



Full wwPDB EM Validation Report ⓘ

Sep 24, 2026 – 02:58 PM EDT

PDB ID : 9ZN2 / pdb_00009zn2
EMDB ID : EMD-74431
Title : Escherichia coli 70S ribosome initiation complex bound to IF1 and extended IF2-GDPCP (70S IC*)
Authors : Basu, R.S.; Valdez, N.A.; Guerra, G.S.; Demo, G.; Gagnon, M.G.
Deposited on : 2025-12-11
Resolution : 3.00 Å(reported)
Based on initial model : 8G7P

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:

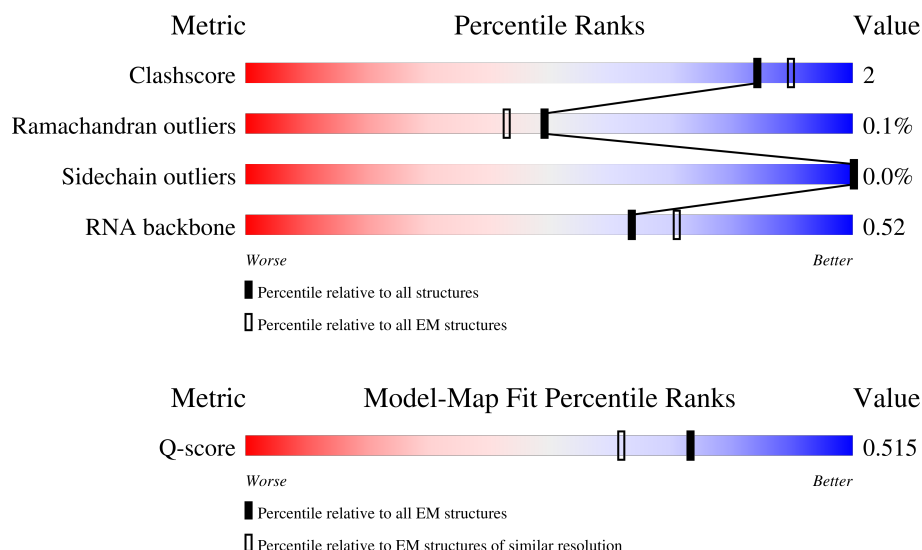
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



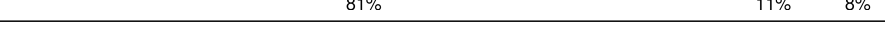
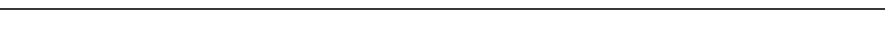
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1542	
2	b	241	
3	c	233	

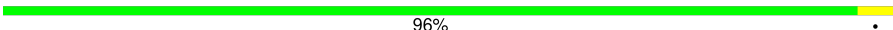
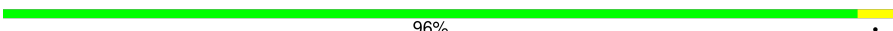
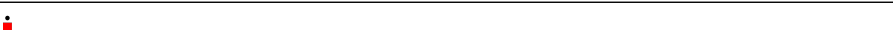
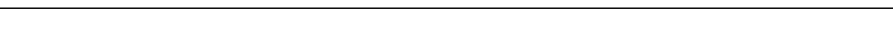
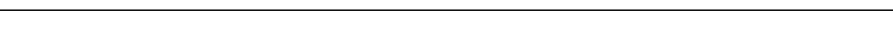
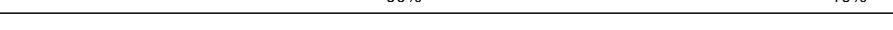
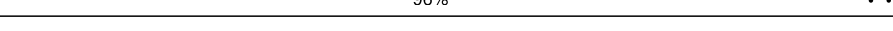
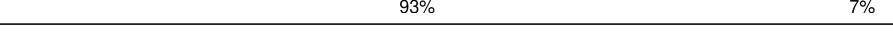
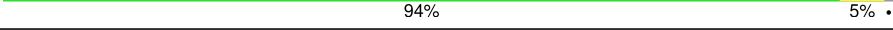
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Mol	Chain	Length	Quality of chain
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	101	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	w	24	
23	v	77	
24	x	890	
25	y	72	
26	A	2904	
27	B	120	
28	C	273	

