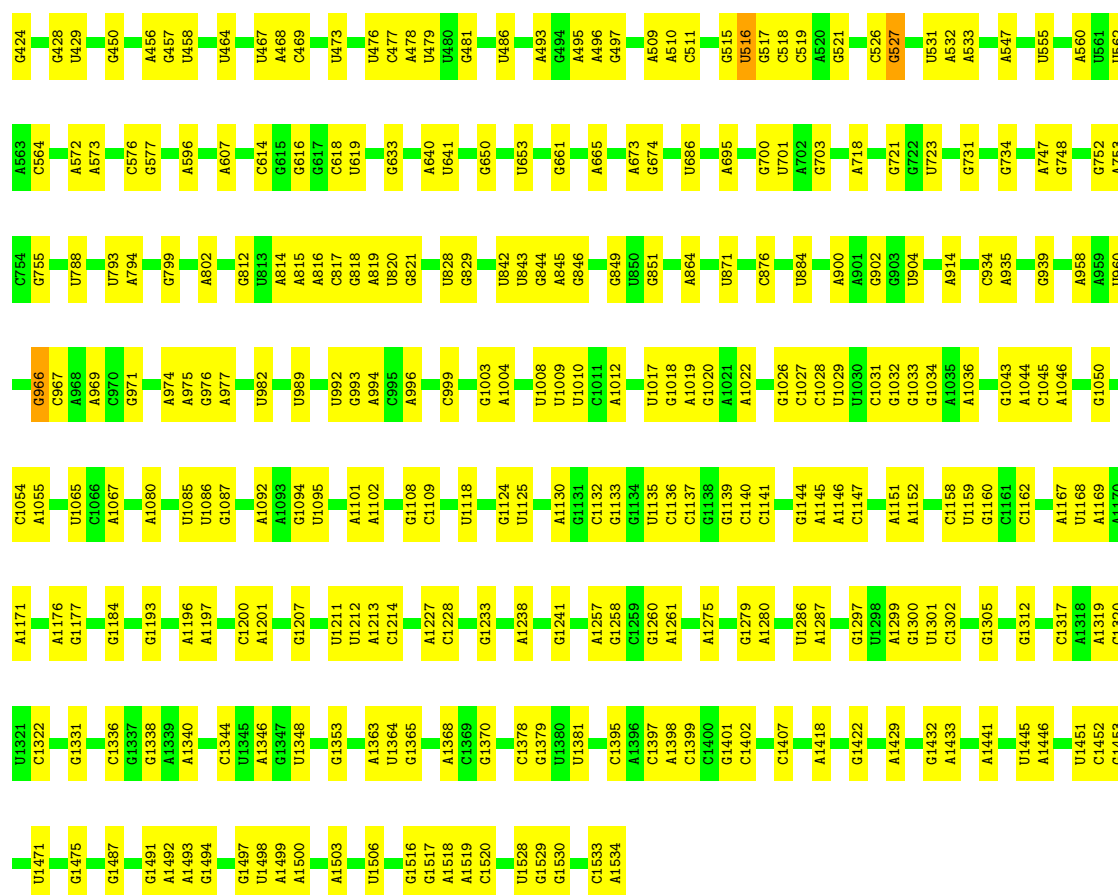


A1490	G1491	G1492	C1493	U1497	C1498	A1502	A1508	A1509	G1510	A1515	U1523	U1524	A1528	G1529	U1648	G1530	C1531	A1532	A1535	G1536	G1537	G1538	A1544	U1554	C1558	U1559	G1560	C1565	A1566	A1569	A1570	U1578	A1579	A1580	G1581	C1582	A1583	U1584	C1585	A1586	G1587	U1588	U1589	A1590	A1603																																					
C1607	A1610	G1613	G1618	A1618	G1622	A1626	A1634	A1635	U1636	A1637	C1638	C1639	C1646	U1647	U1648	G1649	A1655	G1660	A1665	G1666	G1667	A1668	A1669	G1674	U1680	U1683	C1694	G1695	A1698	G1699	A1700	U1709	G1715	U1716	G1724	U1725	U1729	A1731	G1732	G1733	C1734	A1735	G1738	U1742	A1754	A1755	G1756	A1757	A1758	U1759	C1760	G1764	A1773	U1781	U1782	A1791	G1792	G1797	A1800	A1801	A1802	G1807	A1808	A1809	A1810	G1811	A1829	C1833	U1834	G1835	U1841	A1847	A1848	G1849	G1850	G1857	A1858	U1859	U1864	U1865	G1733	A1866
U1991	G1992	U1993	C1996	C1997	G2002	C2021	U2022	C2023	A2030	A2031	G2032	A2033	U2034	C2043	G2049	C2050	A2051	C2055	G2056	G2057	A2060	G2061	A2062	C2069	C2072	U2075	U2076	A2077	U2092	G2093	U2099	G2100	A2101	G2102	A2108	U2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	U2189	G2190	G2193	U2194	A2198	A2199																																	
A2119	G2120	G2121	U2122	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	U2137	G2138	U2139	A2142	C2145	C2146	A2147	G2148	C2153	A2154	A2158	A2163	U2164	C2165	U2166	U2167	A2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	U2181	U2182	U2188	U2189	G2190	G2193	U2194	A2198	A2199																																			
U2203	G2204	A2211	A2212	U2213	A2225	U2229	G2238	U2243	G2246	G2250	G2251	A2266	A2267	A2268	G2269	A2278	G2279	C2283	A2287	A2288	U2296	A2297	G2303	G2304	U2305	A2309	G2315	G2319	U2320	U2321	G2325	G2326	A2327	G2331	C2332	A2333	U2334	A2335	A2336																																											
U2343	U2344	A2345	A2346	C2347	C2350	G2357	G2361	A2376	G2379	G2383	U2384	C2385	A2388	U2402	C2403	A2406	A2407	U2408	G2409	G2410	U2423	C2424	A2425	A2426	G2427	G2428	G2429	A2430	U2431	A2434	A2435	G2436	U2441	G2445	G2446	G2447	A2448	U2457	G2458	A2459	G2464	A2469	G2470																																							
U2473	U2474	C2475	A2476	U2477	C2480	G2484	G2490	U2491	U2492	U2493	G2494	C2498	C2501	G2502	A2503	U2504	G2505	U2506	C2507	C2512	A2513	U2518	C2520	G2529	A2530	A2531	G2535	A2547	U2552	G2553	U2554	A2564	A2565	A2566	G2567	A2572	C2573	G2574	U2580	U2585	U2586																																									
G2599	A2602	U2605	G2608	U2609	C2610	C2611	G2612	U2613	G2621	U2629	G2630	C2636	G2644	G2645	C2646	U2647	G2648	A2654	G2673	G2686	U2689	U2690	U2707	C2716	G2717	G2718	A2725	A2726	U2727	U2728	G2732	A2733	U2739	G2744	A2748	C2752	U2756	A2757																																												
A2765	A2766	U2769	A2776	G2777	A2778	U2779	G2780	C2787	C2793	C2794	U2797	U2798	A2799	G2811	G2812	U2818	G2819	A2820	A2821	G2822	A2823	C2824	G2825	U2833	G2834	A2835	A2860	U2861	G2867	A2879	C2880	U2884	G2885	A2886	A2893	U2898	A2899	A2900	C2901	U2902	U2903																																									

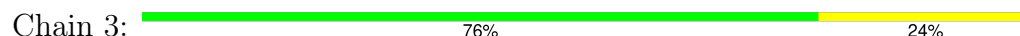
● Molecule 2: 16S Ribosomal RNA

Chain 2:  74% 26%

A1	A2	A3	U4	U5	G6	A7	A8	C9	G22	G39	A44	C47	C48	U49	A50	A51	C52	A53	C54	G61	G68	G69	U70	A71	A72	C73	A74	G75	G76	G79	A80	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95	A120	U121	G122	U123
G127	G128	A129	A130	A131	G141	G144	G145	G146	A149	U154	C163	G164	C169	C189	U173	G177	U180	A181	A182	C183	G184	U185	A192	A195	A196	A197	G202	G203	G204	U209	C210	G211	G212	G213	C214	A223	G226	G240	U244	U245	U246	G247								
G251	G266	C267	A279	C280	G281	G289	A306	C316	G319	A320	C328	A329	C330	C331	G332	C339	G347	G348	G351	C352	A353	C356	U365	A366	U367	C372	G384	G388	A389	U390	A397	G406	A411	A412	G413	A414	U421	C422	A423	G423										



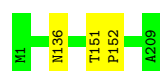
• Molecule 3: 5S Ribosomal RNA



• Molecule 4: 50S ribosomal protein L2



• Molecule 5: 50S ribosomal protein L3



• Molecule 6: 50S ribosomal protein L4





- Molecule 7: 50S ribosomal protein L5

Chain E:  100%

There are no outlier residues recorded for this chain.

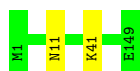
- Molecule 8: 50S ribosomal protein L6

Chain F:  99%



- Molecule 9: 50S ribosomal protein L9

Chain G:  99%



- Molecule 10: 50S ribosomal protein L13

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L14

Chain K:  98%



- Molecule 12: 50S ribosomal protein L15

Chain L:  98%



- Molecule 13: 50S ribosomal protein L16

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 50S ribosomal protein L17

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 50S ribosomal protein L18

Chain O:  98%



- Molecule 16: 50S ribosomal protein L19

Chain P:  99%



- Molecule 17: 50S ribosomal protein L20

Chain Q:  99%



- Molecule 18: 50S ribosomal protein L21

Chain R:  98%



- Molecule 19: 50S ribosomal protein L22

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: 50S ribosomal protein L23

Chain T:  100%


There are no outlier residues recorded for this chain.

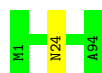
- Molecule 21: 50S ribosomal protein L24

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L25

Chain V:  99% .



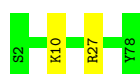
- Molecule 23: 50S ribosomal protein L27

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L28

Chain X:  97% .



- Molecule 25: 50S ribosomal protein L29

Chain Y:  100%

There are no outlier residues recorded for this chain.

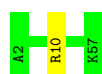
- Molecule 26: 50S ribosomal protein L30

Chain Z:  98% .



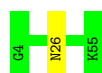
- Molecule 27: 50S ribosomal protein L32

Chain b:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain c:  98% .



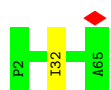
- Molecule 29: 50S ribosomal protein L34

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L35

Chain e:  98%



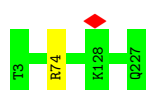
- Molecule 31: 50S ribosomal protein L36

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 30S ribosomal protein S2

Chain g:  100%



- Molecule 33: 30S ribosomal protein S3

Chain h:  98%



- Molecule 34: 30S ribosomal protein S4

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: 30S ribosomal protein S5

Chain j:  99%



- Molecule 36: 30S ribosomal protein S6

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 30S ribosomal protein S7

Chain l:  99%



- Molecule 38: 30S ribosomal protein S8

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S9

Chain n: 98%



- Molecule 40: 30S ribosomal protein S10

Chain o: 98%



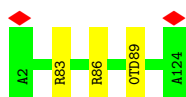
- Molecule 41: 30S ribosomal protein S11

Chain p: 98%



- Molecule 42: 30S ribosomal protein S12

Chain q: 98%



- Molecule 43: 30S ribosomal protein S13

Chain r: 100%



- Molecule 44: 30S ribosomal protein S14

Chain s: 99%



- Molecule 45: 30S ribosomal protein S15

Chain t:  99%



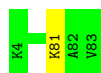
- Molecule 46: 30S ribosomal protein S16

Chain u:  99%



- Molecule 47: 30S ribosomal protein S17

Chain v:  99%



- Molecule 48: 30S ribosomal protein S18

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S19

Chain x:  98%



- Molecule 50: 30S ribosomal protein S20

Chain y:  100%

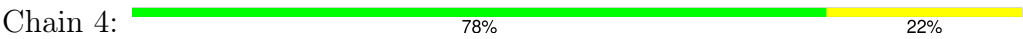
There are no outlier residues recorded for this chain.

- Molecule 51: 30S ribosomal protein S21

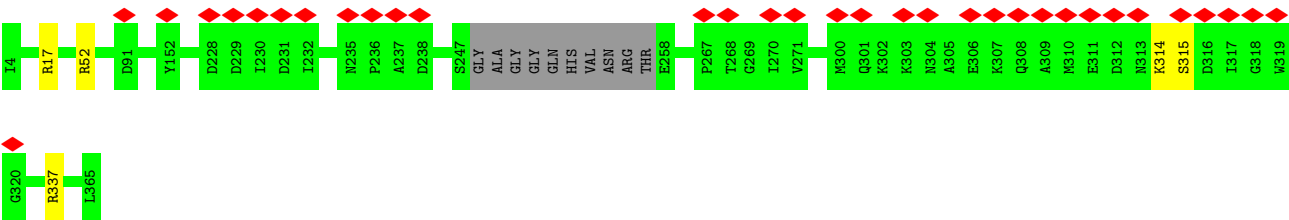
Chain z:  100%

There are no outlier residues recorded for this chain.

