



Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 06:52 pm GMT

PDB ID : 5NP6
EMDB ID : EMD-3618
Title : 70S structure prior to bypassing
Authors : Agirrezabala, X.; Samatova, E.; Klimova, M.; Zamora, M.; Gil-Carton, D.;
Rodnina, M.; Valle, M.
Deposited on : 2017-04-13
Resolution : 3.60 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 : 1.8.4, CSD as541be (2020)
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

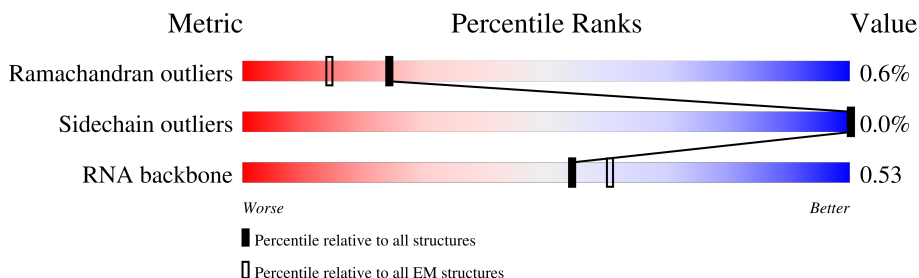
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



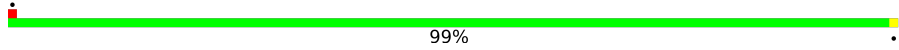
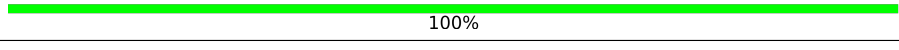
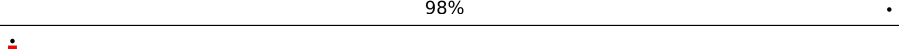
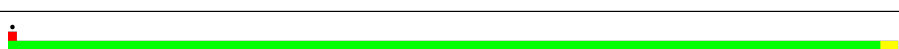

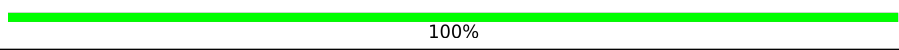
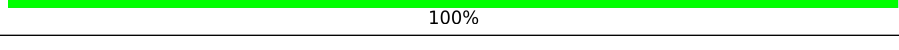
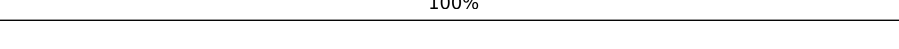


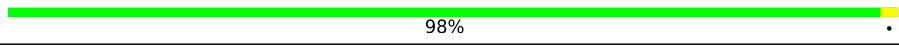
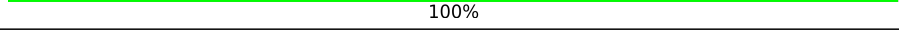
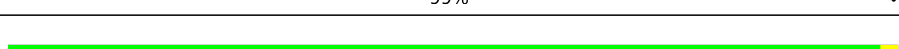
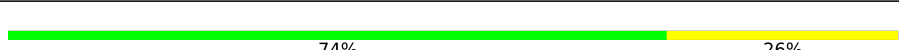

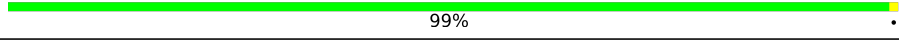
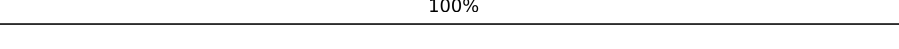

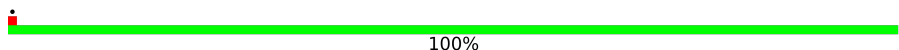
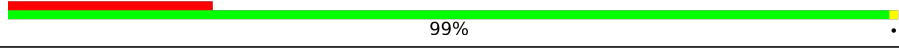
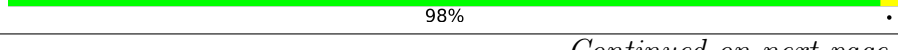



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	29	<div> <div>14%</div> <div>28%</div> <div>55%</div> <div>14%</div> <div>.</div> </div>
2	B	76	<div> <div>74%</div> <div>26%</div> </div>
3	C	46	<div> <div>46%</div> <div>98%</div> <div>.</div> </div>
4	D	1539	<div> <div>76%</div> <div>23%</div> </div>
5	E	218	<div> <div>100%</div> </div>
6	F	206	<div> <div>100%</div> </div>
7	G	205	<div> <div>100%</div> </div>
8	H	157	<div> <div>98%</div> <div>.</div> </div>

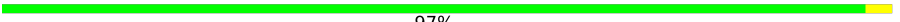
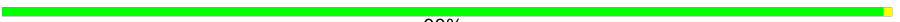








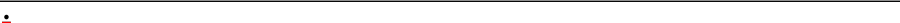

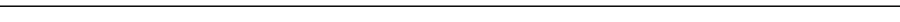


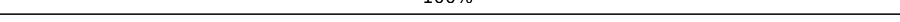
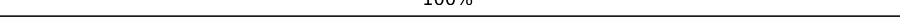
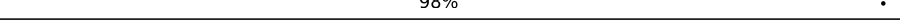
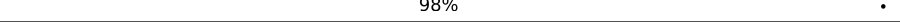
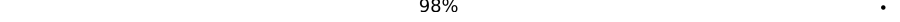
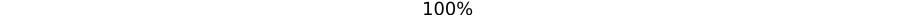
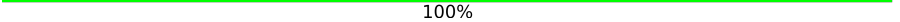
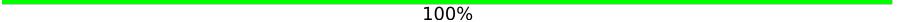
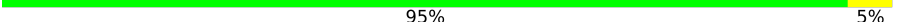
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Mol	Chain	Length	Quality of chain
9	I	100	
10	J	151	
11	K	129	
12	L	127	
13	M	98	
14	N	116	
15	O	123	
16	P	114	
17	Q	101	
18	R	88	
19	S	82	
20	T	80	
21	U	65	
22	V	79	
23	W	85	
24	X	65	
25	Y	2903	
26	Z	120	
27	a	271	
28	b	209	
29	c	201	
30	d	177	
31	e	176	
32	f	149	
33	g	141	

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Mol	Chain	Length	Quality of chain
34	h	142	 97% .
35	i	122	 99% .
36	j	143	 99% .
37	k	136	 100%
38	l	120	 99% .
39	m	116	 99% .
40	n	114	 99% .
41	o	117	 100%
42	p	103	 99% .
43	q	110	 100%
44	r	93	 100%
45	s	102	 100%
46	t	94	 100%
47	u	75	 100%
48	v	77	 100%
49	w	63	 100%
50	x	58	 98% .
51	y	56	 98% .
52	z	50	 98% .
53	0	46	 100%
54	1	64	 100%
55	2	38	 100%
56	3	131	 49% 95% 5%
57	4	66	 100%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146883 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	29	Total	C	N	O	P	0	0
			621	277	111	204	29		

- Molecule 2 is a RNA chain called P-site tRNA-Gly.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	76	Total	C	N	O	P	0	0
			1623	722	291	534	76		

- Molecule 3 is a protein called DNA topoisomerase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	46	Total	C	N	O	S	0	0
			362	222	65	71	4		

- Molecule 4 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1539	Total	C	N	O	P	0	0
			33028	14738	6052	10699	1539		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	35	ALA	-	insertion	UNP P0AG59

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	747	5MC	U	conflict	GB 802133627
Y	887	A	U	conflict	GB 802133627
Y	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	120	A	U	conflict	GB 1146054517

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	s	102	Total	C	N	O		0
			779	492	146	141		0

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	z	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	0	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

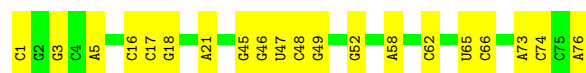
3 Residue-property plots

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.

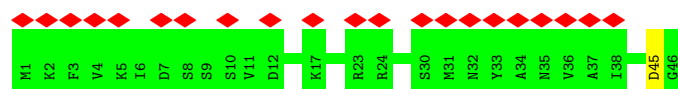
• Molecule 1: mRNA



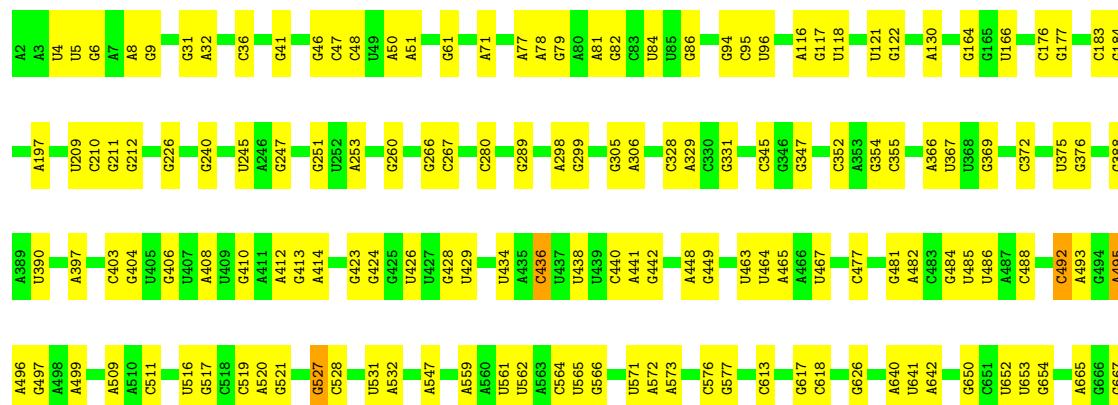
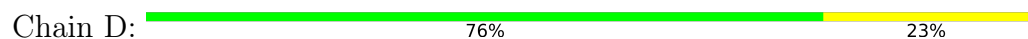
• Molecule 2: P-site tRNA-Gly

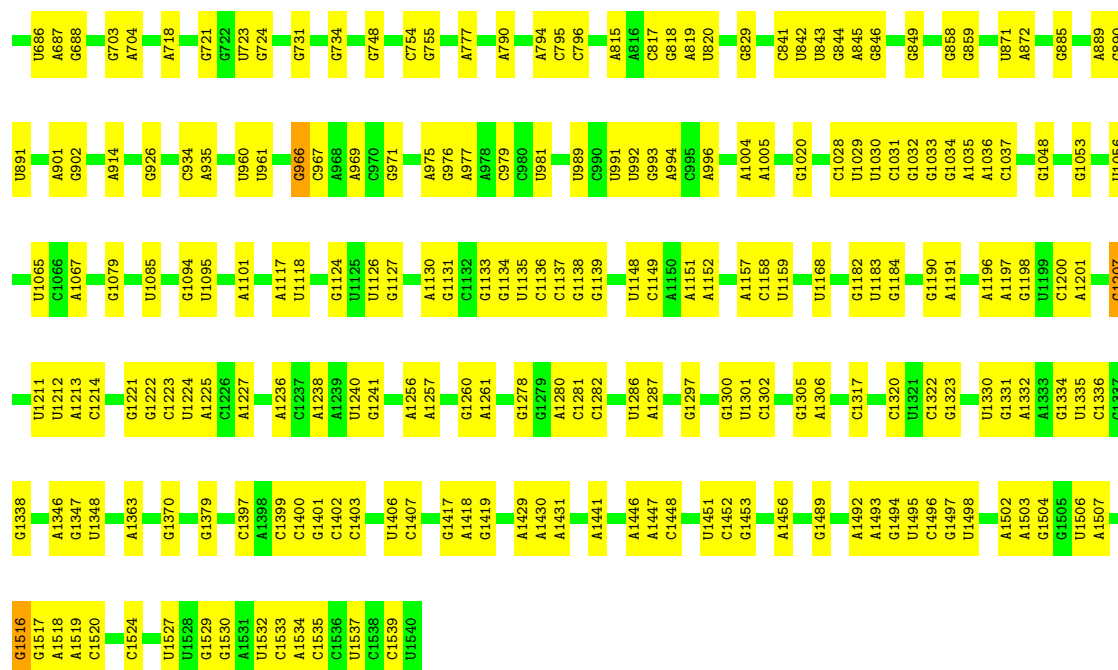


• Molecule 3: DNA topoisomerase small subunit



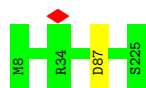
• Molecule 4: 16S ribosomal RNA





- Molecule 5: 30S ribosomal protein S2

Chain E: 100%



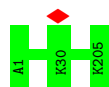
- Molecule 6: 30S ribosomal protein S3

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S ribosomal protein S4

Chain G: 100%



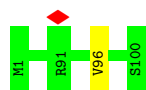
- Molecule 8: 30S ribosomal protein S5

Chain H: 98%



- Molecule 9: 30S ribosomal protein S6

Chain I:  99%



- Molecule 10: 30S ribosomal protein S7

Chain J:  100%

There are no outlier residues recorded for this chain.

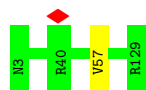
- Molecule 11: 30S ribosomal protein S8

Chain K:  98%



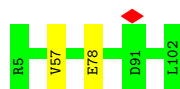
- Molecule 12: 30S ribosomal protein S9

Chain L:  99%



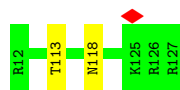
- Molecule 13: 30S ribosomal protein S10

Chain M:  98%



- Molecule 14: 30S ribosomal protein S11

Chain N:  98%



- Molecule 15: 30S ribosomal protein S12

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 30S ribosomal protein S13

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S ribosomal protein S14

Chain Q:  100%

There are no outlier residues recorded for this chain.

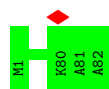
- Molecule 18: 30S ribosomal protein S15

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 30S ribosomal protein S16

Chain S:  100%



- Molecule 20: 30S ribosomal protein S17

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 30S ribosomal protein S18

Chain U:  98%



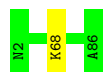
- Molecule 22: 30S ribosomal protein S19

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: 30S ribosomal protein S20

Chain W:  99%



- Molecule 24: 30S ribosomal protein S21

Chain X:  98%



• Molecule 25: 23S ribosomal RNA

Chain Y:



G1	A149	G291	U451	A586	A781	A941	G1062	G1139	U1313	G1491	G1649	G1842
A10	A158	A294	C455	C587	A782	A945	G1063	G1140	C1314	G1492	A1650	G1847
C11	U158	A294	C456	A603	A783	C946	C1084	U1141	C1314	A1493	G1651	A1848
U12	U162	U306	U464	A613	G785	G953	U1066	G1154	C1320	A1494	A1665	
A13	C163	G307	G465	U615	A789	G954	A1067	A1155	A1321	C1498	A1672	G1869
U25	G178	A310	G473	U616	A800	U955	A1069	A1168	U1326	A1504	G1673	G1870
G26	A181	U321	A479	A614	A805	A959	A1070	G1169	A1327	A1505	G1674	A1871
G35	G194	U322	A480	U615	G805	A960	C1072	A1328	U1329	A1508	G1687	A1872
G46	A195	A324	A482	A616	U810	C961	A1073	G1171	C1330	A1509	G1688	G1874
G51	A196	A324	A482	A616	U811	G966	G1074	C1172	G1341	A1515	G1689	G1875
A52	A199	A332	A482	A616	U812	U967	C1076	A1175	G1345	U1523	A1705	A1901
G55	A199	A332	A482	A616	U813	G971	C1077	U1176	C1345	G1524	C1706	G1906
U62	A204	A332	A482	A616	U814	A972	A1078	C1178	A1365	G1529	G1715	
A63	G205	A332	A482	A616	U815	A973	C1079	U1180	G1388	G1530	U1716	
A71	A216	A332	A482	A616	U816	G974	A1081	U1181	G1388	U1534	C1728	U1911
U72	A221	A332	A482	A616	U817	A983	U1082	G1212	A1373	A1535	U1729	A1912
A73	A222	A332	A482	A616	U818	A984	A1083	G1212	A1374	C1536	G1730	A1913
A74	A223	A332	A482	A616	U819	C985	A1084	G1221	U1379	C1537	G1731	3TD1915
G75	U224	A332	A482	A616	U820	C985	U1085	G1221	U1379	G1538	C1732	U1917
G77	A225	A332	A482	A616	U821	C985	A1086	G1221	U1379	U1539	G1733	
G78	A226	A332	A482	A616	U822	C985	A1087	U1234	A1383	G1540	G1734	C1920
C79	A227	A332	A482	A616	U823	C985	U1088	G1235	A1383	U1559	U1736	A1927
G80	C228	A332	A482	A616	U824	C985	A1089	G1236	A1383	G1560	G1737	A1928
G81	C229	A332	A482	A616	U825	C985	U1090	G1237	A1383	G1560	G1738	G1929
U82	G230	A332	A482	A616	U826	C985	U1091	A1247	A1392	A1569	A1755	U1931
G85	A233	A332	A482	A616	U827	C985	U1092	G1248	A1395	U1578	G1756	A1936
A91	C240	A332	A482	A616	U828	C985	U1093	U1249	A1395	U1578	G1757	A1937
U92	A241	A332	A482	A616	U829	C985	U1094	G1250	G1416	U1583	U1758	A1938
U100	G242	A332	A482	A616	U830	C985	U1095	C1251	A1419	U1584	C1764	U1939
A101	G245	A332	A482	A616	U831	C985	U1096	G1252	A1420	C1585	A1773	U1940
U102	G245	A332	A482	A616	U832	C985	U1097	U1253	G1425	A1586	U1781	C1941
A103	G245	A332	A482	A616	U833	C985	U1098	G1254	C1437	G1607	U1782	U1942
A111	G249	A332	A482	A616	U834	C985	U1099	U1255	C1451	A1610	A1783	U1955
U112	G250	A332	A482	A616	U835	C985	U1100	U1256	G1452	A1616	A1784	C1961
U113	G250	A332	A482	A616	U836	C985	U1101	U1257	G1453	A1617	C1800	C1962
U114	G250	A332	A482	A616	U837	C985	U1102	U1258	C1454	A1618	A1801	U1963
A118	G250	A332	A482	A616	U838	C985	U1103	U1259	U1458	A1626	A1802	G1964
A119	G250	A332	A482	A616	U839	C985	U1104	U1260	G1459	G1627	A1808	C1967
U120	G250	A332	A482	A616	U840	C985	U1105	U1261	U1460	A1632	A1816	A1970
A131	G250	A332	A482	A616	U841	C985	U1106	U1262	C1461	A1635	U1971	U1972
U138	G250	A332	A482	A616	U842	C985	U1107	U1263	G1475	U1636	A1829	G1972
U139	G250	A332	A482	A616	U843	C985	U1108	U1264	U1481	A1637	C1833	C1990
C140	G250	A332	A482	A616	U844	C985	U1109	U1265	G1482	U1648	U1834	U1991
A142	G250	A332	A482	A616	U845	C985	U1110	U1266	A1490		G1835	G1992





- Molecule 30: 50S ribosomal protein L5

Chain d: 100%

There are no outlier residues recorded for this chain.

