



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 08:27 pm GMT

PDB ID : 8CD1
EMDB ID : EMD-16566
Title : 70S-PHIKZ014
Authors : Gerovac, M.; Vogel, J.
Deposited on : 2023-01-29
Resolution : 3.00 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.dev113
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) : 2.39

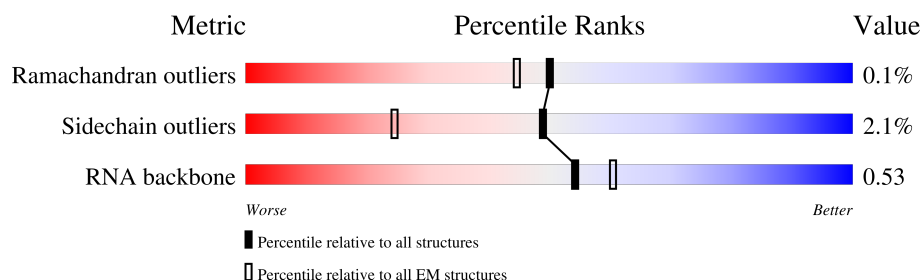
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	2	60	
2	4	44	
3	5	64	
4	6	38	
5	A	2888	
6	B	120	
7	C	273	
8	D	211	

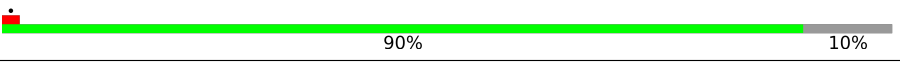
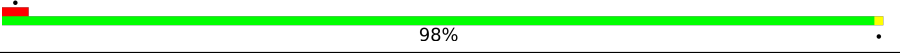
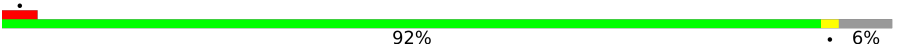

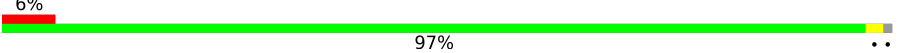
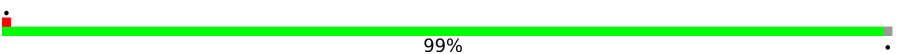

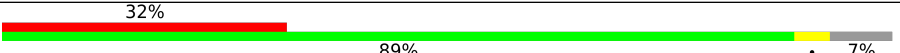
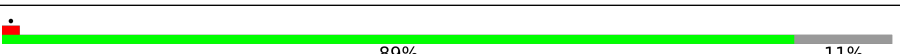
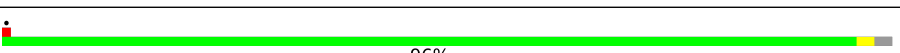
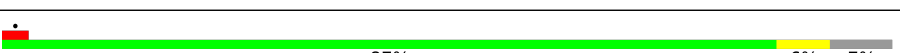
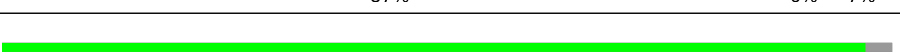
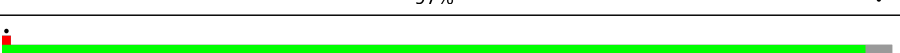
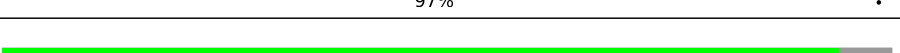
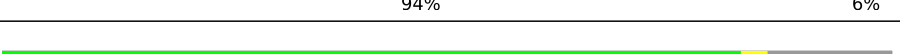

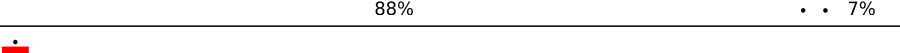
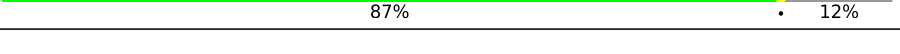
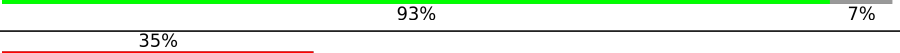
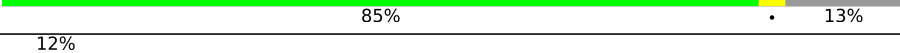
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	Dt	76	
10	E	200	
11	F	179	
12	G	177	
13	H	148	
14	J	142	
15	K	122	
16	L	144	
17	Le	71	
18	M	137	
19	N	129	
20	O	116	
21	P	116	
22	Q	118	
23	R	103	
24	S	110	
25	T	99	
26	U	104	
27	V	204	
28	W	85	
29	X	78	
30	Y	63	
31	Z	58	
32	a	1526	
33	b	246	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	228	
35	d	206	
36	e	166	
37	f	139	
38	g	156	
39	h	130	
40	i	130	
41	j	103	
42	k	129	
43	l	123	
44	m	118	
45	n	101	
46	o	89	
47	p	83	
48	q	88	
49	r	76	
50	s	91	
51	t	91	
52	u	71	
53	v	370	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 144789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	53	Total	C	N	O	S	0	0
			423	254	90	78	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	44	Total	C	N	O	S	1	0
			376	228	91	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	38	Total	C	N	O	S	0	0
			303	184	69	46	4		

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2883	Total	C	N	O	P	0	0
			61859	27600	11347	20030	2882		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	120	Total	C	N	O	P	0	0
			2555	1141	455	839	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	271	Total	C	N	O	S	0	0
			2048	1258	422	362	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	207	Total	C	N	O	S	0	0
			1549	960	297	287	5		

- Molecule 9 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Dt	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	199	Total	C	N	O	S	0	0
			1509	948	281	278	2		

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	174	Total	C	N	O	S	0	0
			1288	811	228	246	3		

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	173	Total	C	N	O	S	0	0
			1294	815	238	239	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	H	78	Total	C	N	O	0	0
			577	363	104	110		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	141	Total	C	N	O	S	0	0
			1122	713	205	201	3		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	120	Total	C	N	O	S	0	0
			922	576	178	162	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	143	Total	C	N	O	S	0	0
			1055	648	213	192	2		

- Molecule 17 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Le	68	Total	C	N	O	S	0	0
			531	334	95	96	6		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	135	Total	C	N	O	S	0	0
			1069	679	209	178	3		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	118	Total	C	N	O	S	0	0
			945	590	190	160	5		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	113	Total	C	N	O	S	0	0
			891	563	168	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	117	Total	C	N	O		0	0
			936	592	196	148			

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	102	Total	C	N	O	S	0	0
			801	509	154	136	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	109	Total	C	N	O	S	0	0
			825	510	160	152	3		

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	92	Total	C	N	O		0	0
			701	449	124	128			

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	103	Total	C	N	O	S	0	0
			800	503	152	143	2		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total	C	N	O	S	0	0
			1396	887	254	253	2		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	76	Total	C	N	O	0	0
			575	364	111	100		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	X	77	Total	C	N	O	S	0
			626	389	134	101	2	0

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	59	Total	C	N	O	S	0
			473	291	94	87	1	0

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	57	Total	C	N	O	S	0
			445	277	87	79	2	0

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	a	1526	Total	C	N	O	P	0
			32744	14606	6011	10602	1525	0

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	b	234	Total	C	N	O	S	0
			1821	1145	329	337	10	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	205	Total	C	N	O	S	0
			1627	1028	307	287	5	0

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1603	991	311	296	5		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	156	Total	C	N	O	S	0	0
			1145	720	209	210	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	105	Total	C	N	O	S	0	0
			853	531	158	159	5		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	154	Total	C	N	O	S	0	0
			1190	747	227	211	5		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1010	625	203	181	1		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	96	Total	C	N	O	S	0	0
			765	479	143	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	115	Total	C	N	O	S	0	0
			838	517	163	156	2		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	121	Total	C	N	O	S	0	0
			949	582	196	167	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	110	Total	C	N	O	S	0	0
			859	524	174	157	4		

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	98	Total	C	N	O	S	0	0
			777	479	163	132	3		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	86	Total	C	N	O	S	0	0
			686	425	134	126	1		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	p	78	Total	C	N	O	0	0
			610	381	121	108		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	76	Total	C	N	O	S	0	0
			619	387	120	110	2		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	71	Total	C	N	O	S	0	0
			566	361	107	97	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	80	Total	C	N	O	S	0	0
			635	405	121	106	3		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	85	Total	C	N	O	S	0	0
			654	404	135	113	2		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	62	Total	C	N	O	S	0	0
			519	320	112	86	1		

- Molecule 53 is a protein called PHIKZ014.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	271	Total	C	N	O	S	0	0
			2262	1436	410	409	7		

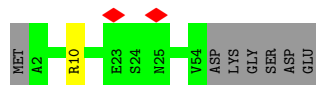
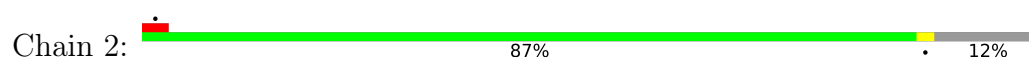
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	150	Total	Mg	0
			150	150	
54	C	1	Total	Mg	0
			1	1	
54	D	1	Total	Mg	0
			1	1	
54	P	1	Total	Mg	0
			1	1	
54	U	1	Total	Mg	0
			1	1	
54	a	17	Total	Mg	0
			17	17	

3 Residue-property plots [i](#)

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

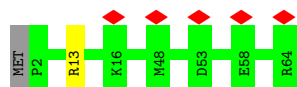
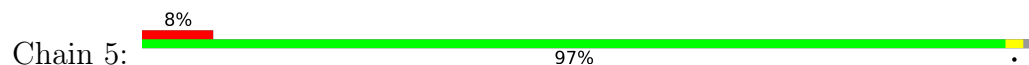
- Molecule 1: 50S ribosomal protein L32



- Molecule 2: 50S ribosomal protein L34



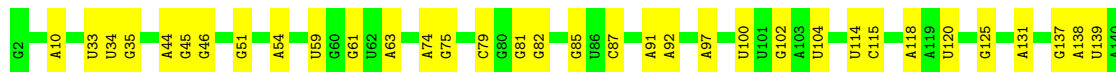
- Molecule 3: 50S ribosomal protein L35



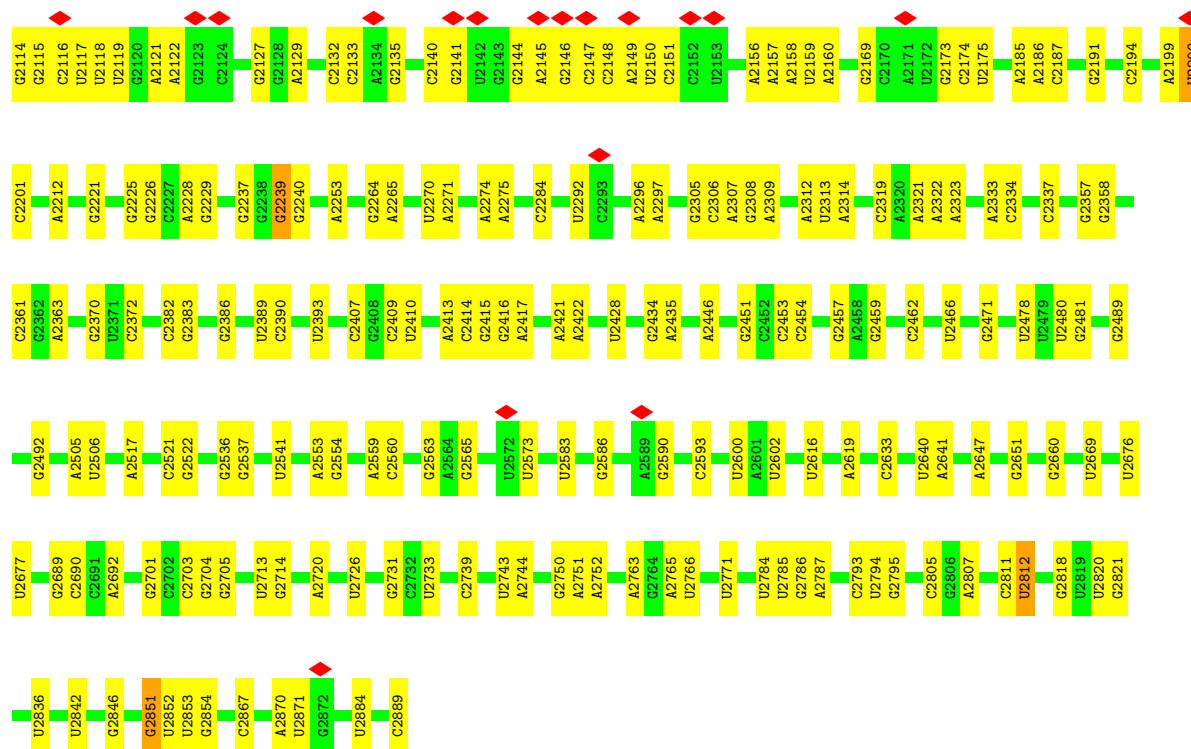
- Molecule 4: 50S ribosomal protein L36



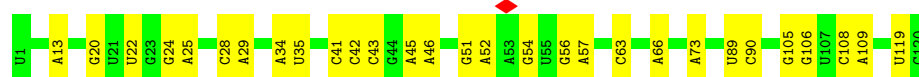
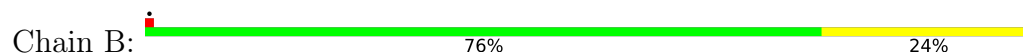
- Molecule 5: 23S rRNA