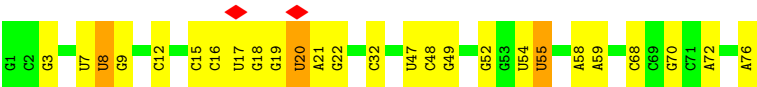
- Molecule 52: mRNA



• Molecule 53: Peptide chain release factor 2



• Molecule 54: P-tRNA



• Molecule 55: FME-PHE-PHE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.027	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	421.12, 421.12, 421.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.645, 1.645, 1.645	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 6MZ, 4OC, 2MG, 5MC, MG, OMC, 0TD, PSU, UR3, H2U, 1MG, 4SU, 2MA, OMU, ZN, OMG, G7M, 3TD, FME, 5MU

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	1	1.05	1/69286 (0.0%)	1.14	0/108087
2	2	0.95	0/36590	1.13	0/57074
3	3	0.94	0/2872	1.12	0/4478
4	B	0.49	0/2121	0.62	0/2852
5	C	0.47	0/1586	0.64	0/2134
6	D	0.45	0/1571	0.59	0/2113
7	E	0.47	0/1434	0.61	0/1926
8	F	0.45	0/1333	0.57	0/1805
9	G	0.41	0/1122	0.61	0/1515
10	J	0.50	0/1152	0.57	0/1551
11	K	0.43	0/955	0.61	0/1279
12	L	0.45	0/1062	0.62	0/1413
13	M	0.46	0/1093	0.60	0/1460
14	N	0.44	0/964	0.65	0/1289
15	O	0.42	0/902	0.57	0/1209
16	P	0.48	0/929	0.61	0/1242
17	Q	0.49	0/960	0.54	0/1278
18	R	0.52	0/829	0.65	0/1107
19	S	0.45	0/864	0.59	0/1156
20	T	0.44	0/752	0.60	0/1005
21	U	0.47	0/796	0.61	0/1062
22	V	0.47	0/766	0.59	0/1025
23	W	0.48	0/589	0.58	0/779
24	X	0.48	0/635	0.61	0/848
25	Y	0.43	0/502	0.55	0/667
26	Z	0.42	0/452	0.62	0/605
27	b	0.46	0/450	0.62	0/599
28	c	0.47	0/433	0.59	0/576
29	d	0.48	0/380	0.62	0/498
30	e	0.47	0/513	0.61	0/676
31	f	0.49	0/303	0.59	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.42	0/1791	0.58	0/2413
33	h	0.44	0/1663	0.57	0/2241
34	i	0.42	0/1665	0.56	0/2227
35	j	0.44	0/1165	0.59	0/1568
36	k	0.45	0/867	0.59	0/1171
37	l	0.41	0/1195	0.55	0/1602
38	m	0.44	0/989	0.56	0/1326
39	n	0.43	0/1034	0.61	0/1375
40	o	0.40	0/800	0.65	0/1082
41	p	0.40	0/893	0.53	0/1205
42	q	0.46	0/960	0.61	0/1286
43	r	0.41	0/909	0.60	0/1215
44	s	0.41	0/817	0.54	0/1088
45	t	0.43	0/722	0.55	0/964
46	u	0.40	0/659	0.57	0/884
47	v	0.47	0/657	0.69	0/881
48	w	0.44	0/553	0.56	0/743
49	x	0.39	0/680	0.52	0/915
50	y	0.42	0/675	0.49	0/895
51	z	0.41	0/597	0.55	0/792
52	4	0.57	0/203	1.06	0/312
53	7	0.41	0/2831	0.63	0/3815
54	5	0.54	0/1704	1.01	0/2654
55	6	0.48	0/23	0.30	0/29
All	All	0.88	1/158248 (0.0%)	1.01	0/236388

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1313	U	O3'-P	-5.94	1.54	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
4	B	269/271 (99%)	243 (90%)	25 (9%)	1 (0%)	30	67
5	C	207/209 (99%)	197 (95%)	9 (4%)	1 (0%)	25	62
6	D	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
7	E	175/177 (99%)	157 (90%)	18 (10%)	0	100	100
8	F	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
9	G	147/149 (99%)	130 (88%)	17 (12%)	0	100	100
10	J	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
11	K	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
12	L	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
13	M	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
14	N	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
15	O	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
16	P	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
19	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
20	T	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
21	U	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
22	V	92/94 (98%)	84 (91%)	8 (9%)	0	100	100
23	W	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
26	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
27	b	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
28	c	50/52 (96%)	48 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
30	e	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	8	38
31	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	g	223/225 (99%)	205 (92%)	18 (8%)	0	100	100
33	h	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
34	i	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
35	j	154/156 (99%)	138 (90%)	16 (10%)	0	100	100
36	k	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
37	l	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
38	m	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
39	n	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
40	o	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
41	p	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
42	q	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
43	r	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
44	s	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
45	t	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
46	u	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
47	v	78/80 (98%)	69 (88%)	9 (12%)	0	100	100
48	w	64/66 (97%)	64 (100%)	0	0	100	100
49	x	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
50	y	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
51	z	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
53	7	348/362 (96%)	326 (94%)	21 (6%)	1 (0%)	37	71
55	6	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5893/6006 (98%)	5480 (93%)	409 (7%)	4 (0%)	50	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	225	MET
53	7	315	SER
5	C	152	PRO

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Mol	Chain	Res	Type
30	e	32	ILE

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	
4	B	216/216 (100%)	212 (98%)	4 (2%)	52	69
5	C	164/164 (100%)	162 (99%)	2 (1%)	67	78
6	D	165/165 (100%)	163 (99%)	2 (1%)	67	78
7	E	148/148 (100%)	148 (100%)	0	100	100
8	F	136/136 (100%)	134 (98%)	2 (2%)	60	74
9	G	114/114 (100%)	112 (98%)	2 (2%)	54	71
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	104/104 (100%)	102 (98%)	2 (2%)	52	69
12	L	103/103 (100%)	100 (97%)	3 (3%)	37	58
13	M	109/109 (100%)	109 (100%)	0	100	100
14	N	99/99 (100%)	99 (100%)	0	100	100
15	O	86/86 (100%)	84 (98%)	2 (2%)	45	64
16	P	99/99 (100%)	98 (99%)	1 (1%)	73	81
17	Q	89/89 (100%)	88 (99%)	1 (1%)	70	79
18	R	84/84 (100%)	82 (98%)	2 (2%)	44	63
19	S	93/93 (100%)	93 (100%)	0	100	100
20	T	81/81 (100%)	81 (100%)	0	100	100
21	U	84/84 (100%)	84 (100%)	0	100	100
22	V	78/78 (100%)	77 (99%)	1 (1%)	65	76
23	W	58/58 (100%)	58 (100%)	0	100	100
24	X	67/67 (100%)	65 (97%)	2 (3%)	36	57
25	Y	54/54 (100%)	54 (100%)	0	100	100
26	Z	48/48 (100%)	47 (98%)	1 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	47/47 (100%)	46 (98%)	1 (2%)	48	66
28	c	47/47 (100%)	46 (98%)	1 (2%)	48	66
29	d	38/38 (100%)	38 (100%)	0	100	100
30	e	51/51 (100%)	51 (100%)	0	100	100
31	f	34/34 (100%)	34 (100%)	0	100	100
32	g	187/187 (100%)	186 (100%)	1 (0%)	86	90
33	h	171/171 (100%)	167 (98%)	4 (2%)	45	64
34	i	172/172 (100%)	172 (100%)	0	100	100
35	j	119/119 (100%)	117 (98%)	2 (2%)	56	72
36	k	91/91 (100%)	91 (100%)	0	100	100
37	l	124/124 (100%)	123 (99%)	1 (1%)	79	84
38	m	104/104 (100%)	104 (100%)	0	100	100
39	n	105/105 (100%)	102 (97%)	3 (3%)	37	58
40	o	86/86 (100%)	84 (98%)	2 (2%)	45	64
41	p	90/90 (100%)	88 (98%)	2 (2%)	47	65
42	q	102/102 (100%)	100 (98%)	2 (2%)	50	68
43	r	94/94 (100%)	94 (100%)	0	100	100
44	s	83/83 (100%)	82 (99%)	1 (1%)	67	78
45	t	76/76 (100%)	75 (99%)	1 (1%)	65	76
46	u	65/65 (100%)	64 (98%)	1 (2%)	60	74
47	v	74/74 (100%)	73 (99%)	1 (1%)	62	75
48	w	57/57 (100%)	57 (100%)	0	100	100
49	x	72/72 (100%)	70 (97%)	2 (3%)	38	59
50	y	65/65 (100%)	65 (100%)	0	100	100
51	z	60/60 (100%)	60 (100%)	0	100	100
53	7	301/308 (98%)	297 (99%)	4 (1%)	65	76
55	6	2/2 (100%)	0	2 (100%)	0	0
All	All	4912/4919 (100%)	4854 (99%)	58 (1%)	66	78

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	80	ARG

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Mol	Chain	Res	Type
4	B	130	LEU
4	B	225	MET
4	B	260	ASN
5	C	136	ASN
5	C	151	THR
6	D	44	ARG
6	D	163	ASN
8	F	73	ASN
8	F	176	LYS
9	G	11	ASN
9	G	41	LYS
11	K	17	ARG
11	K	49	ARG
12	L	36	LYS
12	L	48	ARG
12	L	126	ARG
15	O	25	ARG
15	O	94	ARG
16	P	51	ARG
17	Q	92	ARG
18	R	51	VAL
18	R	80	ARG
22	V	24	ASN
24	X	10	LYS
24	X	27	ARG
26	Z	31	ARG
27	b	10	ARG
28	c	26	ASN
32	g	74	ARG
33	h	72	ARG
33	h	164	ARG
33	h	172	ARG
33	h	179	ARG
35	j	29	ARG
35	j	132	ASN
37	l	130	ASN
39	n	106	ARG
39	n	113	ARG
39	n	130	ARG
40	o	5	ARG
40	o	9	ARG
41	p	13	ARG

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Mol	Chain	Res	Type
41	p	56	ARG
42	q	83	ARG
42	q	86	ARG
44	s	69	ARG
45	t	20	ASN
46	u	1	MET
47	v	81	LYS
49	x	32	ARG
49	x	78	ARG
53	7	17	ARG
53	7	52	ARG
53	7	314	LYS
53	7	337	ARG
55	6	78	PHE
55	6	79	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	70	ASN
4	B	86	ASN
4	B	251	GLN
4	B	260	ASN
5	C	136	ASN
6	D	163	ASN
8	F	88	GLN
8	F	104	ASN
8	F	116	GLN
9	G	18	GLN
15	O	29	HIS
15	O	38	GLN
15	O	61	GLN
17	Q	72	ASN
17	Q	81	ASN
18	R	6	GLN
19	S	60	HIS
19	S	61	ASN
20	T	28	ASN
21	U	46	GLN
21	U	54	GLN
22	V	24	ASN
23	W	50	ASN

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Mol	Chain	Res	Type
25	Y	15	ASN
28	c	26	ASN
28	c	45	GLN
32	g	178	ASN
34	i	116	GLN
35	j	12	GLN
35	j	132	ASN
36	k	46	GLN
36	k	63	ASN
37	l	28	ASN
37	l	130	ASN
39	n	50	GLN
41	p	15	GLN
42	q	5	ASN
43	r	14	HIS
45	t	20	ASN
45	t	37	ASN
45	t	40	GLN
45	t	80	GLN
48	w	31	ASN
49	x	52	HIS
50	y	48	GLN
50	y	52	ASN
53	7	38	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	770 (26%)	14 (0%)
2	2	1529/1534 (99%)	392 (25%)	6 (0%)
3	3	119/120 (99%)	29 (24%)	0
52	4	8/9 (88%)	2 (25%)	0
54	5	74/76 (97%)	24 (32%)	1 (1%)
All	All	4628/4642 (99%)	1217 (26%)	21 (0%)

All (1217) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	10	A
1	1	23	G

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Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	35	G
1	1	36	G
1	1	46	G
1	1	51	G
1	1	55	G
1	1	60	G
1	1	61	C
1	1	62	U
1	1	63	A
1	1	64	A
1	1	71	A
1	1	73	A
1	1	74	A
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	87	U
1	1	88	G
1	1	93	G
1	1	96	C
1	1	100	U
1	1	101	A
1	1	102	U
1	1	103	A
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	126	A
1	1	136	G
1	1	137	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	153	U
1	1	156	A
1	1	163	C
1	1	171	U
1	1	172	A

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Mol	Chain	Res	Type
1	1	181	A
1	1	184	C
1	1	196	A
1	1	199	A
1	1	204	A
1	1	209	C
1	1	215	G
1	1	216	A
1	1	222	A
1	1	223	A
1	1	228	C
1	1	229	C
1	1	233	A
1	1	239	C
1	1	245	G
1	1	248	G
1	1	250	G
1	1	252	G
1	1	265	A
1	1	266	G
1	1	270	A
1	1	271	G
1	1	275	C
1	1	276	U
1	1	277	G
1	1	278	A
1	1	279	A
1	1	284	U
1	1	285	G
1	1	287	G
1	1	292	U
1	1	295	G
1	1	311	A
1	1	312	G
1	1	315	G
1	1	323	C
1	1	329	G
1	1	330	A
1	1	332	A
1	1	338	G
1	1	345	A
1	1	347	A

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Mol	Chain	Res	Type
1	1	352	A
1	1	353	C
1	1	354	A
1	1	360	U
1	1	361	G
1	1	367	G
1	1	370	G
1	1	371	A
1	1	372	G
1	1	380	G
1	1	386	G
1	1	387	U
1	1	391	A
1	1	396	G
1	1	405	U
1	1	411	G
1	1	424	G
1	1	438	G
1	1	448	U
1	1	449	A
1	1	451	U
1	1	454	A
1	1	455	C
1	1	456	C
1	1	457	A
1	1	475	C
1	1	479	A
1	1	481	G
1	1	489	G
1	1	491	G
1	1	501	A
1	1	505	A
1	1	508	A
1	1	509	C
1	1	510	C
1	1	513	A
1	1	516	C
1	1	518	G
1	1	530	G
1	1	531	C
1	1	532	A
1	1	533	G