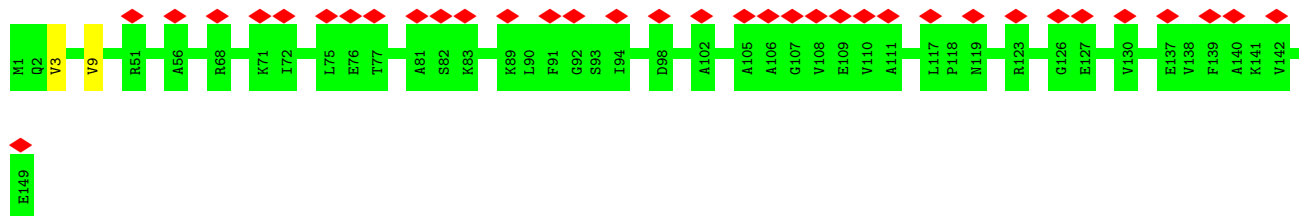
- Molecule 31: 50S ribosomal protein L6

Chain e: 100%



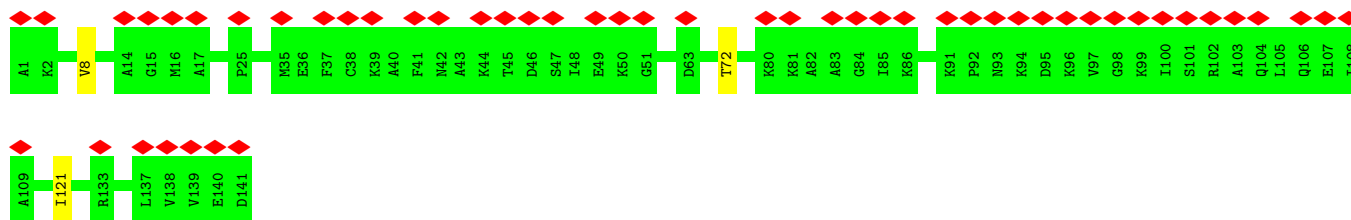
- Molecule 32: 50S ribosomal protein L9

Chain f: 23% 99%



- Molecule 33: 50S ribosomal protein L11

Chain g: 36% 98%



- Molecule 34: 50S ribosomal protein L13

Chain h: 97%



- Molecule 35: 50S ribosomal protein L14

Chain i: 99%



- Molecule 36: 50S ribosomal protein L15

Chain j:  99%



- Molecule 37: 50S ribosomal protein L16

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 50S ribosomal protein L17

Chain l:  99%



- Molecule 39: 50S ribosomal protein L18

Chain m:  99%



- Molecule 40: 50S ribosomal protein L19

Chain n:  99%



- Molecule 41: 50S ribosomal protein L20

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 50S ribosomal protein L21

Chain p:  99%



- Molecule 43: 50S ribosomal protein L22

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L23

Chain r:  100%



- Molecule 45: 50S ribosomal protein L24

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L25

Chain t:  100%


There are no outlier residues recorded for this chain.

- Molecule 47: 50S ribosomal protein L27

Chain u:  100%



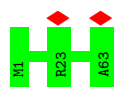
- Molecule 48: 50S ribosomal protein L28

Chain v:  100%

There are no outlier residues recorded for this chain.

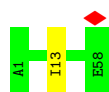
- Molecule 49: 50S ribosomal protein L29

Chain w:  100%



- Molecule 50: 50S ribosomal protein L30

Chain x:  98%



- Molecule 51: 50S ribosomal protein L32

Chain y: 98%



- Molecule 52: 50S ribosomal protein L33

Chain z: 98%



- Molecule 53: 50S ribosomal protein L34

Chain 0: 100%



- Molecule 54: 50S ribosomal protein L35

Chain 1: 100%

There are no outlier residues recorded for this chain.

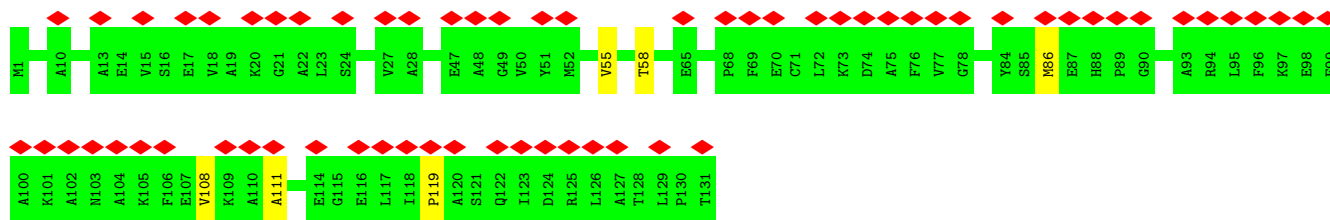
- Molecule 55: 50S ribosomal protein L36

Chain 2: 100%

There are no outlier residues recorded for this chain.

- Molecule 56: 50S ribosomal protein L10

Chain 3: 49% 95% 5%



- Molecule 57: 50S ribosomal protein L31

Chain 4:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction inside Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0045	Depositor
Map size (\AA)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, UR3, 7MG, 1MG, 6MZ, 2MG, MA6, 3TD, OMC, H2U, 5MU, 2MA, 5MC, OMG, PSU, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	1/694 (0.1%)	1.52	15/1078 (1.4%)
2	B	0.38	1/1812 (0.1%)	0.83	0/2822
3	C	0.29	0/365	0.56	0/485
4	D	0.29	1/36700 (0.0%)	0.82	7/57246 (0.0%)
5	E	0.30	0/1735	0.46	0/2338
6	F	0.28	0/1651	0.49	0/2225
7	G	0.31	0/1665	0.48	0/2227
8	H	0.28	0/1154	0.51	0/1554
9	I	0.28	0/835	0.51	0/1128
10	J	0.26	0/1195	0.43	0/1602
11	K	0.37	1/989 (0.1%)	0.50	0/1326
12	L	0.30	0/1034	0.53	0/1375
13	M	0.37	1/796 (0.1%)	0.50	0/1077
14	N	0.35	1/885 (0.1%)	0.51	0/1195
15	O	0.30	0/969	0.50	0/1300
16	P	0.26	0/892	0.46	0/1193
17	Q	0.27	0/811	0.47	0/1081
18	R	0.27	0/722	0.46	0/964
19	S	0.30	0/659	0.49	0/884
20	T	0.29	0/657	0.52	0/881
21	U	0.29	0/511	0.49	0/689
22	V	0.27	0/652	0.46	0/877
23	W	0.29	0/671	0.45	0/888
24	X	0.30	0/500	0.53	0/668
25	Y	0.30	2/69244 (0.0%)	0.84	26/108021 (0.0%)
26	Z	0.32	1/2876 (0.0%)	0.81	2/4483 (0.0%)
27	a	0.36	0/2121	0.51	0/2852
28	b	0.28	0/1586	0.49	0/2134
29	c	0.40	1/1571 (0.1%)	0.45	0/2113
30	d	0.27	0/1434	0.46	0/1926
31	e	0.26	0/1343	0.47	0/1816
32	f	0.30	0/1122	0.47	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.27	0/1046	0.50	0/1410
34	h	0.27	0/1152	0.46	0/1551
35	i	0.28	0/947	0.49	0/1268
36	j	0.34	0/1054	0.55	0/1403
37	k	0.29	0/1093	0.48	0/1460
38	l	0.27	0/973	0.45	0/1301
39	m	0.26	0/902	0.46	0/1209
40	n	0.34	0/929	0.49	0/1242
41	o	0.34	0/960	0.41	0/1278
42	p	0.28	0/829	0.51	0/1107
43	q	0.27	0/864	0.51	0/1156
44	r	0.26	0/744	0.45	0/994
45	s	0.32	0/787	0.49	0/1051
46	t	0.28	0/766	0.46	0/1025
47	u	0.29	0/582	0.47	0/769
48	v	0.27	0/635	0.45	0/848
49	w	0.35	0/510	0.44	0/677
50	x	0.25	0/453	0.45	0/605
51	y	0.25	0/450	0.46	0/599
52	z	0.26	0/416	0.48	0/554
53	0	0.27	0/380	0.46	0/498
54	1	0.26	0/513	0.56	0/676
55	2	0.28	0/303	0.51	0/397
56	3	0.28	0/1001	0.51	0/1350
57	4	0.27	0/531	0.47	0/709
All	All	0.30	10/158671 (0.0%)	0.76	50/237100 (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
1	A	3	3
5	E	0	1
23	W	0	1
40	n	0	1
56	3	0	2
All	All	3	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-11.91	1.46	1.61
25	Y	1	G	OP3-P	-10.62	1.48	1.61
26	Z	1	U	OP3-P	-10.58	1.48	1.61
2	B	1	C	OP3-P	-10.57	1.48	1.61
29	c	128	ALA	C-N	10.24	1.53	1.34
4	D	1489	G	O3'-P	-9.70	1.49	1.61
11	K	55	LYS	C-N	7.79	1.49	1.34
13	M	78	GLU	C-N	7.42	1.48	1.34
25	Y	2508	G	O3'-P	6.40	1.68	1.61
14	N	113	THR	C-N	6.19	1.46	1.34

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	G	N1-C6-O6	-9.46	114.22	119.90
4	D	436	C	N3-C2-O2	-8.68	115.82	121.90
4	D	495	A	O4'-C1'-N9	8.13	114.71	108.20
25	Y	1941	C	C2-N1-C1'	7.93	127.53	118.80
4	D	492	C	N3-C2-O2	-7.78	116.45	121.90
25	Y	1104	C	N3-C2-O2	-7.73	116.49	121.90
26	Z	36	C	C2-N1-C1'	7.30	126.83	118.80
1	A	18	C	N3-C2-O2	-7.23	116.84	121.90
4	D	492	C	N1-C2-O2	7.09	123.16	118.90
4	D	492	C	C6-N1-C2	-6.89	117.54	120.30
25	Y	1104	C	N1-C2-O2	6.83	123.00	118.90
1	A	16	G	N1-C6-O6	-6.65	115.91	119.90
1	A	13	U	O4'-C1'-N1	6.64	113.51	108.20
1	A	14	C	N3-C2-O2	-6.60	117.28	121.90
4	D	754	C	C2-N1-C1'	6.47	125.92	118.80
1	A	10	C	N3-C2-O2	-6.31	117.48	121.90
25	Y	1941	C	N1-C2-O2	6.27	122.66	118.90
1	A	15	G	C5-C6-O6	6.20	132.32	128.60
1	A	11	C	N3-C2-O2	-6.11	117.62	121.90
25	Y	1313	U	C2-N1-C1'	6.03	124.94	117.70
25	Y	1920	C	C2-N1-C1'	5.98	125.38	118.80
1	A	17	G	N1-C6-O6	-5.94	116.33	119.90
25	Y	1081	U	C2-N1-C1'	5.80	124.66	117.70
1	A	18	C	N1-C2-O2	5.75	122.35	118.90
25	Y	1941	C	C6-N1-C1'	-5.66	114.00	120.80
25	Y	924	G	N3-C4-N9	-5.62	122.62	126.00
25	Y	1081	U	N3-C2-O2	-5.61	118.27	122.20
1	A	15	G	P-O3'-C3'	5.48	126.28	119.70
1	A	15	G	N3-C2-N2	-5.48	116.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	854	C	N3-C2-O2	-5.48	118.06	121.90
1	A	16	G	O4'-C1'-N9	5.43	112.55	108.20
25	Y	1941	C	N3-C2-O2	-5.40	118.12	121.90
25	Y	1326	U	C2-N1-C1'	5.39	124.17	117.70
25	Y	114	U	C2-N1-C1'	5.34	124.11	117.70
25	Y	1099	G	C6-C5-N7	-5.34	127.20	130.40
26	Z	36	C	C6-N1-C2	-5.33	118.17	120.30
1	A	13	U	C3'-C2'-C1'	5.29	105.73	101.50
25	Y	2592	G	C4-N9-C1'	5.27	133.35	126.50
25	Y	2592	G	C8-N9-C1'	-5.27	120.15	127.00
25	Y	62	U	C2-N1-C1'	5.23	123.98	117.70
1	A	14	C	N1-C2-O2	5.22	122.03	118.90
25	Y	2244	U	C5-C4-O4	-5.21	122.77	125.90
25	Y	1314	C	C2-N1-C1'	5.21	124.53	118.80
25	Y	1099	G	C4-N9-C1'	5.18	133.23	126.50
4	D	754	C	C6-N1-C1'	-5.14	114.63	120.80
25	Y	2244	U	N3-C4-O4	5.13	122.99	119.40
25	Y	1081	U	N1-C2-O2	5.02	126.32	122.80
25	Y	1920	C	C6-N1-C1'	-5.02	114.77	120.80
25	Y	1099	G	N3-C4-N9	5.01	129.01	126.00
25	Y	2025	C	C2-N1-C1'	5.01	124.31	118.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	15	G	C4',C2',C3'

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	3	58	THR	Peptide
56	3	86	MET	Peptide
1	A	13	U	Sidechain
1	A	17	G	Sidechain
1	A	18	C	Sidechain
5	E	87	ASP	Peptide
23	W	68	LYS	Peptide
40	n	33	GLU	Peptide

5.2 Too-close contacts ⓘ

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	
3	C	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	5	31
5	E	216/218 (99%)	177 (82%)	39 (18%)	0	100	100
6	F	204/206 (99%)	178 (87%)	26 (13%)	0	100	100
7	G	203/205 (99%)	162 (80%)	41 (20%)	0	100	100
8	H	155/157 (99%)	128 (83%)	24 (16%)	3 (2%)	6	35
9	I	98/100 (98%)	79 (81%)	18 (18%)	1 (1%)	13	46
10	J	149/151 (99%)	124 (83%)	25 (17%)	0	100	100
11	K	127/129 (98%)	107 (84%)	19 (15%)	1 (1%)	16	51
12	L	125/127 (98%)	95 (76%)	29 (23%)	1 (1%)	16	51
13	M	96/98 (98%)	75 (78%)	20 (21%)	1 (1%)	13	46
14	N	114/116 (98%)	97 (85%)	16 (14%)	1 (1%)	14	48
15	O	121/123 (98%)	101 (84%)	20 (16%)	0	100	100
16	P	112/114 (98%)	91 (81%)	21 (19%)	0	100	100
17	Q	99/101 (98%)	75 (76%)	24 (24%)	0	100	100
18	R	86/88 (98%)	66 (77%)	20 (23%)	0	100	100
19	S	80/82 (98%)	66 (82%)	14 (18%)	0	100	100
20	T	78/80 (98%)	69 (88%)	9 (12%)	0	100	100
21	U	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	8	38
22	V	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
23	W	83/85 (98%)	66 (80%)	17 (20%)	0	100	100
24	X	63/65 (97%)	41 (65%)	21 (33%)	1 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	a	269/271 (99%)	241 (90%)	28 (10%)	0	100	100
28	b	207/209 (99%)	184 (89%)	23 (11%)	0	100	100
29	c	199/201 (99%)	172 (86%)	26 (13%)	1 (0%)	25	59
30	d	175/177 (99%)	151 (86%)	24 (14%)	0	100	100
31	e	174/176 (99%)	153 (88%)	21 (12%)	0	100	100
32	f	147/149 (99%)	121 (82%)	24 (16%)	2 (1%)	9	40
33	g	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	5	32
34	h	140/142 (99%)	129 (92%)	7 (5%)	4 (3%)	3	27
35	i	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	16	51
36	j	141/143 (99%)	121 (86%)	18 (13%)	2 (1%)	9	40
37	k	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
38	l	118/120 (98%)	98 (83%)	19 (16%)	1 (1%)	16	51
39	m	114/116 (98%)	92 (81%)	21 (18%)	1 (1%)	14	48
40	n	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
41	o	115/117 (98%)	92 (80%)	23 (20%)	0	100	100
42	p	101/103 (98%)	89 (88%)	11 (11%)	1 (1%)	13	46
43	q	108/110 (98%)	92 (85%)	16 (15%)	0	100	100
44	r	91/93 (98%)	74 (81%)	17 (19%)	0	100	100
45	s	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
46	t	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
47	u	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
48	v	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
49	w	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
50	x	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	7	35
51	y	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	6	35
52	z	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	5	33
53	0	44/46 (96%)	35 (80%)	9 (20%)	0	100	100
54	1	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
55	2	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
56	3	129/131 (98%)	102 (79%)	23 (18%)	4 (3%)	3	26
57	4	64/66 (97%)	53 (83%)	11 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5891/5995 (98%)	4979 (84%)	878 (15%)	34 (1%)	24	55