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Mol	Chain	Length	Quality of chain
29	D	209	 96% .
30	E	201	 96% .
31	F	179	 79% 20% .
32	G	177	 85% 13% .
33	H	149	 5% 87% 13% .
34	L	142	 92% 8% .
35	M	123	 93% 7% .
36	N	144	 97% .
37	O	136	 96% .
38	P	127	 91% . 7%
39	Q	117	 93% 6% .
40	R	115	 96% . .
41	S	118	 94% 5% .
42	T	103	 90% 10% .
43	U	110	 96% . .
44	V	100	 88% 5% 7% .
45	W	104	 91% 7% .
46	X	94	 93% 7% .
47	Y	85	 85% . 12%
48	Z	78	 94% 5% .
49	1	63	 90% 6% .
50	2	59	 86% 8% 5% .
51	3	70	 74% 11% 14% .
52	4	57	 93% 7% .
53	5	55	 75% 15% 11% .

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Mol	Chain	Length	Quality of chain
54	6	46	100%
55	7	65	95% ..
56	8	38	95% 5%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 145464 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1522	Total	C	N	O	P	0	0
			32672	14579	5993	10578	1522		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	b	224	Total	C	N	O	0	0
			1103	655	224	224		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1536	977	281	276	2		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1637	1021	315	298	3		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	f	103	Total	C	N	O	0	0
			511	305	103	103		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			961	588	185	185	3		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			972	611	172	183	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	i	127	Total	C	N	O	0	0
			956	595	193	168		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	98	Total	C	N	O	0	0
			662	418	122	122		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			853	525	168	157	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP A7ZSI6

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			930	574	188	163	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			858	530	174	151	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			776	480	161	132	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			639	399	120	119	1		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	80	Total	C	N	O		0	0
			629	395	123	111			

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	77	Total	C	N	O	S	0	0
			624	394	117	110	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	66	Total	C	N	O		0	0
			327	195	66	66			

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			629	399	120	108	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	u	64	Total	C	N	O	0	0
			319	191	64	64		

- Molecule 22 is a RNA chain called 24MF mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	4	Total	C	N	O	P	0	0
			87	39	17	27	4		

- Molecule 23 is a RNA chain called initiator tRNA fMet, DNA (5'-R(P*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
23	v	76	Total	C	N	O	P	S	0	0
			1624	725	294	528	76	1		

- Molecule 24 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	595	Total	C	N	O	S	0	0
			4413	2752	782	863	16		

- Molecule 25 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	y	72	Total	C	N	O	S	0	0
			577	361	104	108	4		

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2845	Total	C	N	O	P	0	0
			61097	27261	11245	19746	2845		

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	119	Total	C	N	O	P	0	0
			2551	1136	468	828	119		

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	208	Total	C	N	O	S	0	0
			1558	975	287	293	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1404	896	246	256	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	149	Total	C	N	O	S	0	0
			833	508	161	163	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	141	Total	C	N	O	S	0	0
			1116	706	211	195	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 37 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	P	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	113	Total	C	N	O	S	0	0
			904	567	176	160	1		

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

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

- Molecule 42 is a protein called Ribosomal protein L21.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	93	Total	C	N	O	S	0	0
			735	464	139	131	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
45	W	102	Total	C	N	O	0	0
			771	488	146	137		

- Molecule 46 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	X	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	Y	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

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

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	61	Total	C	N	O	S	0	0
			492	302	96	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	56	Total	C	N	O	S	0	0
			435	272	84	77	2		

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	60	Total	C	N	O	S	0	0
			432	267	78	81	6		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	53	Total	C	N	O	S	0	0
			417	251	89	76	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	5	49	Total	C	N	O	0	0
			405	261	74	70		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