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Mol	Chain	Res	Type
1	1	540	C
1	1	543	G
1	1	544	C
1	1	545	U
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	550	C
1	1	562	U
1	1	563	A
1	1	573	U
1	1	575	A
1	1	586	A
1	1	603	A
1	1	605	G
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	622	G
1	1	623	C
1	1	627	A
1	1	628	G
1	1	637	A
1	1	645	C
1	1	646	U
1	1	653	U
1	1	654	A
1	1	655	A
1	1	665	U
1	1	670	A
1	1	686	U
1	1	704	G
1	1	709	U
1	1	710	U
1	1	711	G
1	1	726	G
1	1	728	G
1	1	729	G
1	1	730	A
1	1	734	A

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Mol	Chain	Res	Type
1	1	747	5MU
1	1	748	G
1	1	752	A
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	783	A
1	1	784	G
1	1	785	G
1	1	789	A
1	1	794	A
1	1	805	G
1	1	811	U
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
1	1	831	G
1	1	846	U
1	1	856	G
1	1	858	G
1	1	859	G
1	1	860	U
1	1	866	A
1	1	869	G
1	1	877	A
1	1	878	A
1	1	880	G
1	1	882	G
1	1	883	G
1	1	884	U
1	1	885	C
1	1	888	C
1	1	890	C
1	1	891	G
1	1	893	C
1	1	894	U
1	1	895	U

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Mol	Chain	Res	Type
1	1	896	A
1	1	897	C
1	1	898	C
1	1	899	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	918	A
1	1	932	U
1	1	934	U
1	1	941	A
1	1	946	C
1	1	957	C
1	1	959	A
1	1	961	C
1	1	962	G
1	1	973	A
1	1	974	G
1	1	980	A
1	1	983	A
1	1	989	G
1	1	990	A
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1012	U
1	1	1013	C
1	1	1020	A
1	1	1024	G
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1042	G
1	1	1046	A
1	1	1047	G
1	1	1049	C
1	1	1051	G
1	1	1057	A
1	1	1059	G
1	1	1060	U
1	1	1061	U

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Mol	Chain	Res	Type
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1071	G
1	1	1072	C
1	1	1074	G
1	1	1075	C
1	1	1076	C
1	1	1078	U
1	1	1083	U
1	1	1084	A
1	1	1085	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1090	A
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1102	C
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1113	U
1	1	1115	G
1	1	1117	C
1	1	1119	U
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1135	C
1	1	1136	G
1	1	1141	U
1	1	1142	A
1	1	1151	A
1	1	1156	A
1	1	1157	G
1	1	1158	C
1	1	1161	C

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Mol	Chain	Res	Type
1	1	1168	G
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1180	U
1	1	1182	G
1	1	1186	G
1	1	1205	A
1	1	1212	G
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1294	U
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1306	C
1	1	1312	U
1	1	1321	A
1	1	1326	U
1	1	1329	U
1	1	1332	G
1	1	1341	G
1	1	1342	A
1	1	1352	U
1	1	1355	G
1	1	1360	G
1	1	1365	A

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Mol	Chain	Res	Type
1	1	1368	G
1	1	1374	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1395	A
1	1	1396	U
1	1	1397	U
1	1	1403	A
1	1	1407	G
1	1	1408	G
1	1	1409	U
1	1	1410	G
1	1	1411	U
1	1	1415	U
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1421	G
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1451	C
1	1	1452	G
1	1	1455	G
1	1	1458	U
1	1	1460	U
1	1	1461	C
1	1	1475	G
1	1	1476	U
1	1	1479	G
1	1	1482	G
1	1	1483	G
1	1	1490	A
1	1	1491	G
1	1	1493	C
1	1	1497	U
1	1	1498	C
1	1	1502	A
1	1	1508	A
1	1	1509	A

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Mol	Chain	Res	Type
1	1	1510	G
1	1	1515	A
1	1	1523	U
1	1	1524	G
1	1	1528	A
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1538	G
1	1	1544	A
1	1	1554	U
1	1	1558	C
1	1	1560	G
1	1	1565	C
1	1	1566	A
1	1	1569	A
1	1	1570	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1582	C
1	1	1583	A
1	1	1584	U
1	1	1585	C
1	1	1586	A
1	1	1587	G
1	1	1588	G
1	1	1589	U
1	1	1590	A
1	1	1603	A
1	1	1607	C
1	1	1610	A
1	1	1613	G
1	1	1622	G
1	1	1626	A
1	1	1634	A
1	1	1635	A
1	1	1636	U
1	1	1637	A
1	1	1639	C

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Mol	Chain	Res	Type
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1655	A
1	1	1660	G
1	1	1665	A
1	1	1667	G
1	1	1669	A
1	1	1674	G
1	1	1680	U
1	1	1693	U
1	1	1695	G
1	1	1698	A
1	1	1700	A
1	1	1709	U
1	1	1715	G
1	1	1716	U
1	1	1724	G
1	1	1725	U
1	1	1729	U
1	1	1730	C
1	1	1731	G
1	1	1732	C
1	1	1733	G
1	1	1735	A
1	1	1738	G
1	1	1742	U
1	1	1754	A
1	1	1755	A
1	1	1756	G
1	1	1758	U
1	1	1760	C
1	1	1764	C
1	1	1773	A
1	1	1781	U
1	1	1782	U
1	1	1791	A
1	1	1792	G
1	1	1797	G
1	1	1800	C
1	1	1801	A

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Mol	Chain	Res	Type
1	1	1802	A
1	1	1807	G
1	1	1808	A
1	1	1809	A
1	1	1811	G
1	1	1816	C
1	1	1820	U
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1841	U
1	1	1847	A
1	1	1848	A
1	1	1849	G
1	1	1850	G
1	1	1857	G
1	1	1858	A
1	1	1859	U
1	1	1864	U
1	1	1865	U
1	1	1866	A
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1873	G
1	1	1876	A
1	1	1884	G
1	1	1885	A
1	1	1888	G
1	1	1900	A
1	1	1903	G
1	1	1905	C
1	1	1906	G
1	1	1907	G
1	1	1913	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1926	U
1	1	1927	A
1	1	1929	G
1	1	1930	G

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Mol	Chain	Res	Type
1	1	1931	U
1	1	1936	A
1	1	1937	A
1	1	1955	U
1	1	1964	G
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1975	G
1	1	1982	U
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1996	C
1	1	1997	C
1	1	2002	G
1	1	2021	C
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2034	U
1	1	2043	C
1	1	2049	G
1	1	2051	A
1	1	2055	C
1	1	2056	G
1	1	2057	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2072	C
1	1	2075	U
1	1	2077	A
1	1	2092	U
1	1	2093	G
1	1	2099	U
1	1	2101	A
1	1	2102	G
1	1	2108	A

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Mol	Chain	Res	Type
1	1	2111	U
1	1	2112	G
1	1	2113	U
1	1	2114	A
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2122	U
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2130	U
1	1	2131	U
1	1	2133	G
1	1	2134	A
1	1	2137	U
1	1	2138	G
1	1	2139	U
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2148	G
1	1	2153	C
1	1	2154	A
1	1	2158	A
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2167	U
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2174	C
1	1	2176	A
1	1	2178	C
1	1	2181	U

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Mol	Chain	Res	Type
1	1	2182	U
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2199	A
1	1	2203	U
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2243	U
1	1	2246	G
1	1	2250	G
1	1	2266	A
1	1	2267	A
1	1	2269	G
1	1	2278	A
1	1	2279	G
1	1	2283	C
1	1	2287	A
1	1	2288	A
1	1	2296	U
1	1	2297	A
1	1	2303	G
1	1	2305	U
1	1	2309	A
1	1	2315	G
1	1	2319	G
1	1	2320	U
1	1	2321	U
1	1	2325	G
1	1	2327	A
1	1	2331	G
1	1	2333	A
1	1	2335	A
1	1	2336	A

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Mol	Chain	Res	Type
1	1	2343	U
1	1	2344	U
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2379	G
1	1	2383	G
1	1	2385	C
1	1	2388	A
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2408	U
1	1	2410	G
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2434	A
1	1	2436	G
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2459	A
1	1	2464	G
1	1	2469	A
1	1	2470	G
1	1	2473	U
1	1	2475	C
1	1	2476	A
1	1	2477	U
1	1	2480	C
1	1	2484	G
1	1	2490	G

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Mol	Chain	Res	Type
1	1	2491	U
1	1	2492	U
1	1	2494	G
1	1	2498	OMC
1	1	2501	C
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2507	C
1	1	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2530	A
1	1	2531	A
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2564	A
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2586	U
1	1	2599	G
1	1	2602	A
1	1	2608	G
1	1	2609	U
1	1	2610	C
1	1	2611	C
1	1	2613	U
1	1	2621	G
1	1	2629	U
1	1	2630	G
1	1	2636	C
1	1	2644	G
1	1	2646	C
1	1	2648	G
1	1	2654	A

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Mol	Chain	Res	Type
1	1	2673	G
1	1	2686	G
1	1	2689	U
1	1	2690	U
1	1	2707	U
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2728	U
1	1	2732	G
1	1	2733	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2752	C
1	1	2757	A
1	1	2765	A
1	1	2766	A
1	1	2769	U
1	1	2776	A
1	1	2777	G
1	1	2778	A
1	1	2780	G
1	1	2787	C
1	1	2793	C
1	1	2794	C
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2811	G
1	1	2812	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2860	A
1	1	2861	U
1	1	2867	G

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Mol	Chain	Res	Type
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2884	U
1	1	2885	G
1	1	2886	A
1	1	2893	A
1	1	2898	U
1	1	2900	A
1	1	2901	C
2	2	2	A
2	2	3	A
2	2	4	U
2	2	5	U
2	2	6	G
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	39	G
2	2	44	A
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	61	G
2	2	68	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	79	G
2	2	81	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	87	C

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Mol	Chain	Res	Type
2	2	88	U
2	2	89	U
2	2	91	U
2	2	92	U
2	2	94	G
2	2	95	C
2	2	120	A
2	2	121	U
2	2	122	G
2	2	123	U
2	2	127	G
2	2	129	A
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	146	G
2	2	149	A
2	2	154	U
2	2	163	C
2	2	164	G
2	2	169	C
2	2	173	U
2	2	177	G
2	2	180	U
2	2	181	A
2	2	182	A
2	2	183	C
2	2	185	U
2	2	192	A
2	2	195	A
2	2	197	A
2	2	202	G
2	2	203	G
2	2	204	G
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	213	G
2	2	214	C
2	2	223	A

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Mol	Chain	Res	Type
2	2	226	G
2	2	240	G
2	2	244	U
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	281	G
2	2	289	G
2	2	306	A
2	2	316	C
2	2	319	G
2	2	320	A
2	2	328	C
2	2	329	A
2	2	330	C
2	2	332	G
2	2	339	C
2	2	347	G
2	2	348	G
2	2	351	G
2	2	352	C
2	2	353	A
2	2	354	G
2	2	356	A
2	2	365	U
2	2	366	A
2	2	367	U
2	2	372	C
2	2	384	G
2	2	388	G
2	2	390	U
2	2	397	A
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C

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Mol	Chain	Res	Type
2	2	424	G
2	2	428	G
2	2	429	U
2	2	450	G
2	2	456	A
2	2	457	G
2	2	458	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	473	U
2	2	476	U
2	2	477	C
2	2	478	A
2	2	479	U
2	2	481	G
2	2	486	U
2	2	493	A
2	2	495	A
2	2	496	A
2	2	497	G
2	2	509	A
2	2	510	A
2	2	511	C
2	2	515	G
2	2	517	G
2	2	518	C
2	2	519	C
2	2	521	G
2	2	526	C
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	547	A
2	2	555	U
2	2	560	A
2	2	562	U
2	2	564	C
2	2	572	A
2	2	573	A

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Mol	Chain	Res	Type
2	2	576	C
2	2	577	G
2	2	596	A
2	2	607	A
2	2	614	C
2	2	616	G
2	2	618	C
2	2	619	U
2	2	633	G
2	2	640	A
2	2	641	U
2	2	650	G
2	2	653	U
2	2	661	G
2	2	665	A
2	2	673	A
2	2	674	G
2	2	686	U
2	2	695	A
2	2	700	G
2	2	701	U
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	752	G
2	2	753	A
2	2	755	G
2	2	788	U
2	2	793	U
2	2	794	A
2	2	799	G
2	2	802	A
2	2	812	G
2	2	814	A
2	2	815	A
2	2	816	A
2	2	817	C

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Mol	Chain	Res	Type
2	2	818	G
2	2	819	A
2	2	820	U
2	2	821	G
2	2	828	U
2	2	829	G
2	2	842	U
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	849	G
2	2	851	G
2	2	864	A
2	2	871	U
2	2	876	C
2	2	884	U
2	2	900	A
2	2	902	G
2	2	904	U
2	2	914	A
2	2	934	C
2	2	935	A
2	2	939	G
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	969	A
2	2	971	G
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	989	U
2	2	992	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	999	C
2	2	1003	G
2	2	1004	A

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Mol	Chain	Res	Type
2	2	1008	U
2	2	1009	U
2	2	1010	U
2	2	1012	A
2	2	1017	U
2	2	1018	G
2	2	1019	A
2	2	1020	G
2	2	1022	A
2	2	1026	G
2	2	1027	C
2	2	1028	C
2	2	1029	U
2	2	1031	C
2	2	1032	G
2	2	1033	G
2	2	1034	G
2	2	1036	A
2	2	1043	G
2	2	1044	A
2	2	1045	C
2	2	1046	A
2	2	1050	G
2	2	1054	C
2	2	1055	A
2	2	1065	U
2	2	1067	A
2	2	1080	A
2	2	1085	U
2	2	1086	U
2	2	1087	G
2	2	1092	A
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1102	A
2	2	1108	G
2	2	1118	U
2	2	1124	G
2	2	1125	U
2	2	1130	A
2	2	1132	C