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	45	ASP
34	h	81	ILE
52	z	4	ILE
8	H	122	VAL
39	m	35	ILE
13	M	57	VAL
21	U	17	VAL
34	h	137	PRO
56	3	108	VAL
56	3	119	PRO
8	H	25	LYS
12	L	57	VAL
35	i	35	VAL
56	3	111	ALA
11	K	48	PHE
33	g	8	VAL
33	g	72	THR
14	N	118	ASN
24	X	10	PRO
32	f	9	VAL
34	h	136	GLN
38	l	70	THR
36	j	111	ILE
29	c	83	VAL
33	g	121	ILE
56	3	55	VAL
8	H	93	VAL
9	I	96	VAL
32	f	3	VAL
34	h	100	VAL
36	j	85	VAL
51	y	2	VAL
42	p	54	VAL
50	x	13	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	
3	C	42/42 (100%)	42 (100%)	0	100	100
5	E	180/180 (100%)	180 (100%)	0	100	100
6	F	170/170 (100%)	170 (100%)	0	100	100
7	G	172/172 (100%)	172 (100%)	0	100	100
8	H	114/119 (96%)	114 (100%)	0	100	100
9	I	87/87 (100%)	87 (100%)	0	100	100
10	J	124/124 (100%)	124 (100%)	0	100	100
11	K	104/104 (100%)	104 (100%)	0	100	100
12	L	105/105 (100%)	105 (100%)	0	100	100
13	M	86/86 (100%)	86 (100%)	0	100	100
14	N	89/89 (100%)	89 (100%)	0	100	100
15	O	103/103 (100%)	103 (100%)	0	100	100
16	P	92/92 (100%)	92 (100%)	0	100	100
17	Q	79/83 (95%)	79 (100%)	0	100	100
18	R	76/76 (100%)	76 (100%)	0	100	100
19	S	65/65 (100%)	65 (100%)	0	100	100
20	T	74/74 (100%)	74 (100%)	0	100	100
21	U	48/56 (86%)	48 (100%)	0	100	100
22	V	70/70 (100%)	70 (100%)	0	100	100
23	W	65/65 (100%)	65 (100%)	0	100	100
24	X	44/55 (80%)	44 (100%)	0	100	100
27	a	216/216 (100%)	214 (99%)	2 (1%)	75	87
28	b	164/164 (100%)	164 (100%)	0	100	100
29	c	165/165 (100%)	165 (100%)	0	100	100
30	d	148/148 (100%)	148 (100%)	0	100	100
31	e	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	f	114/114 (100%)	114 (100%)	0	100	100
33	g	109/109 (100%)	109 (100%)	0	100	100
34	h	116/116 (100%)	116 (100%)	0	100	100
35	i	103/103 (100%)	103 (100%)	0	100	100
36	j	102/102 (100%)	102 (100%)	0	100	100
37	k	109/109 (100%)	109 (100%)	0	100	100
38	l	100/100 (100%)	100 (100%)	0	100	100
39	m	86/86 (100%)	86 (100%)	0	100	100
40	n	99/99 (100%)	99 (100%)	0	100	100
41	o	89/89 (100%)	89 (100%)	0	100	100
42	p	84/84 (100%)	84 (100%)	0	100	100
43	q	93/93 (100%)	93 (100%)	0	100	100
44	r	80/80 (100%)	80 (100%)	0	100	100
45	s	83/83 (100%)	83 (100%)	0	100	100
46	t	78/78 (100%)	78 (100%)	0	100	100
47	u	57/57 (100%)	57 (100%)	0	100	100
48	v	67/67 (100%)	67 (100%)	0	100	100
49	w	55/55 (100%)	55 (100%)	0	100	100
50	x	48/48 (100%)	48 (100%)	0	100	100
51	y	47/47 (100%)	47 (100%)	0	100	100
52	z	45/45 (100%)	45 (100%)	0	100	100
53	0	38/38 (100%)	38 (100%)	0	100	100
54	1	51/51 (100%)	51 (100%)	0	100	100
55	2	34/34 (100%)	34 (100%)	0	100	100
56	3	100/100 (100%)	100 (100%)	0	100	100
57	4	59/59 (100%)	59 (100%)	0	100	100
All	All	4865/4893 (99%)	4863 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	a	85	ASN
27	a	259	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	28/29 (96%)	14 (50%)	8 (28%)
2	B	75/76 (98%)	18 (24%)	3 (4%)
25	Y	2898/2903 (99%)	673 (23%)	123 (4%)
26	Z	119/120 (99%)	22 (18%)	6 (5%)
4	D	1535/1539 (99%)	327 (21%)	58 (3%)
All	All	4655/4667 (99%)	1054 (22%)	198 (4%)

All (1054) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	A
1	A	7	U
1	A	8	A
1	A	15	G
1	A	16	G
1	A	20	A
1	A	22	C
1	A	23	U
1	A	24	A
1	A	25	U
1	A	26	A
1	A	27	G
1	A	28	A
1	A	29	A
2	B	3	G
2	B	5	A
2	B	16	C
2	B	17	C
2	B	18	G
2	B	21	A
2	B	46	G
2	B	47	U
2	B	48	C
2	B	49	G
2	B	52	G
2	B	58	A
2	B	62	C

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Mol	Chain	Res	Type
2	B	65	U
2	B	66	C
2	B	73	A
2	B	74	C
2	B	76	A
4	D	4	U
4	D	6	G
4	D	8	A
4	D	9	G
4	D	31	G
4	D	32	A
4	D	36	C
4	D	41	G
4	D	46	G
4	D	47	C
4	D	48	C
4	D	50	A
4	D	51	A
4	D	61	G
4	D	71	A
4	D	77	A
4	D	78	A
4	D	79	G
4	D	81	A
4	D	82	G
4	D	84	U
4	D	86	G
4	D	94	G
4	D	96	U
4	D	116	A
4	D	117	G
4	D	118	U
4	D	121	U
4	D	122	G
4	D	130	A
4	D	164	G
4	D	166	U
4	D	177	G
4	D	183	C
4	D	184	G
4	D	197	A
4	D	209	U

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Mol	Chain	Res	Type
4	D	210	C
4	D	211	G
4	D	212	G
4	D	226	G
4	D	240	G
4	D	245	U
4	D	247	G
4	D	251	G
4	D	253	A
4	D	260	G
4	D	266	G
4	D	267	C
4	D	280	C
4	D	289	G
4	D	299	G
4	D	305	G
4	D	306	A
4	D	328	C
4	D	329	A
4	D	331	G
4	D	345	C
4	D	347	G
4	D	352	C
4	D	354	G
4	D	355	C
4	D	366	A
4	D	367	U
4	D	369	G
4	D	372	C
4	D	376	G
4	D	388	G
4	D	390	U
4	D	397	A
4	D	404	G
4	D	406	G
4	D	408	A
4	D	410	G
4	D	412	A
4	D	413	G
4	D	414	A
4	D	423	G
4	D	424	G

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Mol	Chain	Res	Type
4	D	426	U
4	D	429	U
4	D	434	U
4	D	436	C
4	D	438	U
4	D	440	C
4	D	441	A
4	D	442	G
4	D	449	G
4	D	463	U
4	D	465	A
4	D	467	U
4	D	477	C
4	D	481	G
4	D	482	A
4	D	484	G
4	D	485	U
4	D	486	U
4	D	488	C
4	D	492	C
4	D	493	A
4	D	495	A
4	D	496	A
4	D	497	G
4	D	499	A
4	D	509	A
4	D	511	C
4	D	517	G
4	D	519	C
4	D	520	A
4	D	521	G
4	D	527	7MG
4	D	528	C
4	D	531	U
4	D	532	A
4	D	547	A
4	D	559	A
4	D	562	U
4	D	564	C
4	D	565	U
4	D	566	G
4	D	571	U

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Mol	Chain	Res	Type
4	D	572	A
4	D	573	A
4	D	576	C
4	D	577	G
4	D	613	C
4	D	618	C
4	D	626	G
4	D	640	A
4	D	641	U
4	D	642	A
4	D	650	G
4	D	653	U
4	D	654	G
4	D	665	A
4	D	667	G
4	D	687	A
4	D	688	G
4	D	703	G
4	D	704	A
4	D	718	A
4	D	721	G
4	D	723	U
4	D	724	G
4	D	731	G
4	D	734	G
4	D	748	G
4	D	755	G
4	D	777	A
4	D	790	A
4	D	794	A
4	D	795	C
4	D	796	C
4	D	815	A
4	D	817	C
4	D	818	G
4	D	819	A
4	D	820	U
4	D	829	G
4	D	842	U
4	D	843	U
4	D	844	G
4	D	845	A

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Mol	Chain	Res	Type
4	D	846	G
4	D	849	G
4	D	858	G
4	D	859	G
4	D	872	A
4	D	885	G
4	D	890	G
4	D	891	U
4	D	901	A
4	D	902	G
4	D	914	A
4	D	926	G
4	D	934	C
4	D	935	A
4	D	960	U
4	D	961	U
4	D	966	2MG
4	D	969	A
4	D	971	G
4	D	975	A
4	D	976	G
4	D	977	A
4	D	979	C
4	D	981	U
4	D	989	U
4	D	992	U
4	D	993	G
4	D	994	A
4	D	996	A
4	D	1004	A
4	D	1005	A
4	D	1020	G
4	D	1028	C
4	D	1029	U
4	D	1030	U
4	D	1031	C
4	D	1032	G
4	D	1033	G
4	D	1034	G
4	D	1035	A
4	D	1036	A
4	D	1037	C

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Mol	Chain	Res	Type
4	D	1048	G
4	D	1053	G
4	D	1056	U
4	D	1065	U
4	D	1067	A
4	D	1079	G
4	D	1085	U
4	D	1094	G
4	D	1095	U
4	D	1101	A
4	D	1117	A
4	D	1118	U
4	D	1124	G
4	D	1126	U
4	D	1127	G
4	D	1130	A
4	D	1131	G
4	D	1133	G
4	D	1134	G
4	D	1135	U
4	D	1136	C
4	D	1137	C
4	D	1138	G
4	D	1139	G
4	D	1149	C
4	D	1151	A
4	D	1152	A
4	D	1157	A
4	D	1158	C
4	D	1159	U
4	D	1168	U
4	D	1183	U
4	D	1184	G
4	D	1191	A
4	D	1196	A
4	D	1197	A
4	D	1198	G
4	D	1200	C
4	D	1201	A
4	D	1207	2MG
4	D	1212	U
4	D	1213	A

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Mol	Chain	Res	Type
4	D	1214	C
4	D	1222	G
4	D	1223	C
4	D	1224	U
4	D	1225	A
4	D	1227	A
4	D	1236	A
4	D	1238	A
4	D	1240	U
4	D	1241	G
4	D	1256	A
4	D	1257	A
4	D	1260	G
4	D	1261	A
4	D	1278	G
4	D	1280	A
4	D	1282	C
4	D	1286	U
4	D	1287	A
4	D	1297	G
4	D	1300	G
4	D	1301	U
4	D	1302	C
4	D	1306	A
4	D	1317	C
4	D	1320	C
4	D	1322	C
4	D	1323	G
4	D	1331	G
4	D	1332	A
4	D	1334	G
4	D	1335	U
4	D	1336	C
4	D	1338	G
4	D	1346	A
4	D	1347	G
4	D	1348	U
4	D	1363	A
4	D	1370	G
4	D	1379	G
4	D	1397	C
4	D	1400	C

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Mol	Chain	Res	Type
4	D	1401	G
4	D	1403	C
4	D	1406	U
4	D	1417	G
4	D	1418	A
4	D	1419	G
4	D	1429	A
4	D	1431	A
4	D	1441	A
4	D	1446	A
4	D	1448	C
4	D	1452	C
4	D	1453	G
4	D	1456	A
4	D	1492	A
4	D	1493	A
4	D	1494	G
4	D	1495	U
4	D	1496	C
4	D	1497	G
4	D	1502	A
4	D	1503	A
4	D	1504	G
4	D	1506	U
4	D	1507	A
4	D	1516	2MG
4	D	1517	G
4	D	1520	C
4	D	1524	C
4	D	1527	U
4	D	1529	G
4	D	1530	G
4	D	1532	U
4	D	1533	C
4	D	1534	A
4	D	1535	C
4	D	1537	U
4	D	1539	C
25	Y	10	A
25	Y	12	U
25	Y	13	A
25	Y	26	G

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Mol	Chain	Res	Type
25	Y	35	G
25	Y	46	G
25	Y	51	G
25	Y	52	A
25	Y	55	G
25	Y	63	A
25	Y	71	A
25	Y	72	U
25	Y	74	A
25	Y	75	G
25	Y	78	U
25	Y	80	G
25	Y	82	U
25	Y	85	G
25	Y	91	A
25	Y	92	U
25	Y	100	U
25	Y	101	A
25	Y	102	U
25	Y	103	A
25	Y	112	U
25	Y	113	U
25	Y	114	U
25	Y	118	A
25	Y	120	U
25	Y	131	A
25	Y	138	U
25	Y	139	U
25	Y	140	C
25	Y	141	G
25	Y	142	A
25	Y	149	A
25	Y	158	U
25	Y	162	U
25	Y	163	C
25	Y	178	G
25	Y	181	A
25	Y	194	G
25	Y	196	A
25	Y	199	A
25	Y	204	A
25	Y	205	G

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Mol	Chain	Res	Type
25	Y	216	A
25	Y	221	A
25	Y	222	A
25	Y	223	A
25	Y	224	U
25	Y	226	A
25	Y	228	C
25	Y	229	C
25	Y	230	G
25	Y	233	A
25	Y	241	A
25	Y	242	G
25	Y	245	G
25	Y	248	G
25	Y	250	G
25	Y	255	A
25	Y	266	G
25	Y	276	U
25	Y	277	G
25	Y	278	A
25	Y	279	A
25	Y	280	U
25	Y	281	C
25	Y	282	A
25	Y	285	G
25	Y	286	U
25	Y	291	G
25	Y	294	A
25	Y	306	U
25	Y	307	G
25	Y	310	A
25	Y	321	U
25	Y	323	C
25	Y	324	A
25	Y	329	G
25	Y	330	A
25	Y	332	A
25	Y	340	A
25	Y	358	U
25	Y	361	G
25	Y	362	A
25	Y	366	C

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Mol	Chain	Res	Type
25	Y	370	G
25	Y	372	G
25	Y	373	U
25	Y	386	G
25	Y	387	U
25	Y	389	G
25	Y	396	G
25	Y	402	A
25	Y	403	U
25	Y	404	A
25	Y	405	U
25	Y	406	G
25	Y	412	A
25	Y	421	C
25	Y	422	A
25	Y	424	G
25	Y	430	A
25	Y	451	U
25	Y	455	C
25	Y	456	C
25	Y	457	A
25	Y	464	U
25	Y	465	G
25	Y	473	G
25	Y	479	A
25	Y	480	A
25	Y	481	G
25	Y	482	A
25	Y	491	G
25	Y	503	A
25	Y	505	A
25	Y	508	A
25	Y	509	C
25	Y	510	C
25	Y	518	G
25	Y	527	C
25	Y	528	A
25	Y	529	A
25	Y	531	C
25	Y	532	A
25	Y	543	G
25	Y	545	U

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Mol	Chain	Res	Type
25	Y	546	U
25	Y	547	A
25	Y	548	G
25	Y	550	C
25	Y	556	A
25	Y	563	A
25	Y	568	U
25	Y	569	U
25	Y	570	G
25	Y	572	A
25	Y	573	U
25	Y	575	A
25	Y	586	A
25	Y	587	C
25	Y	603	A
25	Y	613	A
25	Y	614	A
25	Y	615	U
25	Y	616	A
25	Y	627	A
25	Y	637	A
25	Y	645	C
25	Y	646	U
25	Y	647	G
25	Y	653	U
25	Y	654	A
25	Y	655	A
25	Y	670	A
25	Y	676	A
25	Y	677	A
25	Y	686	U
25	Y	687	C
25	Y	705	A
25	Y	715	A
25	Y	717	C
25	Y	729	G
25	Y	730	A
25	Y	736	C
25	Y	747	5MC
25	Y	748	G
25	Y	752	A
25	Y	757	G

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Mol	Chain	Res	Type
25	Y	764	A
25	Y	765	C
25	Y	775	G
25	Y	776	G
25	Y	781	A
25	Y	782	A
25	Y	784	G
25	Y	785	G
25	Y	789	A
25	Y	800	A
25	Y	805	G
25	Y	811	U
25	Y	812	C
25	Y	819	A
25	Y	827	U
25	Y	828	U
25	Y	844	A
25	Y	845	A
25	Y	846	U
25	Y	860	U
25	Y	878	A
25	Y	883	G
25	Y	887	A
25	Y	888	C
25	Y	890	C
25	Y	891	G
25	Y	895	U
25	Y	896	A
25	Y	897	C
25	Y	904	G
25	Y	907	G
25	Y	910	A
25	Y	914	G
25	Y	915	C
25	Y	932	U
25	Y	933	A
25	Y	941	A
25	Y	945	A
25	Y	946	C
25	Y	953	G
25	Y	959	A
25	Y	961	C

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Mol	Chain	Res	Type
25	Y	966	G
25	Y	967	U
25	Y	972	A
25	Y	973	A
25	Y	974	G
25	Y	983	A
25	Y	985	C
25	Y	995	C
25	Y	996	A
25	Y	997	G
25	Y	1005	C
25	Y	1008	A
25	Y	1009	A
25	Y	1012	U
25	Y	1013	C
25	Y	1021	A
25	Y	1022	G
25	Y	1023	U
25	Y	1025	G
25	Y	1026	G
25	Y	1033	U
25	Y	1034	G
25	Y	1046	A
25	Y	1047	G
25	Y	1053	C
25	Y	1054	A
25	Y	1056	G
25	Y	1057	A
25	Y	1058	U
25	Y	1060	U
25	Y	1061	U
25	Y	1062	G
25	Y	1063	G
25	Y	1065	U
25	Y	1066	U
25	Y	1068	G
25	Y	1069	A
25	Y	1070	A
25	Y	1071	G
25	Y	1072	C
25	Y	1073	A
25	Y	1075	C