C1984	G1844	G1709	G1558	G1243	G1100	C972	C841	G659	A519	A390	A265	A141
C1993	G1850	A1710	A1559	C1244	A1101	A973	U842	A660	A520	A381	G266	C142
A2008	U1851	A1711	A1560	A1249	G1102	A980	G843	G671	G521	U385	C267	U144
U2009	A1852	A1714	U1573	G1253	G1114	A986	G845	G672	A523	U386	A145	G146
C2010	A1853	U1715	U1574	G1257	A1117	A999	G847	C673	A534	G387	U271	G147
U2015	C1857	U1716	C1575	A1266	G1118	U1002	G848	U676	C535	U390	A273	U148
G2016	C1861	U1717	A1576	G1267	A1119	U1003	A850	G687	U536	G391	U281	A149
A2017	U1873	C1721	A1580	G1268	A1120	U1010	A855	A708	U537	A395	U285	A160
A2018	C1874	U1724	A1598	G1269	A1121	G1012	U866	G716	U538	U396	U289	A161
G2019	G1875	U1731	A1600	A1261	C1125	U1013	U870	A720	U539	G397	A294	C163
A2020	U1876	U1440	C1575	A1262	A1133	G1016	G877	G747	U540	G398	A299	A165
C2023	U1877	U1441	A1576	U1263	A1146	U1017	C878	A754	C550	G400	C299	U166
U2028	U1735	G1442	G1603	C1276	A1147	A1036	C879	G755	A553	A403	A305	C172
A2029	A1741	U1445	U1606	G1283	G1148	U1037	A880	G743	U557	A406	A314	A173
U2030	A1742	G1446	C1607	A1287	C1149	U1049	U876	G765	U558	U407	U315	A181
A2039	U1745	C1448	A1608	A1288	G1154	G1031	C878	G766	A564	C408	A316	G194
C2042	U1749	C1449	G1609	U1300	G1162	U1036	C879	G768	A565	A414	G317	A195
G2043	G1750	U1454	U1614	C1301	U1163	A1037	A889	U769	A576	U428	U321	A196
A2047	G1751	G1469	A1627	G1311	A1164	G1048	A889	A772	A576	A431	G322	A199
A2049	G1756	C1474	C1628	U1316	A1165	G1049	U883	G774	A586	A444	G323	U202
U2055	U1760	C1474	C1629	U1321	G1166	U1050	U884	G775	A593	A445	A324	G205
G2056	C1761	U1480	G1634	G1321	U1167	U1051	A885	G783	A599	C600	G337	G215
C2060	A1771	A1481	C1636	U1339	A1169	G1063	A889	G784	A599	C601	G338	A216
U2063	A1772	U1484	U1638	C1349	C1170	C1064	A889	A792	A599	U603	A351	G220
A2064	A1773	A1496	G1639	U1352	G1193	C1065	A889	A793	A599	A604	A351	A222
U2067	A1778	G1497	U1639	A1352	G1199	A1067	A889	G795	A599	A604	G342	A227
U2068	C1787	G1508	A1654	A1353	G1214	C1068	A889	C802	A599	A604	U347	C228
G2080	A1788	A1509	A1654	A1354	U1218	G1068	A889	C802	A599	A604	U348	C229
G2081	A1795	U1510	G1664	A1355	G1223	A1076	A889	C802	A599	A604	U349	G230
A2082	A1796	G1511	G1672	A1356	G1224	A1077	A889	C802	A599	A604	G350	A233
C2083	A1797	A1512	C1673	U1366	G1225	A1078	A889	C802	A599	A604	A351	U240
U2094	G1798	G1516	U1673	G1367	G1226	A1079	A889	C802	A599	A604	A351	A241
U2095	C1803	U1522	U1683	A1370	A1228	A1080	A889	C802	A599	A604	A351	G242
U2096	A1816	U	C1684	A1371	A1229	A1081	A889	C802	A599	A604	A351	U243
G2097	C1817	U	G1685	A1372	G1230	G1082	A889	C802	A599	A604	A351	A244
U2098	G1818	U	G1686	A1373	A1231	G1083	A889	C802	A599	A604	A351	A244
G2099	G1819	A1526	G1687	U1378	G1232	U1084	A889	C802	A599	A604	A351	A244
U2100	C1819	G1527	G1688	A1379	U1085	U1085	A889	C802	A599	A604	A351	A244
A2101	C1820	A1528	A1690	A1380	U1086	A1086	A889	C802	A599	A604	A351	A244
G2102	U1820	U1537	C1698	U1381	A1234	A1086	A889	C802	A599	A604	A351	A244
G2103	A1834	U1537	C1698	A1382	A1235	U1087	A889	C802	A599	A604	A351	A244
U1978	U1837	G1542	A1704	A1390	C1238	U1088	A889	C802	A599	A604	A351	A244
G1979	U1838	A1556	G1705	A1390	G1239	A1088	A889	C802	A599	A604	A351	A244
U1982	C1983	A1557	U1708	U1402	A1240	A1097	A889	C802	A599	A604	A351	A244



• Molecule 6: 5S rRNA



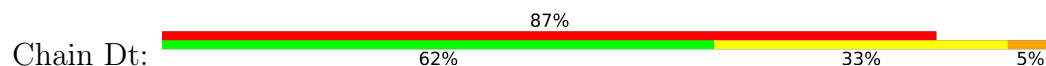
• Molecule 7: 50S ribosomal protein L2

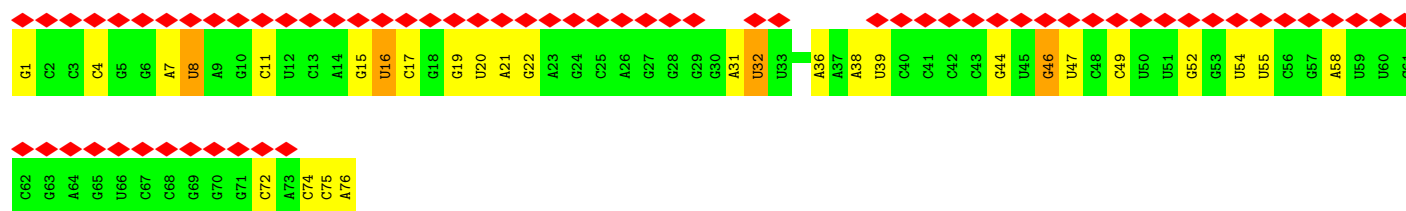


• Molecule 8: 50S ribosomal protein L3



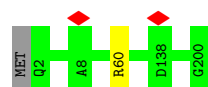
• Molecule 9: tRNA





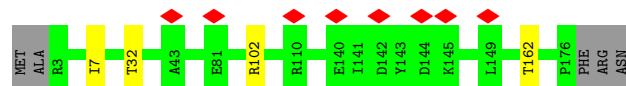
- Molecule 10: 50S ribosomal protein L4

Chain E: 99%



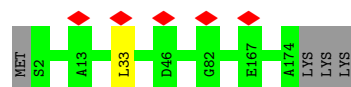
- Molecule 11: 50S ribosomal protein L5

Chain F: 95%



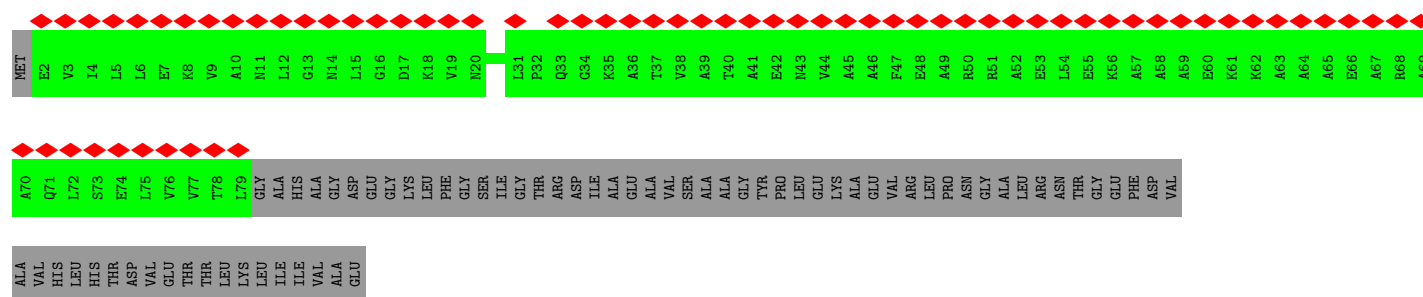
- Molecule 12: 50S ribosomal protein L6

Chain G: 97%



- Molecule 13: 50S ribosomal protein L9

Chain H: 45% 53% 47%



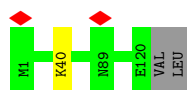
- Molecule 14: 50S ribosomal protein L13

Chain J: 96%



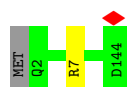
- Molecule 15: 50S ribosomal protein L14

Chain K:  98%



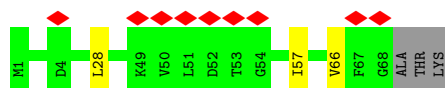
- Molecule 16: 50S ribosomal protein L15

Chain L:  99%



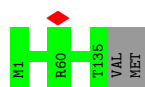
- Molecule 17: 50S ribosomal protein L31

Chain Le:  13% 92%




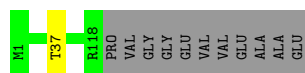
- Molecule 18: 50S ribosomal protein L16

Chain M:  99%



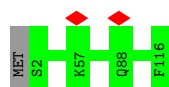
- Molecule 19: 50S ribosomal protein L17

Chain N:  91% 9%



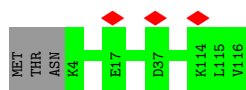
- Molecule 20: 50S ribosomal protein L18

Chain O:  99%



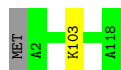
- Molecule 21: 50S ribosomal protein L19

Chain P:  97%



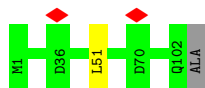
- Molecule 22: 50S ribosomal protein L20

Chain Q: 98%



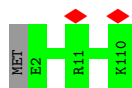
- Molecule 23: 50S ribosomal protein L21

Chain R: 98%



- Molecule 24: Large ribosomal subunit protein uL22

Chain S: 99%



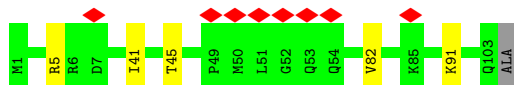
- Molecule 25: 50S ribosomal protein L23

Chain T: 89%



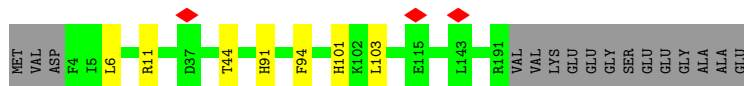
- Molecule 26: 50S ribosomal protein L24

Chain U: 8% 94% 5%




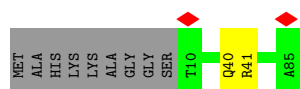
- Molecule 27: 50S ribosomal protein L25

Chain V: 89% 8%



- Molecule 28: 50S ribosomal protein L27

Chain W:  87% 11%




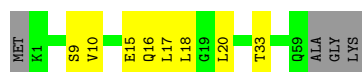
- Molecule 29: 50S ribosomal protein L28

Chain X:  97%



- Molecule 30: 50S ribosomal protein L29

Chain Y:  81% 13% 6%




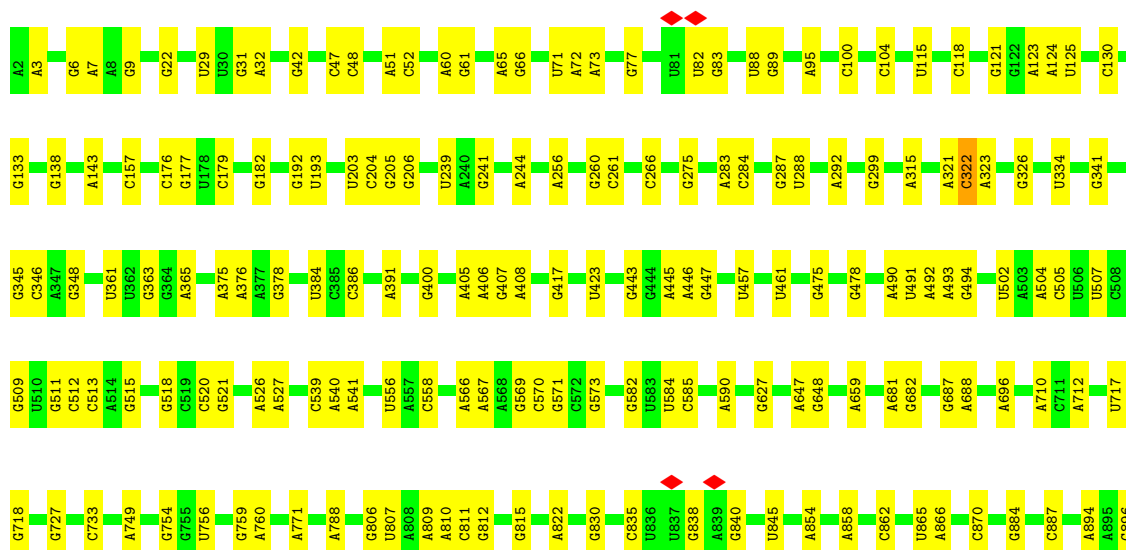
- Molecule 31: 50S ribosomal protein L30

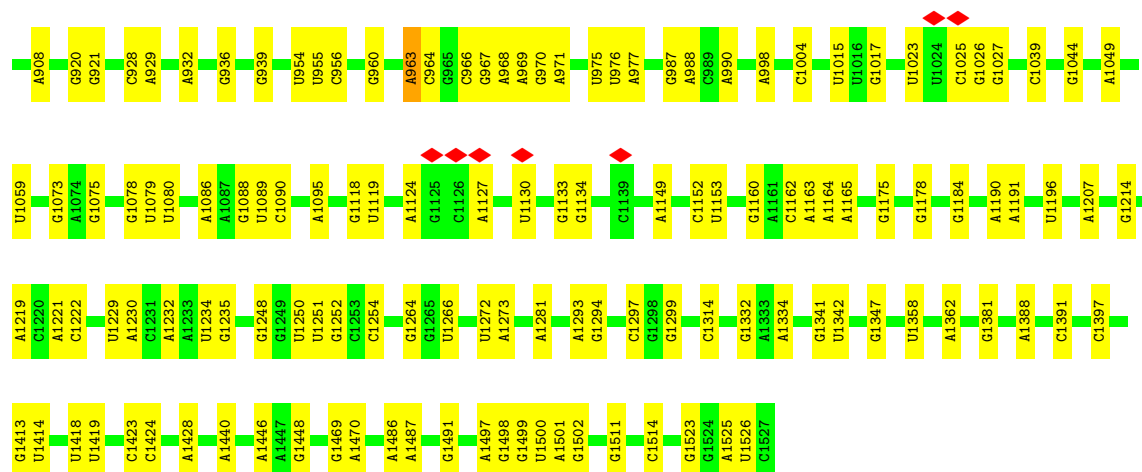
Chain Z:  98%



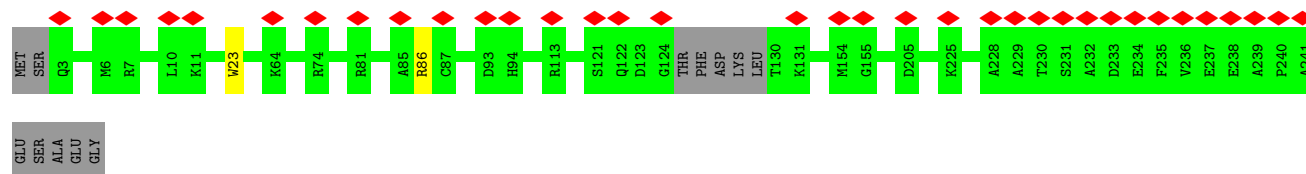
- Molecule 32: 16S rRNA

Chain a:  80% 20%

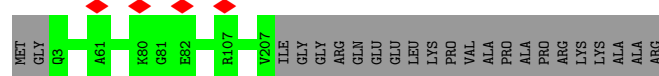
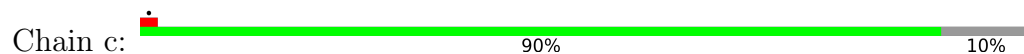




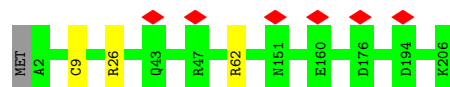
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