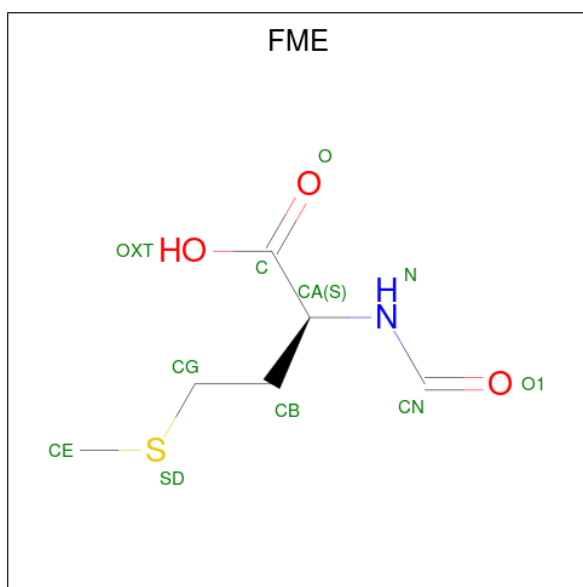
- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

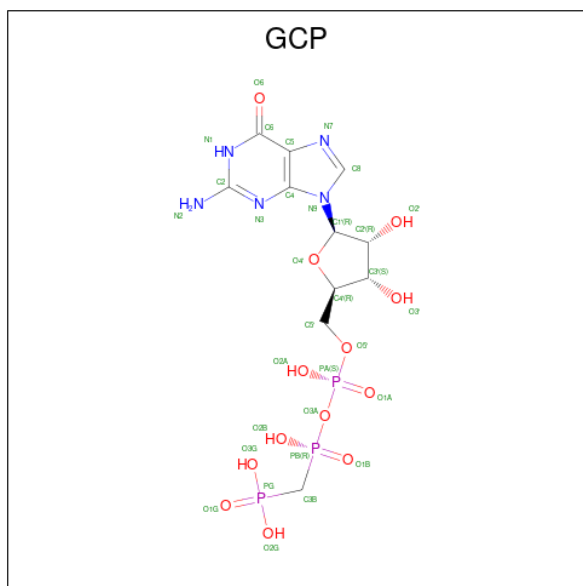
Mol	Chain	Residues	Atoms		AltConf
57	a	56	Total	Mg	0
			56	56	
57	w	1	Total	Mg	0
			1	1	
57	x	1	Total	Mg	0
			1	1	
57	A	237	Total	Mg	0
			237	237	
57	B	3	Total	Mg	0
			3	3	
57	D	1	Total	Mg	0
			1	1	
57	S	1	Total	Mg	0
			1	1	
57	4	1	Total	Mg	0
			1	1	

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
58	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
59	x	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total 1	Zn 1	0
60	8	1	Total 1	Zn 1	0