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Mol	Chain	Res	Type
25	Y	1076	C
25	Y	1077	A
25	Y	1078	U
25	Y	1079	C
25	Y	1081	U
25	Y	1082	U
25	Y	1085	A
25	Y	1087	G
25	Y	1088	A
25	Y	1089	A
25	Y	1095	A
25	Y	1097	U
25	Y	1101	U
25	Y	1103	A
25	Y	1104	C
25	Y	1105	U
25	Y	1106	G
25	Y	1108	U
25	Y	1109	C
25	Y	1110	G
25	Y	1112	G
25	Y	1119	U
25	Y	1126	A
25	Y	1131	G
25	Y	1132	U
25	Y	1134	A
25	Y	1135	C
25	Y	1136	G
25	Y	1139	G
25	Y	1141	U
25	Y	1142	A
25	Y	1154	G
25	Y	1155	A
25	Y	1169	A
25	Y	1171	G
25	Y	1172	C
25	Y	1175	A
25	Y	1176	U
25	Y	1177	G
25	Y	1178	C
25	Y	1180	U
25	Y	1181	U

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Mol	Chain	Res	Type
25	Y	1212	G
25	Y	1221	C
25	Y	1235	G
25	Y	1237	A
25	Y	1247	A
25	Y	1248	G
25	Y	1249	U
25	Y	1251	C
25	Y	1252	G
25	Y	1253	A
25	Y	1255	U
25	Y	1256	G
25	Y	1257	C
25	Y	1265	A
25	Y	1270	C
25	Y	1271	G
25	Y	1272	A
25	Y	1273	U
25	Y	1280	G
25	Y	1284	A
25	Y	1288	G
25	Y	1300	G
25	Y	1301	A
25	Y	1306	C
25	Y	1321	A
25	Y	1327	A
25	Y	1328	A
25	Y	1329	U
25	Y	1330	C
25	Y	1341	G
25	Y	1345	C
25	Y	1365	A
25	Y	1368	G
25	Y	1374	G
25	Y	1378	A
25	Y	1379	U
25	Y	1383	A
25	Y	1386	C
25	Y	1392	A
25	Y	1395	A
25	Y	1416	G
25	Y	1419	A

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Mol	Chain	Res	Type
25	Y	1420	A
25	Y	1425	G
25	Y	1437	C
25	Y	1451	C
25	Y	1452	G
25	Y	1454	C
25	Y	1458	U
25	Y	1459	G
25	Y	1460	U
25	Y	1461	C
25	Y	1475	G
25	Y	1481	U
25	Y	1482	G
25	Y	1490	A
25	Y	1491	G
25	Y	1493	C
25	Y	1494	A
25	Y	1498	C
25	Y	1504	A
25	Y	1505	A
25	Y	1509	A
25	Y	1515	A
25	Y	1524	G
25	Y	1529	G
25	Y	1530	G
25	Y	1534	U
25	Y	1535	A
25	Y	1536	C
25	Y	1537	G
25	Y	1538	G
25	Y	1540	G
25	Y	1559	U
25	Y	1560	G
25	Y	1569	A
25	Y	1578	U
25	Y	1584	U
25	Y	1585	C
25	Y	1587	G
25	Y	1607	C
25	Y	1610	A
25	Y	1616	A
25	Y	1617	C

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Mol	Chain	Res	Type
25	Y	1627	G
25	Y	1632	A
25	Y	1635	A
25	Y	1637	A
25	Y	1648	U
25	Y	1649	G
25	Y	1651	G
25	Y	1665	A
25	Y	1672	A
25	Y	1673	G
25	Y	1674	G
25	Y	1687	G
25	Y	1698	A
25	Y	1699	G
25	Y	1706	C
25	Y	1715	G
25	Y	1716	U
25	Y	1729	U
25	Y	1730	C
25	Y	1731	G
25	Y	1732	C
25	Y	1733	G
25	Y	1735	A
25	Y	1736	U
25	Y	1738	G
25	Y	1755	A
25	Y	1758	U
25	Y	1764	C
25	Y	1773	A
25	Y	1781	U
25	Y	1782	U
25	Y	1784	A
25	Y	1800	C
25	Y	1801	A
25	Y	1802	A
25	Y	1808	A
25	Y	1816	C
25	Y	1829	A
25	Y	1833	C
25	Y	1835	2MG
25	Y	1842	G
25	Y	1848	A

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Mol	Chain	Res	Type
25	Y	1869	G
25	Y	1871	A
25	Y	1873	G
25	Y	1876	A
25	Y	1901	A
25	Y	1906	G
25	Y	1912	A
25	Y	1913	A
25	Y	1914	C
25	Y	1927	A
25	Y	1928	A
25	Y	1929	G
25	Y	1930	G
25	Y	1931	U
25	Y	1936	A
25	Y	1937	A
25	Y	1938	A
25	Y	1939	5MU
25	Y	1940	U
25	Y	1941	C
25	Y	1942	C
25	Y	1943	U
25	Y	1955	U
25	Y	1962	5MC
25	Y	1964	G
25	Y	1967	C
25	Y	1970	A
25	Y	1971	U
25	Y	1972	G
25	Y	1990	C
25	Y	1991	U
25	Y	1993	U
25	Y	1997	C
25	Y	2002	G
25	Y	2005	A
25	Y	2006	C
25	Y	2007	U
25	Y	2020	A
25	Y	2022	U
25	Y	2023	C
25	Y	2031	A
25	Y	2033	A

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Mol	Chain	Res	Type
25	Y	2034	U
25	Y	2036	C
25	Y	2043	C
25	Y	2049	G
25	Y	2051	A
25	Y	2055	C
25	Y	2056	G
25	Y	2060	A
25	Y	2061	G
25	Y	2062	A
25	Y	2063	C
25	Y	2069	7MG
25	Y	2072	C
25	Y	2076	U
25	Y	2092	U
25	Y	2093	G
25	Y	2096	C
25	Y	2107	G
25	Y	2110	G
25	Y	2112	G
25	Y	2113	U
25	Y	2118	U
25	Y	2119	A
25	Y	2120	G
25	Y	2122	U
25	Y	2123	G
25	Y	2124	G
25	Y	2125	G
25	Y	2127	G
25	Y	2128	G
25	Y	2131	U
25	Y	2132	U
25	Y	2133	G
25	Y	2134	A
25	Y	2135	A
25	Y	2136	G
25	Y	2138	G
25	Y	2140	G
25	Y	2145	C
25	Y	2146	C
25	Y	2147	A
25	Y	2149	U

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Mol	Chain	Res	Type
25	Y	2150	C
25	Y	2152	G
25	Y	2162	G
25	Y	2163	A
25	Y	2164	C
25	Y	2166	U
25	Y	2168	G
25	Y	2171	A
25	Y	2172	U
25	Y	2173	A
25	Y	2174	C
25	Y	2175	C
25	Y	2177	C
25	Y	2178	C
25	Y	2188	U
25	Y	2198	A
25	Y	2199	A
25	Y	2204	G
25	Y	2211	A
25	Y	2213	U
25	Y	2214	C
25	Y	2225	A
25	Y	2238	G
25	Y	2239	G
25	Y	2249	U
25	Y	2250	G
25	Y	2266	A
25	Y	2268	A
25	Y	2278	A
25	Y	2279	G
25	Y	2283	C
25	Y	2287	A
25	Y	2288	A
25	Y	2297	A
25	Y	2305	U
25	Y	2311	A
25	Y	2318	G
25	Y	2320	U
25	Y	2325	G
25	Y	2327	A
25	Y	2328	A
25	Y	2333	A

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Mol	Chain	Res	Type
25	Y	2337	G
25	Y	2340	A
25	Y	2345	G
25	Y	2347	C
25	Y	2354	C
25	Y	2361	G
25	Y	2379	G
25	Y	2382	G
25	Y	2383	G
25	Y	2385	C
25	Y	2388	A
25	Y	2402	U
25	Y	2403	C
25	Y	2406	A
25	Y	2407	A
25	Y	2423	U
25	Y	2424	C
25	Y	2425	A
25	Y	2428	G
25	Y	2429	G
25	Y	2430	A
25	Y	2441	U
25	Y	2445	2MG
25	Y	2447	G
25	Y	2448	A
25	Y	2449	H2U
25	Y	2452	C
25	Y	2473	U
25	Y	2475	C
25	Y	2476	A
25	Y	2478	A
25	Y	2492	U
25	Y	2496	C
25	Y	2497	A
25	Y	2499	C
25	Y	2500	U
25	Y	2501	C
25	Y	2502	G
25	Y	2504	PSU
25	Y	2505	G
25	Y	2506	U
25	Y	2507	C

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Mol	Chain	Res	Type
25	Y	2518	A
25	Y	2520	C
25	Y	2530	A
25	Y	2531	A
25	Y	2535	G
25	Y	2543	G
25	Y	2547	A
25	Y	2554	U
25	Y	2567	G
25	Y	2573	C
25	Y	2576	G
25	Y	2577	A
25	Y	2581	G
25	Y	2584	U
25	Y	2585	U
25	Y	2586	U
25	Y	2597	G
25	Y	2602	A
25	Y	2603	G
25	Y	2609	U
25	Y	2610	C
25	Y	2612	C
25	Y	2613	U
25	Y	2614	A
25	Y	2615	U
25	Y	2630	G
25	Y	2644	G
25	Y	2645	G
25	Y	2646	C
25	Y	2655	G
25	Y	2656	U
25	Y	2682	A
25	Y	2689	U
25	Y	2690	U
25	Y	2714	G
25	Y	2716	C
25	Y	2725	A
25	Y	2726	A
25	Y	2731	G
25	Y	2733	A
25	Y	2744	G
25	Y	2751	G

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Mol	Chain	Res	Type
25	Y	2758	A
25	Y	2764	A
25	Y	2765	A
25	Y	2776	A
25	Y	2778	A
25	Y	2779	U
25	Y	2780	G
25	Y	2781	A
25	Y	2790	U
25	Y	2791	G
25	Y	2793	C
25	Y	2794	C
25	Y	2797	U
25	Y	2798	U
25	Y	2799	A
25	Y	2800	A
25	Y	2808	G
25	Y	2809	A
25	Y	2818	U
25	Y	2820	A
25	Y	2821	A
25	Y	2825	G
25	Y	2833	U
25	Y	2834	G
25	Y	2848	G
25	Y	2849	U
25	Y	2859	G
25	Y	2861	U
25	Y	2866	U
25	Y	2867	G
25	Y	2868	A
25	Y	2873	A
25	Y	2879	A
25	Y	2880	C
25	Y	2884	U
25	Y	2893	A
25	Y	2894	G
25	Y	2900	A
25	Y	2903	U
26	Z	2	G
26	Z	4	C
26	Z	9	G

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Mol	Chain	Res	Type
26	Z	13	G
26	Z	14	U
26	Z	15	A
26	Z	35	C
26	Z	36	C
26	Z	37	C
26	Z	42	C
26	Z	44	G
26	Z	45	A
26	Z	51	G
26	Z	57	A
26	Z	66	A
26	Z	67	G
26	Z	88	C
26	Z	89	U
26	Z	90	C
26	Z	108	A
26	Z	109	A
26	Z	120	A

All (198) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	15	G
1	A	22	C
1	A	23	U
1	A	24	A
1	A	25	U
1	A	26	A
1	A	27	G
1	A	28	A
2	B	17	C
2	B	45	G
2	B	47	U
4	D	5	U
4	D	81	A
4	D	95	C
4	D	116	A
4	D	176	C
4	D	183	C
4	D	298	A
4	D	375	U

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Mol	Chain	Res	Type
4	D	403	C
4	D	413	G
4	D	428	G
4	D	448	A
4	D	464	U
4	D	492	C
4	D	519	C
4	D	561	U
4	D	564	C
4	D	617	G
4	D	640	A
4	D	641	U
4	D	652	U
4	D	686	U
4	D	703	G
4	D	723	U
4	D	841	C
4	D	871	U
4	D	889	A
4	D	890	G
4	D	960	U
4	D	991	U
4	D	1094	G
4	D	1134	G
4	D	1148	U
4	D	1151	A
4	D	1182	G
4	D	1183	U
4	D	1190	G
4	D	1196	A
4	D	1200	C
4	D	1211	U
4	D	1221	G
4	D	1240	U
4	D	1256	A
4	D	1281	C
4	D	1300	G
4	D	1301	U
4	D	1305	G
4	D	1330	U
4	D	1331	G
4	D	1347	G

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Mol	Chain	Res	Type
4	D	1399	C
4	D	1417	G
4	D	1430	A
4	D	1447	A
4	D	1451	U
4	D	1492	A
4	D	1493	A
4	D	1494	G
25	Y	12	U
25	Y	25	U
25	Y	51	G
25	Y	91	A
25	Y	100	U
25	Y	111	A
25	Y	223	A
25	Y	227	A
25	Y	240	C
25	Y	279	A
25	Y	280	U
25	Y	328	U
25	Y	339	U
25	Y	369	U
25	Y	372	G
25	Y	401	A
25	Y	402	A
25	Y	404	A
25	Y	421	C
25	Y	455	C
25	Y	464	U
25	Y	481	G
25	Y	490	C
25	Y	507	A
25	Y	546	U
25	Y	549	G
25	Y	555	G
25	Y	569	U
25	Y	614	A
25	Y	636	G
25	Y	669	G
25	Y	704	G
25	Y	774	G
25	Y	810	U

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Mol	Chain	Res	Type
25	Y	859	G
25	Y	889	C
25	Y	894	U
25	Y	896	A
25	Y	931	U
25	Y	960	A
25	Y	966	G
25	Y	971	G
25	Y	984	A
25	Y	1020	A
25	Y	1046	A
25	Y	1055	G
25	Y	1060	U
25	Y	1071	G
25	Y	1076	C
25	Y	1094	U
25	Y	1103	A
25	Y	1104	C
25	Y	1109	C
25	Y	1111	A
25	Y	1130	U
25	Y	1168	G
25	Y	1171	G
25	Y	1176	U
25	Y	1234	U
25	Y	1236	G
25	Y	1320	C
25	Y	1327	A
25	Y	1328	A
25	Y	1373	A
25	Y	1378	A
25	Y	1453	A
25	Y	1508	A
25	Y	1523	U
25	Y	1583	A
25	Y	1584	U
25	Y	1626	A
25	Y	1672	A
25	Y	1705	A
25	Y	1715	G
25	Y	1728	C
25	Y	1730	C

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Mol	Chain	Res	Type
25	Y	1757	A
25	Y	1834	U
25	Y	1847	G
25	Y	1875	G
25	Y	1930	G
25	Y	1941	C
25	Y	1942	C
25	Y	1961	C
25	Y	2006	C
25	Y	2019	A
25	Y	2048	G
25	Y	2050	C
25	Y	2112	G
25	Y	2121	G
25	Y	2122	U
25	Y	2123	G
25	Y	2127	G
25	Y	2149	U
25	Y	2212	A
25	Y	2248	C
25	Y	2286	G
25	Y	2326	C
25	Y	2405	G
25	Y	2406	A
25	Y	2423	U
25	Y	2428	G
25	Y	2495	G
25	Y	2496	C
25	Y	2499	C
25	Y	2566	A
25	Y	2580	PSU
25	Y	2583	G
25	Y	2602	A
25	Y	2629	U
25	Y	2643	G
25	Y	2644	G
25	Y	2655	G
25	Y	2790	U
25	Y	2798	U
25	Y	2808	G
25	Y	2820	A
25	Y	2824	C

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Mol	Chain	Res	Type
25	Y	2832	U
25	Y	2848	G
25	Y	2858	C
25	Y	2867	G
25	Y	2893	A
26	Z	3	C
26	Z	12	C
26	Z	44	G
26	Z	66	A
26	Z	87	U
26	Z	88	C

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

35 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
25	PSU	Y	2457	25	18,21,22	1.01	1 (5%)	22,30,33	1.84	4 (18%)
4	5MC	D	1407	4	18,22,23	3.74	7 (38%)	26,32,35	1.04	1 (3%)
25	5MU	Y	1939	25	19,22,23	4.76	7 (36%)	28,32,35	3.56	9 (32%)
25	PSU	Y	2604	25	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)
25	PSU	Y	1917	25	18,21,22	1.05	1 (5%)	22,30,33	1.81	5 (22%)
4	PSU	D	516	4	18,21,22	1.09	1 (5%)	22,30,33	1.84	6 (27%)
25	5MC	Y	1962	25	18,22,23	3.81	7 (38%)	26,32,35	1.08	2 (7%)
25	PSU	Y	1911	25	18,21,22	1.03	1 (5%)	22,30,33	1.85	5 (22%)
25	OMC	Y	2498	25	19,22,23	3.01	7 (36%)	26,31,34	0.70	0
25	1MG	Y	745	25	18,26,27	2.73	5 (27%)	19,39,42	1.44	4 (21%)
25	2MG	Y	1835	25	18,26,27	2.62	7 (38%)	16,38,41	1.42	4 (25%)
25	PSU	Y	2504	25	18,21,22	1.02	2 (11%)	22,30,33	1.94	5 (22%)
4	7MG	D	527	4	22,26,27	3.82	10 (45%)	29,39,42	2.09	9 (31%)
25	OMG	Y	2251	2,25	18,26,27	2.62	8 (44%)	19,38,41	1.77	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MA6	D	1518	4	18,26,27	1.02	2 (11%)	19,38,41	2.53	2 (10%)
25	7MG	Y	2069	25	22,26,27	3.74	10 (45%)	29,39,42	1.98	8 (27%)
4	2MG	D	1207	4	18,26,27	2.64	7 (38%)	16,38,41	1.34	3 (18%)
25	2MA	Y	2503	25	19,25,26	3.29	6 (31%)	21,37,40	1.49	3 (14%)
4	UR3	D	1498	4	19,22,23	2.74	8 (42%)	26,32,35	1.23	1 (3%)
25	6MZ	Y	2030	25	18,25,26	2.14	3 (16%)	16,36,39	2.14	3 (18%)
25	5MC	Y	747	25	18,22,23	3.78	7 (38%)	26,32,35	1.05	2 (7%)
4	4OC	D	1402	4	20,23,24	0.79	0	26,32,35	1.15	2 (7%)
25	PSU	Y	2605	25	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
25	OMU	Y	2552	25	19,22,23	3.02	8 (42%)	26,31,34	1.66	4 (15%)
25	PSU	Y	955	25	18,21,22	1.07	1 (5%)	22,30,33	1.81	5 (22%)
25	PSU	Y	2580	25	18,21,22	0.98	1 (5%)	22,30,33	1.84	4 (18%)
25	6MZ	Y	1618	25	18,25,26	2.18	3 (16%)	16,36,39	1.75	3 (18%)
4	2MG	D	1516	4	18,26,27	2.65	7 (38%)	16,38,41	1.31	3 (18%)
4	MA6	D	1519	4	18,26,27	1.01	2 (11%)	19,38,41	2.56	2 (10%)
25	3TD	Y	1915	25	18,22,23	4.40	5 (27%)	22,32,35	1.61	3 (13%)
25	2MG	Y	2445	25	18,26,27	2.64	7 (38%)	16,38,41	1.37	4 (25%)
4	5MC	D	967	4	18,22,23	3.77	7 (38%)	26,32,35	1.09	2 (7%)
25	PSU	Y	746	25	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
25	H2U	Y	2449	25	18,21,22	3.00	5 (27%)	21,30,33	2.11	5 (23%)
4	2MG	D	966	4	18,26,27	2.66	7 (38%)	16,38,41	1.41	4 (25%)