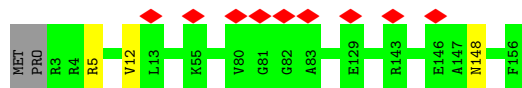


• Molecule 37: 30S ribosomal protein S6

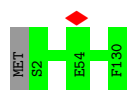




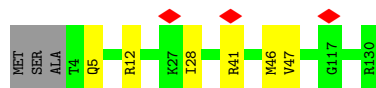
- Molecule 38: 30S ribosomal protein S7



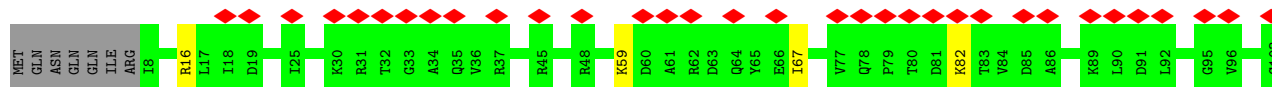
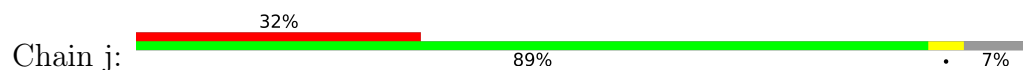
- Molecule 39: 30S ribosomal protein S8



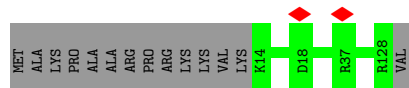
- Molecule 40: 30S ribosomal protein S9



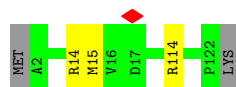
- Molecule 41: 30S ribosomal protein S10



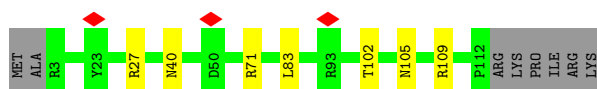
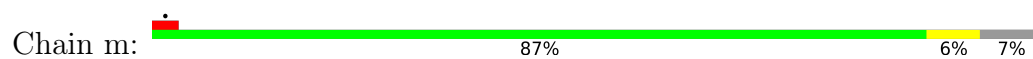
- Molecule 42: 30S ribosomal protein S11



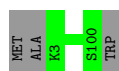
- Molecule 43: 30S ribosomal protein S12



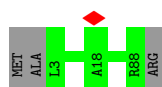
- Molecule 44: 30S ribosomal protein S13



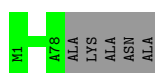
- Molecule 45: 30S ribosomal protein S14



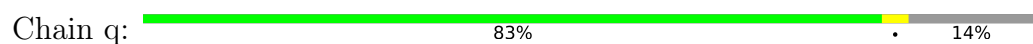
- Molecule 46: 30S ribosomal protein S15



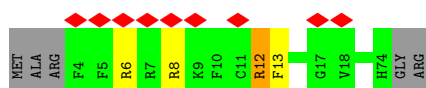
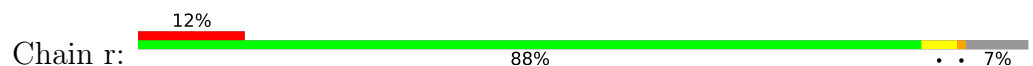
- Molecule 47: 30S ribosomal protein S16



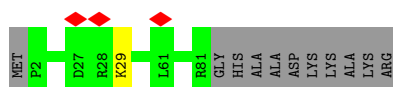
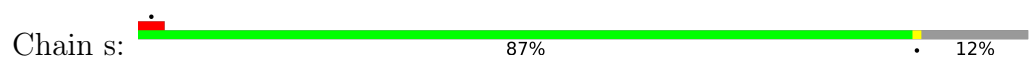
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19




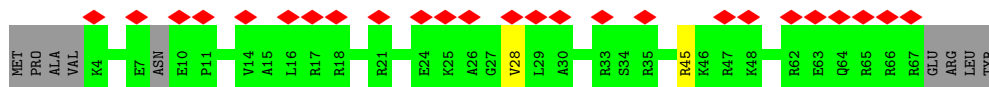
- Molecule 51: 30S ribosomal protein S20

Chain t:  93% 7%



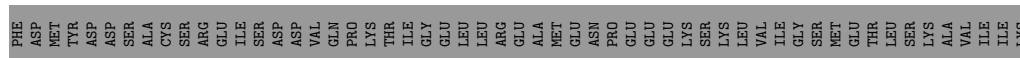
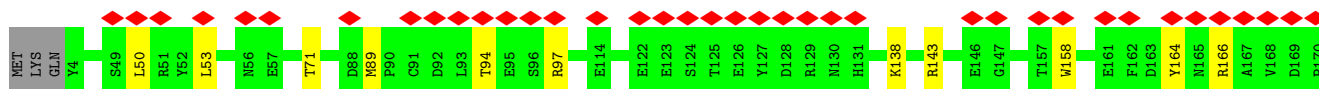
- Molecule 52: 30S ribosomal protein S21

Chain u:  35% 85% 13%



- Molecule 53: PHIKZ014

Chain v:  12% 69% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169672	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 ($e^-/\text{\AA}^2$)	88.28	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	26.120	Depositor
Minimum map value	-7.773	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.894	Depositor
Recommended contour level	3.46	Depositor
Map size (Å)	544.512, 544.512, 544.512	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	0.24	0/429	0.62	0/572
2	4	0.25	0/379	0.77	0/496
3	5	0.24	0/511	0.66	0/668
4	6	0.26	0/304	0.70	0/399
5	A	0.25	4/69275 (0.0%)	0.84	62/108063 (0.1%)
6	B	0.24	0/2855	0.85	3/4447 (0.1%)
7	C	0.26	0/2084	0.64	0/2800
8	D	0.26	0/1572	0.61	0/2118
9	Dt	0.36	1/1813 (0.1%)	0.99	12/2823 (0.4%)
10	E	0.25	0/1529	0.56	0/2060
11	F	0.27	0/1304	0.58	0/1766
12	G	0.26	0/1311	0.58	0/1767
13	H	0.26	0/580	0.52	0/781
14	J	0.26	0/1148	0.56	0/1549
15	K	0.26	0/931	0.65	0/1247
16	L	0.26	0/1067	0.63	0/1422
17	Le	0.28	0/542	0.57	0/728
18	M	0.26	0/1089	0.62	0/1456
19	N	0.25	0/960	0.63	0/1282
20	O	0.25	0/888	0.63	0/1183
21	P	0.25	0/900	0.61	0/1203
22	Q	0.25	0/946	0.64	0/1257
23	R	0.26	0/814	0.60	0/1091
24	S	0.25	0/829	0.59	0/1104
25	T	0.26	0/710	0.52	0/953
26	U	0.27	0/808	0.58	0/1079
27	V	0.25	0/1419	0.56	0/1925
28	W	0.27	0/583	0.64	0/774
29	X	0.24	0/637	0.68	0/849
30	Y	0.34	0/474	0.60	0/632
31	Z	0.24	0/449	0.61	0/602
32	a	0.23	0/36667	0.81	12/57202 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.25	0/1849	0.55	0/2486
34	c	0.24	0/1656	0.60	0/2232
35	d	0.25	0/1622	0.60	0/2171
36	e	0.27	0/1159	0.62	1/1559 (0.1%)
37	f	0.25	0/867	0.57	0/1167
38	g	0.25	0/1207	0.59	0/1616
39	h	0.25	0/993	0.55	0/1332
40	i	0.26	0/1022	0.68	0/1365
41	j	0.26	0/775	0.60	0/1046
42	k	0.25	0/854	0.59	0/1159
43	l	0.27	0/963	0.68	0/1292
44	m	0.24	0/867	0.63	0/1165
45	n	0.25	0/787	0.64	0/1048
46	o	0.24	0/693	0.54	0/926
47	p	0.27	0/621	0.64	0/837
48	q	0.25	0/627	0.64	0/844
49	r	0.27	0/575	2.14	2/771 (0.3%)
50	s	0.23	0/649	0.58	0/874
51	t	0.25	0/661	0.54	0/881
52	u	0.25	0/524	0.66	0/689
53	v	0.26	0/2323	0.60	0/3138
All	All	0.25	5/157101 (0.0%)	0.79	92/234896 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	1	0
8	D	0	1
23	R	0	1
49	r	0	1
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Dt	1	G	OP3-P	-10.53	1.48	1.61
5	A	1897	G	C8-N7	-9.41	1.25	1.30
5	A	1897	G	N7-C5	-6.26	1.35	1.39
5	A	1897	G	C6-N1	-5.93	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1909	G	N1-C2	-5.50	1.33	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r	12	ARG	O-C-N	-56.80	31.82	122.70
5	A	1897	G	N7-C8-N9	12.70	119.45	113.10
5	A	1897	G	C8-N9-C4	-10.79	102.08	106.40
5	A	1909	G	N1-C2-N2	-10.28	106.94	116.20
5	A	1896	C	C5-C6-N1	9.41	125.71	121.00
5	A	1897	G	C4-N9-C1'	9.13	138.37	126.50
5	A	877	C	C6-N1-C2	-9.06	116.67	120.30
5	A	2239	G	O4'-C1'-N9	8.76	115.21	108.20
5	A	1897	G	C6-C5-N7	-8.60	125.24	130.40
5	A	1909	G	N3-C2-N2	8.19	125.63	119.90
5	A	1909	G	C5-C6-N1	-7.75	107.63	111.50
5	A	1895	C	N3-C4-C5	7.68	124.97	121.90
5	A	1300	U	C2-N1-C1'	7.41	126.59	117.70
5	A	818	U	C2-N1-C1'	7.37	126.54	117.70
5	A	535	C	C6-N1-C2	-7.31	117.38	120.30
5	A	1897	G	N3-C4-N9	7.28	130.37	126.00
5	A	1897	G	N3-C4-C5	-7.15	125.02	128.60
5	A	2851	G	N3-C4-N9	7.08	130.25	126.00
5	A	1895	C	C2-N1-C1'	-7.07	111.03	118.80
9	Dt	8	U	C2-N1-C1'	7.05	126.16	117.70
5	A	1897	G	N1-C2-N2	-6.99	109.91	116.20
5	A	877	C	N1-C2-O2	6.99	123.09	118.90
5	A	1909	G	C8-N9-C4	-6.84	103.67	106.40
5	A	877	C	N3-C2-O2	-6.83	117.12	121.90
5	A	2812	U	N3-C2-O2	-6.69	117.52	122.20
49	r	12	ARG	C-N-CA	-6.69	104.98	121.70
5	A	1896	C	C2-N1-C1'	6.68	126.15	118.80
36	e	47	VAL	CG1-CB-CG2	6.68	121.58	110.90
5	A	1761	C	C6-N1-C2	-6.57	117.67	120.30
5	A	1909	G	C2-N3-C4	-6.57	108.62	111.90
5	A	1896	C	C6-N1-C2	-6.54	117.68	120.30
5	A	2100	U	C2-N1-C1'	6.54	125.54	117.70
5	A	1724	U	N3-C2-O2	-6.52	117.63	122.20
32	a	104	C	N1-C2-O2	6.42	122.75	118.90
9	Dt	32	U	C6-N1-C2	-6.30	117.22	121.00
5	A	1897	G	C4-C5-C6	6.28	122.56	118.80
5	A	2851	G	C4-N9-C1'	6.23	134.60	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Dt	36	A	OP1-P-O3'	6.19	118.83	105.20
9	Dt	38	A	OP1-P-O3'	6.19	118.81	105.20
32	a	130	C	C6-N1-C2	-6.16	117.83	120.30
9	Dt	46	G	OP1-P-OP2	6.16	128.84	119.60
9	Dt	31	A	OP1-P-O3'	6.16	118.74	105.20
5	A	2851	G	C8-N9-C1'	-6.06	119.12	127.00
5	A	2812	U	N1-C2-O2	5.92	126.95	122.80
5	A	1897	G	C8-N9-C1'	-5.88	119.35	127.00
5	A	1909	G	N1-C2-N3	5.87	127.42	123.90
32	a	963	A	O4'-C1'-N9	5.87	112.89	108.20
32	a	104	C	C6-N1-C2	-5.83	117.97	120.30
32	a	104	C	N3-C2-O2	-5.74	117.88	121.90
9	Dt	32	U	N3-C2-O2	-5.73	118.19	122.20
32	a	1341	G	P-O3'-C3'	5.68	126.51	119.70
5	A	1896	C	N1-C2-O2	5.67	122.30	118.90
6	B	108	C	C6-N1-C2	-5.66	118.03	120.30
32	a	104	C	C2-N1-C1'	5.65	125.01	118.80
32	a	987	G	C4-N9-C1'	5.63	133.82	126.50
5	A	1724	U	C6-N1-C2	-5.60	117.64	121.00
5	A	1896	C	N3-C4-N4	5.58	121.91	118.00
5	A	1897	G	N1-C2-N3	5.58	127.25	123.90
6	B	119	U	N3-C2-O2	-5.56	118.31	122.20
9	Dt	16	U	OP1-P-OP2	5.55	127.93	119.60
5	A	836	U	N3-C2-O2	-5.50	118.35	122.20
5	A	535	C	C6-N1-C1'	5.45	127.34	120.80
5	A	1166	G	C4-N9-C1'	5.44	133.57	126.50
5	A	1724	U	N1-C2-O2	5.41	126.59	122.80
9	Dt	54	U	OP1-P-O3'	5.41	117.10	105.20
5	A	922	G	C4-N9-C1'	5.39	133.51	126.50
5	A	2023	C	C6-N1-C2	-5.38	118.15	120.30
5	A	1415	C	C6-N1-C2	-5.36	118.16	120.30
5	A	2812	U	C6-N1-C2	-5.36	117.79	121.00
5	A	1909	G	N1-C6-O6	5.33	123.10	119.90
5	A	1895	C	C4-C5-C6	-5.29	114.76	117.40
9	Dt	8	U	OP1-P-OP2	5.28	127.52	119.60
5	A	1897	G	C5-N7-C8	-5.27	101.66	104.30
5	A	1051	U	P-O3'-C3'	5.25	126.00	119.70
32	a	203	U	C2-N1-C1'	5.19	123.92	117.70
5	A	910	C	C6-N1-C2	-5.17	118.23	120.30
6	B	119	U	N1-C2-O2	5.10	126.37	122.80
32	a	322	C	P-O3'-C3'	5.09	125.81	119.70
5	A	360	C	P-O3'-C3'	5.09	125.81	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2583	U	N3-C2-O2	-5.09	118.64	122.20
5	A	2030	U	C2-N1-C1'	5.08	123.80	117.70
9	Dt	32	U	C5-C6-N1	5.08	125.24	122.70
9	Dt	7	A	OP1-P-O3'	-5.08	94.03	105.20
5	A	836	U	N1-C2-O2	5.08	126.35	122.80
5	A	1724	U	C5-C6-N1	5.07	125.24	122.70
5	A	1898	U	O5'-P-OP1	-5.07	101.13	105.70
5	A	1896	C	C2-N3-C4	5.06	122.43	119.90
5	A	1301	C	C6-N1-C2	-5.05	118.28	120.30
32	a	987	G	C8-N9-C1'	-5.03	120.46	127.00
5	A	1818	G	N3-C4-N9	5.02	129.01	126.00
32	a	976	U	P-O3'-C3'	5.01	125.72	119.70
5	A	2200	U	P-O3'-C3'	5.01	125.71	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1897	G	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	151	THR	Peptide
23	R	51	LEU	Peptide
49	r	12	ARG	Mainchain