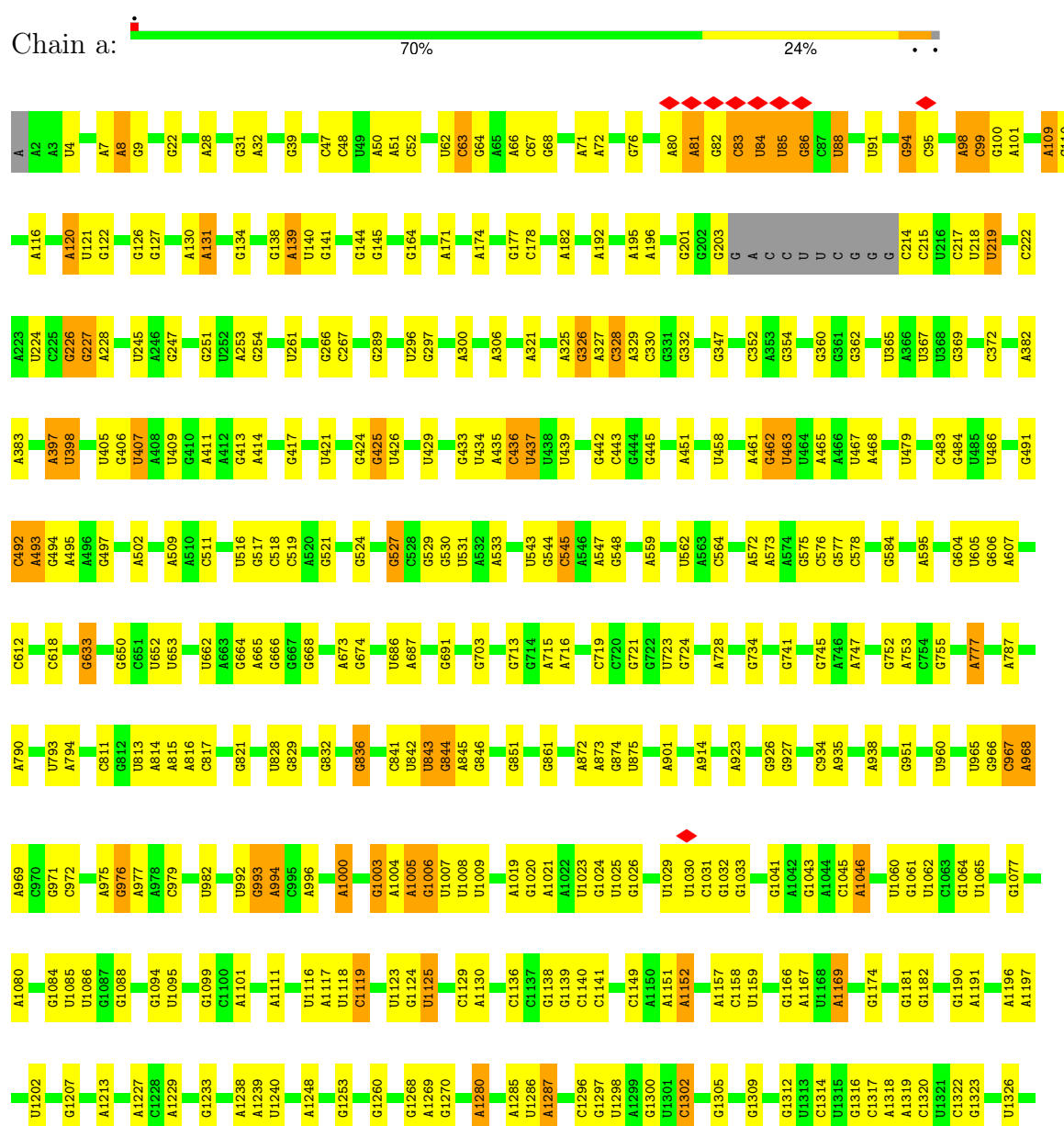
- Molecule 61 is water.

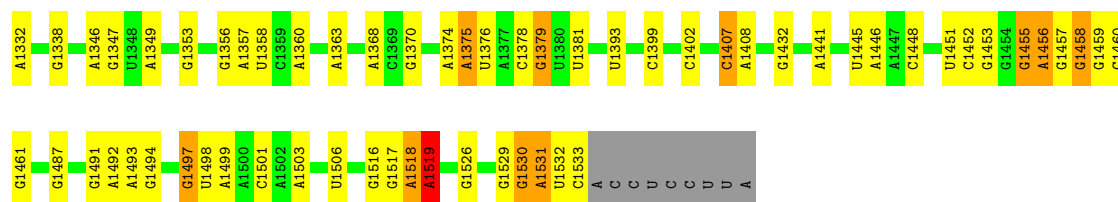
Mol	Chain	Residues	Atoms		AltConf
61	a	22	Total 22	O 22	0
61	A	245	Total 245	O 245	0
61	C	2	Total 2	O 2	0
61	P	1	Total 1	O 1	0
61	U	2	Total 2	O 2	0
61	4	2	Total 2	O 2	0

3 Residue-property plots

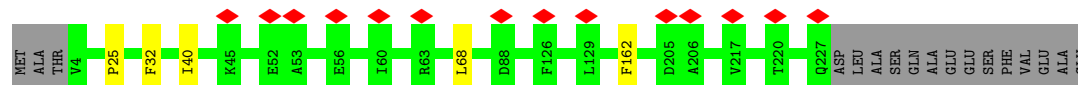
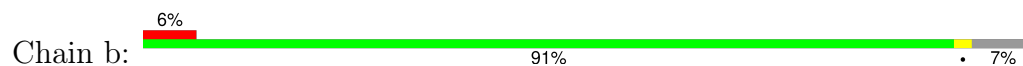
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S Ribosomal RNA