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
25	PSU	Y	2457	25	-	0/7/25/26	0/2/2/2
4	5MC	D	1407	4	-	1/7/25/26	0/2/2/2
25	5MU	Y	1939	25	-	2/7/25/26	0/2/2/2
25	PSU	Y	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	Y	1917	25	-	0/7/25/26	0/2/2/2
4	PSU	D	516	4	-	0/7/25/26	0/2/2/2
25	5MC	Y	1962	25	-	3/7/25/26	0/2/2/2
25	PSU	Y	1911	25	-	1/7/25/26	0/2/2/2
25	OMC	Y	2498	25	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	1MG	Y	745	25	-	0/3/25/26	0/3/3/3
25	2MG	Y	1835	25	-	2/5/27/28	0/3/3/3
25	PSU	Y	2504	25	-	2/7/25/26	0/2/2/2
4	7MG	D	527	4	-	3/7/37/38	0/3/3/3
25	OMG	Y	2251	2,25	-	1/5/27/28	0/3/3/3
4	MA6	D	1518	4	-	4/7/29/30	0/3/3/3
25	7MG	Y	2069	25	-	2/7/37/38	0/3/3/3
4	2MG	D	1207	4	-	2/5/27/28	0/3/3/3
25	2MA	Y	2503	25	-	2/3/25/26	0/3/3/3
4	UR3	D	1498	4	-	2/7/25/26	0/2/2/2
25	6MZ	Y	2030	25	-	3/5/27/28	0/3/3/3
25	5MC	Y	747	25	-	3/7/25/26	0/2/2/2
4	4OC	D	1402	4	-	4/9/29/30	0/2/2/2
25	PSU	Y	2605	25	-	0/7/25/26	0/2/2/2
25	OMU	Y	2552	25	-	5/9/27/28	0/2/2/2
25	PSU	Y	955	25	-	2/7/25/26	0/2/2/2
25	PSU	Y	2580	25	-	0/7/25/26	0/2/2/2
25	6MZ	Y	1618	25	-	0/5/27/28	0/3/3/3
4	2MG	D	1516	4	-	2/5/27/28	0/3/3/3
4	MA6	D	1519	4	-	6/7/29/30	0/3/3/3
25	3TD	Y	1915	25	-	3/7/25/26	0/2/2/2
25	2MG	Y	2445	25	-	2/5/27/28	0/3/3/3
4	5MC	D	967	4	-	0/7/25/26	0/2/2/2
25	PSU	Y	746	25	-	4/7/25/26	0/2/2/2
25	H2U	Y	2449	25	-	2/7/38/39	0/2/2/2
4	2MG	D	966	4	-	2/5/27/28	0/3/3/3

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	1915	3TD	C6-C5	13.21	1.50	1.35
25	Y	1939	5MU	C2-N1	11.02	1.56	1.38
25	Y	1939	5MU	C6-N1	10.16	1.55	1.38
25	Y	1939	5MU	C4-C5	9.99	1.61	1.44
4	D	527	7MG	C8-N9	9.93	1.51	1.46
4	D	1407	5MC	C6-C5	9.82	1.50	1.34
25	Y	1915	3TD	C2-N1	9.71	1.49	1.37
25	Y	2069	7MG	C8-N9	9.51	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	1962	5MC	C6-C5	9.39	1.50	1.34
25	Y	747	5MC	C6-C5	9.35	1.50	1.34
4	D	967	5MC	C6-C5	9.31	1.49	1.34
25	Y	2449	H2U	C2-N1	9.06	1.48	1.35
25	Y	2503	2MA	C4-N3	8.75	1.49	1.35
25	Y	1618	6MZ	C6-N6	7.90	1.48	1.35
25	Y	1939	5MU	C4-N3	-7.71	1.24	1.38
25	Y	2030	6MZ	C6-N6	7.70	1.47	1.35
25	Y	745	1MG	C2-N2	7.44	1.47	1.34
25	Y	1962	5MC	C4-N3	7.24	1.46	1.34
25	Y	2069	7MG	C5-N7	7.24	1.43	1.35
4	D	967	5MC	C4-N3	7.19	1.46	1.34
25	Y	747	5MC	C4-N3	7.11	1.46	1.34
25	Y	2503	2MA	C2-N3	7.08	1.46	1.34
4	D	527	7MG	C5-N7	7.01	1.43	1.35
25	Y	2552	OMU	C2-N3	6.98	1.50	1.38
4	D	1498	UR3	C2-N1	6.94	1.48	1.38
25	Y	2552	OMU	C2-N1	6.90	1.49	1.38
25	Y	1962	5MC	C2-N3	6.57	1.49	1.36
4	D	1407	5MC	C4-N3	6.57	1.45	1.34
25	Y	747	5MC	C2-N3	6.46	1.49	1.36
4	D	967	5MC	C2-N3	6.43	1.49	1.36
25	Y	2449	H2U	C2-N3	6.40	1.49	1.38
25	Y	2498	OMC	C6-C5	6.39	1.49	1.35
25	Y	2498	OMC	C2-N3	6.34	1.49	1.36
4	D	1516	2MG	C2-N2	6.32	1.47	1.33
4	D	1207	2MG	C2-N2	6.29	1.47	1.33
25	Y	2445	2MG	C2-N2	6.29	1.47	1.33
4	D	966	2MG	C2-N2	6.28	1.47	1.33
25	Y	1835	2MG	C2-N2	6.24	1.47	1.33
4	D	1498	UR3	C6-C5	6.23	1.49	1.35
4	D	527	7MG	C2-N3	6.12	1.47	1.33
25	Y	2498	OMC	C4-N3	6.00	1.46	1.34
4	D	1407	5MC	C2-N3	5.99	1.48	1.36
25	Y	2069	7MG	C2-N3	5.98	1.47	1.33
25	Y	1915	3TD	C6-N1	5.95	1.46	1.36
4	D	527	7MG	C4-N9	5.92	1.44	1.37
25	Y	745	1MG	C2-N3	5.83	1.45	1.34
25	Y	1939	5MU	C6-C5	5.73	1.44	1.34
25	Y	2552	OMU	C6-C5	5.64	1.48	1.35
25	Y	2503	2MA	C2-N1	5.63	1.44	1.34
4	D	527	7MG	C4-N3	5.62	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	2069	7MG	C4-N9	5.57	1.44	1.37
25	Y	2069	7MG	C4-N3	5.56	1.47	1.34
25	Y	2251	OMG	C2-N3	5.43	1.46	1.33
25	Y	1835	2MG	C4-N3	5.17	1.49	1.37
25	Y	1915	3TD	C2-N3	5.15	1.50	1.38
4	D	1207	2MG	C4-N3	5.14	1.49	1.37
4	D	1516	2MG	C4-N3	5.13	1.49	1.37
25	Y	745	1MG	C4-N3	5.11	1.49	1.37
25	Y	2445	2MG	C4-N3	5.07	1.49	1.37
4	D	966	2MG	C4-N3	5.05	1.49	1.37
25	Y	2503	2MA	C6-N1	5.04	1.43	1.33
4	D	1498	UR3	C2-N3	5.03	1.48	1.39
25	Y	2251	OMG	C4-N3	4.98	1.49	1.37
4	D	1407	5MC	C6-N1	4.91	1.46	1.38
25	Y	1962	5MC	C4-N4	4.90	1.46	1.34
25	Y	2449	H2U	C4-N3	4.88	1.45	1.37
25	Y	747	5MC	C4-N4	4.87	1.46	1.34
4	D	967	5MC	C4-N4	4.82	1.46	1.34
25	Y	2251	OMG	C2-N2	4.80	1.45	1.34
4	D	1407	5MC	C4-N4	4.78	1.46	1.34
4	D	527	7MG	C2-N2	4.78	1.45	1.34
25	Y	747	5MC	C6-N1	4.65	1.46	1.38
25	Y	2069	7MG	C2-N2	4.64	1.45	1.34
25	Y	1962	5MC	C6-N1	4.61	1.45	1.38
4	D	966	2MG	C2-N1	4.58	1.44	1.36
4	D	1516	2MG	C2-N1	4.57	1.44	1.36
4	D	967	5MC	C6-N1	4.56	1.45	1.38
25	Y	2445	2MG	C2-N1	4.51	1.43	1.36
4	D	1207	2MG	C2-N1	4.50	1.43	1.36
4	D	967	5MC	C2-N1	4.43	1.49	1.40
25	Y	1962	5MC	C2-N1	4.43	1.49	1.40
25	Y	747	5MC	C2-N1	4.42	1.49	1.40
25	Y	1835	2MG	C2-N1	4.40	1.43	1.36
25	Y	2552	OMU	C4-N3	4.04	1.45	1.38
4	D	1407	5MC	C2-N1	3.98	1.48	1.40
25	Y	2498	OMC	C4-N4	3.95	1.43	1.33
25	Y	2251	OMG	C6-N1	3.81	1.43	1.37
4	D	527	7MG	C2-N1	3.71	1.46	1.37
25	Y	2498	OMC	C2-N1	3.70	1.48	1.40
25	Y	2069	7MG	C2-N1	3.67	1.46	1.37
25	Y	2498	OMC	C6-N1	3.63	1.46	1.38
4	D	966	2MG	C6-N1	3.57	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1516	2MG	C6-N1	3.46	1.43	1.37
25	Y	2445	2MG	C6-N1	3.45	1.43	1.37
25	Y	746	PSU	C6-C5	3.44	1.39	1.35
4	D	1207	2MG	C6-N1	3.44	1.43	1.37
4	D	516	PSU	C6-C5	3.38	1.39	1.35
25	Y	2069	7MG	C5-C6	3.37	1.52	1.43
25	Y	955	PSU	C6-C5	3.31	1.39	1.35
25	Y	1835	2MG	C6-N1	3.30	1.42	1.37
4	D	527	7MG	C5-C6	3.30	1.52	1.43
25	Y	1917	PSU	C6-C5	3.29	1.39	1.35
25	Y	2604	PSU	C6-C5	3.28	1.39	1.35
25	Y	2069	7MG	C6-N1	3.27	1.44	1.38
25	Y	1911	PSU	C6-C5	3.27	1.39	1.35
25	Y	2605	PSU	C6-C5	3.23	1.39	1.35
4	D	527	7MG	C6-N1	3.21	1.44	1.38
25	Y	1915	3TD	C4-N3	3.16	1.47	1.40
25	Y	2251	OMG	C5-C6	3.16	1.53	1.47
4	D	1407	5MC	O2-C2	-3.13	1.17	1.23
4	D	966	2MG	C5-C6	3.12	1.53	1.47
25	Y	747	5MC	O2-C2	-3.05	1.18	1.23
4	D	967	5MC	O2-C2	-3.05	1.18	1.23
25	Y	1835	2MG	O6-C6	-3.04	1.17	1.23
4	D	1498	UR3	C6-N1	3.04	1.45	1.38
25	Y	2580	PSU	C6-C5	3.03	1.38	1.35
25	Y	2457	PSU	C6-C5	3.02	1.38	1.35
4	D	1207	2MG	C5-C6	3.02	1.53	1.47
25	Y	1962	5MC	O2-C2	-3.01	1.18	1.23
4	D	1516	2MG	C5-C6	3.01	1.53	1.47
25	Y	2445	2MG	C5-C6	3.01	1.53	1.47
25	Y	1618	6MZ	C2-N3	2.99	1.36	1.32
25	Y	2030	6MZ	C2-N3	2.94	1.36	1.32
25	Y	2445	2MG	O6-C6	-2.91	1.17	1.23
25	Y	1835	2MG	C5-C6	2.90	1.53	1.47
4	D	1516	2MG	O6-C6	-2.87	1.17	1.23
4	D	966	2MG	O6-C6	-2.87	1.17	1.23
25	Y	2552	OMU	O4-C4	-2.86	1.18	1.24
4	D	1207	2MG	O6-C6	-2.84	1.17	1.23
25	Y	2498	OMC	O2-C2	-2.83	1.18	1.23
25	Y	2552	OMU	C6-N1	2.83	1.44	1.38
4	D	966	2MG	C5-C4	-2.77	1.36	1.43
25	Y	1835	2MG	C5-C4	-2.75	1.36	1.43
25	Y	2445	2MG	C5-C4	-2.72	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1516	2MG	C5-C4	-2.70	1.36	1.43
25	Y	2251	OMG	C2-N1	2.70	1.44	1.37
25	Y	2503	2MA	C6-C5	2.70	1.53	1.43
25	Y	2030	6MZ	C5-C4	-2.68	1.33	1.40
4	D	1207	2MG	C5-C4	-2.67	1.36	1.43
25	Y	2251	OMG	C5-C4	-2.65	1.36	1.43
4	D	1518	MA6	C5-C4	-2.59	1.34	1.40
25	Y	1618	6MZ	C5-C4	-2.57	1.34	1.40
4	D	527	7MG	O6-C6	-2.55	1.18	1.23
25	Y	1939	5MU	O4-C4	-2.53	1.18	1.23
25	Y	745	1MG	C5-C4	-2.51	1.36	1.43
4	D	1519	MA6	C5-C4	-2.50	1.34	1.40
25	Y	2069	7MG	O6-C6	-2.46	1.18	1.23
25	Y	745	1MG	C6-N1	2.42	1.43	1.39
25	Y	2503	2MA	C6-N6	-2.37	1.25	1.34
25	Y	2504	PSU	C6-C5	2.33	1.38	1.35
25	Y	2449	H2U	O4-C4	-2.32	1.18	1.23
25	Y	2449	H2U	O2-C2	-2.29	1.18	1.23
25	Y	2552	OMU	C5-C4	2.28	1.48	1.43
25	Y	1939	5MU	O2-C2	-2.26	1.18	1.23
25	Y	2552	OMU	O2-C2	-2.25	1.18	1.23
4	D	1498	UR3	C5-C4	2.25	1.49	1.43
25	Y	2251	OMG	O6-C6	-2.20	1.18	1.23
4	D	1498	UR3	C4-N3	2.18	1.45	1.40
25	Y	2504	PSU	C4-C5	-2.14	1.38	1.44
4	D	1498	UR3	O4-C4	-2.14	1.18	1.23
4	D	1518	MA6	C2-N3	2.12	1.35	1.32
4	D	1519	MA6	C2-N3	2.11	1.35	1.32
4	D	1498	UR3	O2-C2	-2.10	1.18	1.22