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	51/60 (85%)	49 (96%)	2 (4%)	0	100	100
2	4	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
3	5	61/64 (95%)	54 (88%)	7 (12%)	0	100	100
4	6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
8	D	205/211 (97%)	184 (90%)	21 (10%)	0	100	100
10	E	197/200 (98%)	190 (96%)	7 (4%)	0	100	100
11	F	172/179 (96%)	155 (90%)	17 (10%)	0	100	100
12	G	171/177 (97%)	164 (96%)	7 (4%)	0	100	100
13	H	76/148 (51%)	76 (100%)	0	0	100	100
14	J	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
15	K	118/122 (97%)	111 (94%)	7 (6%)	0	100	100
16	L	141/144 (98%)	130 (92%)	11 (8%)	0	100	100
17	Le	66/71 (93%)	59 (89%)	6 (9%)	1 (2%)	8	36
18	M	133/137 (97%)	132 (99%)	1 (1%)	0	100	100
19	N	116/129 (90%)	105 (90%)	11 (10%)	0	100	100
20	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
21	P	111/116 (96%)	104 (94%)	7 (6%)	0	100	100
22	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
23	R	100/103 (97%)	93 (93%)	7 (7%)	0	100	100
24	S	107/110 (97%)	107 (100%)	0	0	100	100
25	T	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	12	44
26	U	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
27	V	186/204 (91%)	173 (93%)	13 (7%)	0	100	100
28	W	74/85 (87%)	57 (77%)	17 (23%)	0	100	100
29	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
30	Y	57/63 (90%)	54 (95%)	2 (4%)	1 (2%)	7	32
31	Z	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
33	b	230/246 (94%)	214 (93%)	16 (7%)	0	100	100
34	c	203/228 (89%)	188 (93%)	15 (7%)	0	100	100
35	d	203/206 (98%)	190 (94%)	13 (6%)	0	100	100
36	e	154/166 (93%)	141 (92%)	13 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	f	103/139 (74%)	98 (95%)	5 (5%)	0	100	100
38	g	152/156 (97%)	147 (97%)	5 (3%)	0	100	100
39	h	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
40	i	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	16	51
41	j	94/103 (91%)	88 (94%)	6 (6%)	0	100	100
42	k	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
43	l	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
44	m	108/118 (92%)	103 (95%)	5 (5%)	0	100	100
45	n	96/101 (95%)	91 (95%)	5 (5%)	0	100	100
46	o	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
47	p	76/83 (92%)	73 (96%)	3 (4%)	0	100	100
48	q	74/88 (84%)	72 (97%)	2 (3%)	0	100	100
49	r	67/76 (88%)	65 (97%)	1 (2%)	1 (2%)	8	36
50	s	78/91 (86%)	71 (91%)	7 (9%)	0	100	100
51	t	83/91 (91%)	83 (100%)	0	0	100	100
52	u	58/71 (82%)	56 (97%)	1 (2%)	1 (2%)	7	33
53	v	269/370 (73%)	264 (98%)	5 (2%)	0	100	100
All	All	5794/6327 (92%)	5463 (94%)	325 (6%)	6 (0%)	50	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	T	71	ARG
30	Y	10	VAL
40	i	28	ILE
49	r	13	PHE
17	Le	66	VAL
52	u	28	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	46/52 (88%)	45 (98%)	1 (2%)	47	76
2	4	38/37 (103%)	37 (97%)	1 (3%)	41	72
3	5	54/55 (98%)	53 (98%)	1 (2%)	52	79
4	6	33/34 (97%)	32 (97%)	1 (3%)	36	69
7	C	206/213 (97%)	204 (99%)	2 (1%)	73	88
8	D	157/162 (97%)	155 (99%)	2 (1%)	65	85
10	E	155/158 (98%)	154 (99%)	1 (1%)	84	93
11	F	124/153 (81%)	120 (97%)	4 (3%)	34	67
12	G	133/141 (94%)	132 (99%)	1 (1%)	79	90
13	H	55/107 (51%)	55 (100%)	0	100	100
14	J	118/119 (99%)	114 (97%)	4 (3%)	32	66
15	K	100/102 (98%)	99 (99%)	1 (1%)	73	88
16	L	104/106 (98%)	103 (99%)	1 (1%)	73	88
17	Le	59/61 (97%)	57 (97%)	2 (3%)	32	66
18	M	108/110 (98%)	108 (100%)	0	100	100
19	N	97/104 (93%)	96 (99%)	1 (1%)	73	88
20	O	86/87 (99%)	86 (100%)	0	100	100
21	P	94/98 (96%)	94 (100%)	0	100	100
22	Q	87/88 (99%)	86 (99%)	1 (1%)	70	87
23	R	82/86 (95%)	82 (100%)	0	100	100
24	S	86/87 (99%)	86 (100%)	0	100	100
25	T	73/82 (89%)	70 (96%)	3 (4%)	26	60
26	U	88/88 (100%)	83 (94%)	5 (6%)	17	49
27	V	143/164 (87%)	136 (95%)	7 (5%)	21	54
28	W	56/61 (92%)	54 (96%)	2 (4%)	30	64
29	X	65/67 (97%)	64 (98%)	1 (2%)	60	83
30	Y	52/55 (94%)	45 (86%)	7 (14%)	3	14
31	Z	48/49 (98%)	48 (100%)	0	100	100
33	b	191/202 (95%)	189 (99%)	2 (1%)	73	88
34	c	165/187 (88%)	165 (100%)	0	100	100
35	d	166/174 (95%)	163 (98%)	3 (2%)	54	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	114/124 (92%)	112 (98%)	2 (2%)	54	80
37	f	88/119 (74%)	87 (99%)	1 (1%)	70	87
38	g	116/122 (95%)	113 (97%)	3 (3%)	41	72
39	h	108/109 (99%)	108 (100%)	0	100	100
40	i	104/106 (98%)	99 (95%)	5 (5%)	21	55
41	j	85/92 (92%)	81 (95%)	4 (5%)	22	56
42	k	84/98 (86%)	84 (100%)	0	100	100
43	l	105/107 (98%)	102 (97%)	3 (3%)	37	70
44	m	92/99 (93%)	85 (92%)	7 (8%)	11	37
45	n	78/82 (95%)	78 (100%)	0	100	100
46	o	73/75 (97%)	73 (100%)	0	100	100
47	p	61/65 (94%)	61 (100%)	0	100	100
48	q	70/79 (89%)	67 (96%)	3 (4%)	25	58
49	r	56/64 (88%)	54 (96%)	2 (4%)	30	64
50	s	69/78 (88%)	68 (99%)	1 (1%)	62	83
51	t	67/70 (96%)	67 (100%)	0	100	100
52	u	51/60 (85%)	50 (98%)	1 (2%)	50	78
53	v	242/335 (72%)	227 (94%)	15 (6%)	15	45
All	All	4732/5173 (92%)	4631 (98%)	101 (2%)	49	77

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	10	ARG
2	4	42	LEU
3	5	13	ARG
4	6	37	GLN
7	C	79	GLU
7	C	258	THR
8	D	13	THR
8	D	34	ARG
10	E	60	ARG
11	F	7	ILE
11	F	32	THR
11	F	102	ARG
11	F	162	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	G	33	LEU
14	J	45	THR
14	J	50	THR
14	J	116	ARG
14	J	141	LYS
15	K	40	LYS
16	L	7	ARG
17	Le	28	LEU
17	Le	57	ILE
19	N	37	THR
22	Q	103	LYS
25	T	5	ARG
25	T	8	LYS
25	T	40	LEU
26	U	5	ARG
26	U	41	ILE
26	U	45	THR
26	U	82	VAL
26	U	91	LYS
27	V	6	LEU
27	V	11	ARG
27	V	44	THR
27	V	91	HIS
27	V	94	PHE
27	V	101	HIS
27	V	103	LEU
28	W	40	GLN
28	W	41	ARG
29	X	27	ARG
30	Y	9	SER
30	Y	15	GLU
30	Y	16	GLN
30	Y	17	LEU
30	Y	18	LEU
30	Y	20	LEU
30	Y	33	THR
33	b	23	TRP
33	b	86	ARG
35	d	9	CYS
35	d	26	ARG
35	d	62	ARG
36	e	27	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	e	158	ARG
37	f	9	LEU
38	g	5	ARG
38	g	12	VAL
38	g	148	ASN
40	i	5	GLN
40	i	12	ARG
40	i	41	ARG
40	i	46	MET
40	i	47	VAL
41	j	16	ARG
41	j	59	LYS
41	j	67	ILE
41	j	82	LYS
43	l	14	ARG
43	l	15	MET
43	l	114	ARG
44	m	27	ARG
44	m	40	ASN
44	m	71	ARG
44	m	83	LEU
44	m	102	THR
44	m	105	ASN
44	m	109	ARG
48	q	54	ASN
48	q	65	ARG
48	q	68	ARG
49	r	6	ARG
49	r	8	ARG
50	s	29	LYS
52	u	45	ARG
53	v	50	LEU
53	v	53	LEU
53	v	71	THR
53	v	89	MET
53	v	94	THR
53	v	97	ARG
53	v	138	LYS
53	v	143	ARG
53	v	158	TRP
53	v	164	TYR
53	v	166	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	v	177	LYS
53	v	234	ARG
53	v	259	THR
53	v	268	ASP

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

Mol	Chain	Res	Type
2	4	26	ASN
7	C	261	ASN
8	D	150	GLN
12	G	60	GLN
14	J	58	ASN
15	K	88	ASN
16	L	54	GLN
22	Q	37	GLN
22	Q	101	ASN
23	R	66	HIS
26	U	44	HIS
28	W	29	GLN
30	Y	12	GLN
30	Y	16	GLN
31	Z	43	ASN
33	b	3	GLN
33	b	24	ASN
36	e	147	ASN
38	g	153	HIS
40	i	75	GLN
46	o	61	ASN
53	v	102	ASN
53	v	116	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1525/1526 (99%)	301 (19%)	0
5	A	2880/2888 (99%)	707 (24%)	49 (1%)
6	B	119/120 (99%)	26 (21%)	2 (1%)
9	Dt	75/76 (98%)	23 (30%)	0
All	All	4599/4610 (99%)	1057 (22%)	51 (1%)