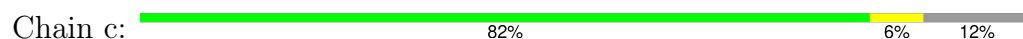




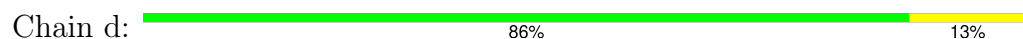
• Molecule 2: 30S ribosomal protein S2



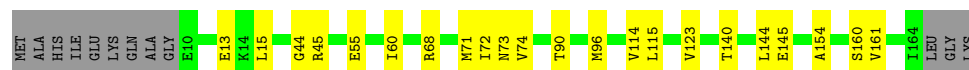
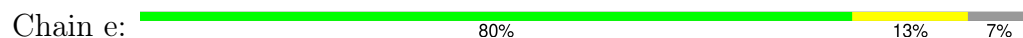
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: Small ribosomal subunit protein uS4



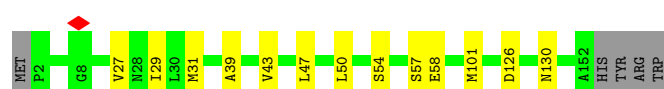
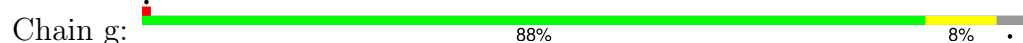
• Molecule 5: Small ribosomal subunit protein uS5



• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



- Molecule 8: Small ribosomal subunit protein uS8

Chain h:  88% 12%



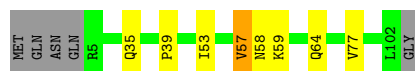
- Molecule 9: Small ribosomal subunit protein uS9

Chain i:  82% 15%



- Molecule 10: Small ribosomal subunit protein uS10

Chain j:  87% 7% 5%



- Molecule 11: Small ribosomal subunit protein uS11

Chain k:  74% 15% 10%



- Molecule 12: Small ribosomal subunit protein uS12

Chain l:  90% 8% ..



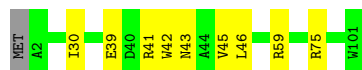
- Molecule 13: Small ribosomal subunit protein uS13

Chain m:  86% 11%



- Molecule 14: Small ribosomal subunit protein uS14

Chain n:  90% 9%



- Molecule 15: Small ribosomal subunit protein uS15

Chain o:  81% 18%



- Molecule 16: Small ribosomal subunit protein bS16

Chain p:  88% 10%



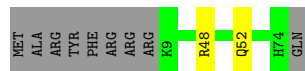
- Molecule 17: Small ribosomal subunit protein uS17

Chain q:  81% 11% 8%



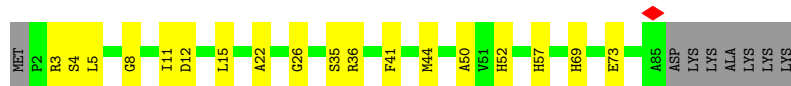
- Molecule 18: Small ribosomal subunit protein bS18