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	1939	5MU	C5-C4-N3	12.07	125.62	115.31
4	D	1519	MA6	N1-C6-N6	-9.48	107.08	117.06
25	Y	1939	5MU	C5-C6-N1	-9.27	113.80	123.34
4	D	1518	MA6	N1-C6-N6	-8.87	107.72	117.06
25	Y	2449	H2U	C4-N3-C2	-7.37	119.67	125.79
4	D	1518	MA6	N3-C2-N1	-5.70	119.77	128.68
25	Y	2030	6MZ	N3-C2-N1	-5.51	120.06	128.68
4	D	1519	MA6	N3-C2-N1	-5.50	120.08	128.68
25	Y	1618	6MZ	N3-C2-N1	-5.47	120.13	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	2030	6MZ	C9-N6-C6	-5.33	118.28	122.87
25	Y	2552	OMU	C4-N3-C2	-4.99	120.00	126.58
25	Y	1939	5MU	O4-C4-C5	-4.93	119.19	124.90
4	D	527	7MG	C5-C6-N1	4.88	119.59	110.99
25	Y	1915	3TD	N1-C2-N3	4.85	119.97	116.14
25	Y	2604	PSU	C4-N3-C2	-4.83	119.38	126.34
25	Y	1911	PSU	C4-N3-C2	-4.82	119.39	126.34
25	Y	1939	5MU	C4-N3-C2	-4.77	121.17	127.35
25	Y	2504	PSU	N1-C2-N3	4.77	120.53	115.13
25	Y	2605	PSU	C4-N3-C2	-4.75	119.49	126.34
25	Y	2069	7MG	C5-C6-N1	4.74	119.35	110.99
25	Y	1917	PSU	C4-N3-C2	-4.73	119.53	126.34
25	Y	746	PSU	C4-N3-C2	-4.70	119.56	126.34
25	Y	1911	PSU	N1-C2-N3	4.70	120.45	115.13
25	Y	2604	PSU	N1-C2-N3	4.68	120.43	115.13
25	Y	955	PSU	N1-C2-N3	4.63	120.38	115.13
25	Y	2457	PSU	C4-N3-C2	-4.61	119.69	126.34
25	Y	2605	PSU	N1-C2-N3	4.61	120.35	115.13
4	D	516	PSU	C4-N3-C2	-4.59	119.72	126.34
25	Y	955	PSU	C4-N3-C2	-4.59	119.73	126.34
4	D	527	7MG	C5-C4-N3	-4.56	119.45	128.13
25	Y	2503	2MA	C2-N3-C4	4.55	119.22	115.52
25	Y	1917	PSU	N1-C2-N3	4.55	120.29	115.13
25	Y	2504	PSU	C4-N3-C2	-4.54	119.80	126.34
25	Y	2580	PSU	C4-N3-C2	-4.51	119.83	126.34
25	Y	746	PSU	N1-C2-N3	4.51	120.24	115.13
4	D	516	PSU	N1-C2-N3	4.50	120.22	115.13
25	Y	2457	PSU	N1-C2-N3	4.44	120.16	115.13
4	D	527	7MG	C2-N3-C4	4.43	120.18	112.30
25	Y	2580	PSU	N1-C2-N3	4.41	120.13	115.13
4	D	1498	UR3	C4-N3-C2	-4.40	120.42	124.56
25	Y	1939	5MU	N3-C2-N1	4.35	120.67	114.89
25	Y	1939	5MU	C5M-C5-C4	4.26	123.45	118.77
25	Y	2069	7MG	C5-C4-N3	-4.18	120.17	128.13
25	Y	2069	7MG	C2-N3-C4	4.15	119.69	112.30
25	Y	1939	5MU	C5M-C5-C6	-3.99	117.52	122.85
25	Y	745	1MG	C5-C6-N1	3.98	119.89	113.90
25	Y	1915	3TD	C4-N3-C2	-3.82	120.46	124.61
25	Y	2251	OMG	CM2-O2'-C2'	3.62	124.03	114.52
25	Y	2504	PSU	C6-C5-C4	3.59	120.71	118.20
25	Y	1835	2MG	C5-C6-N1	3.56	120.24	113.95
4	D	967	5MC	C5-C6-N1	-3.51	119.72	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	2552	OMU	N3-C2-N1	3.51	119.55	114.89
25	Y	2251	OMG	C5-C6-N1	3.46	120.06	113.95
4	D	966	2MG	C5-C6-N1	3.45	120.04	113.95
4	D	1407	5MC	C5-C6-N1	-3.41	119.83	123.34
25	Y	2445	2MG	C5-C6-N1	3.40	119.95	113.95
4	D	1207	2MG	C5-C6-N1	3.39	119.94	113.95
4	D	527	7MG	C4-C5-N7	3.36	110.19	105.53
4	D	527	7MG	N9-C4-N3	3.33	130.44	125.47
4	D	1516	2MG	C5-C6-N1	3.32	119.81	113.95
25	Y	2449	H2U	N3-C2-N1	3.31	120.15	116.65
25	Y	1618	6MZ	C9-N6-C6	-3.30	120.03	122.87
25	Y	1962	5MC	C5-C6-N1	-3.29	119.95	123.34
25	Y	2552	OMU	C5-C4-N3	3.16	119.57	114.84
25	Y	747	5MC	C5-C6-N1	-3.12	120.12	123.34
25	Y	2030	6MZ	C1'-N9-C4	-3.09	121.22	126.64
25	Y	2069	7MG	C4-C5-N7	3.07	109.79	105.53
25	Y	2069	7MG	C5-C4-N9	3.02	110.27	106.35
4	D	527	7MG	O6-C6-C5	-2.98	120.24	127.54
4	D	527	7MG	C2-N1-C6	-2.97	119.68	125.10
25	Y	2449	H2U	O2-C2-N1	-2.97	119.38	123.11
4	D	527	7MG	C5-C4-N9	2.90	110.11	106.35
25	Y	746	PSU	O2-C2-N1	-2.89	119.61	122.79
25	Y	2069	7MG	O6-C6-C5	-2.88	120.47	127.54
25	Y	2449	H2U	C5-C4-N3	2.86	119.86	116.65
25	Y	2069	7MG	C2-N1-C6	-2.86	119.89	125.10
4	D	1402	4OC	C2'-C1'-N1	-2.85	108.70	114.22
25	Y	2552	OMU	O4-C4-C5	-2.84	120.16	125.16
25	Y	2251	OMG	C2-N1-C6	-2.83	119.89	125.10
25	Y	2503	2MA	N3-C2-N1	-2.80	120.62	125.73
25	Y	2457	PSU	C6-C5-C4	2.76	120.12	118.20
25	Y	2069	7MG	N9-C4-N3	2.74	129.57	125.47
25	Y	2251	OMG	C8-N7-C5	2.74	108.21	102.99
25	Y	1911	PSU	O2-C2-N1	-2.73	119.79	122.79
4	D	516	PSU	O2-C2-N1	-2.71	119.80	122.79
25	Y	2457	PSU	O2-C2-N1	-2.65	119.87	122.79
4	D	966	2MG	C8-N7-C5	2.65	108.03	102.99
25	Y	745	1MG	O6-C6-C5	-2.59	119.60	124.19
25	Y	1917	PSU	O2-C2-N1	-2.59	119.94	122.79
25	Y	2605	PSU	O2-C2-N1	-2.59	119.94	122.79
25	Y	2449	H2U	C5-C6-N1	2.58	120.13	111.61
25	Y	955	PSU	O2-C2-N1	-2.58	119.95	122.79
25	Y	2580	PSU	O2-C2-N1	-2.58	119.95	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	2604	PSU	O2-C2-N1	-2.58	119.95	122.79
25	Y	2504	PSU	O2-C2-N1	-2.58	119.95	122.79
4	D	1516	2MG	C8-N7-C5	2.57	107.88	102.99
25	Y	1939	5MU	O4-C4-N3	-2.57	115.20	120.12
25	Y	2504	PSU	C6-N1-C2	-2.56	120.06	122.68
4	D	516	PSU	C6-C5-C4	2.56	119.99	118.20
25	Y	2445	2MG	C8-N7-C5	2.56	107.86	102.99
25	Y	745	1MG	C8-N7-C5	2.55	107.85	102.99
4	D	1207	2MG	C8-N7-C5	2.53	107.80	102.99
25	Y	1835	2MG	C8-N7-C5	2.51	107.77	102.99
25	Y	1939	5MU	O2-C2-N1	-2.51	119.46	122.79
25	Y	955	PSU	C6-N1-C2	-2.50	120.13	122.68
25	Y	1915	3TD	C6-C5-C4	2.50	119.94	118.22
25	Y	2580	PSU	C6-C5-C4	2.47	119.92	118.20
25	Y	1962	5MC	CM5-C5-C6	-2.45	119.58	122.85
25	Y	2503	2MA	CM2-C2-N3	2.43	120.93	117.16
25	Y	1835	2MG	O6-C6-C5	-2.39	119.70	124.37
25	Y	2604	PSU	C6-C5-C4	2.32	119.82	118.20
25	Y	747	5MC	CM5-C5-C6	-2.29	119.79	122.85
4	D	1402	4OC	C6-C5-C4	2.27	119.73	116.96
25	Y	745	1MG	CM1-N1-C6	2.27	120.65	117.55
4	D	516	PSU	O4'-C1'-C2'	2.25	108.32	105.14
25	Y	2445	2MG	O6-C6-C5	-2.24	119.99	124.37
4	D	966	2MG	O6-C6-C5	-2.24	119.99	124.37
25	Y	2605	PSU	C6-N1-C2	-2.24	120.39	122.68
25	Y	1911	PSU	C6-N1-C2	-2.23	120.40	122.68
25	Y	2605	PSU	C6-C5-C4	2.23	119.75	118.20
25	Y	2251	OMG	O6-C6-C5	-2.22	120.03	124.37
4	D	1516	2MG	O6-C6-C5	-2.20	120.08	124.37
25	Y	2604	PSU	C6-N1-C2	-2.20	120.44	122.68
4	D	527	7MG	N9-C8-N7	2.19	106.51	103.38
4	D	1207	2MG	O6-C6-C5	-2.16	120.15	124.37
25	Y	1917	PSU	C6-C5-C4	2.14	119.70	118.20
4	D	966	2MG	CM2-N2-C2	-2.11	119.20	123.86
4	D	967	5MC	CM5-C5-C6	-2.11	120.03	122.85
25	Y	1917	PSU	C6-N1-C2	-2.09	120.54	122.68
4	D	516	PSU	C6-N1-C2	-2.09	120.55	122.68
25	Y	2445	2MG	CM2-N2-C2	-2.09	119.25	123.86
25	Y	1835	2MG	CM2-N2-C2	-2.05	119.33	123.86
25	Y	1618	6MZ	C1'-N9-C4	-2.04	123.06	126.64
25	Y	1911	PSU	C6-C5-C4	2.03	119.62	118.20
25	Y	746	PSU	C6-C5-C4	2.01	119.60	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	955	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	527	7MG	C3'-C4'-C5'-O5'
4	D	1207	2MG	C3'-C4'-C5'-O5'
4	D	1402	4OC	O4'-C4'-C5'-O5'
4	D	1402	4OC	C1'-C2'-O2'-CM2
4	D	1498	UR3	O4'-C1'-N1-C2
4	D	1516	2MG	O4'-C4'-C5'-O5'
4	D	1516	2MG	C3'-C4'-C5'-O5'
4	D	1519	MA6	C3'-C4'-C5'-O5'
4	D	1519	MA6	C5-C6-N6-C9
4	D	1519	MA6	C5-C6-N6-C10
4	D	1519	MA6	N1-C6-N6-C9
25	Y	746	PSU	C2'-C1'-C5-C4
25	Y	1915	3TD	C2'-C1'-C5-C4
25	Y	1915	3TD	O4'-C1'-C5-C4
25	Y	1915	3TD	O4'-C1'-C5-C6
25	Y	1962	5MC	C3'-C4'-C5'-O5'
25	Y	2030	6MZ	N1-C6-N6-C9
25	Y	2030	6MZ	O4'-C4'-C5'-O5'
25	Y	2030	6MZ	C3'-C4'-C5'-O5'
25	Y	2251	OMG	C3'-C2'-O2'-CM2
25	Y	2445	2MG	C3'-C4'-C5'-O5'
25	Y	2449	H2U	O4'-C4'-C5'-O5'
25	Y	2504	PSU	C3'-C4'-C5'-O5'
25	Y	2504	PSU	O4'-C4'-C5'-O5'
25	Y	2552	OMU	O4'-C1'-N1-C2
25	Y	2552	OMU	O4'-C1'-N1-C6
25	Y	747	5MC	C3'-C4'-C5'-O5'
4	D	1498	UR3	O4'-C1'-N1-C6
25	Y	1962	5MC	C4'-C5'-O5'-P
4	D	1402	4OC	C3'-C4'-C5'-O5'
25	Y	746	PSU	O4'-C4'-C5'-O5'
25	Y	1939	5MU	C3'-C4'-C5'-O5'
25	Y	1939	5MU	O4'-C4'-C5'-O5'
25	Y	2449	H2U	C3'-C4'-C5'-O5'
25	Y	747	5MC	O4'-C4'-C5'-O5'
4	D	966	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	D	966	2MG	C3'-C4'-C5'-O5'
4	D	1519	MA6	O4'-C4'-C5'-O5'
25	Y	746	PSU	C3'-C4'-C5'-O5'
25	Y	1835	2MG	O4'-C4'-C5'-O5'
25	Y	1835	2MG	C3'-C4'-C5'-O5'
25	Y	2445	2MG	O4'-C4'-C5'-O5'
25	Y	2552	OMU	O4'-C4'-C5'-O5'
4	D	1519	MA6	N1-C6-N6-C10
4	D	527	7MG	O4'-C4'-C5'-O5'
4	D	1207	2MG	O4'-C4'-C5'-O5'
4	D	1518	MA6	O4'-C4'-C5'-O5'
25	Y	1962	5MC	O4'-C4'-C5'-O5'
4	D	1518	MA6	C5-C6-N6-C10
25	Y	2552	OMU	C4'-C5'-O5'-P
4	D	1518	MA6	C5-C6-N6-C9
25	Y	2069	7MG	C4'-C5'-O5'-P
25	Y	2503	2MA	C4'-C5'-O5'-P
25	Y	2498	OMC	O4'-C4'-C5'-O5'
25	Y	2498	OMC	C4'-C5'-O5'-P
4	D	527	7MG	C4'-C5'-O5'-P
25	Y	746	PSU	O4'-C1'-C5-C4
25	Y	955	PSU	O4'-C1'-C5-C4
25	Y	1911	PSU	O4'-C1'-C5-C4
25	Y	2552	OMU	C3'-C4'-C5'-O5'
25	Y	2069	7MG	O4'-C4'-C5'-O5'
4	D	1407	5MC	C2'-C1'-N1-C2
4	D	1518	MA6	C3'-C4'-C5'-O5'
25	Y	747	5MC	C2'-C1'-N1-C2
25	Y	955	PSU	O4'-C1'-C5-C6
4	D	1402	4OC	C3'-C2'-O2'-CM2
25	Y	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

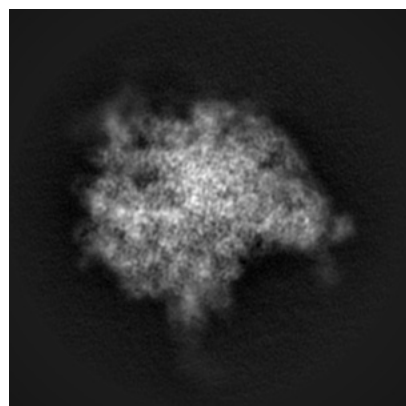
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3618. These allow visual inspection of the internal detail of the map and identification of artifacts.

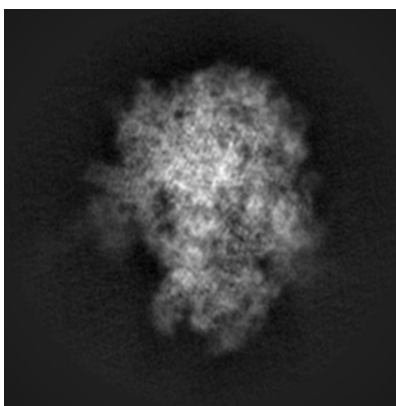
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

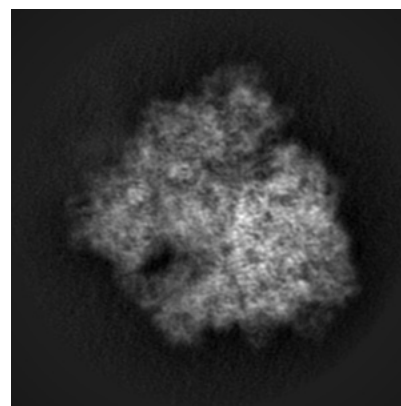
6.1.1 Primary map



X

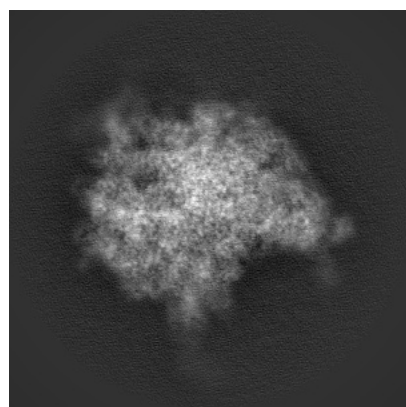


Y

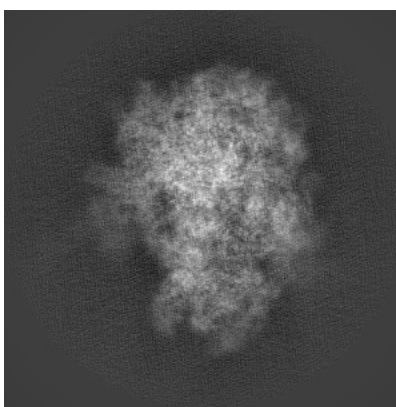


Z

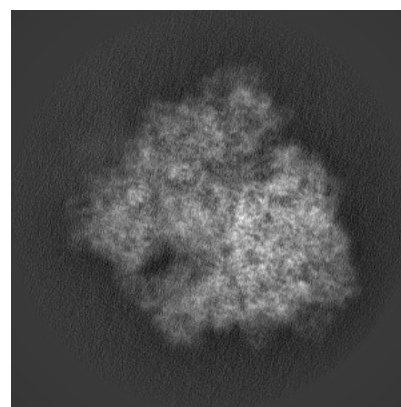
6.1.2 Raw map



X



Y

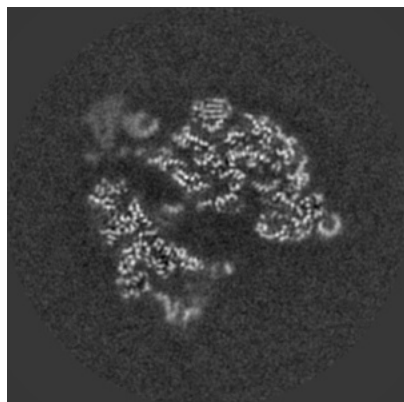


Z

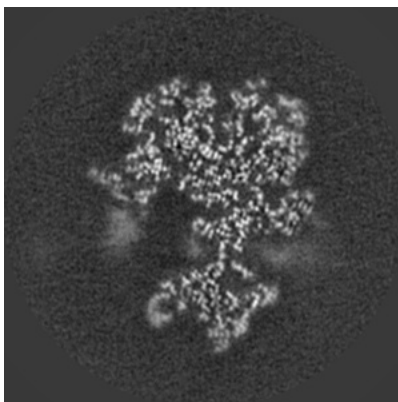
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