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Mol	Chain	Res	Type
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1144	G
2	2	1145	A
2	2	1146	A
2	2	1147	C
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1162	C
2	2	1167	A
2	2	1168	U
2	2	1169	A
2	2	1171	A
2	2	1176	A
2	2	1177	G
2	2	1184	G
2	2	1193	G
2	2	1196	A
2	2	1197	A
2	2	1200	C
2	2	1201	A
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1227	A
2	2	1228	C
2	2	1233	G
2	2	1238	A
2	2	1241	G
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A

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Mol	Chain	Res	Type
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1300	G
2	2	1301	U
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1319	A
2	2	1320	C
2	2	1322	C
2	2	1331	G
2	2	1336	C
2	2	1338	G
2	2	1340	A
2	2	1344	C
2	2	1346	A
2	2	1348	U
2	2	1353	G
2	2	1363	A
2	2	1364	U
2	2	1365	G
2	2	1368	A
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1395	C
2	2	1397	C
2	2	1398	A
2	2	1399	C
2	2	1401	G
2	2	1418	A
2	2	1422	G
2	2	1429	A
2	2	1432	G
2	2	1433	A

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Mol	Chain	Res	Type
2	2	1441	A
2	2	1445	U
2	2	1446	A
2	2	1451	U
2	2	1452	C
2	2	1453	G
2	2	1471	U
2	2	1475	G
2	2	1487	G
2	2	1491	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1500	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1520	C
2	2	1528	U
2	2	1529	G
2	2	1530	G
2	2	1533	C
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	12	C
3	3	13	G
3	3	17	C
3	3	20	G
3	3	33	G
3	3	34	A
3	3	35	C
3	3	36	C
3	3	37	C
3	3	40	U
3	3	42	C
3	3	44	G
3	3	53	A
3	3	54	G
3	3	56	G

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Mol	Chain	Res	Type
3	3	57	A
3	3	58	A
3	3	66	A
3	3	68	C
3	3	74	U
3	3	88	C
3	3	89	U
3	3	90	C
3	3	91	C
3	3	99	A
3	3	109	A
3	3	119	A
52	4	19	U
52	4	21	A
54	5	3	G
54	5	7	U
54	5	8	4SU
54	5	9	G
54	5	12	C
54	5	15	C
54	5	16	C
54	5	17	U
54	5	18	G
54	5	19	G
54	5	20	H2U
54	5	21	A
54	5	22	G
54	5	47	U
54	5	48	C
54	5	49	G
54	5	52	G
54	5	55	PSU
54	5	58	A
54	5	59	A
54	5	68	C
54	5	70	G
54	5	72	A
54	5	76	A

All (21) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
1	1	140	C
1	1	323	C
1	1	329	G
1	1	404	A
1	1	546	U
1	1	613	A
1	1	784	G
1	1	894	U
1	1	1069	A
1	1	1379	U
1	1	1636	U
1	1	2146	C
1	1	2425	A
1	1	2756	U
2	2	210	C
2	2	428	G
2	2	496	A
2	2	516	PSU
2	2	1109	C
2	2	1145	A
54	5	17	U

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

40 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	PSU	1	2457	1	18,21,22	1.19	3 (16%)	21,30,33	2.05	6 (28%)
2	MA6	2	1518	2	19,26,27	1.76	2 (10%)	18,38,41	2.72	3 (16%)
2	4OC	2	1402	2	20,23,24	2.92	8 (40%)	25,32,35	1.31	3 (12%)
2	2MG	2	1516	2	18,26,27	2.63	7 (38%)	16,38,41	1.62	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	4SU	5	8	54	18,21,22	3.68	7 (38%)	25,30,33	2.20	5 (20%)
2	5MC	2	967	2	19,22,23	3.72	8 (42%)	26,32,35	1.25	2 (7%)
55	FME	6	77	55	8,9,10	0.70	0	8,9,11	1.27	1 (12%)
1	2MG	1	2445	1	18,26,27	2.48	6 (33%)	16,38,41	1.54	3 (18%)
1	OMU	1	2552	1	19,22,23	2.81	8 (42%)	25,31,34	2.10	5 (20%)
1	6MZ	1	1618	1	17,25,26	1.83	3 (17%)	15,36,39	2.24	3 (20%)
1	PSU	1	1917	1	18,21,22	1.09	1 (5%)	21,30,33	2.08	4 (19%)
1	G7M	1	2069	1	20,26,27	2.29	6 (30%)	16,39,42	1.39	3 (18%)
2	2MG	2	1207	2	18,26,27	2.50	7 (38%)	16,38,41	2.20	5 (31%)
2	5MC	2	1407	2	19,22,23	3.69	8 (42%)	26,32,35	1.12	2 (7%)
1	3TD	1	1915	1	19,22,23	4.31	5 (26%)	23,32,35	1.98	4 (17%)
1	OMG	1	2251	54,1	19,26,27	2.33	8 (42%)	21,38,41	1.41	4 (19%)
2	2MG	2	966	2	18,26,27	2.60	7 (38%)	16,38,41	1.59	4 (25%)
54	4OC	5	32	54	20,23,24	3.02	8 (40%)	25,32,35	1.00	2 (8%)
1	PSU	1	2580	1	18,21,22	1.13	3 (16%)	21,30,33	2.34	6 (28%)
54	PSU	5	55	54	18,21,22	1.18	1 (5%)	21,30,33	1.64	4 (19%)
42	0TD	q	89	42	8,9,10	1.47	0	6,11,13	3.05	3 (50%)
1	5MU	1	1939	1	19,22,23	4.66	7 (36%)	27,32,35	3.98	10 (37%)
1	PSU	1	2605	1	18,21,22	1.11	2 (11%)	21,30,33	2.16	5 (23%)
1	PSU	1	955	1	18,21,22	1.00	1 (5%)	21,30,33	1.85	4 (19%)
1	2MG	1	1835	1	18,26,27	2.49	7 (38%)	16,38,41	1.51	5 (31%)
2	PSU	2	516	2	18,21,22	1.04	2 (11%)	21,30,33	2.03	4 (19%)
1	5MU	1	747	1	19,22,23	4.70	7 (36%)	27,32,35	4.06	10 (37%)
1	1MG	1	745	1	19,26,27	2.77	5 (26%)	18,39,42	1.65	4 (22%)
54	H2U	5	20	54	18,21,22	3.31	5 (27%)	19,30,33	1.36	3 (15%)
1	PSU	1	1911	1	18,21,22	1.06	1 (5%)	21,30,33	2.19	4 (19%)
1	PSU	1	746	1	18,21,22	1.11	2 (11%)	21,30,33	1.85	5 (23%)
1	PSU	1	2504	1	18,21,22	1.11	1 (5%)	21,30,33	1.97	4 (19%)
2	UR3	2	1498	2	19,22,23	2.39	6 (31%)	26,32,35	1.53	3 (11%)
54	5MU	5	54	54	19,22,23	4.82	7 (36%)	27,32,35	3.43	9 (33%)
1	5MC	1	1962	1	19,22,23	3.56	8 (42%)	26,32,35	1.24	3 (11%)
1	6MZ	1	2030	1	17,25,26	1.76	3 (17%)	15,36,39	2.68	4 (26%)
2	MA6	2	1519	2	19,26,27	1.68	2 (10%)	18,38,41	3.12	3 (16%)
1	OMC	1	2498	1	19,22,23	2.85	7 (36%)	25,31,34	0.89	0
1	2MA	1	2503	1	18,25,26	3.27	6 (33%)	20,37,40	1.60	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G7M	2	527	2	20,26,27	3.86	9 (45%)	16,39,42	1.11	2 (12%)

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	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	1/7/29/30	0/3/3/3
2	4OC	2	1402	2	-	4/9/29/30	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
54	4SU	5	8	54	-	4/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
55	FME	6	77	55	-	2/7/9/11	-
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2552	1	-	1/9/27/28	0/2/2/2
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	0/3/25/26	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	4/7/25/26	0/2/2/2
1	OMG	1	2251	54,1	-	2/5/27/28	0/3/3/3
2	2MG	2	966	2	-	3/5/27/28	0/3/3/3
54	4OC	5	32	54	-	0/9/29/30	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
54	PSU	5	55	54	-	2/7/25/26	0/2/2/2
42	0TD	q	89	42	-	3/7/12/14	-
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	PSU	2	516	2	-	2/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
54	H2U	5	20	54	-	4/7/38/39	0/2/2/2
1	PSU	1	1911	1	-	1/7/25/26	0/2/2/2
1	PSU	1	746	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
54	5MU	5	54	54	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	3/5/27/28	0/3/3/3
2	MA6	2	1519	2	-	3/7/29/30	0/3/3/3
1	OMC	1	2498	1	-	1/9/27/28	0/2/2/2
1	2MA	1	2503	1	-	2/3/25/26	0/3/3/3
2	G7M	2	527	2	-	2/3/25/26	0/3/3/3