All (1057) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	A
5	A	33	U
5	A	34	U
5	A	35	G
5	A	44	A
5	A	45	G
5	A	46	G
5	A	51	G
5	A	54	A
5	A	59	U
5	A	61	G
5	A	63	A
5	A	74	A
5	A	75	G
5	A	79	C
5	A	82	G
5	A	85	G
5	A	91	A
5	A	92	A
5	A	97	A
5	A	100	U
5	A	102	G
5	A	104	U
5	A	114	U
5	A	115	C
5	A	118	A
5	A	120	U
5	A	125	G
5	A	131	A
5	A	137	G
5	A	138	A
5	A	139	U
5	A	141	A
5	A	142	C
5	A	144	U
5	A	146	G
5	A	147	G
5	A	149	A
5	A	150	U
5	A	160	A
5	A	162	U
5	A	163	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	164	C
5	A	165	A
5	A	166	U
5	A	172	C
5	A	173	A
5	A	181	A
5	A	194	G
5	A	196	A
5	A	199	A
5	A	202	U
5	A	205	G
5	A	215	G
5	A	216	A
5	A	220	G
5	A	222	A
5	A	227	A
5	A	228	C
5	A	230	G
5	A	233	A
5	A	240	U
5	A	241	A
5	A	242	G
5	A	243	U
5	A	244	A
5	A	248	G
5	A	249	C
5	A	252	G
5	A	255	A
5	A	265	A
5	A	266	G
5	A	267	C
5	A	271	U
5	A	273	A
5	A	281	U
5	A	285	U
5	A	289	G
5	A	294	A
5	A	299	C
5	A	305	A
5	A	315	U
5	A	316	A
5	A	317	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	318	U
5	A	321	G
5	A	322	U
5	A	323	G
5	A	324	A
5	A	325	U
5	A	335	C
5	A	337	C
5	A	338	G
5	A	339	A
5	A	342	G
5	A	347	U
5	A	348	U
5	A	349	U
5	A	350	G
5	A	351	A
5	A	353	G
5	A	358	A
5	A	359	U
5	A	360	C
5	A	361	A
5	A	374	C
5	A	376	C
5	A	377	G
5	A	380	A
5	A	381	A
5	A	385	U
5	A	387	G
5	A	390	U
5	A	391	G
5	A	395	A
5	A	396	U
5	A	397	G
5	A	398	G
5	A	399	G
5	A	400	G
5	A	403	A
5	A	406	A
5	A	407	U
5	A	408	C
5	A	414	A
5	A	428	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	431	C
5	A	435	C
5	A	438	A
5	A	445	A
5	A	447	C
5	A	448	A
5	A	461	A
5	A	464	G
5	A	466	C
5	A	471	A
5	A	472	G
5	A	481	A
5	A	485	G
5	A	496	A
5	A	499	A
5	A	500	C
5	A	509	G
5	A	519	A
5	A	521	G
5	A	522	C
5	A	523	A
5	A	534	A
5	A	535	C
5	A	536	U
5	A	537	U
5	A	538	G
5	A	539	U
5	A	540	U
5	A	541	A
5	A	550	C
5	A	553	A
5	A	557	U
5	A	558	U
5	A	562	A
5	A	563	U
5	A	564	A
5	A	565	A
5	A	576	A
5	A	586	A
5	A	593	A
5	A	594	G
5	A	599	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	601	C
5	A	603	U
5	A	604	A
5	A	610	U
5	A	611	A
5	A	618	G
5	A	622	A
5	A	627	A
5	A	635	U
5	A	636	A
5	A	647	U
5	A	659	G
5	A	660	A
5	A	671	G
5	A	672	G
5	A	673	C
5	A	676	U
5	A	687	G
5	A	708	A
5	A	716	G
5	A	720	A
5	A	737	U
5	A	738	G
5	A	743	G
5	A	747	G
5	A	754	A
5	A	755	C
5	A	765	G
5	A	766	G
5	A	767	A
5	A	769	U
5	A	772	A
5	A	774	G
5	A	775	G
5	A	783	A
5	A	784	G
5	A	793	U
5	A	795	G
5	A	802	C
5	A	817	U
5	A	824	G
5	A	827	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	833	G
5	A	836	U
5	A	841	C
5	A	843	G
5	A	844	G
5	A	846	G
5	A	848	G
5	A	850	A
5	A	855	A
5	A	866	U
5	A	870	G
5	A	875	A
5	A	877	C
5	A	878	C
5	A	880	G
5	A	881	A
5	A	889	A
5	A	899	A
5	A	904	C
5	A	908	U
5	A	911	C
5	A	921	C
5	A	922	G
5	A	931	A
5	A	935	A
5	A	936	C
5	A	949	A
5	A	951	C
5	A	952	G
5	A	954	C
5	A	963	A
5	A	964	A
5	A	972	C
5	A	973	A
5	A	980	A
5	A	986	A
5	A	999	A
5	A	1002	U
5	A	1003	U
5	A	1011	A
5	A	1012	G
5	A	1013	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1016	U
5	A	1017	A
5	A	1023	U
5	A	1031	G
5	A	1036	A
5	A	1037	G
5	A	1048	G
5	A	1050	U
5	A	1051	U
5	A	1052	G
5	A	1057	A
5	A	1058	G
5	A	1060	A
5	A	1061	G
5	A	1063	A
5	A	1064	G
5	A	1066	C
5	A	1068	C
5	A	1076	A
5	A	1077	G
5	A	1078	A
5	A	1079	A
5	A	1080	A
5	A	1082	C
5	A	1084	U
5	A	1085	A
5	A	1086	A
5	A	1088	A
5	A	1097	G
5	A	1100	G
5	A	1101	A
5	A	1102	G
5	A	1114	G
5	A	1117	A
5	A	1119	A
5	A	1120	U
5	A	1124	A
5	A	1125	C
5	A	1133	A
5	A	1146	A
5	A	1148	G
5	A	1149	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1154	G
5	A	1162	G
5	A	1164	A
5	A	1167	U
5	A	1168	G
5	A	1170	C
5	A	1171	G
5	A	1191	A
5	A	1192	A
5	A	1193	G
5	A	1198	U
5	A	1199	G
5	A	1214	A
5	A	1218	U
5	A	1223	G
5	A	1225	G
5	A	1228	A
5	A	1232	G
5	A	1233	A
5	A	1234	A
5	A	1238	C
5	A	1240	A
5	A	1243	G
5	A	1244	C
5	A	1249	A
5	A	1253	G
5	A	1256	A
5	A	1258	G
5	A	1259	A
5	A	1261	A
5	A	1263	U
5	A	1276	C
5	A	1283	G
5	A	1287	A
5	A	1288	A
5	A	1301	C
5	A	1311	G
5	A	1316	U
5	A	1321	G
5	A	1339	U
5	A	1349	C
5	A	1352	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1354	A
5	A	1355	A
5	A	1363	C
5	A	1365	A
5	A	1366	U
5	A	1367	G
5	A	1370	A
5	A	1373	C
5	A	1379	A
5	A	1380	A
5	A	1382	A
5	A	1390	A
5	A	1402	U
5	A	1403	G
5	A	1404	C
5	A	1408	G
5	A	1414	A
5	A	1415	C
5	A	1422	G
5	A	1424	C
5	A	1434	U
5	A	1440	U
5	A	1441	U
5	A	1442	G
5	A	1445	U
5	A	1447	U
5	A	1448	C
5	A	1449	C
5	A	1454	U
5	A	1469	G
5	A	1474	C
5	A	1480	U
5	A	1481	A
5	A	1484	U
5	A	1496	A
5	A	1497	G
5	A	1508	G
5	A	1509	A
5	A	1511	G
5	A	1512	A
5	A	1516	G
5	A	1528	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1537	U
5	A	1542	G
5	A	1556	A
5	A	1558	G
5	A	1559	A
5	A	1560	A
5	A	1573	U
5	A	1574	U
5	A	1576	A
5	A	1580	A
5	A	1597	C
5	A	1598	A
5	A	1600	A
5	A	1602	C
5	A	1603	G
5	A	1606	A
5	A	1608	A
5	A	1609	G
5	A	1614	U
5	A	1628	C
5	A	1629	C
5	A	1634	C
5	A	1636	C
5	A	1637	U
5	A	1638	U
5	A	1639	G
5	A	1654	A
5	A	1663	G
5	A	1664	G
5	A	1673	C
5	A	1683	U
5	A	1685	G
5	A	1686	G
5	A	1689	G
5	A	1690	A
5	A	1698	C
5	A	1704	A
5	A	1705	G
5	A	1708	U
5	A	1711	A
5	A	1714	A
5	A	1716	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1717	U
5	A	1720	U
5	A	1721	C
5	A	1724	U
5	A	1731	U
5	A	1732	G
5	A	1735	U
5	A	1741	A
5	A	1742	A
5	A	1745	U
5	A	1749	A
5	A	1750	G
5	A	1751	G
5	A	1756	U
5	A	1760	A
5	A	1771	A
5	A	1773	A
5	A	1778	A
5	A	1787	C
5	A	1788	A
5	A	1795	A
5	A	1797	A
5	A	1798	G
5	A	1803	C
5	A	1816	A
5	A	1820	C
5	A	1834	A
5	A	1837	G
5	A	1838	U
5	A	1844	G
5	A	1850	G
5	A	1851	U
5	A	1853	A
5	A	1861	C
5	A	1873	U
5	A	1875	G
5	A	1892	C
5	A	1893	G
5	A	1897	G
5	A	1898	U
5	A	1899	A
5	A	1901	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1902	U
5	A	1906	A
5	A	1916	G
5	A	1917	G
5	A	1918	U
5	A	1924	A
5	A	1925	A
5	A	1942	U
5	A	1949	C
5	A	1950	U
5	A	1951	G
5	A	1954	C
5	A	1957	A
5	A	1958	U
5	A	1959	G
5	A	1967	G
5	A	1968	A
5	A	1969	U
5	A	1978	U
5	A	1979	G
5	A	1982	U
5	A	1983	C
5	A	1984	C
5	A	1993	C
5	A	2008	A
5	A	2010	C
5	A	2015	U
5	A	2017	A
5	A	2018	A
5	A	2020	A
5	A	2028	U
5	A	2030	U
5	A	2039	A
5	A	2042	C
5	A	2043	G
5	A	2047	A
5	A	2048	G
5	A	2049	A
5	A	2055	U
5	A	2056	G
5	A	2060	C
5	A	2063	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2064	A
5	A	2067	G
5	A	2068	U
5	A	2080	G
5	A	2082	A
5	A	2083	C
5	A	2094	C
5	A	2095	U
5	A	2097	G
5	A	2098	U
5	A	2099	G
5	A	2101	A
5	A	2103	G
5	A	2106	A
5	A	2113	A
5	A	2114	G
5	A	2115	G
5	A	2116	C
5	A	2117	U
5	A	2118	U
5	A	2119	U
5	A	2121	A
5	A	2122	A
5	A	2127	G
5	A	2129	A
5	A	2132	C
5	A	2133	C
5	A	2135	G
5	A	2140	C
5	A	2141	G
5	A	2144	G
5	A	2145	A
5	A	2146	G
5	A	2147	C
5	A	2148	C
5	A	2149	A
5	A	2150	U
5	A	2151	C
5	A	2156	A
5	A	2157	A
5	A	2158	A
5	A	2159	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2160	A
5	A	2169	G
5	A	2173	G
5	A	2174	C
5	A	2175	U
5	A	2185	A
5	A	2186	A
5	A	2187	C
5	A	2191	G
5	A	2194	C
5	A	2199	A
5	A	2201	C
5	A	2212	A
5	A	2221	G
5	A	2225	G
5	A	2226	G
5	A	2229	G
5	A	2237	G
5	A	2239	G
5	A	2240	G
5	A	2253	A
5	A	2264	G
5	A	2265	A
5	A	2270	U
5	A	2271	A
5	A	2274	A
5	A	2275	A
5	A	2284	C
5	A	2292	U
5	A	2296	A
5	A	2297	A
5	A	2305	G
5	A	2306	C
5	A	2307	A
5	A	2308	G
5	A	2309	A
5	A	2312	A
5	A	2313	U
5	A	2314	A
5	A	2319	C
5	A	2321	A
5	A	2322	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2323	A
5	A	2333	A
5	A	2334	C
5	A	2337	C
5	A	2357	G
5	A	2358	G
5	A	2361	C
5	A	2363	A
5	A	2370	G
5	A	2372	C
5	A	2382	C
5	A	2383	G
5	A	2386	G
5	A	2389	U
5	A	2390	C
5	A	2393	U
5	A	2407	C
5	A	2409	C
5	A	2410	U
5	A	2413	A
5	A	2414	C
5	A	2415	G
5	A	2416	G
5	A	2417	A
5	A	2421	A
5	A	2422	A
5	A	2428	U
5	A	2434	G
5	A	2435	A
5	A	2446	A
5	A	2451	G
5	A	2453	C
5	A	2454	C
5	A	2457	G
5	A	2459	G
5	A	2462	C
5	A	2466	U
5	A	2471	G
5	A	2478	U
5	A	2480	U
5	A	2481	G
5	A	2489	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2492	G
5	A	2505	A
5	A	2506	U
5	A	2517	A
5	A	2521	C
5	A	2522	G
5	A	2537	G
5	A	2541	U
5	A	2553	A
5	A	2554	G
5	A	2559	A
5	A	2560	C
5	A	2563	G
5	A	2565	G
5	A	2573	U
5	A	2586	G
5	A	2590	G
5	A	2593	C
5	A	2600	U
5	A	2602	U
5	A	2616	U
5	A	2619	A
5	A	2633	C
5	A	2640	U
5	A	2641	A
5	A	2647	A
5	A	2651	G
5	A	2660	G
5	A	2669	U
5	A	2676	U
5	A	2677	U
5	A	2689	G
5	A	2690	C
5	A	2692	A
5	A	2701	G
5	A	2703	C
5	A	2704	G
5	A	2705	G
5	A	2713	U
5	A	2714	G
5	A	2720	A
5	A	2726	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	2731	G
5	A	2733	U
5	A	2739	C
5	A	2743	U
5	A	2744	A
5	A	2751	A
5	A	2752	A
5	A	2763	A
5	A	2765	A
5	A	2766	U
5	A	2771	U
5	A	2784	U
5	A	2785	U
5	A	2786	G
5	A	2787	A
5	A	2794	U
5	A	2795	G
5	A	2805	C
5	A	2807	A
5	A	2811	C
5	A	2812	U
5	A	2818	G
5	A	2820	U
5	A	2821	G
5	A	2836	U
5	A	2842	U
5	A	2846	G
5	A	2851	G
5	A	2852	U
5	A	2854	G
5	A	2867	C
5	A	2870	A
5	A	2871	U
5	A	2884	U
5	A	2889	C
6	B	13	A
6	B	20	G
6	B	22	U
6	B	24	G
6	B	25	A
6	B	28	C
6	B	29	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	35	U
6	B	41	C
6	B	42	C
6	B	43	C
6	B	45	A
6	B	46	A
6	B	51	G
6	B	52	A
6	B	54	G
6	B	56	G
6	B	57	A
6	B	63	C
6	B	66	A
6	B	73	A
6	B	89	U
6	B	90	C
6	B	105	G
6	B	106	G
6	B	109	A
9	Dt	4	C
9	Dt	8	U
9	Dt	11	C
9	Dt	15	G
9	Dt	16	U
9	Dt	17	C
9	Dt	19	G
9	Dt	20	U
9	Dt	21	A
9	Dt	22	G
9	Dt	32	U
9	Dt	39	U
9	Dt	44	G
9	Dt	46	G
9	Dt	47	U
9	Dt	49	C
9	Dt	52	G
9	Dt	55	U
9	Dt	58	A
9	Dt	72	C
9	Dt	74	C
9	Dt	75	C
9	Dt	76	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	3	A
32	a	6	G
32	a	7	A
32	a	9	G
32	a	22	G
32	a	29	U
32	a	31	G
32	a	32	A
32	a	42	G
32	a	47	C
32	a	48	C
32	a	51	A
32	a	52	C
32	a	60	A
32	a	61	G
32	a	65	A
32	a	66	G
32	a	71	U
32	a	72	A
32	a	73	A
32	a	77	G
32	a	82	U
32	a	83	G
32	a	88	U
32	a	89	G
32	a	95	A
32	a	100	C
32	a	115	U
32	a	118	C
32	a	121	G
32	a	123	A
32	a	124	A
32	a	125	U
32	a	133	G
32	a	138	G
32	a	143	A
32	a	157	C
32	a	176	C
32	a	177	G
32	a	179	C
32	a	182	G
32	a	192	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	193	U
32	a	204	C
32	a	205	G
32	a	206	G
32	a	239	U
32	a	241	G
32	a	244	A
32	a	256	A
32	a	260	G
32	a	261	C
32	a	266	C
32	a	275	G
32	a	283	A
32	a	284	C
32	a	287	G
32	a	288	U
32	a	292	A
32	a	299	G
32	a	315	A
32	a	321	A
32	a	322	C
32	a	323	A
32	a	326	G
32	a	334	U
32	a	341	G
32	a	345	G
32	a	346	C
32	a	348	G
32	a	361	U
32	a	363	G
32	a	365	A
32	a	375	A
32	a	376	A
32	a	378	G
32	a	384	U
32	a	386	C
32	a	391	A
32	a	400	G
32	a	405	A
32	a	406	A
32	a	407	G
32	a	408	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	417	G
32	a	423	U
32	a	443	G
32	a	445	A
32	a	446	A
32	a	447	G
32	a	457	U
32	a	461	U
32	a	475	G
32	a	478	G
32	a	490	A
32	a	491	U
32	a	492	A
32	a	493	A
32	a	494	G
32	a	502	U
32	a	504	A
32	a	505	C
32	a	507	U
32	a	509	G
32	a	511	G
32	a	512	C
32	a	513	C
32	a	515	G
32	a	518	G
32	a	520	C
32	a	521	G
32	a	526	A
32	a	527	A
32	a	539	C
32	a	540	A
32	a	541	A
32	a	556	U
32	a	558	C
32	a	566	A
32	a	567	A
32	a	569	G
32	a	570	C
32	a	571	G
32	a	573	G
32	a	582	G
32	a	584	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	585	C
32	a	590	A
32	a	627	G
32	a	647	A
32	a	648	G
32	a	659	A
32	a	681	A
32	a	682	G
32	a	687	G
32	a	688	A
32	a	696	A
32	a	710	A
32	a	712	A
32	a	717	U
32	a	718	G
32	a	727	G
32	a	733	C
32	a	749	A
32	a	754	G
32	a	756	U
32	a	759	G
32	a	760	A
32	a	771	A
32	a	788	A
32	a	806	G
32	a	807	U
32	a	809	A
32	a	810	A
32	a	811	C
32	a	812	G
32	a	815	G
32	a	822	A
32	a	830	G
32	a	835	C
32	a	838	G
32	a	840	G
32	a	845	U
32	a	854	A
32	a	858	A
32	a	862	C
32	a	865	U
32	a	866	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	870	C
32	a	884	G
32	a	887	C
32	a	894	A
32	a	896	G
32	a	908	A
32	a	920	G
32	a	921	G
32	a	928	C
32	a	929	A
32	a	932	A
32	a	936	G
32	a	939	G
32	a	954	U
32	a	955	U
32	a	956	C
32	a	960	G
32	a	963	A
32	a	964	C
32	a	966	C
32	a	967	G
32	a	968	A
32	a	969	A
32	a	970	G
32	a	971	A
32	a	975	U
32	a	977	A
32	a	988	A
32	a	990	A
32	a	998	A
32	a	1004	C
32	a	1015	U
32	a	1017	G
32	a	1023	U
32	a	1025	C
32	a	1026	G
32	a	1027	G
32	a	1039	C
32	a	1044	G
32	a	1049	A
32	a	1059	U
32	a	1073	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1075	G
32	a	1078	G
32	a	1079	U
32	a	1080	U
32	a	1086	A
32	a	1088	G
32	a	1089	U
32	a	1090	C
32	a	1095	A
32	a	1118	G
32	a	1119	U
32	a	1124	A
32	a	1127	A
32	a	1130	U
32	a	1133	G
32	a	1134	G
32	a	1149	A
32	a	1152	C
32	a	1153	U
32	a	1160	G
32	a	1162	C
32	a	1163	A
32	a	1164	A
32	a	1165	A
32	a	1175	G
32	a	1178	G
32	a	1184	G
32	a	1190	A
32	a	1191	A
32	a	1196	U
32	a	1207	A
32	a	1214	G
32	a	1219	A
32	a	1221	A
32	a	1222	C
32	a	1229	U
32	a	1230	A
32	a	1232	A
32	a	1234	U
32	a	1235	G
32	a	1248	G
32	a	1250	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1251	U
32	a	1252	G
32	a	1254	C
32	a	1264	G
32	a	1266	U
32	a	1272	U
32	a	1273	A
32	a	1281	A
32	a	1293	A
32	a	1294	G
32	a	1297	C
32	a	1299	G
32	a	1314	C
32	a	1332	G
32	a	1334	A
32	a	1342	U
32	a	1347	G
32	a	1358	U
32	a	1362	A
32	a	1381	G
32	a	1388	A
32	a	1391	C
32	a	1397	C
32	a	1413	G
32	a	1414	U
32	a	1418	U
32	a	1419	U
32	a	1423	C
32	a	1424	C
32	a	1428	A
32	a	1440	A
32	a	1446	A
32	a	1448	G
32	a	1469	G
32	a	1470	A
32	a	1486	A
32	a	1487	A
32	a	1491	G
32	a	1497	A
32	a	1498	G
32	a	1499	G
32	a	1500	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1501	A
32	a	1502	G
32	a	1511	G
32	a	1514	C
32	a	1523	G
32	a	1525	A
32	a	1526	U