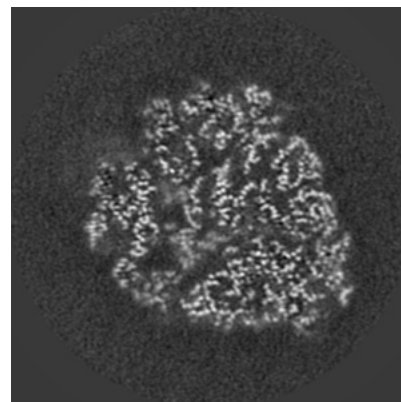
6.2.1 Primary map



X Index: 170

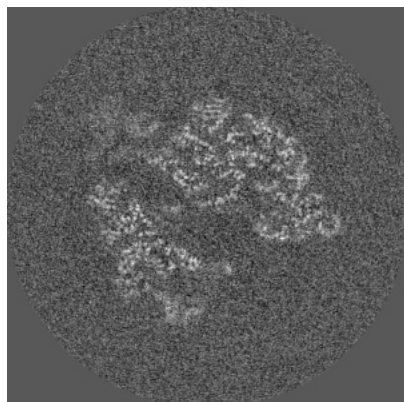


Y Index: 170

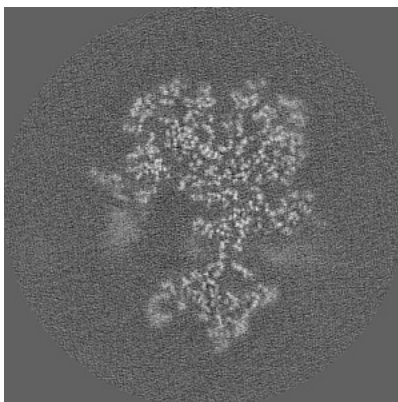


Z Index: 170

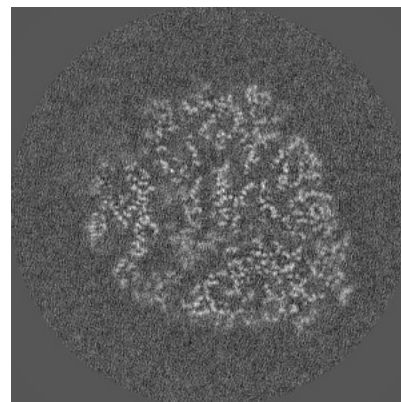
6.2.2 Raw map



X Index: 170



Y Index: 170

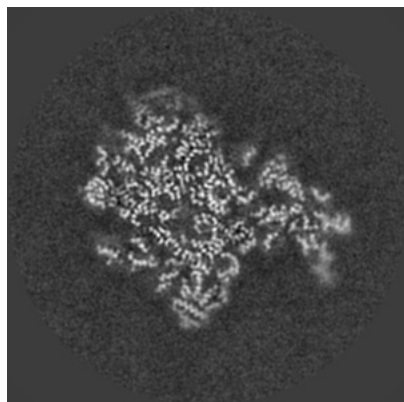


Z Index: 170

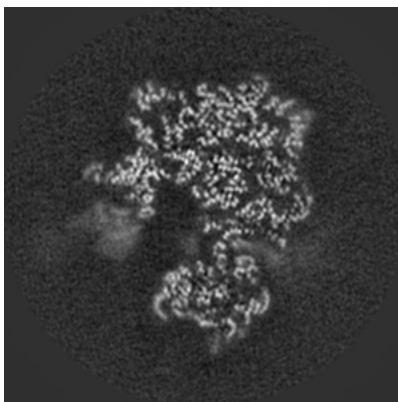
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

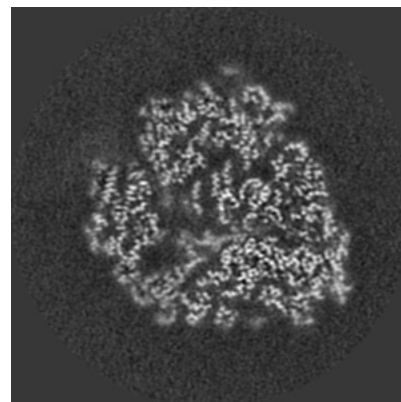
6.3.1 Primary map



X Index: 196

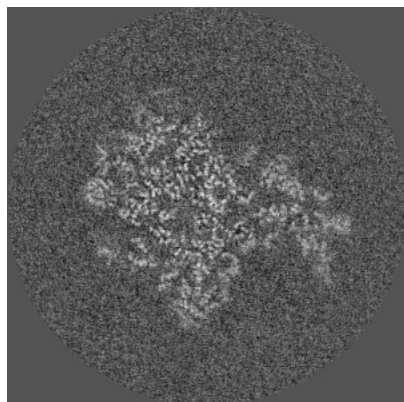


Y Index: 163

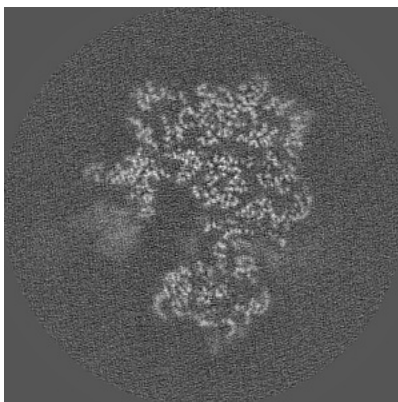


Z Index: 166

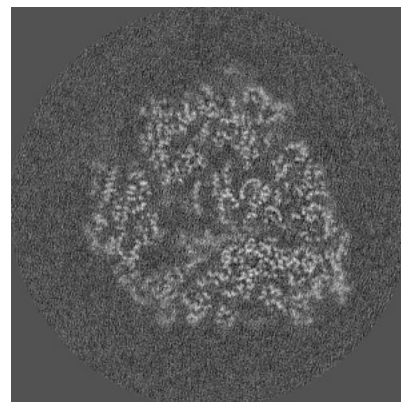
6.3.2 Raw map



X Index: 196



Y Index: 163

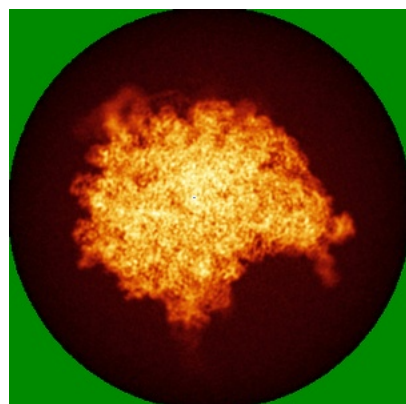


Z Index: 166

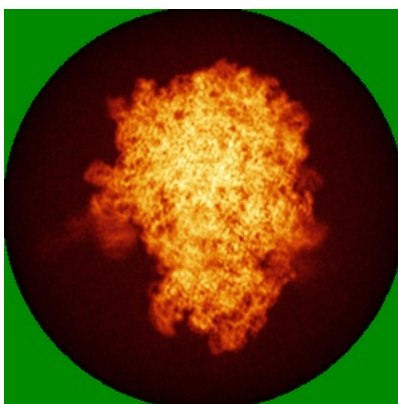
The images above show the largest variance slices of the map in three orthogonal directions.

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

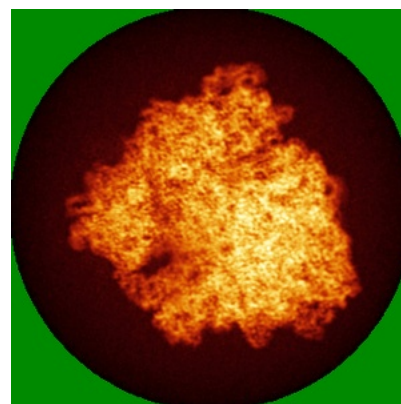
6.4.1 Primary map



X

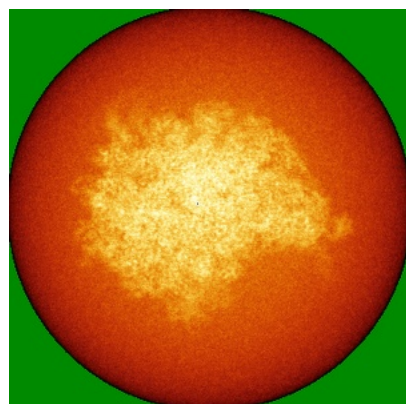


Y

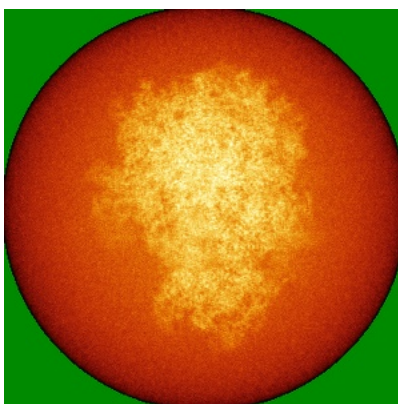


Z

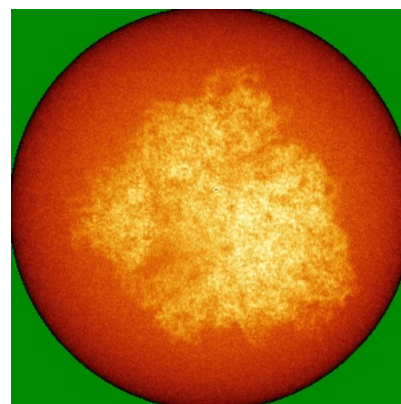
6.4.2 Raw map



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



X



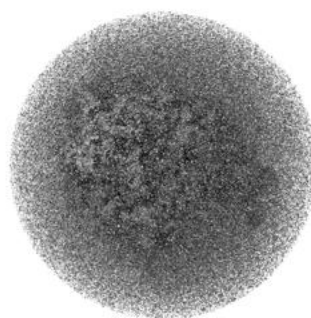
Y



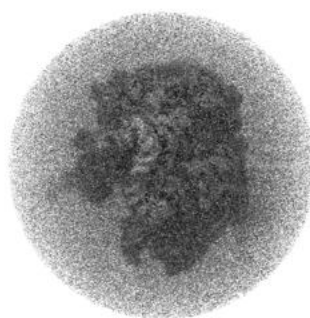
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

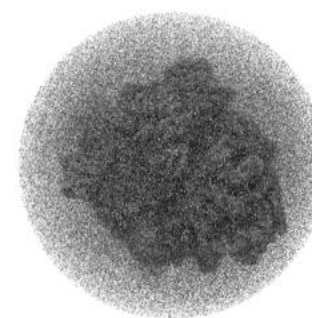
6.5.2 Raw map



X



Y



Z

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.

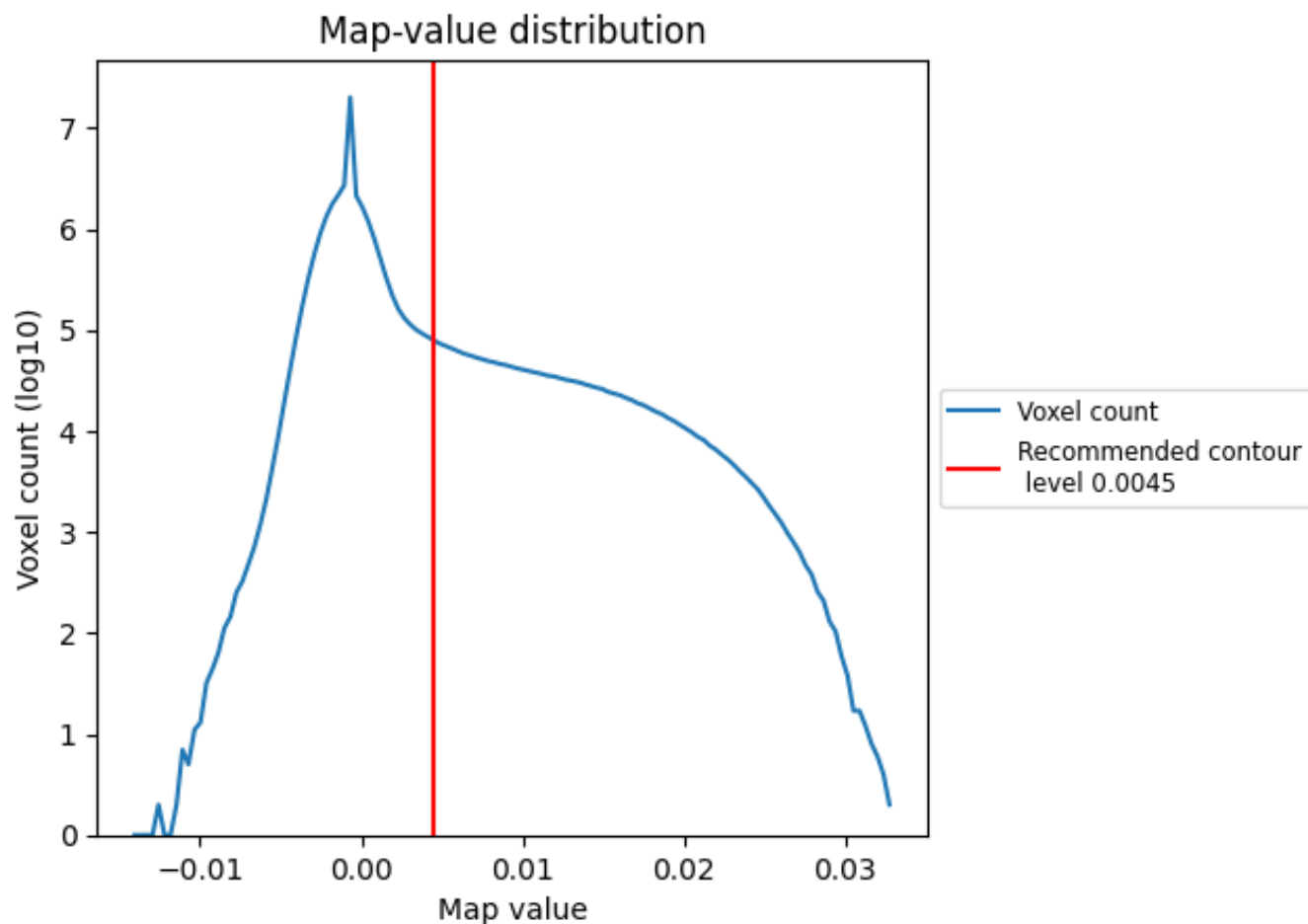
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

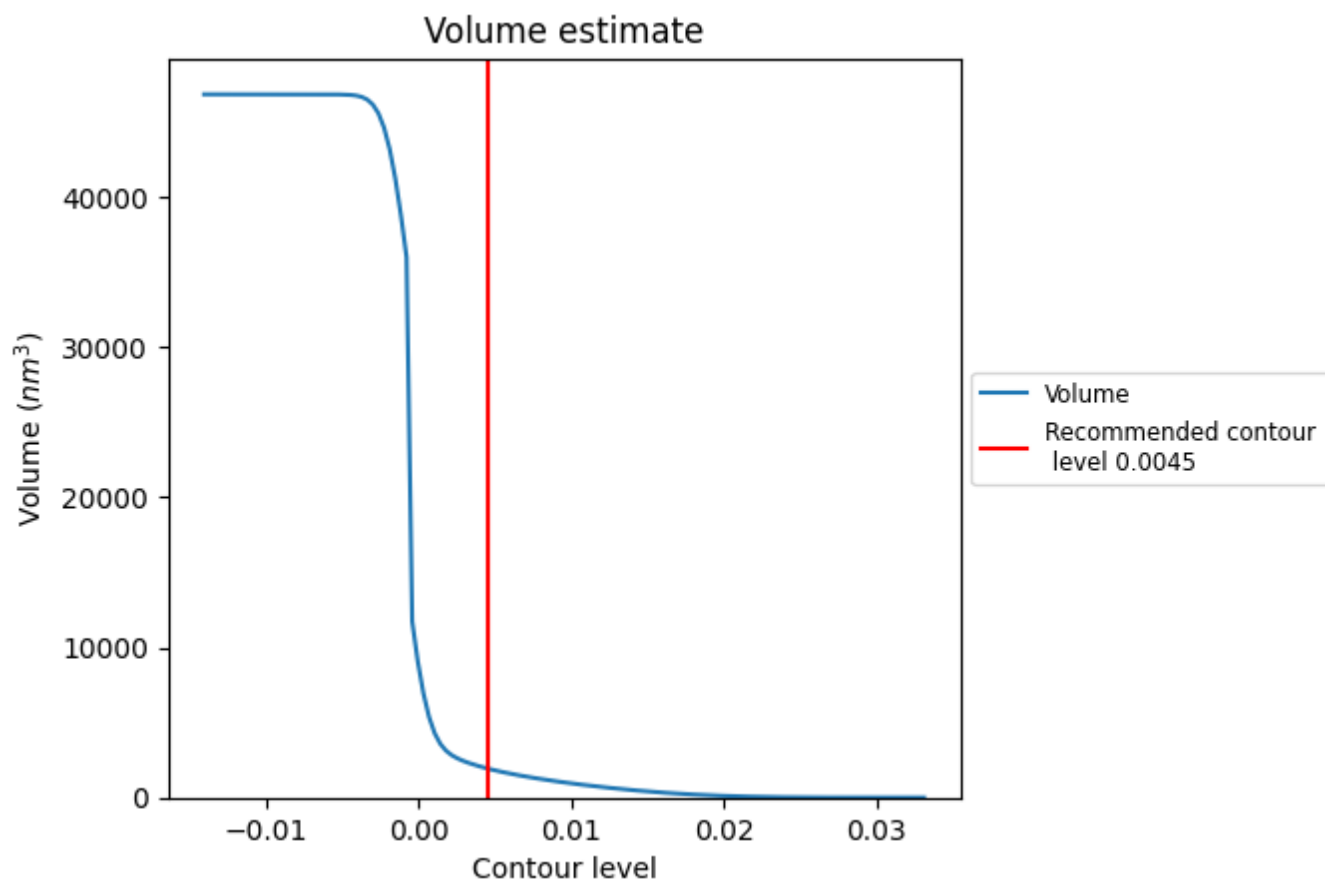
This section contains the results of statistical analysis of the map.

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.