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	13.54	1.50	1.35
54	5	54	5MU	C2-N1	11.31	1.56	1.38
54	5	20	H2U	C2-N1	10.61	1.50	1.35
1	1	747	5MU	C2-N1	10.48	1.54	1.38
54	5	54	5MU	C6-N1	10.46	1.55	1.38
1	1	1939	5MU	C2-N1	10.10	1.54	1.38
2	2	527	G7M	C8-N7	10.03	1.51	1.33
1	1	747	5MU	C4-C5	9.92	1.61	1.44
54	5	54	5MU	C4-C5	9.81	1.60	1.44
1	1	747	5MU	C6-N1	9.78	1.54	1.38
1	1	1939	5MU	C6-N1	9.73	1.54	1.38
1	1	1939	5MU	C4-C5	9.64	1.60	1.44
1	1	1915	3TD	C2-N1	9.62	1.49	1.37
2	2	527	G7M	C8-N9	9.31	1.50	1.33
2	2	967	5MC	C6-C5	9.08	1.49	1.34
2	2	1407	5MC	C6-C5	8.75	1.48	1.34
1	1	1939	5MU	C4-N3	-8.33	1.23	1.38
1	1	2503	2MA	C4-N3	8.30	1.48	1.35
1	1	1962	5MC	C6-C5	8.29	1.48	1.34
1	1	747	5MU	C4-N3	-8.20	1.23	1.38
54	5	8	4SU	C2-N1	7.88	1.50	1.38
54	5	8	4SU	C4-N3	7.87	1.45	1.37
54	5	54	5MU	C4-N3	-7.86	1.24	1.38
1	1	745	1MG	C2-N2	7.36	1.47	1.34
1	1	1962	5MC	C4-N3	7.00	1.45	1.34
54	5	32	4OC	C4-N3	6.94	1.44	1.32
2	2	967	5MC	C4-N3	6.83	1.45	1.34
1	1	2503	2MA	C2-N3	6.82	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1516	2MG	C2-N2	6.77	1.47	1.33
2	2	1402	4OC	C4-N3	6.72	1.44	1.32
54	5	20	H2U	C2-N3	6.71	1.49	1.38
2	2	966	2MG	C2-N2	6.58	1.47	1.33
2	2	1407	5MC	C4-N3	6.47	1.44	1.34
1	1	1835	2MG	C2-N2	6.28	1.46	1.33
1	1	2445	2MG	C2-N2	6.27	1.46	1.33
1	1	2552	OMU	C2-N3	6.21	1.48	1.38
1	1	2498	OMC	C6-C5	6.20	1.49	1.35
1	1	745	1MG	C2-N3	6.16	1.43	1.33
1	1	2552	OMU	C2-N1	6.06	1.48	1.38
54	5	32	4OC	C6-C5	6.05	1.49	1.35
2	2	1207	2MG	C2-N2	6.02	1.46	1.33
1	1	1618	6MZ	C6-C5	-6.02	1.35	1.44
1	1	2498	OMC	C2-N3	5.95	1.48	1.36
2	2	967	5MC	C2-N3	5.95	1.48	1.36
2	2	1402	4OC	C2-N3	5.87	1.48	1.36
54	5	8	4SU	C6-C5	5.85	1.48	1.35
54	5	32	4OC	C2-N3	5.81	1.47	1.36
1	1	1962	5MC	C2-N3	5.81	1.47	1.36
1	1	1939	5MU	C6-C5	5.79	1.44	1.34
1	1	2503	2MA	C2-N1	5.78	1.44	1.34
1	1	1915	3TD	C6-N1	5.77	1.45	1.36
2	2	1407	5MC	C5-C4	5.76	1.48	1.44
2	2	1407	5MC	C2-N3	5.74	1.47	1.36
2	2	1518	MA6	C6-C5	-5.68	1.36	1.44
54	5	8	4SU	C2-N3	5.65	1.47	1.38
54	5	8	4SU	C4-S4	-5.63	1.58	1.68
2	2	1498	UR3	C2-N1	5.62	1.46	1.38
1	1	2030	6MZ	C6-C5	-5.58	1.36	1.44
54	5	54	5MU	C6-C5	5.51	1.43	1.34
2	2	1498	UR3	C6-C5	5.50	1.47	1.35
1	1	2498	OMC	C4-N3	5.48	1.45	1.34
2	2	1402	4OC	C6-C5	5.44	1.47	1.35
1	1	2552	OMU	C6-C5	5.38	1.47	1.35
1	1	747	5MU	C6-C5	5.37	1.43	1.34
2	2	527	G7M	C2-N3	5.34	1.46	1.33
2	2	1519	MA6	C6-C5	-5.19	1.36	1.44
1	1	2069	G7M	C4-N3	5.16	1.49	1.37
2	2	966	2MG	C4-N3	5.15	1.49	1.37
2	2	967	5MC	C5-C4	5.08	1.48	1.44
54	5	20	H2U	C4-N3	5.04	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2069	G7M	C2-N3	4.99	1.45	1.33
1	1	2251	OMG	C2-N3	4.95	1.45	1.33
1	1	2445	2MG	C4-N3	4.94	1.49	1.37
2	2	1516	2MG	C4-N3	4.92	1.49	1.37
1	1	1962	5MC	C5-C4	4.86	1.47	1.44
1	1	1835	2MG	C4-N3	4.84	1.48	1.37
1	1	1915	3TD	C2-N3	4.84	1.48	1.38
1	1	745	1MG	C4-N3	4.76	1.48	1.37
2	2	527	G7M	C2-N2	4.74	1.45	1.34
2	2	967	5MC	C4-N4	4.71	1.46	1.34
1	1	1962	5MC	C4-N4	4.70	1.46	1.34
2	2	1407	5MC	C4-N4	4.69	1.46	1.34
1	1	2503	2MA	C6-N1	4.67	1.42	1.33
1	1	2251	OMG	C4-N3	4.56	1.48	1.37
1	1	2251	OMG	C2-N2	4.54	1.44	1.34
2	2	1402	4OC	C2-N1	4.45	1.49	1.40
2	2	1207	2MG	C4-N3	4.44	1.47	1.37
2	2	1498	UR3	C2-N3	4.40	1.47	1.39
2	2	967	5MC	C2-N1	4.35	1.49	1.40
2	2	967	5MC	C6-N1	4.35	1.45	1.38
2	2	1407	5MC	C6-N1	4.29	1.45	1.38
2	2	1407	5MC	C2-N1	4.24	1.49	1.40
1	1	2069	G7M	C2-N2	4.23	1.44	1.34
54	5	32	4OC	C2-N1	4.16	1.48	1.40
2	2	1516	2MG	C2-N1	4.15	1.43	1.36
54	5	55	PSU	C6-C5	4.11	1.39	1.35
2	2	1519	MA6	C6-N6	4.06	1.46	1.37
2	2	966	2MG	C2-N1	4.03	1.43	1.36
1	1	1962	5MC	C6-N1	4.03	1.44	1.38
54	5	32	4OC	C4-N4	3.98	1.44	1.36
2	2	527	G7M	C6-N1	3.95	1.43	1.37
2	2	1518	MA6	C6-N6	3.92	1.46	1.37
2	2	1207	2MG	C2-N1	3.90	1.42	1.36
1	1	1835	2MG	C2-N1	3.83	1.42	1.36
2	2	1402	4OC	C4-N4	3.74	1.43	1.36
2	2	527	G7M	C4-N3	3.63	1.46	1.37
1	1	1962	5MC	C2-N1	3.62	1.47	1.40
54	5	32	4OC	C5-C4	3.57	1.48	1.41
1	1	2552	OMU	C4-N3	3.56	1.44	1.38
1	1	2504	PSU	C6-C5	3.53	1.39	1.35
1	1	2445	2MG	C5-C4	-3.53	1.34	1.43
1	1	2445	2MG	C2-N1	3.52	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2498	OMC	O2-C2	-3.47	1.17	1.23
2	2	1207	2MG	C5-C4	-3.46	1.34	1.43
1	1	2498	OMC	C4-N4	3.45	1.42	1.33
2	2	527	G7M	C2-N1	3.43	1.46	1.37
1	1	745	1MG	C5-C4	-3.42	1.34	1.43
1	1	2498	OMC	C6-N1	3.40	1.46	1.38
2	2	1407	5MC	O2-C2	-3.39	1.17	1.23
1	1	2498	OMC	C2-N1	3.36	1.47	1.40
1	1	1962	5MC	O2-C2	-3.36	1.17	1.23
1	1	2552	OMU	O4-C4	-3.30	1.18	1.24
54	5	8	4SU	C5-C4	3.30	1.46	1.42
1	1	746	PSU	C6-C5	3.29	1.38	1.35
2	2	1516	2MG	C5-C4	-3.29	1.34	1.43
1	1	1835	2MG	C5-C4	-3.23	1.35	1.43
1	1	1915	3TD	C4-N3	3.17	1.47	1.40
2	2	966	2MG	C5-C4	-3.17	1.35	1.43
2	2	967	5MC	O2-C2	-3.15	1.17	1.23
1	1	2552	OMU	O2-C2	-3.14	1.17	1.23
1	1	2251	OMG	C5-C4	-3.12	1.35	1.43
1	1	2457	PSU	C6-C5	3.10	1.38	1.35
1	1	1911	PSU	C6-C5	3.08	1.38	1.35
1	1	2069	G7M	C5-C6	3.06	1.53	1.45
1	1	2605	PSU	C6-C5	3.05	1.38	1.35
2	2	1402	4OC	C5-C4	3.03	1.47	1.41
2	2	1516	2MG	C6-N1	3.02	1.42	1.37
54	5	32	4OC	C6-N1	3.02	1.45	1.38
1	1	2445	2MG	O6-C6	-3.01	1.16	1.23
2	2	1207	2MG	C5-C6	3.01	1.53	1.47
2	2	1207	2MG	C6-N1	3.00	1.42	1.37
1	1	1939	5MU	O2-C2	-2.96	1.17	1.23
1	1	747	5MU	O2-C2	-2.93	1.17	1.23
1	1	1917	PSU	C6-C5	2.92	1.38	1.35
1	1	747	5MU	O4-C4	-2.92	1.18	1.23
2	2	966	2MG	O6-C6	-2.90	1.16	1.23
1	1	1939	5MU	O4-C4	-2.89	1.18	1.23
2	2	1402	4OC	C6-N1	2.89	1.45	1.38
1	1	745	1MG	C2-N1	2.88	1.42	1.37
2	2	1516	2MG	O6-C6	-2.86	1.16	1.23
2	2	1207	2MG	O6-C6	-2.84	1.16	1.23
1	1	955	PSU	C6-C5	2.83	1.38	1.35
1	1	2069	G7M	C6-N1	2.82	1.42	1.37
1	1	2251	OMG	C6-N1	2.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	966	2MG	C6-N1	2.80	1.42	1.37
1	1	2580	PSU	C6-C5	2.79	1.38	1.35
1	1	2030	6MZ	C2-N3	2.78	1.36	1.32
54	5	32	4OC	O2-C2	-2.77	1.18	1.23
1	1	1835	2MG	O6-C6	-2.74	1.17	1.23
2	2	1402	4OC	O2-C2	-2.69	1.18	1.23
54	5	54	5MU	O4-C4	-2.68	1.18	1.23
1	1	1835	2MG	C6-N1	2.67	1.41	1.37
2	2	527	G7M	C5-C6	2.60	1.52	1.45
2	2	1498	UR3	O4-C4	-2.58	1.18	1.23
2	2	1498	UR3	O2-C2	-2.56	1.17	1.22
2	2	516	PSU	C6-C5	2.54	1.38	1.35
2	2	966	2MG	C5-C6	2.52	1.52	1.47
1	1	2503	2MA	C6-N6	-2.52	1.25	1.34
54	5	8	4SU	O2-C2	-2.49	1.18	1.23
1	1	1618	6MZ	C2-N3	2.48	1.35	1.32
1	1	2445	2MG	C6-N1	2.48	1.41	1.37
1	1	1618	6MZ	C6-N1	-2.47	1.30	1.34
1	1	2251	OMG	C2-N1	2.43	1.43	1.37
1	1	1835	2MG	C5-C6	2.43	1.52	1.47
1	1	2069	G7M	O6-C6	-2.42	1.17	1.23
54	5	54	5MU	O2-C2	-2.42	1.18	1.23
2	2	1516	2MG	C5-C6	2.41	1.52	1.47
1	1	2503	2MA	C6-C5	2.40	1.52	1.43
54	5	20	H2U	O4-C4	-2.34	1.18	1.23
1	1	2580	PSU	O4'-C1'	-2.31	1.40	1.43
54	5	20	H2U	O2-C2	-2.26	1.19	1.23
1	1	2251	OMG	O6-C6	-2.25	1.18	1.23
1	1	2552	OMU	C6-N1	2.21	1.43	1.38
2	2	527	G7M	O6-C6	-2.20	1.18	1.23
1	1	2457	PSU	C4-C5	-2.20	1.38	1.44
1	1	2457	PSU	O4'-C1'	-2.19	1.40	1.43
1	1	746	PSU	C4-C5	-2.17	1.38	1.44
1	1	2552	OMU	C5-C4	2.17	1.48	1.43
1	1	2251	OMG	C5-C6	2.16	1.51	1.47
2	2	516	PSU	C4-C5	-2.13	1.38	1.44
1	1	2030	6MZ	C6-N1	-2.12	1.31	1.34
2	2	1498	UR3	C6-N1	2.10	1.43	1.38
1	1	2580	PSU	C4-C5	-2.03	1.38	1.44
1	1	2605	PSU	C4-C5	-2.00	1.38	1.44