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	81	G
5	A	87	C
5	A	114	U
5	A	227	A
5	A	243	U
5	A	266	G
5	A	314	A
5	A	334	A
5	A	348	U
5	A	360	C
5	A	434	A
5	A	444	A
5	A	538	G
5	A	540	U
5	A	774	G
5	A	783	A
5	A	792	A
5	A	840	U
5	A	920	C
5	A	953	U
5	A	963	A
5	A	1003	U
5	A	1016	U
5	A	1051	U
5	A	1169	A
5	A	1232	G
5	A	1233	A
5	A	1378	U
5	A	1448	C
5	A	1627	A
5	A	1653	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1672	G
5	A	1710	A
5	A	1715	U
5	A	1741	A
5	A	1891	G
5	A	1897	G
5	A	1917	G
5	A	2029	A
5	A	2149	A
5	A	2200	U
5	A	2228	A
5	A	2274	A
5	A	2536	G
5	A	2703	C
5	A	2750	G
5	A	2784	U
5	A	2793	C
5	A	2853	U
6	B	34	A
6	B	51	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 171 ligands modelled in this entry, 171 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	11:CYS	C	12:ARG	N	3.53

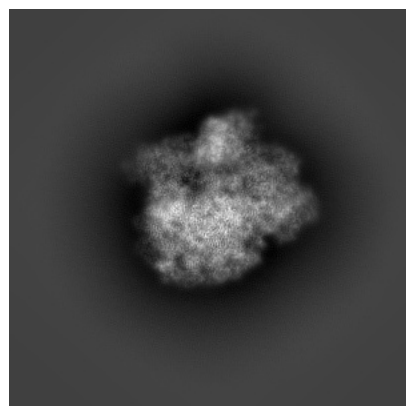
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16566. These allow visual inspection of the internal detail of the map and identification of artifacts.

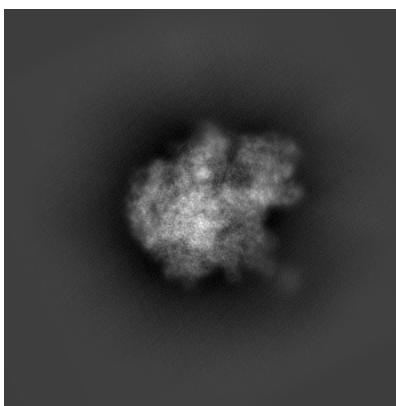
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

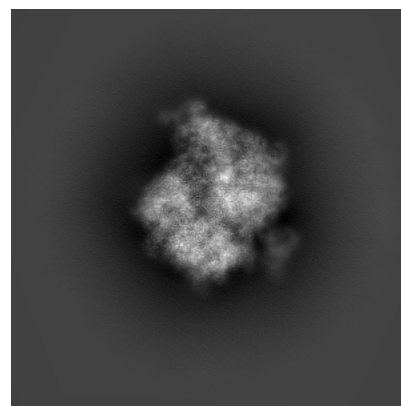
6.1.1 Primary map



X

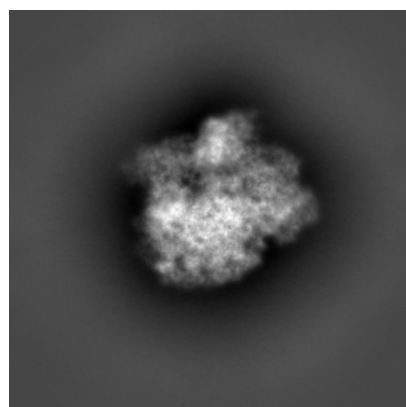


Y

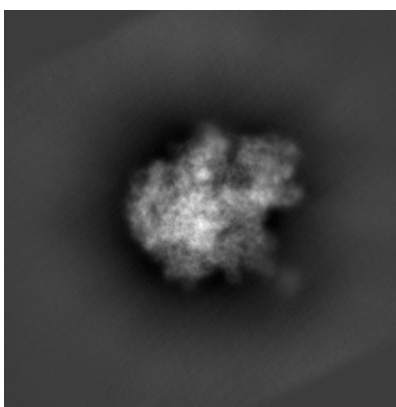


Z

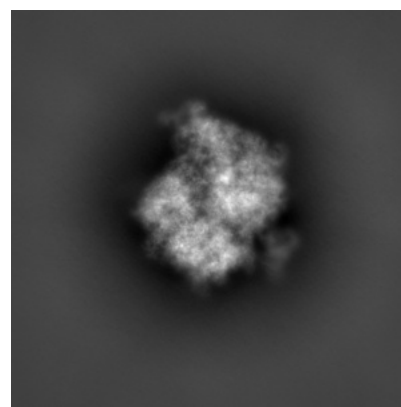
6.1.2 Raw map



X



Y

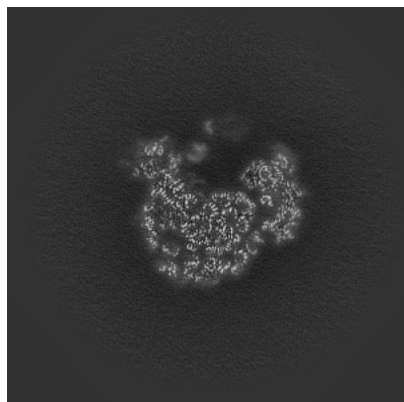


Z

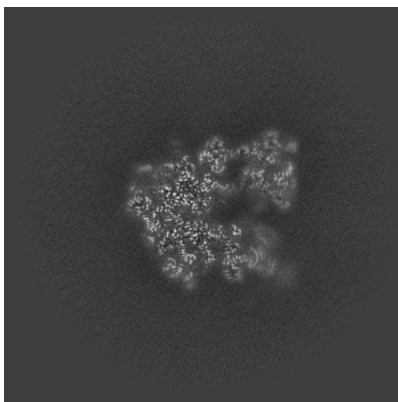
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

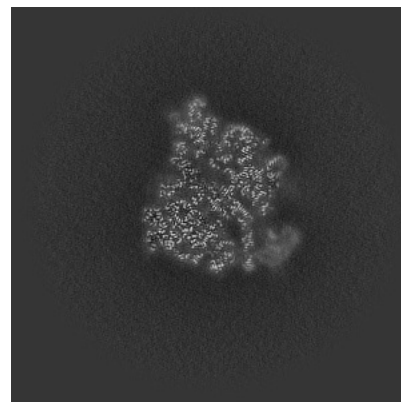
6.2.1 Primary map



X Index: 256

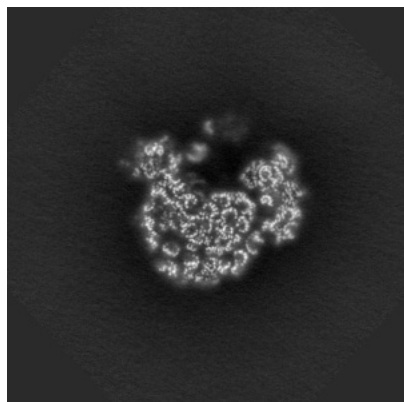


Y Index: 256

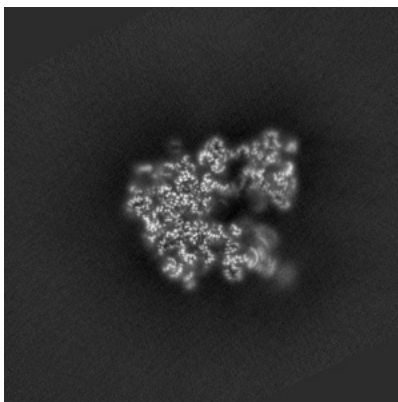


Z Index: 256

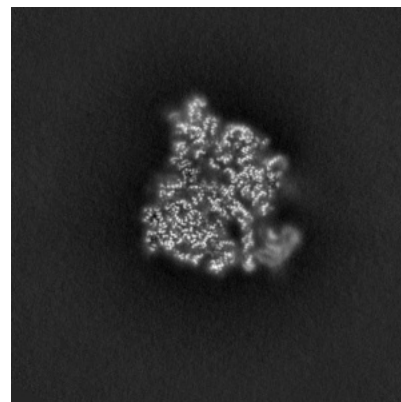
6.2.2 Raw map



X Index: 256



Y Index: 256

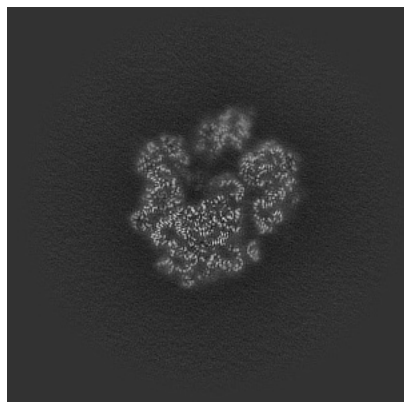


Z Index: 256

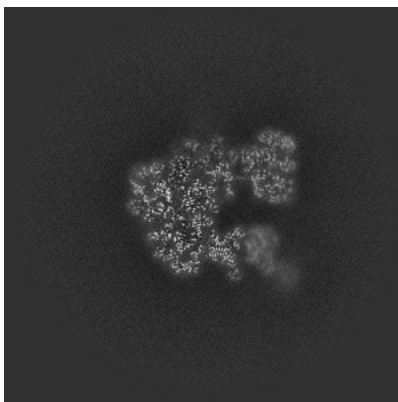
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

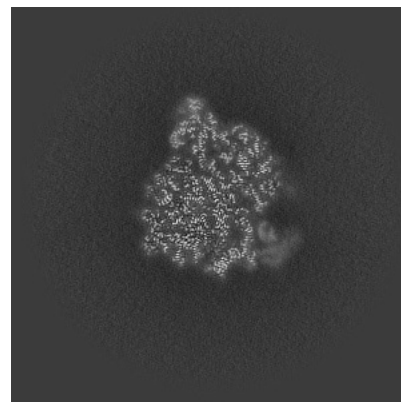
6.3.1 Primary map



X Index: 268

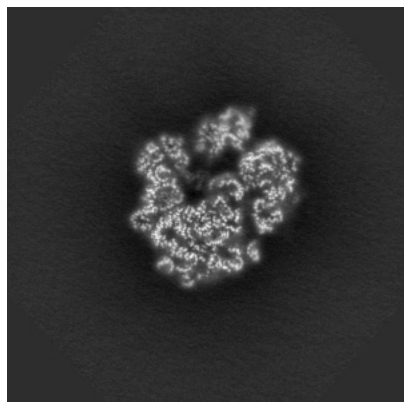


Y Index: 267

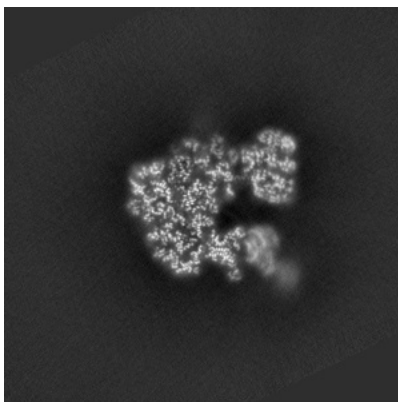


Z Index: 250

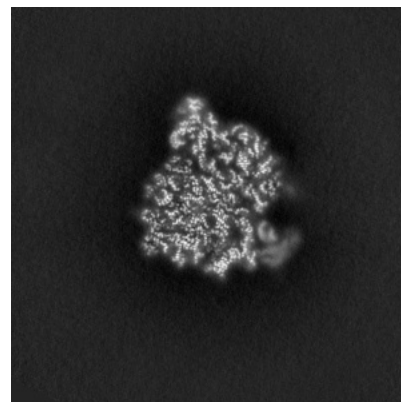
6.3.2 Raw map



X Index: 269



Y Index: 267

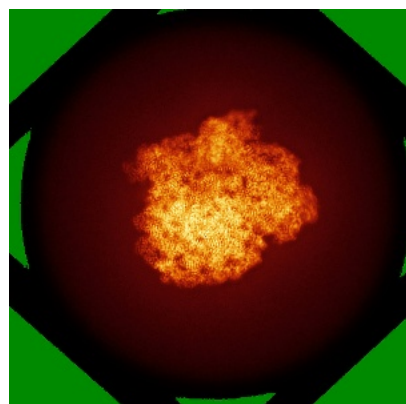


Z Index: 250

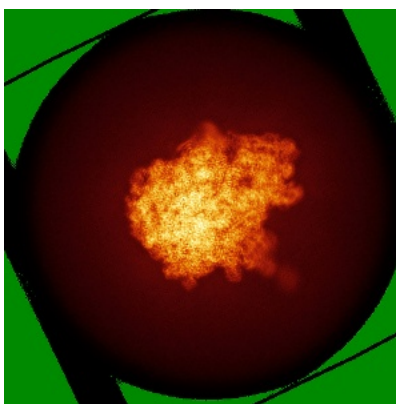
The images above show the largest variance slices of the map in three orthogonal directions.