Chain r:  85% 12%



- Molecule 19: Small ribosomal subunit protein uS19

Chain s:  72% 20% 9%



- Molecule 20: Small ribosomal subunit protein bS20

Chain t:  89% 10%

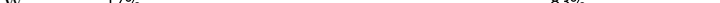


- Molecule 21: Small ribosomal subunit protein bS21

Chain u:  90% 10%



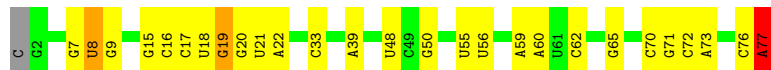
- Molecule 22: 24MF mRNA

Chain w:  17% 83%

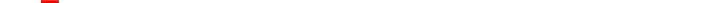


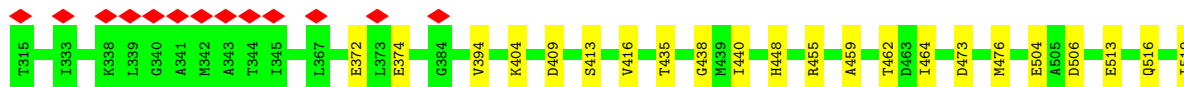
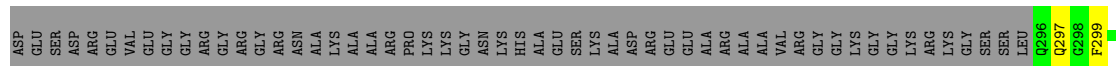
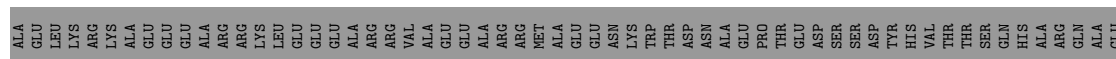
- Molecule 23: initiator tRNA fMet, DNA (5'-R(P*A)-3')

Chain v: 64% 31% ...

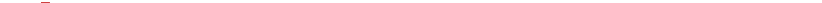


- Molecule 24: Translation initiation factor IF-2

Chain x:  61% 6% 33%



- Molecule 25: Translation initiation factor IF-1

Chain y:  88% 12%



- Molecule 26: 23S Ribosomal RNA

Chain A: 81% 15% . .

U2604	A2435	G2238	G2124	C1962	A1784	G1514	G1256	A	C961	U746	C531	A272	G1
U2605	U2441	G2239	G2125	U1963	C1790	A1515	C1257	A	A973	U747	A532	C275	G2
U2609	G2445	G2250	A2126	G1964	G1797	G1524	A1268	G	G974	A764	U534	U276	A10
U2613	G2448	G2251	G2127	C1967	C1800	A1528	G1271	A	A983	G775	U545	A277	G27
A2614	U2449	G2252	G2128	A1970	A1801	G1529	U1272	A	G989	G776	U546	A278	A28
U2615	G2455	G2253	U2130	U1971	A1808	U1534	U1273	G	A996	A781	A547	A279	
U2629	G2456	G2283	U2132	G1972	A1816	A1536	G1300	C	C1005	A782	G548	U280	U34
G2630	U2457	A2287	A2134	U1991	C1816	C1537	A1301	U	A1009	G784	G549	C281	
C2636	C2467	A2288	A2135	G1992	A1829	G1542	C1315	A	U1012	G785	A563	G307	A71
U2637	G2470	U2291	G2140	U1993	G1835	G1543	G1315	U	C1044	A310	U568	A310	A74
G2638	U2474	G2304	G2144	A2013	G1836	A1544	A1353	A	C1045	A311	U569	A311	G75
G2640	U2475	U2305	C2145	A2014	C1837	G1544	G1358	G	A1046	A84	U573	A320	A84
C2646	C2475	G2306	G2146	C2023	A1848	A1569	A1359	U	A1047	U100	A574	G329	U100
U2647	C2496	G2307	A2147	C2023	A1858	A1572	A1365	C	G1051	U807	A575	A330	A101
G2648	C2497	G2308	G2148	A2030	A1859	A1584	A1383	A	C1052	C812	G601	C331	U102
G2655	C2498	U2312	C2153	A2031	A1871	A1585	A1378	U	U1033	U827	A602	C332	A118
U2656	C2499	G2316	G2157	A2032	G1884	A1586	U1379	G	C1044	U828	A603	C334	A119
A2657	G2502	G2322	A2158	A2033	A1885	G1587	A1384	U	A1046		G604		U120
G2661	U2503	G2325	G2159	G2043	G1906	A1588	A1385	C	G1047	A845	G605	A362	A125
A2662	G2504	G2325	C2160	G2049	G1909	A1589	A1386	C	G1051	U846	U615	A384	U139
G2663	U2505	G2325	G2161	C2055	G1910	A1590	A1387	U	C1052	U847	C624	C385	A101
C2664	C2507	G2333	A2162	G2056	G1911	A1591	A1387	U	C	G859	A627	G386	A142
G2667	G2508	G2347	A2163	A2060	U1912	A1618	A1392	U	A	G864	G628	G396	A149
U2689	A2513	G2361	A2170	G2061	A1913	G1622	U1396	G	G	G881	G629	A404	A163
U2690	A2518	G2375	A2171	A2062	C1914	A1632	G1416	U	A	U884	A637	U405	A181
G2714	G2526	A2376	A2172	G2069	3ID1915	A1647	C1417	U	U	C890	U639	G406	A181
U2720	C2527	A2377	A2173	G2093	A1916	U1648	A1420	G	G		C645	G411	A196
C2723	U2528	G2378	U2181	U2099	U1917	U1649	G1425	U	U	U895	U653	A412	A199
U2724	G2529	G2379	U2182	G2109	A1918	A1650	G1425	C	C	A896	A654	G424	G215
A2725	A2530	C2380	A2183	A2101	A1919	A1650	G1425	U	U	C897	G425	G425	A216
G2726	C2540	G2383	A2184	G2102	C1920	G1674	C1428	U	U	G907	U657	C475	
A2727	U2547	U2384	U2185	C2103	U1923	G1675	C1447	G	A		U658	A479	A219
G2732	U2552	C2385	G2186	C2104	A1927	G1715	G1447	U	G	A910	G659	A480	G220
A2740	A2564	U2402	U2187	G2107	A1928	U1729	G1452	A	A	G914	U686	G481	A221
G2744	A2565	C2403	U2188	G2110	G1930	G1738	G1455	U	C	U931	A693	A482	A223
A2748	G2566	A2406	G2189	G2111	A1936	G1743	G1475	G	G	U934	G700	A483	A233
G2765	G2567	U2419	U2112	G2112	A1937	A1744	U1481	C	C		U934	A504	U234
U2775	U2580	G2204	A2113	U2113	A1938	G1764	G1482	A	A	A945	U714	A505	G245
C2773	U2586	G2204	G2115	G2115	U1939	A1773	G1483	U	U	C946	A730	A505	G248
G2774	G2428	U2210	A2116	A2117	G1948	A1773	A1508	C	A	U955	C740	C509	C249
C2775	G2429	U2211	U2118	U2118	G1954	U1779	A1509	U	U	U958	G745	C510	G266
	A2430	C2214	U2119	U2119	U1955		G1510	U	U			G530	
	G2603	A2225	G2121	G2121	U1956			A1253					