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	747	5MU	C5-C4-N3	12.81	126.46	115.32
1	1	1939	5MU	C5-C4-N3	12.31	126.02	115.32
54	5	54	5MU	C5-C4-N3	11.65	125.44	115.32
1	1	747	5MU	C5-C6-N1	-11.40	110.92	123.31
1	1	1939	5MU	C5-C6-N1	-11.26	111.08	123.31
2	2	1519	MA6	N1-C6-N6	-9.56	105.79	116.83
2	2	1518	MA6	N1-C6-N6	-8.18	107.38	116.83
54	5	54	5MU	C5-C6-N1	-8.11	114.51	123.31
2	2	1519	MA6	N3-C2-N1	-7.34	118.70	128.67
54	5	8	4SU	C4-N3-C2	-7.22	120.39	127.31
1	1	2552	OMU	C4-N3-C2	-6.87	118.08	126.61
2	2	1518	MA6	N3-C2-N1	-6.62	119.69	128.67
1	1	2030	6MZ	N3-C2-N1	-6.58	119.74	128.67
1	1	1618	6MZ	N3-C2-N1	-6.15	120.33	128.67
1	1	2580	PSU	N1-C2-N3	6.01	121.51	115.17
1	1	1939	5MU	C4-N3-C2	-5.92	119.58	127.34
1	1	747	5MU	C4-N3-C2	-5.77	119.78	127.34
1	1	1911	PSU	N1-C2-N3	5.76	121.24	115.17
1	1	1915	3TD	C1'-C5-C4	5.66	126.20	117.61
42	q	89	0TD	OD2-CG-CB	5.66	125.36	113.15
1	1	2605	PSU	N1-C2-N3	5.60	121.07	115.17
1	1	1917	PSU	N1-C2-N3	5.47	120.94	115.17
1	1	2457	PSU	N1-C2-N3	5.40	120.86	115.17
1	1	1939	5MU	O4-C4-C5	-5.36	118.79	124.92
1	1	1911	PSU	C4-N3-C2	-5.30	119.07	126.37
2	2	1207	2MG	N1-C2-N2	5.28	121.95	116.56
1	1	747	5MU	O4-C4-C5	-5.25	118.91	124.92
1	1	1939	5MU	N3-C2-N1	5.25	121.72	114.89
54	5	8	4SU	C5-C4-N3	5.24	119.62	114.75
1	1	2605	PSU	C4-N3-C2	-5.22	119.18	126.37
54	5	54	5MU	O4-C4-C5	-5.18	119.00	124.92
1	1	1915	3TD	N1-C2-N3	5.17	119.89	116.13
2	2	516	PSU	C4-N3-C2	-5.14	119.28	126.37
1	1	1917	PSU	C4-N3-C2	-5.08	119.38	126.37
1	1	2030	6MZ	C9-N6-C6	-5.08	118.14	122.85
2	2	516	PSU	N1-C2-N3	5.08	120.52	115.17
1	1	746	PSU	C4-N3-C2	-5.02	119.46	126.37
1	1	2504	PSU	C4-N3-C2	-5.01	119.47	126.37
1	1	2580	PSU	C4-N3-C2	-5.01	119.47	126.37
1	1	955	PSU	C4-N3-C2	-5.00	119.48	126.37
1	1	2504	PSU	N1-C2-N3	4.95	120.39	115.17
2	2	1498	UR3	C4-N3-C2	-4.88	120.65	124.58
2	2	1519	MA6	C2-N1-C6	4.85	121.59	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	C2-N3-C4	4.79	119.33	115.46
54	5	54	5MU	C5M-C5-C4	4.69	123.79	118.78
1	1	1618	6MZ	C9-N6-C6	-4.68	118.51	122.85
1	1	2457	PSU	C4-N3-C2	-4.68	119.93	126.37
1	1	955	PSU	N1-C2-N3	4.64	120.06	115.17
1	1	747	5MU	C5M-C5-C6	-4.64	116.58	122.85
1	1	746	PSU	N1-C2-N3	4.58	120.00	115.17
1	1	2552	OMU	N3-C2-N1	4.56	120.82	114.89
1	1	747	5MU	N3-C2-N1	4.47	120.71	114.89
1	1	1939	5MU	O2-C2-N1	-4.35	117.14	122.80
1	1	2030	6MZ	C1'-N9-C4	-4.33	119.04	126.64
1	1	745	1MG	C5-C6-N1	4.32	120.21	113.96
1	1	2552	OMU	C5-C4-N3	4.21	120.70	114.80
1	1	747	5MU	C5M-C5-C4	4.17	123.23	118.78
54	5	55	PSU	N1-C2-N3	4.16	119.56	115.17
2	2	1518	MA6	C2-N1-C6	4.12	120.88	116.84
54	5	55	PSU	C4-N3-C2	-4.10	120.73	126.37
1	1	1911	PSU	O2-C2-N1	-4.08	118.58	122.79
2	2	967	5MC	C5-C6-N1	-3.99	118.98	123.31
2	2	1402	4OC	O2-C2-N3	-3.83	116.29	122.33
54	5	54	5MU	N3-C2-N1	3.80	119.83	114.89
54	5	54	5MU	C4-N3-C2	-3.76	122.41	127.34
1	1	2580	PSU	O2-C2-N1	-3.75	118.92	122.79
54	5	54	5MU	C5M-C5-C6	-3.73	117.81	122.85
2	2	966	2MG	C5-C6-N1	3.69	121.12	114.07
1	1	2445	2MG	C5-C6-N1	3.63	121.00	114.07
1	1	2580	PSU	C6-N1-C2	-3.61	119.34	122.69
2	2	1207	2MG	C5-C6-N1	3.59	120.92	114.07
2	2	1516	2MG	C5-C6-N1	3.54	120.83	114.07
42	q	89	0TD	OD1-CG-CB	-3.52	115.07	122.44
2	2	1498	UR3	C5-C4-N3	3.51	119.67	115.04
1	1	2030	6MZ	C6-C5-C4	-3.51	113.95	117.68
54	5	8	4SU	N3-C2-N1	3.48	119.42	114.89
1	1	1915	3TD	C4-N3-C2	-3.45	120.96	124.61
1	1	1939	5MU	C5M-C5-C6	-3.31	118.37	122.85
2	2	1207	2MG	C8-N7-C5	3.31	108.18	102.55
1	1	1917	PSU	O2-C2-N1	-3.30	119.39	122.79
54	5	20	H2U	C5-C6-N1	3.27	121.42	111.52
1	1	1962	5MC	C5-C6-N1	-3.26	119.77	123.31
1	1	2251	OMG	C2-N1-C6	-3.23	119.20	125.11
1	1	1917	PSU	C6-N1-C2	-3.20	119.72	122.69
54	5	8	4SU	C5-C4-S4	-3.19	120.66	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1207	2MG	CM2-N2-C2	-3.18	116.82	123.65
1	1	2580	PSU	C6-C5-C4	3.17	120.31	118.17
1	1	745	1MG	C8-N7-C5	3.16	107.93	102.55
1	1	2251	OMG	C5-C6-N1	3.11	120.00	114.07
1	1	2457	PSU	C6-N1-C2	-3.10	119.81	122.69
54	5	20	H2U	N3-C2-N1	3.10	119.77	116.65
1	1	1835	2MG	C8-N7-C5	3.07	107.78	102.55
1	1	1939	5MU	C6-C5-C4	3.05	120.54	118.02
1	1	1835	2MG	C5-C6-N1	3.05	119.89	114.07
54	5	8	4SU	C1'-N1-C2	3.01	123.00	117.59
1	1	2504	PSU	C6-N1-C2	-3.01	119.90	122.69
2	2	966	2MG	C8-N7-C5	2.98	107.63	102.55
1	1	2251	OMG	C8-N7-C5	2.98	107.62	102.55
1	1	2605	PSU	C6-C5-C4	2.98	120.18	118.17
1	1	2504	PSU	O2-C2-N1	-2.95	119.75	122.79
1	1	2069	G7M	C2-N1-C6	-2.94	119.73	125.11
1	1	1911	PSU	C6-N1-C2	-2.93	119.97	122.69
1	1	2552	OMU	O4-C4-C5	-2.93	120.12	125.16
1	1	747	5MU	O4-C4-N3	-2.92	114.63	120.11
1	1	2445	2MG	O6-C6-C5	-2.87	118.62	124.32
2	2	1516	2MG	C8-N7-C5	2.87	107.43	102.55
1	1	2445	2MG	C8-N7-C5	2.83	107.38	102.55
1	1	2503	2MA	N3-C2-N1	-2.81	120.86	125.77
2	2	1207	2MG	N2-C2-N3	-2.80	116.95	120.51
2	2	1498	UR3	C1'-N1-C2	2.77	121.58	117.04
2	2	1516	2MG	O6-C6-C5	-2.77	118.84	124.32
1	1	745	1MG	O6-C6-C5	-2.75	119.66	124.18
1	1	1962	5MC	C1'-N1-C6	-2.74	116.63	121.15
1	1	2457	PSU	C6-C5-C4	2.74	120.02	118.17
2	2	1516	2MG	N1-C2-N2	2.71	119.33	116.56
2	2	1407	5MC	O2-C2-N3	-2.71	118.06	122.33
54	5	20	H2U	C5-C4-N3	2.65	119.51	116.69
2	2	527	G7M	C2-N1-C6	-2.65	120.26	125.11
1	1	747	5MU	C6-C5-C4	2.64	120.19	118.02
1	1	1939	5MU	O4-C4-N3	-2.62	115.19	120.11
1	1	747	5MU	O2-C2-N1	-2.60	119.42	122.80
54	5	54	5MU	C1'-N1-C2	2.59	122.24	117.59
54	5	55	PSU	C6-N1-C2	-2.59	120.29	122.69
1	1	2605	PSU	C6-N1-C2	-2.58	120.30	122.69
1	1	955	PSU	O2-C2-N1	-2.58	120.13	122.79
1	1	2552	OMU	O2-C2-N1	-2.54	119.49	122.80
2	2	967	5MC	O2-C2-N3	-2.54	118.33	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1407	5MC	C5-C6-N1	-2.54	120.56	123.31
2	2	516	PSU	C6-N1-C2	-2.53	120.34	122.69
2	2	966	2MG	O6-C6-C5	-2.53	119.30	124.32
2	2	1402	4OC	O2-C2-N1	2.47	123.74	118.90
2	2	966	2MG	N1-C2-N2	2.44	119.05	116.56
54	5	54	5MU	O4-C4-N3	-2.42	115.56	120.11
1	1	2580	PSU	O4'-C1'-C2'	2.40	108.48	105.15
1	1	1835	2MG	N1-C2-N2	2.38	119.00	116.56
2	2	1402	4OC	C1'-N1-C2	2.37	123.67	118.44
1	1	2069	G7M	N1-C2-N3	-2.35	119.02	123.32
1	1	2605	PSU	O2-C2-N1	-2.35	120.37	122.79
2	2	527	G7M	O6-C6-N1	-2.33	117.85	120.62
1	1	1835	2MG	CM2-N2-C2	-2.33	118.64	123.65
2	2	516	PSU	O3'-C3'-C4'	2.33	117.76	111.08
54	5	32	4OC	O2-C2-N3	-2.28	118.73	122.33
54	5	32	4OC	C6-C5-C4	2.27	119.74	117.00
1	1	2069	G7M	O6-C6-N1	-2.25	117.95	120.62
1	1	745	1MG	CM1-N1-C6	2.24	120.59	117.54
54	5	55	PSU	O2-C2-N1	-2.22	120.50	122.79
1	1	2251	OMG	O6-C6-C5	-2.22	119.93	124.32
1	1	2457	PSU	O2-C2-N1	-2.18	120.53	122.79
1	1	1939	5MU	C5M-C5-C4	2.16	121.09	118.78
1	1	2457	PSU	O4'-C1'-C2'	2.14	108.11	105.15
1	1	955	PSU	C6-N1-C2	-2.12	120.73	122.69
1	1	1835	2MG	O6-C6-C5	-2.09	120.17	124.32
1	1	1962	5MC	C5-C4-N4	-2.08	118.46	121.39
1	1	746	PSU	O2-C2-N1	-2.08	120.64	122.79
55	6	77	FME	O1-CN-N	-2.07	119.96	125.32
1	1	1618	6MZ	C6-C5-C4	-2.06	115.50	117.68
1	1	746	PSU	C6-N1-C2	-2.04	120.80	122.69
1	1	1915	3TD	O4-C4-N3	-2.03	116.64	120.36
42	q	89	0TD	CSB-SB-CB	2.03	106.01	102.36
1	1	746	PSU	O4-C4-C5	-2.03	118.97	124.01

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	q	89	0TD	CA-CB-SB-CSB
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1915	3TD	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	1	1915	3TD	O4'-C1'-C5-C6
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
54	5	20	H2U	O4'-C1'-N1-C2
54	5	20	H2U	O4'-C1'-N1-C6
55	6	77	FME	O1-CN-N-CA
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
54	5	8	4SU	O4'-C1'-N1-C2
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
54	5	8	4SU	C3'-C4'-C5'-O5'
54	5	20	H2U	O4'-C4'-C5'-O5'
54	5	20	H2U	C3'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
54	5	55	PSU	C3'-C4'-C5'-O5'
55	6	77	FME	CA-CB-CG-SD
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
54	5	8	4SU	O4'-C1'-N1-C6
1	1	2503	2MA	C3'-C4'-C5'-O5'
1	1	2251	OMG	O4'-C4'-C5'-O5'
54	5	55	PSU	O4'-C4'-C5'-O5'
42	q	89	0TD	CG-CB-SB-CSB
1	1	1911	PSU	O4'-C4'-C5'-O5'
54	5	8	4SU	O4'-C4'-C5'-O5'
2	2	966	2MG	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	2552	OMU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	1	2251	OMG	C4'-C5'-O5'-P
1	1	1962	5MC	C2'-C1'-N1-C6
42	q	89	0TD	SB-CB-CG-OD2
1	1	2498	OMC	O4'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C2'-O2'-CM2
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	2030	6MZ	C5-C6-N6-C9
2	2	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

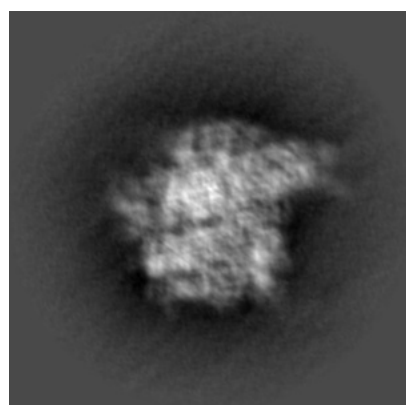
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20188. These allow visual inspection of the internal detail of the map and identification of artifacts.

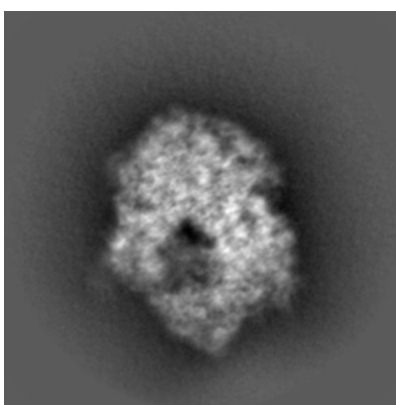
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

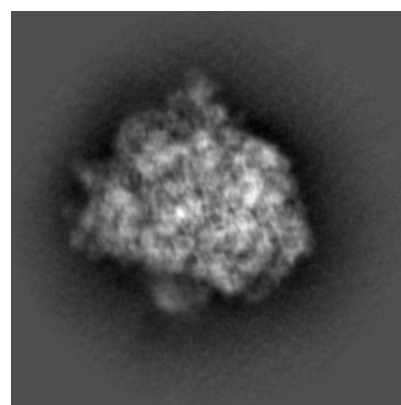
6.1.1 Primary map



X



Y

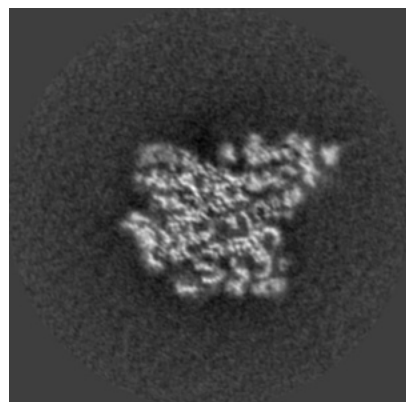


Z

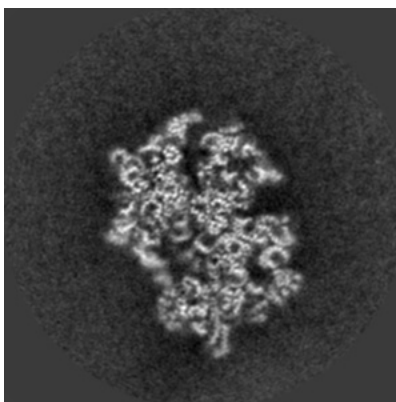
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

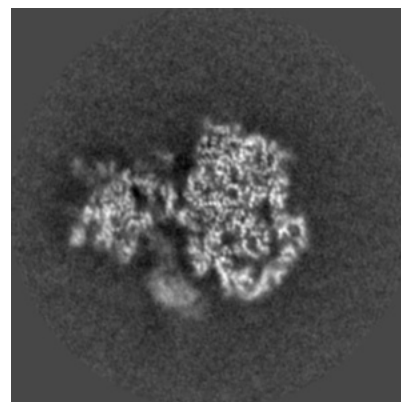
6.2.1 Primary map



X Index: 128



Y Index: 128

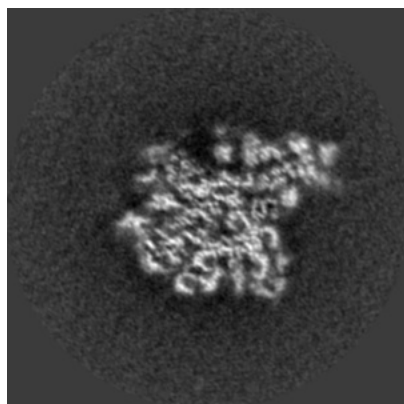


Z Index: 128

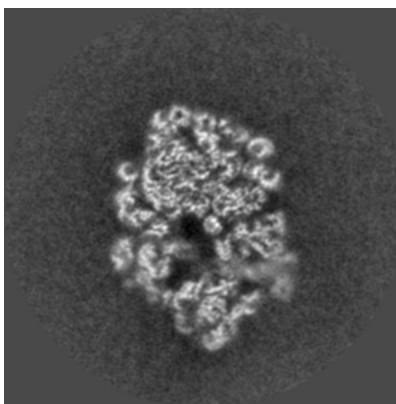
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