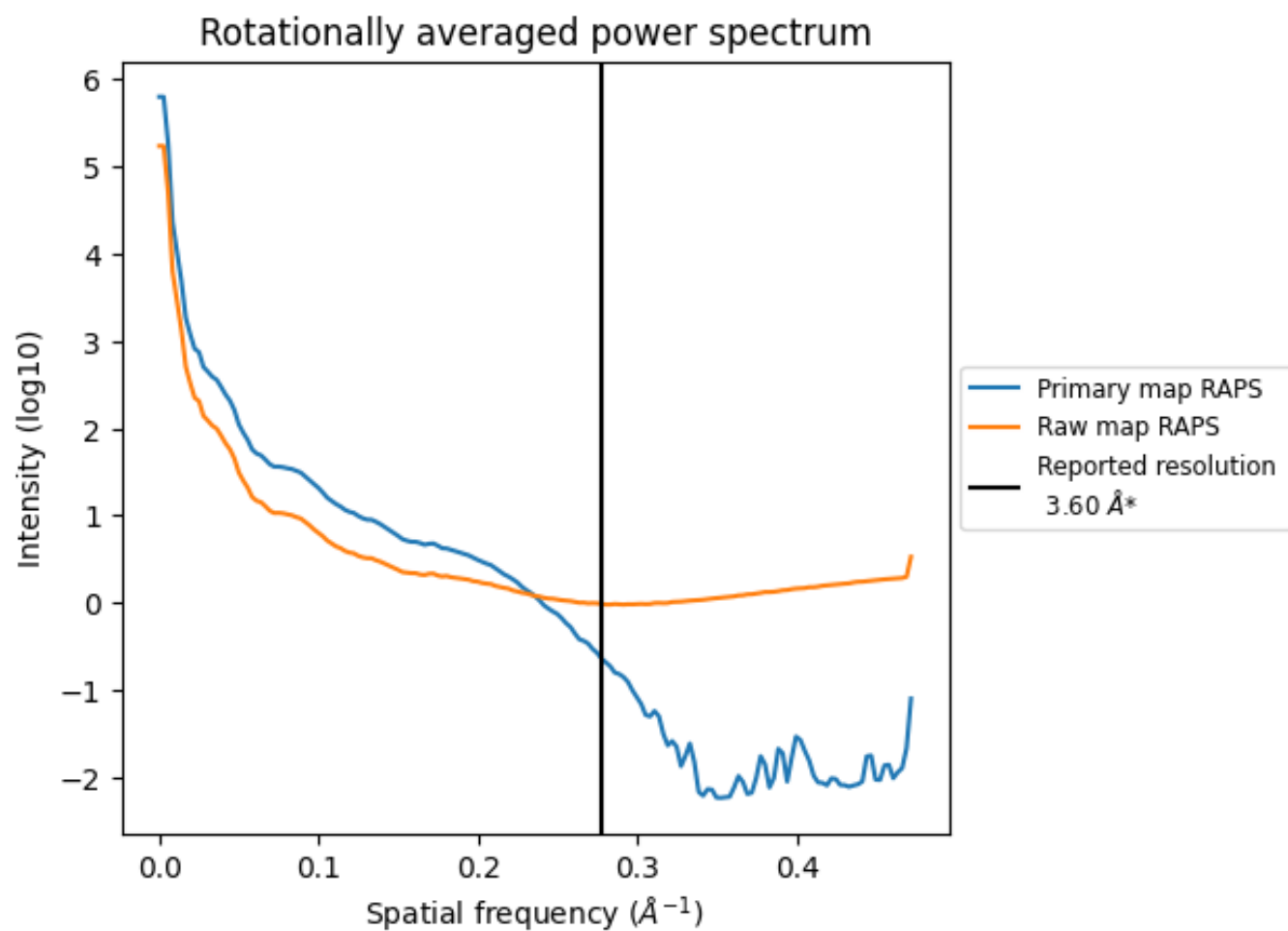
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1939 nm³; this corresponds to an approximate mass of 1751 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 ⓘ

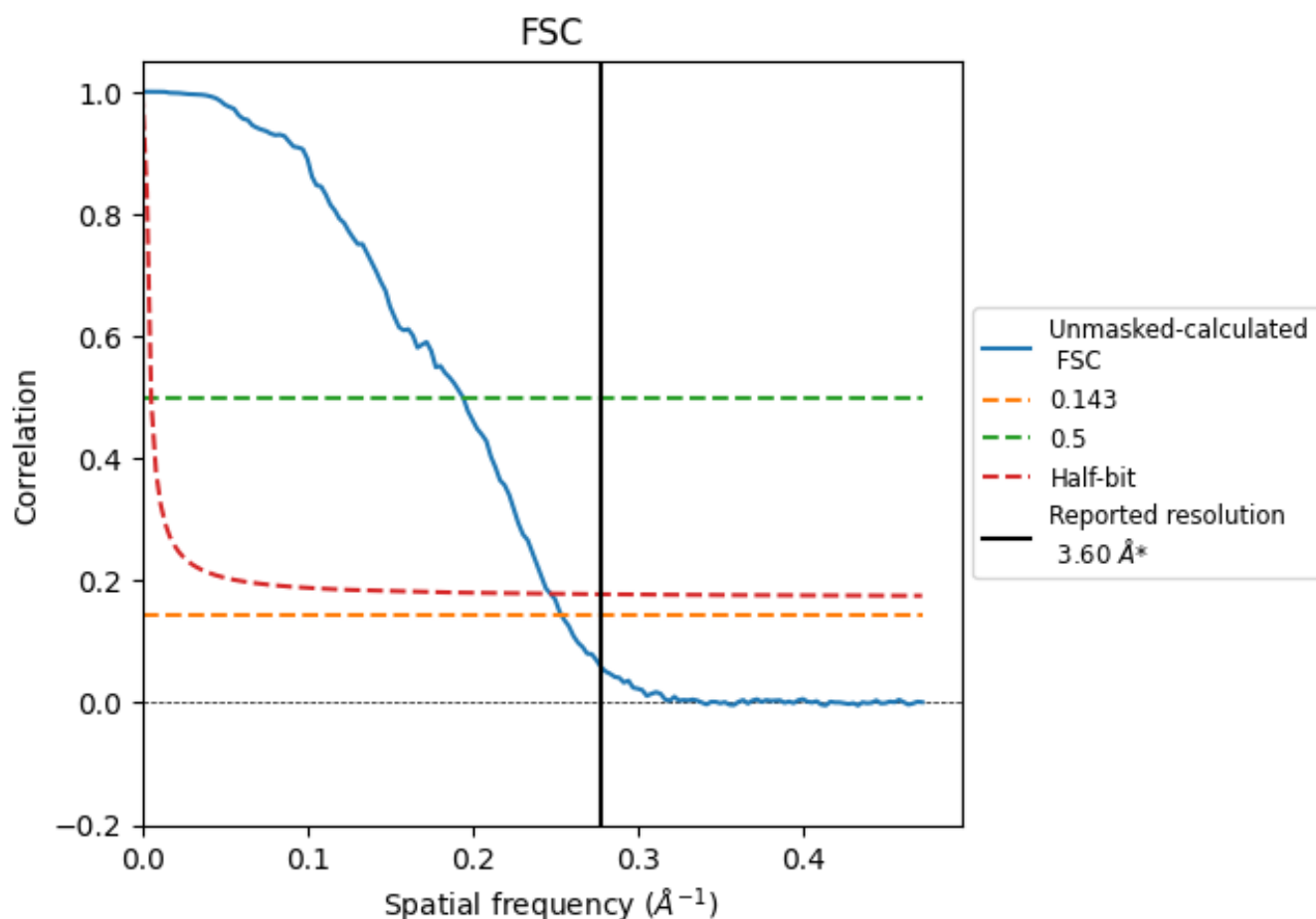


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

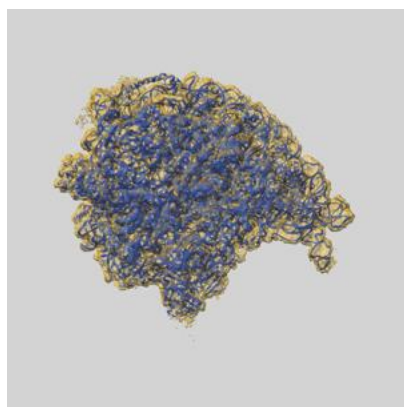
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	5.15	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

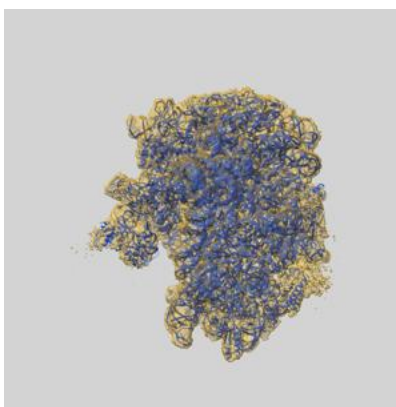
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3618 and PDB model 5NP6. Per-residue inclusion information can be found in section [3](#) on page [14](#).

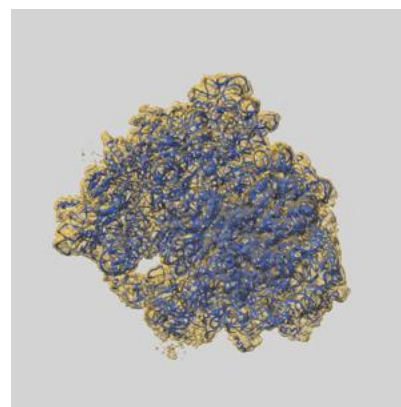
9.1 Map-model overlay [i](#)



X



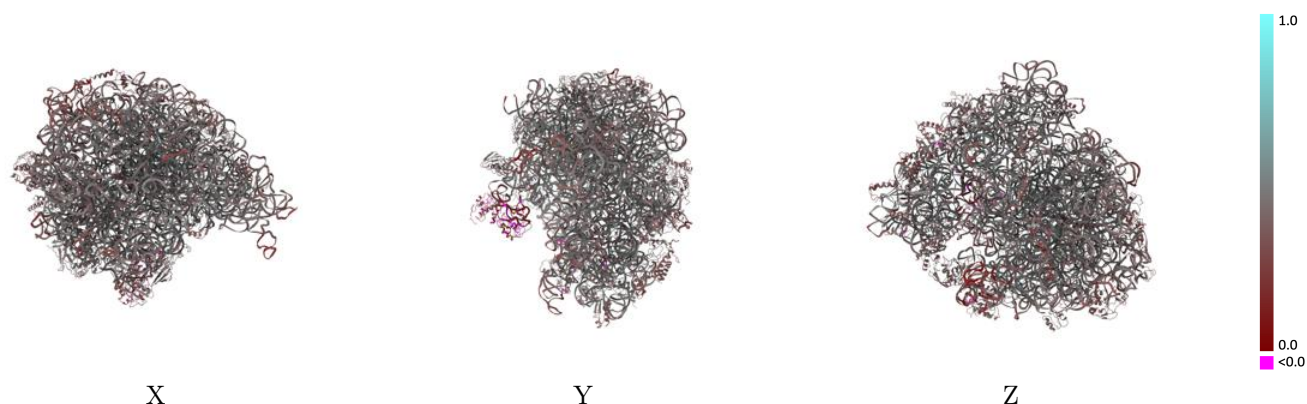
Y



Z

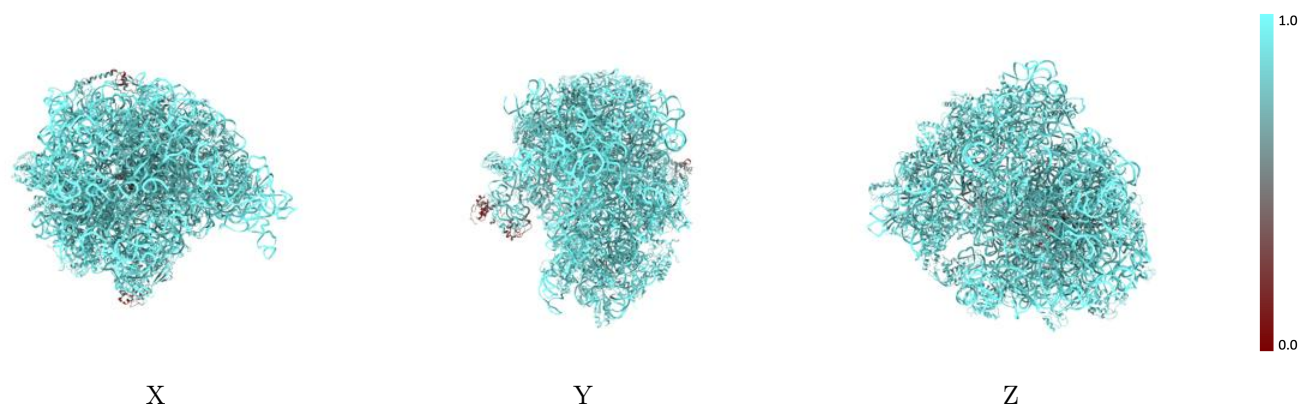
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



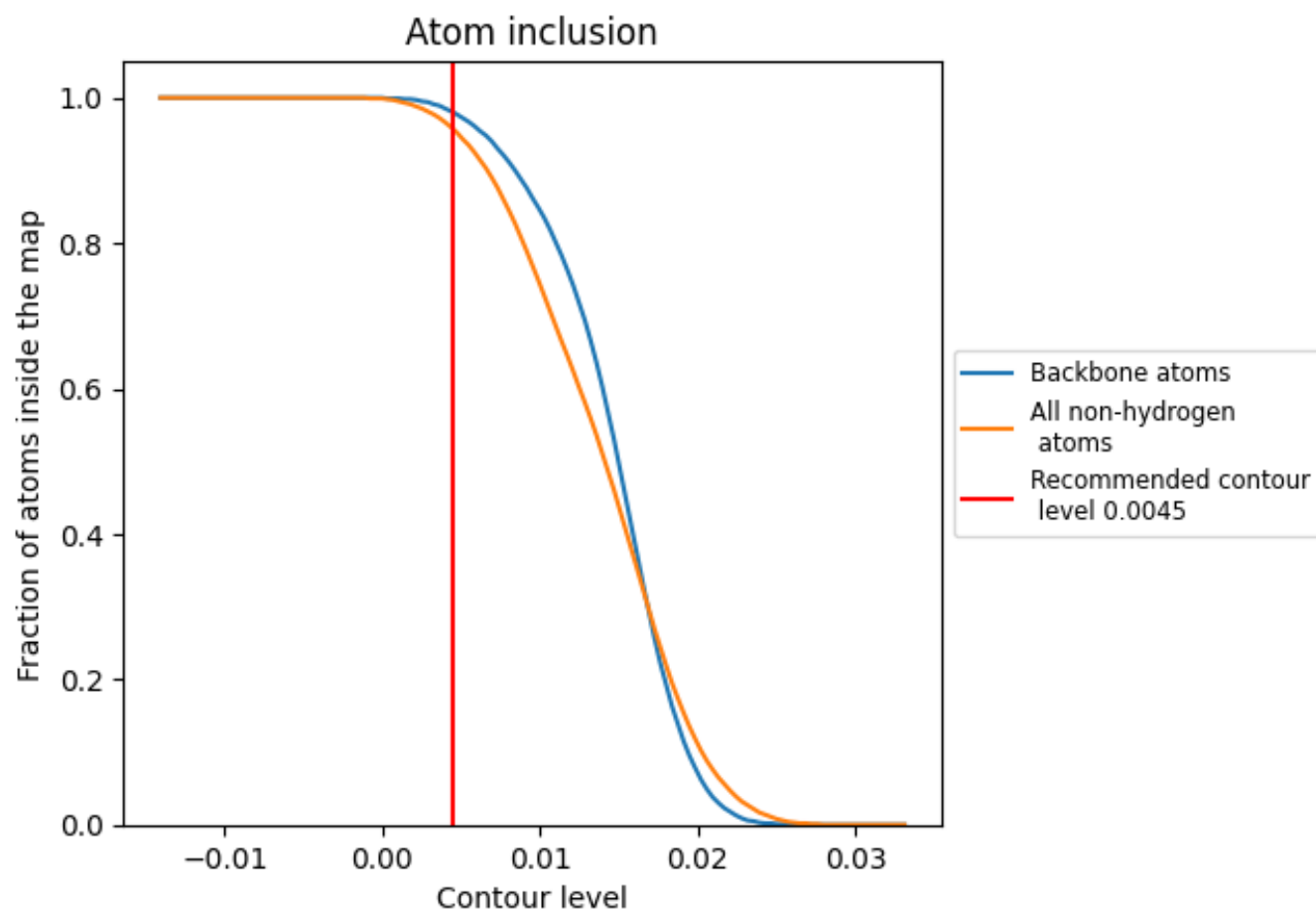
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.4240
0	 0.9210	 0.4360
1	 0.9330	 0.4710
2	 0.9210	 0.4480
3	 0.4620	 0.1670
4	 0.8920	 0.3630
A	 0.6960	 0.1820
B	 0.9690	 0.4010
C	 0.4410	 0.2550
D	 0.9950	 0.4470
E	 0.8690	 0.3620
F	 0.9000	 0.4290
G	 0.8910	 0.3960
H	 0.9250	 0.4340
I	 0.8930	 0.3920
J	 0.9110	 0.3840
K	 0.9180	 0.4360
L	 0.9120	 0.4000
M	 0.8560	 0.3880
N	 0.9290	 0.4190
O	 0.8960	 0.4470
P	 0.9240	 0.3940
Q	 0.9220	 0.4260
R	 0.9270	 0.4020
S	 0.9230	 0.4250
T	 0.9080	 0.4230
U	 0.9280	 0.4170
V	 0.9310	 0.4080
W	 0.9050	 0.3790
X	 0.8340	 0.3030
Y	 0.9920	 0.4310
Z	 0.9950	 0.4310
a	 0.9310	 0.4600
b	 0.9280	 0.4590
c	 0.9090	 0.4070



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Chain	Atom inclusion	Q-score
d	 0.9070	 0.3880
e	 0.9230	 0.4120
f	 0.6130	 0.3260
g	 0.5800	 0.1280
h	 0.9210	 0.4340
i	 0.8990	 0.4500
j	 0.9240	 0.4270
k	 0.9240	 0.4550
l	 0.9390	 0.4370
m	 0.9430	 0.4070
n	 0.9060	 0.4350
o	 0.9310	 0.4240
p	 0.9110	 0.4360
q	 0.8830	 0.4250
r	 0.9020	 0.4080
s	 0.9280	 0.3940
t	 0.9150	 0.4370
u	 0.9160	 0.4570
v	 0.9100	 0.4260
w	 0.8850	 0.3560
x	 0.9200	 0.4370
y	 0.9160	 0.4270
z	 0.8550	 0.4230