- Molecule 27: 5S Ribosomal RNA

Chain B: 78% 19%



- Molecule 28: 50S ribosomal protein L2

Chain C: 88% 11%



- Molecule 29: 50S ribosomal protein L3

Chain D: 96%



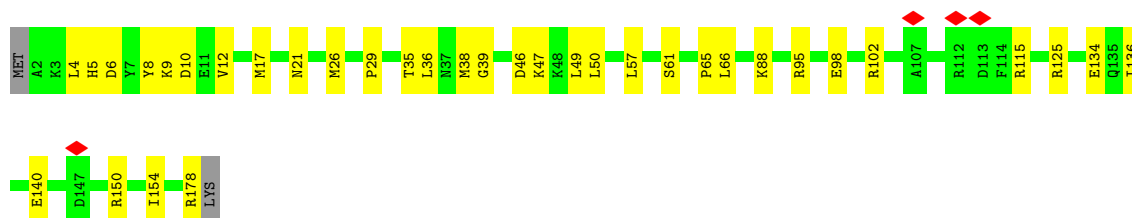
- Molecule 30: Large ribosomal subunit protein uL4

Chain E: 96%



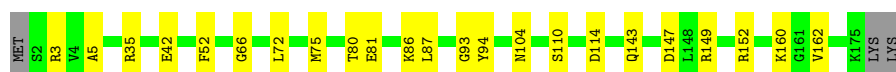
- Molecule 31: Large ribosomal subunit protein uL5