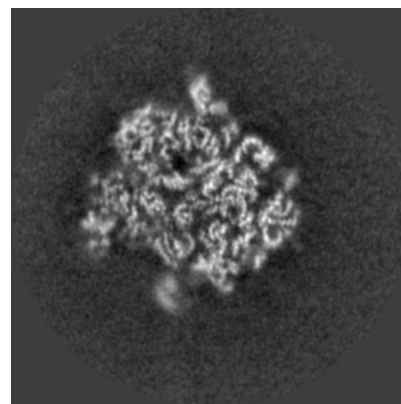
6.3.1 Primary map



X Index: 126



Y Index: 114

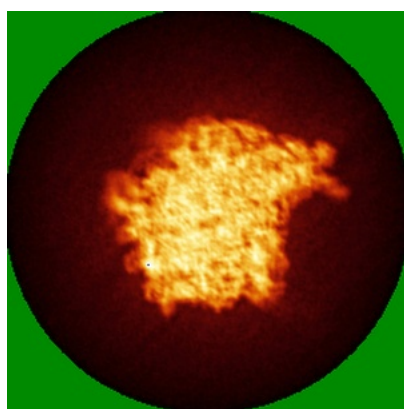


Z Index: 146

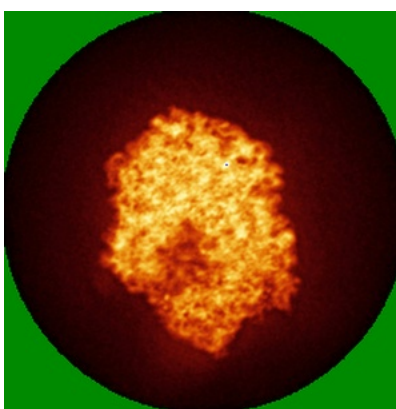
The images above show the largest variance slices of the map in three orthogonal directions.

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

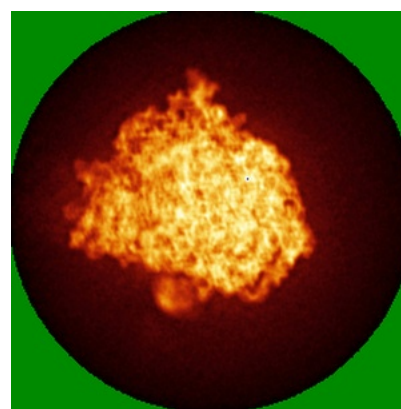
6.4.1 Primary map



X



Y

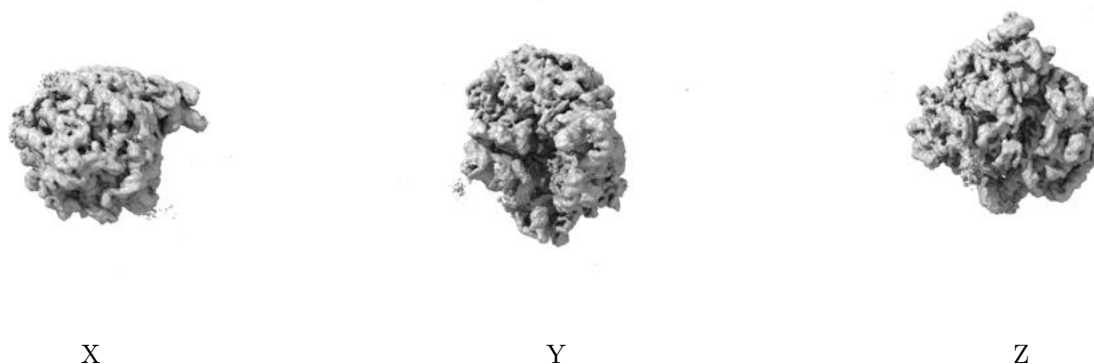


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

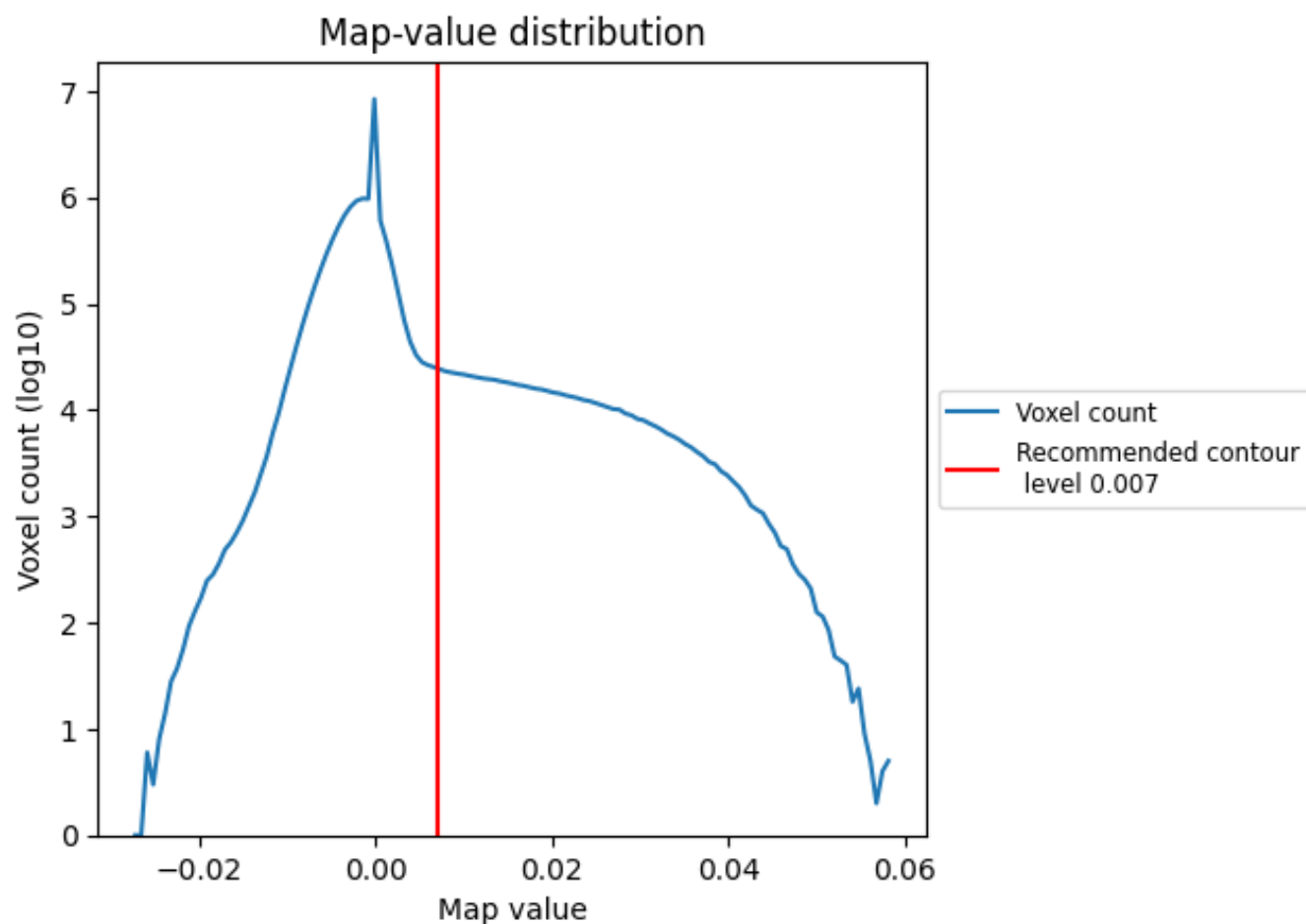
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

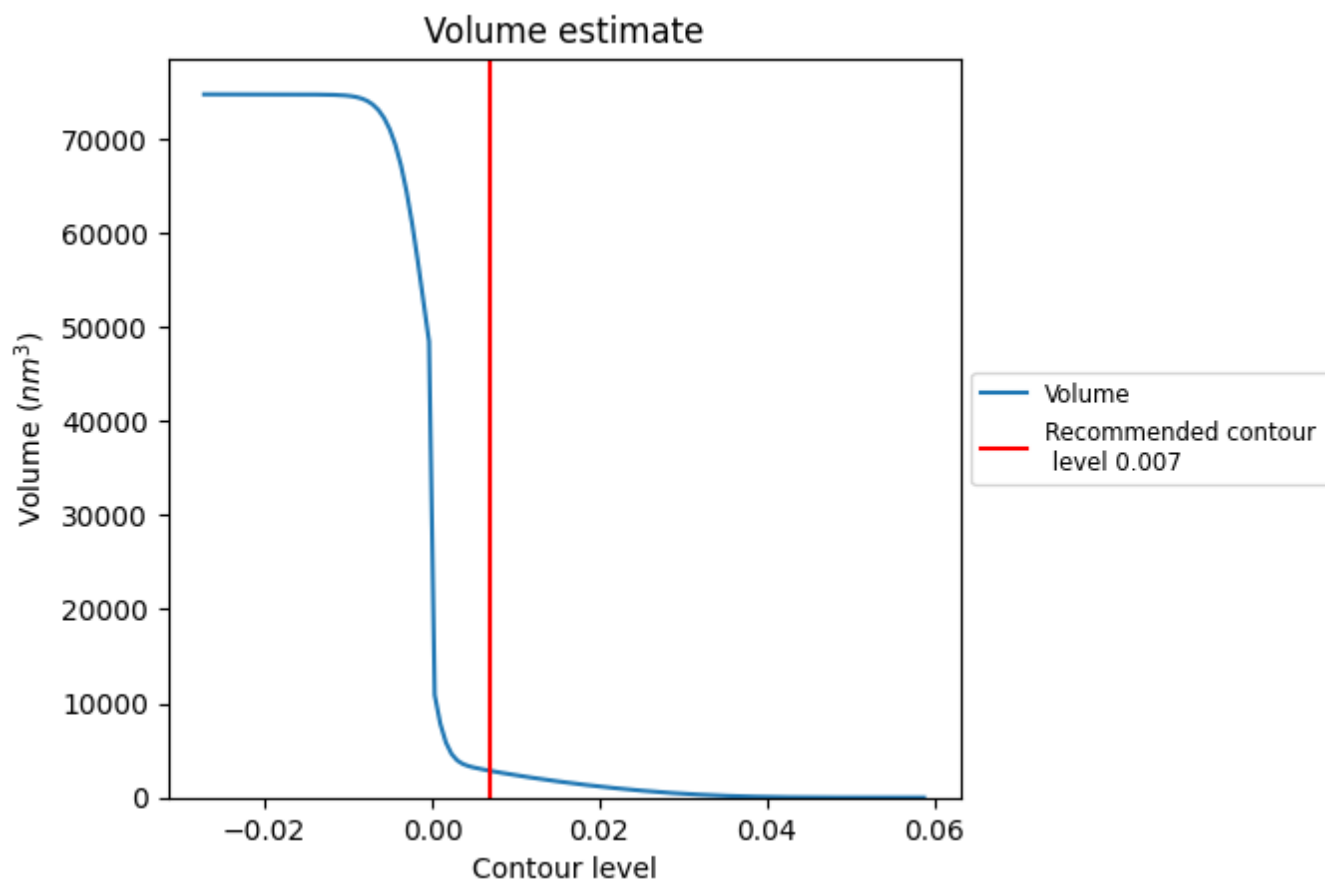
This section contains the results of statistical analysis of the map.

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.