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

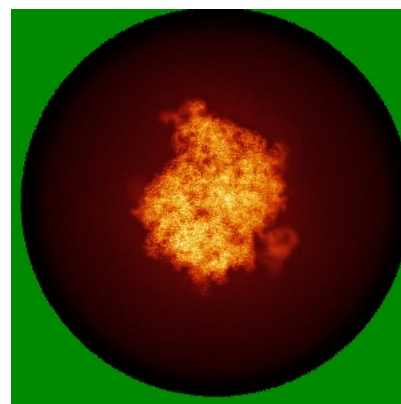
6.4.1 Primary map



X

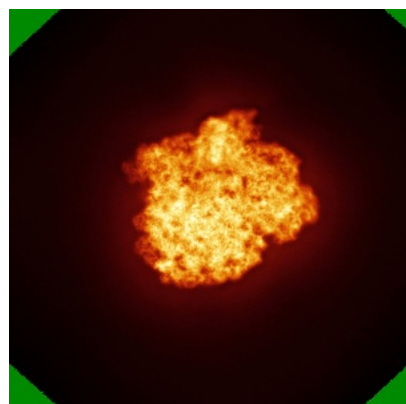


Y

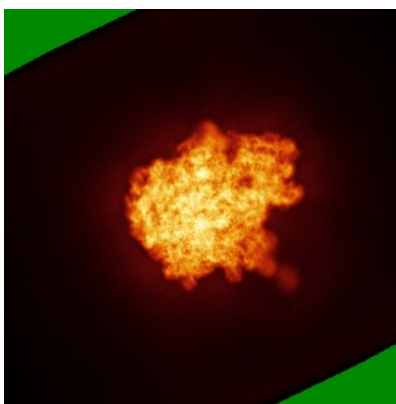


Z

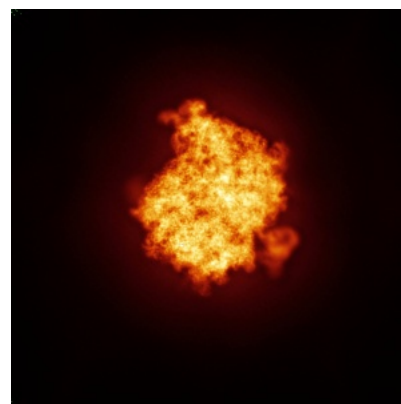
6.4.2 Raw map



X



Y

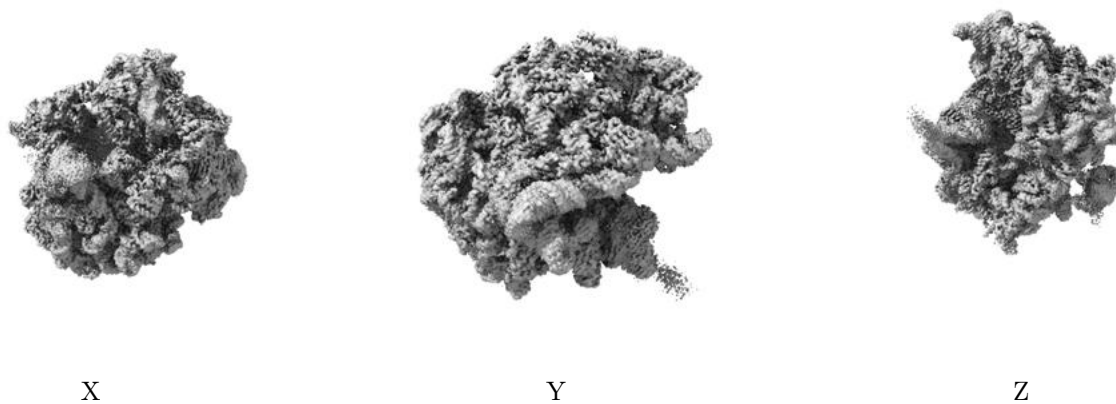


Z

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

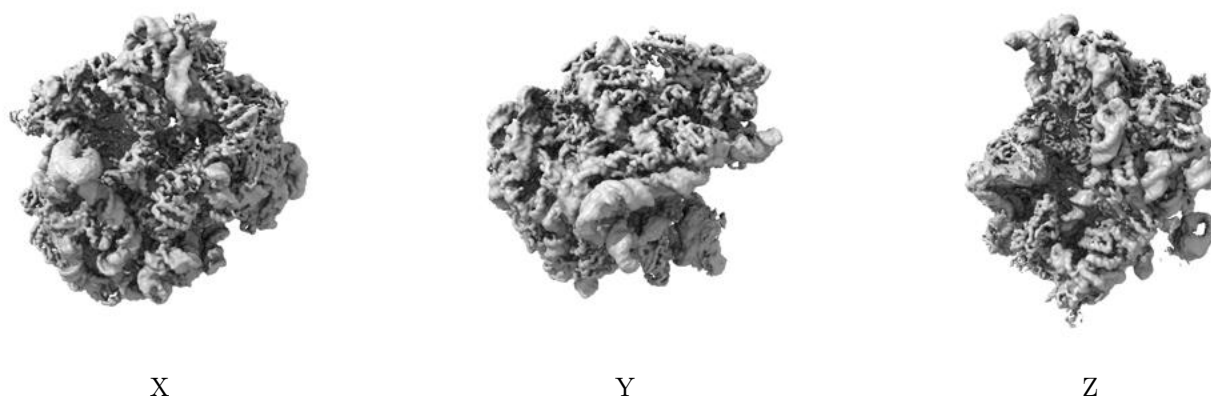
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

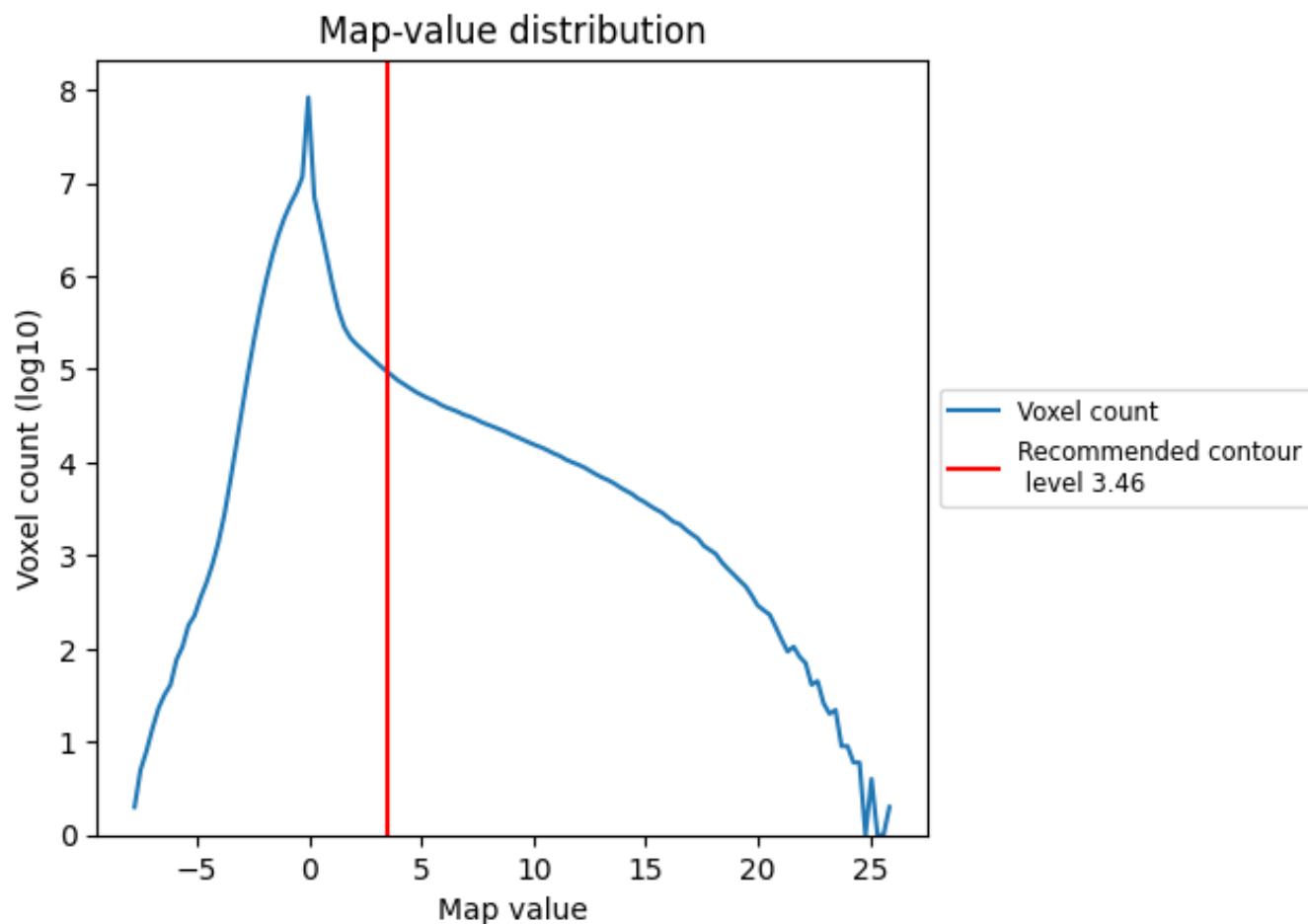
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

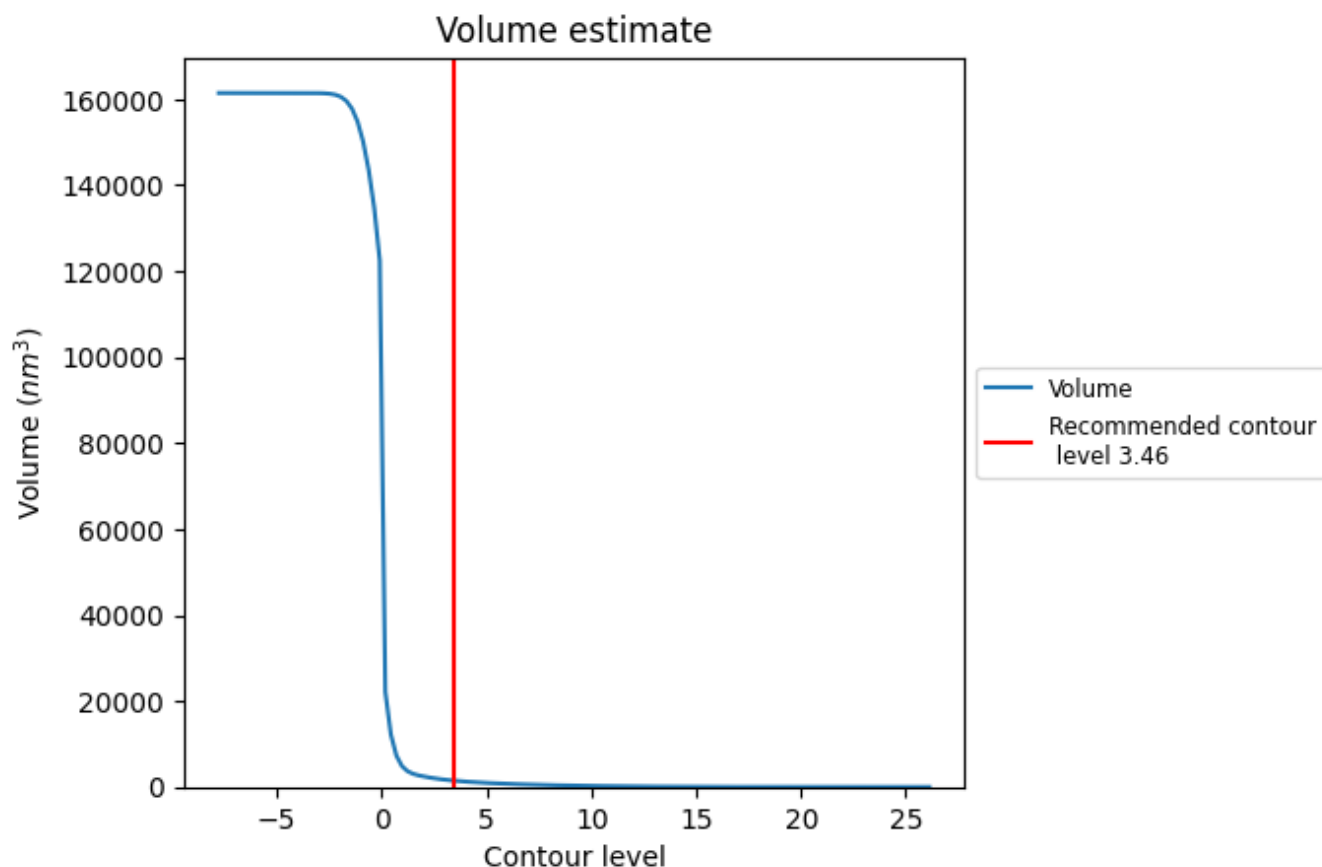
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

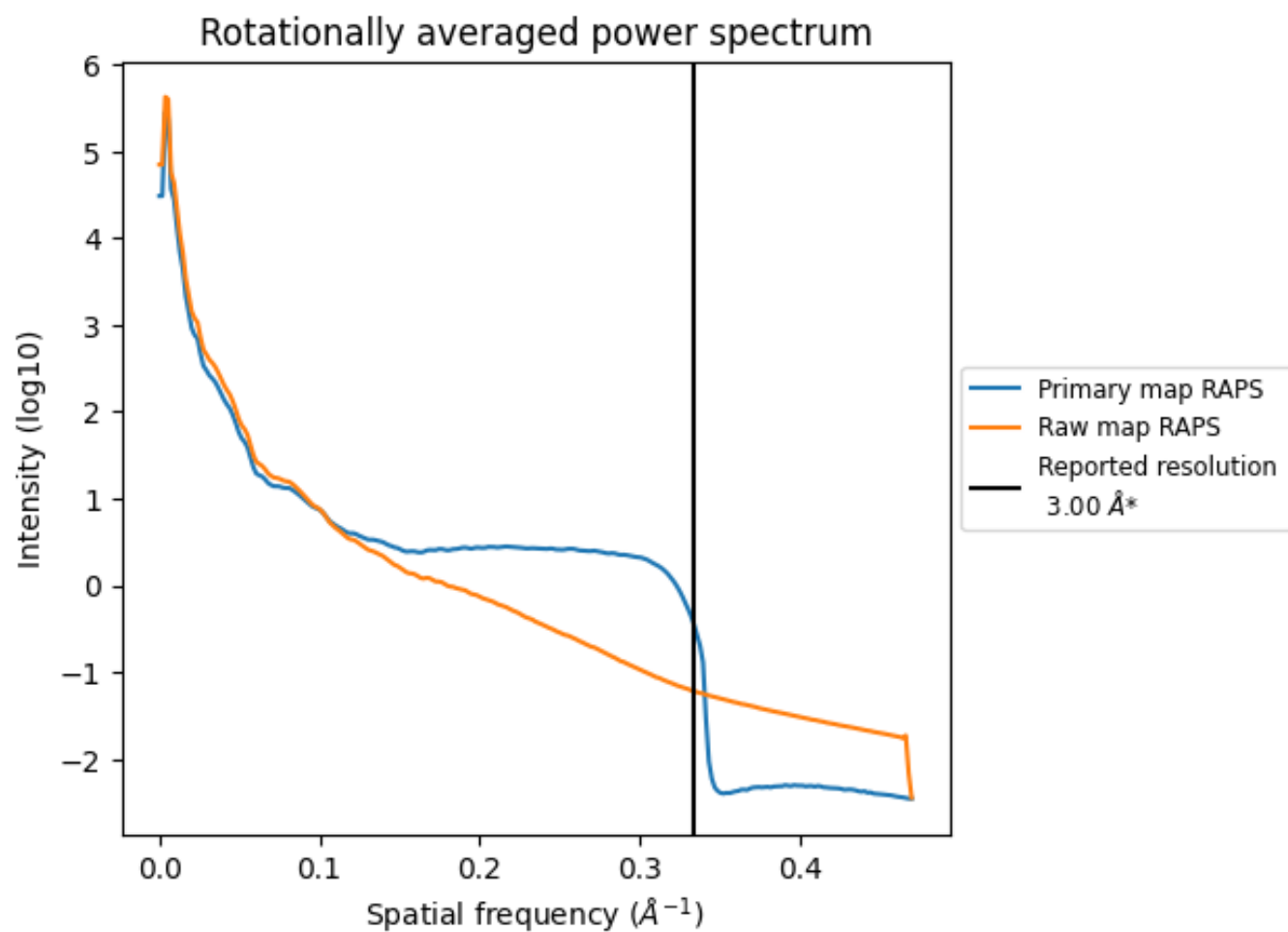
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1459 nm^3 ; this corresponds to an approximate mass of 1318 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 ⓘ