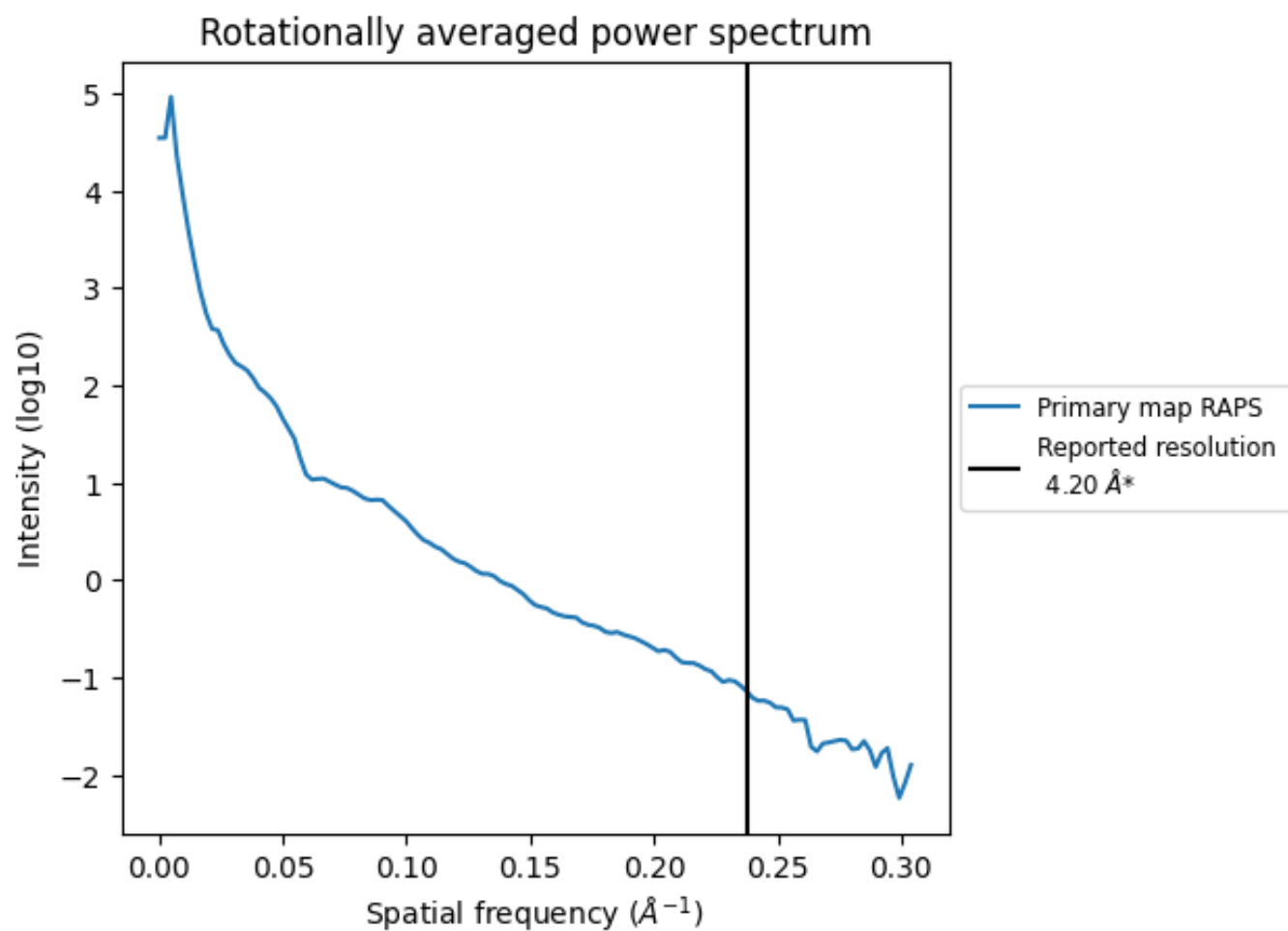
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2833 nm³; this corresponds to an approximate mass of 2559 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 0.238 Å⁻¹

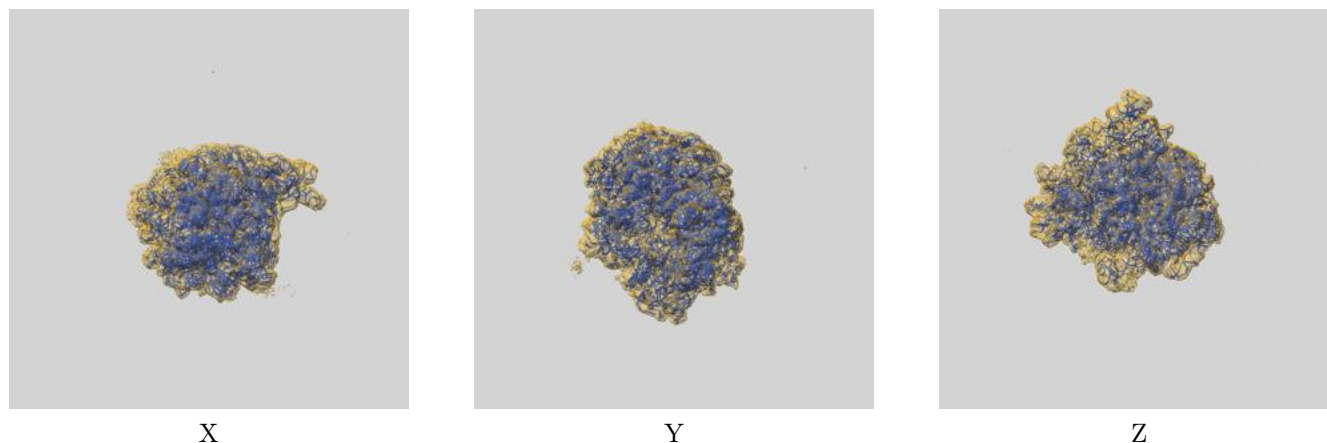
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

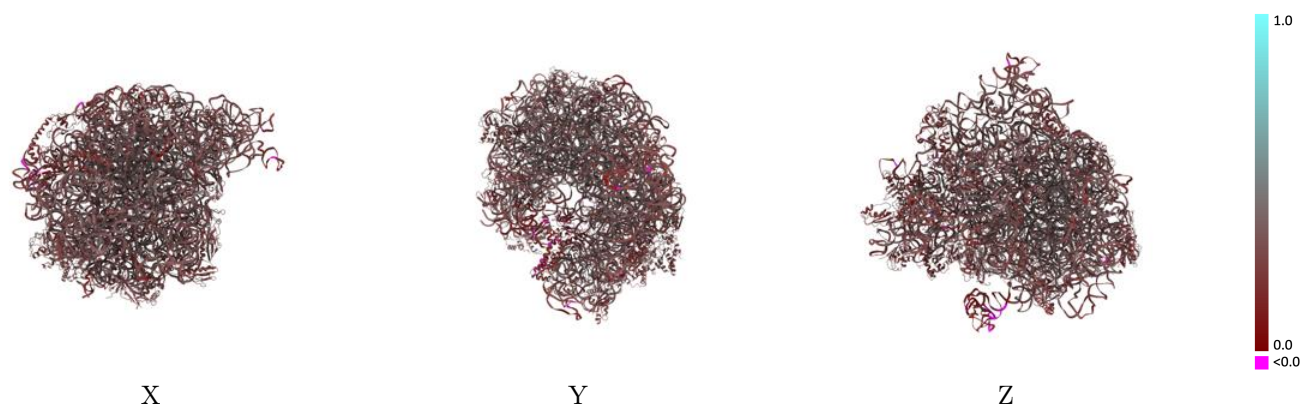
This section contains information regarding the fit between EMDB map EMD-20188 and PDB model 6OST. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



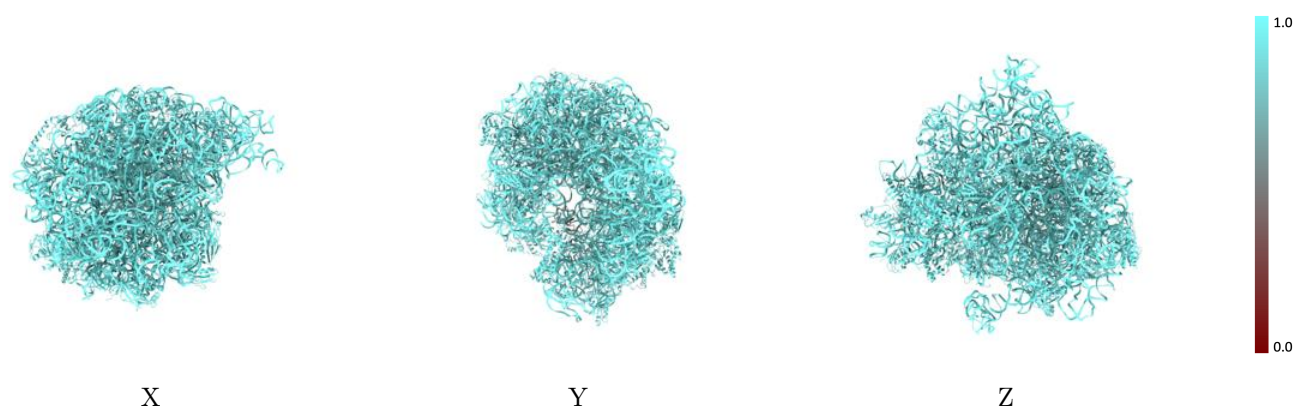
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



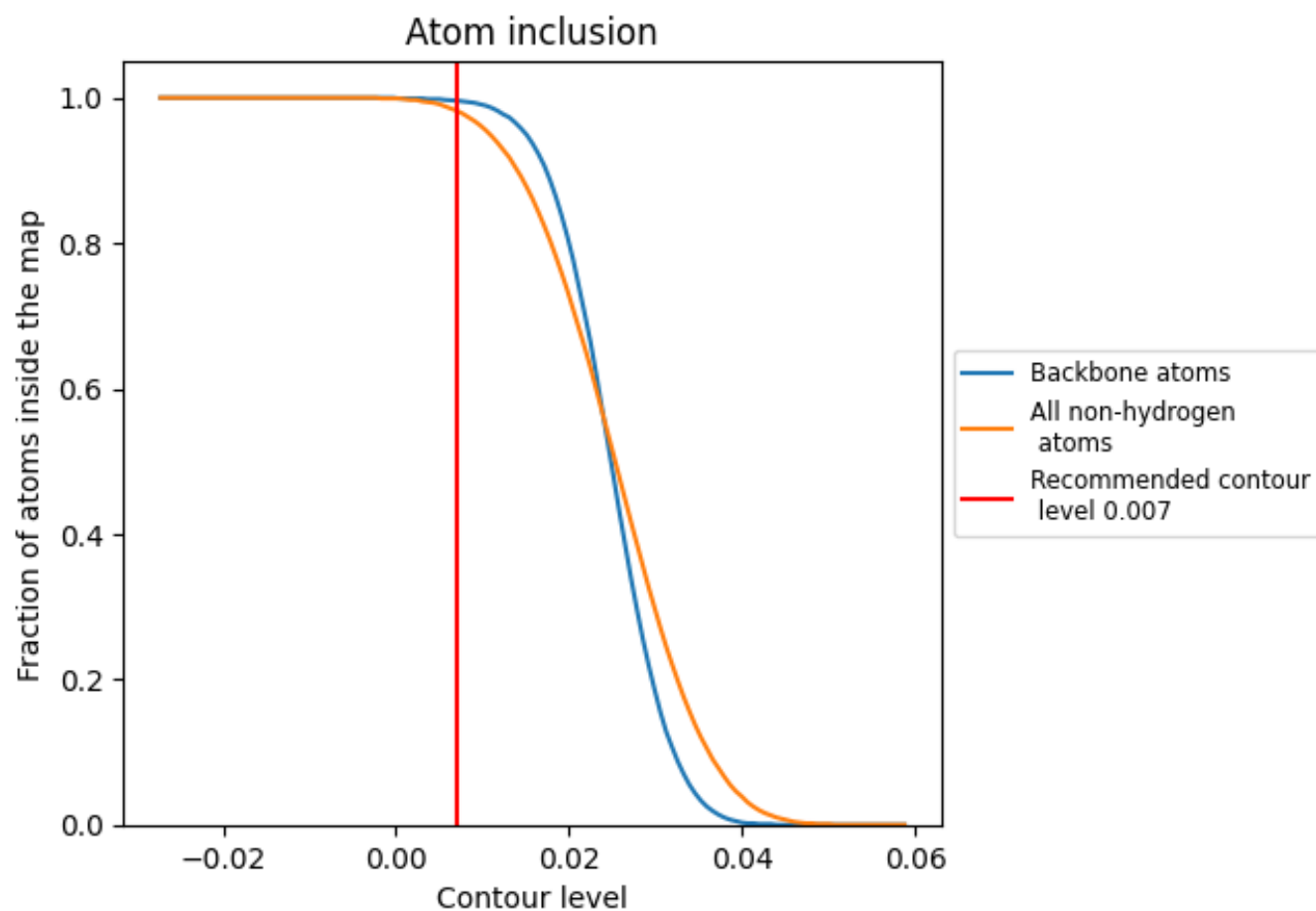
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9820	 0.3180
1	 0.9990	 0.3350
2	 0.9990	 0.3270
3	 1.0000	 0.3160
4	 0.9950	 0.3570
5	 0.9370	 0.2620
6	 0.7190	 0.1580
7	 0.8320	 0.1740
B	 0.9410	 0.3420
C	 0.9580	 0.3320
D	 0.9670	 0.3170
E	 0.9590	 0.2570
F	 0.9750	 0.2860
G	 0.9280	 0.2500
J	 0.9580	 0.3140
K	 0.9350	 0.3410
L	 0.9820	 0.3300
M	 0.9660	 0.3260
N	 0.9870	 0.3080
O	 0.9800	 0.2910
P	 0.9640	 0.3360
Q	 0.9650	 0.2790
R	 0.9670	 0.3250
S	 0.9450	 0.3330
T	 0.9510	 0.3130
U	 0.9870	 0.2940
V	 0.9850	 0.3050
W	 0.9630	 0.3140
X	 0.9480	 0.2990
Y	 0.9780	 0.2440
Z	 0.9630	 0.3160
b	 0.9720	 0.3160
c	 0.9640	 0.3100
d	 0.9520	 0.3280
e	 0.9310	 0.3200



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Chain	Atom inclusion	Q-score
f	 0.9760	 0.3020
g	 0.9350	 0.2730
h	 0.9250	 0.2980
i	 0.9690	 0.2670
j	 0.9510	 0.3080
k	 0.9300	 0.2770
l	 0.9440	 0.2730
m	 0.9570	 0.3140
n	 0.9770	 0.2750
o	 0.9390	 0.2790
p	 0.9310	 0.3070
q	 0.8960	 0.3160
r	 0.9370	 0.2600
s	 0.9630	 0.2830
t	 0.9520	 0.2850
u	 0.9840	 0.3230
v	 0.9640	 0.2900
w	 0.9500	 0.2820
x	 0.9610	 0.2750
y	 0.9600	 0.2660
z	 0.8770	 0.2590