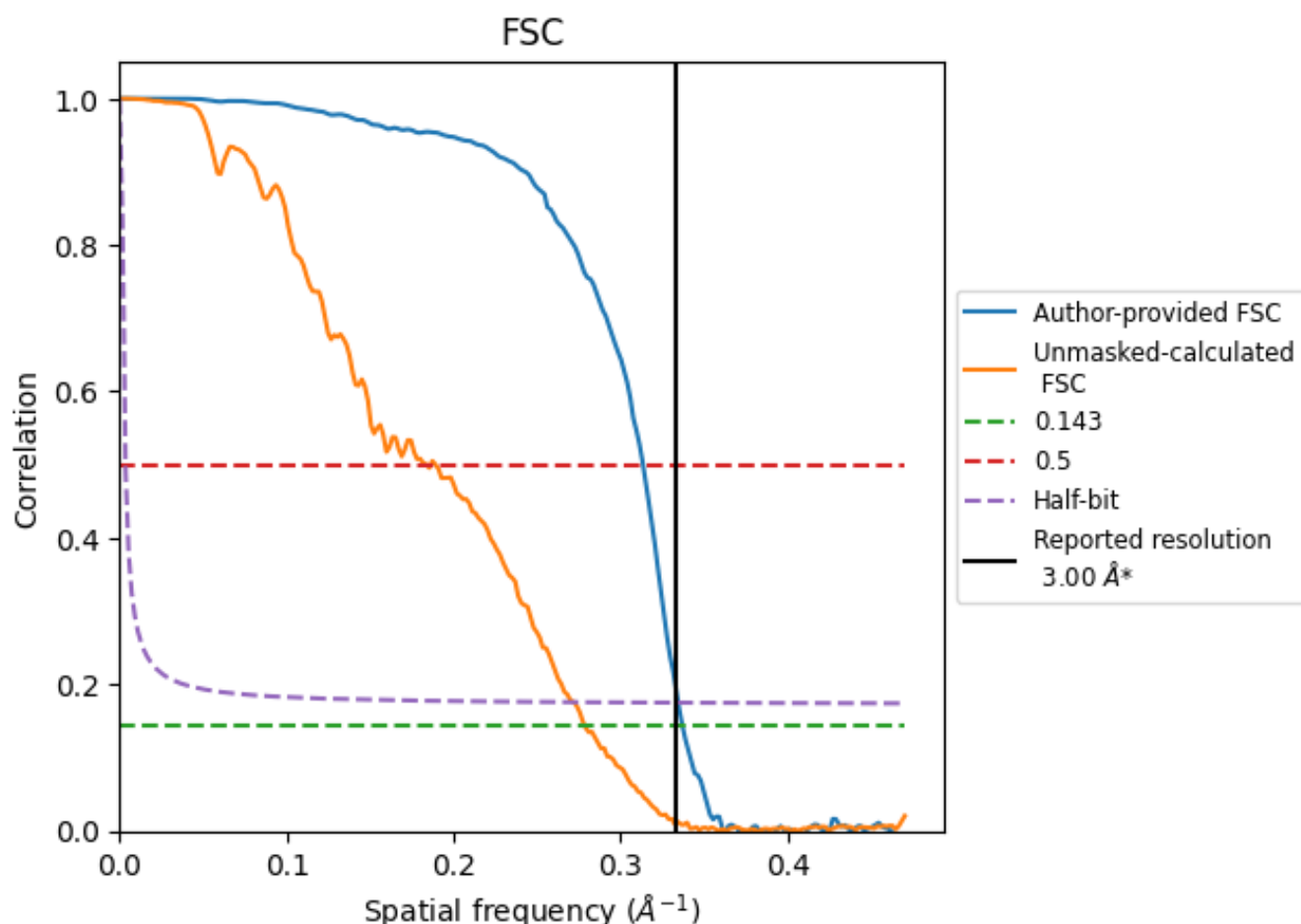


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

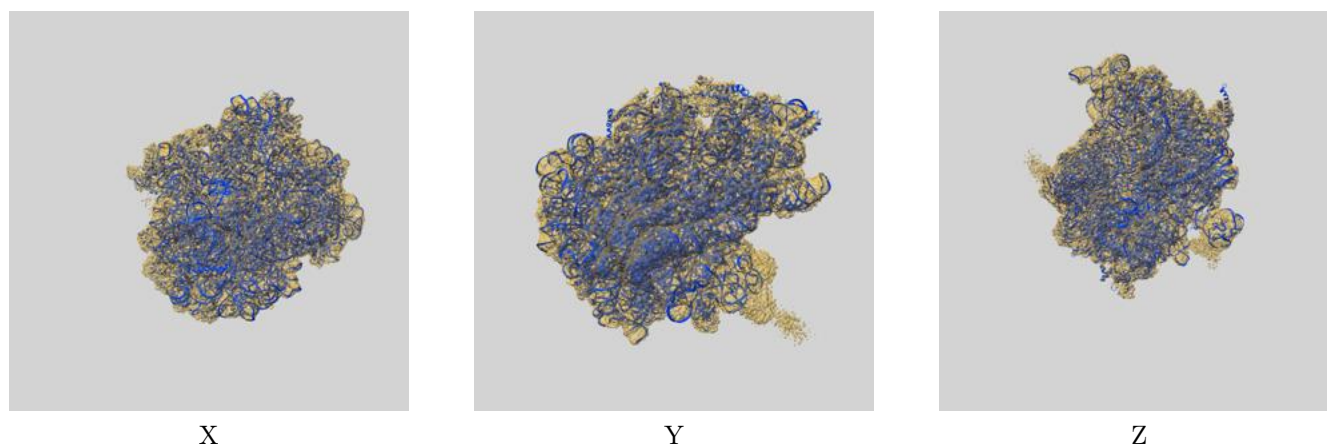
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.19	2.99
Unmasked-calculated*	3.59	5.44	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

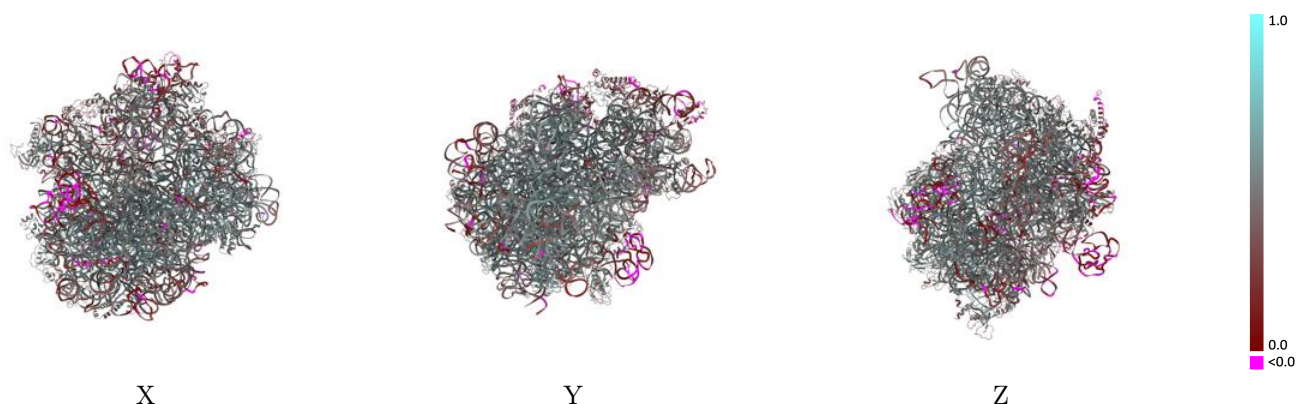
This section contains information regarding the fit between EMDB map EMD-16566 and PDB model 8CD1. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



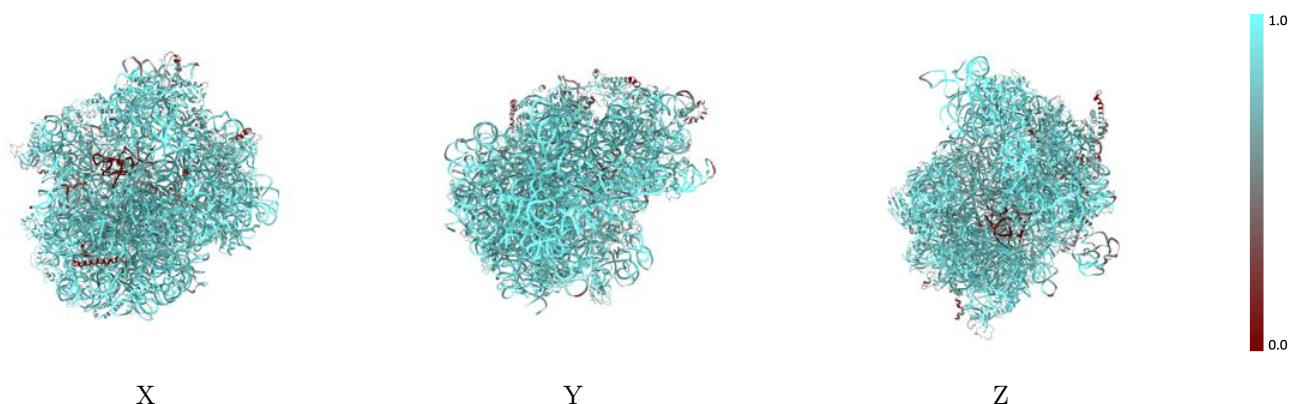
The images above show the 3D surface view of the map at the recommended contour level 3.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



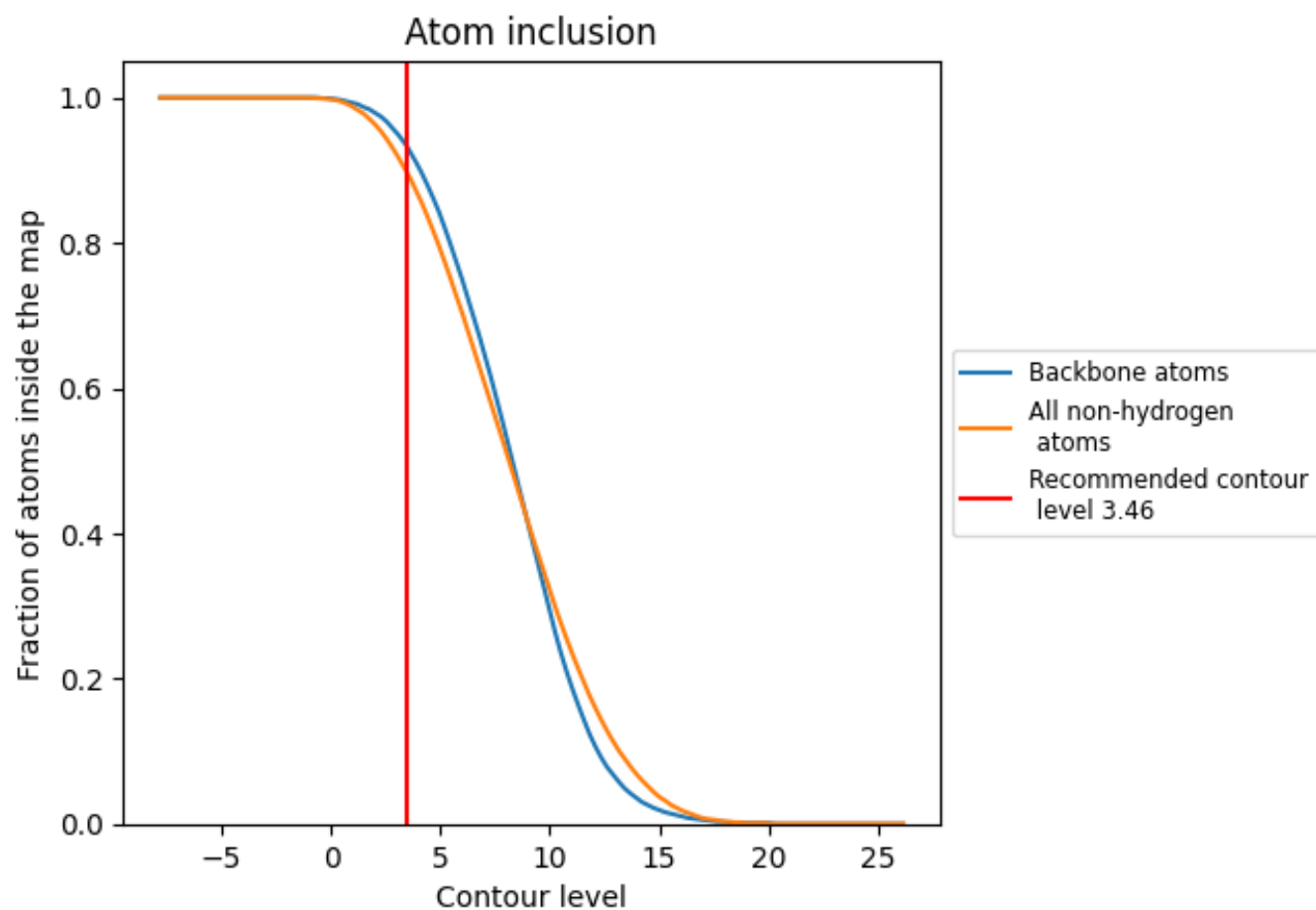
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.46).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (3.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.4610
2	 0.8800	 0.5090
4	 0.9330	 0.5560
5	 0.6800	 0.4950
6	 0.8960	 0.5200
A	 0.9400	 0.4550
B	 0.9300	 0.4200
C	 0.9020	 0.5320
D	 0.8950	 0.5120
Dt	 0.1470	 0.3840
E	 0.8990	 0.5220
F	 0.7810	 0.3700
G	 0.8210	 0.4400
H	 0.1530	 0.2090
J	 0.9060	 0.5310
K	 0.8330	 0.4870
L	 0.8800	 0.4960
Le	 0.7180	 0.3440
M	 0.8750	 0.5400
N	 0.9200	 0.5360
O	 0.8660	 0.4610
P	 0.8550	 0.4940
Q	 0.9290	 0.5520
R	 0.8940	 0.5230
S	 0.8790	 0.5210
T	 0.9020	 0.5250
U	 0.8180	 0.4650
V	 0.8200	 0.4580
W	 0.8750	 0.5090
X	 0.9000	 0.5260
Y	 0.8850	 0.4640
Z	 0.9140	 0.5280
a	 0.9630	 0.4840
b	 0.6390	 0.3340
c	 0.8060	 0.4230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.8360	 0.4510
e	 0.8150	 0.4450
f	 0.7900	 0.4050
g	 0.7650	 0.3770
h	 0.8740	 0.4970
i	 0.8530	 0.4170
j	 0.5110	 0.1420
k	 0.8480	 0.4720
l	 0.8320	 0.4750
m	 0.7860	 0.3550
n	 0.8650	 0.4270
o	 0.8730	 0.4910
p	 0.9250	 0.5130
q	 0.8600	 0.4860
r	 0.8000	 0.4290
s	 0.8260	 0.3850
t	 0.8990	 0.5050
u	 0.4290	 0.3630
v	 0.6920	 0.4530