Chain F: 79% 20%

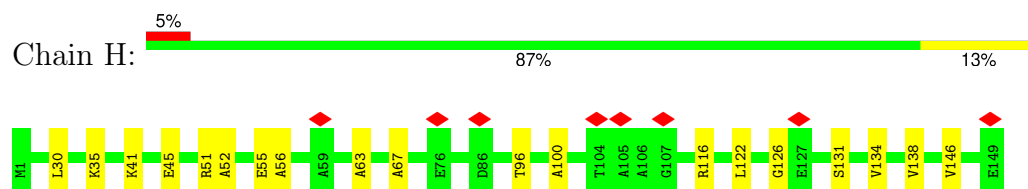


- Molecule 32: Large ribosomal subunit protein uL6

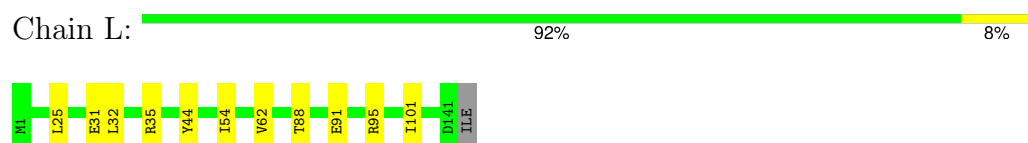
Chain G: 85% 13%



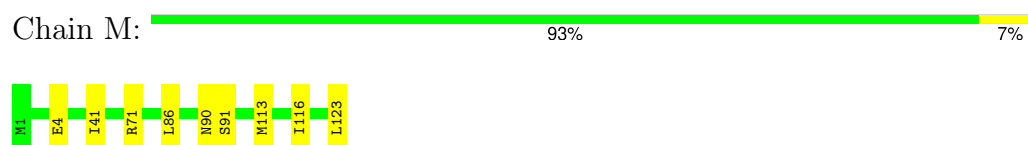
- Molecule 33: Large ribosomal subunit protein bL9



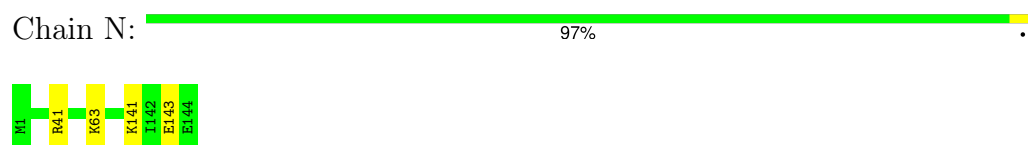
- Molecule 34: Large ribosomal subunit protein uL13



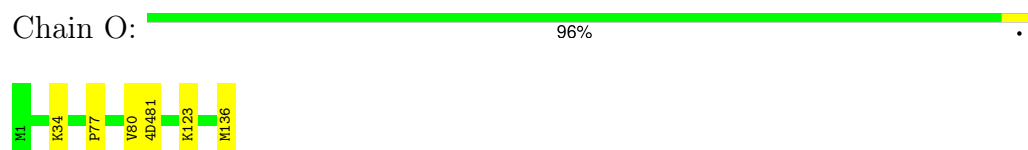
- Molecule 35: Large ribosomal subunit protein uL14



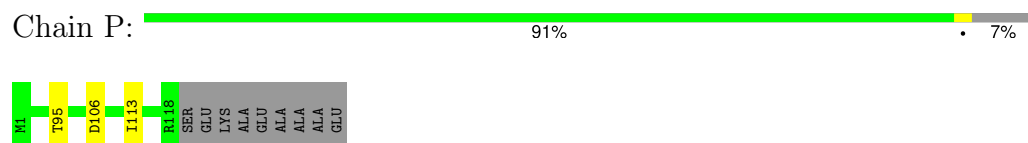
- Molecule 36: 50S ribosomal protein L15



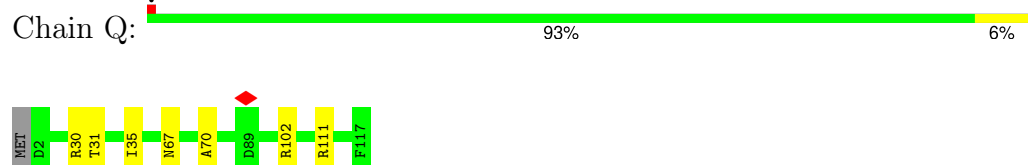
- Molecule 37: Large ribosomal subunit protein uL16



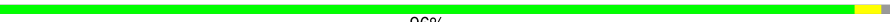
- Molecule 38: Large ribosomal subunit protein bL17



- Molecule 39: Large ribosomal subunit protein uL18



- Molecule 40: Large ribosomal subunit protein bL19

Chain R:  96% ..



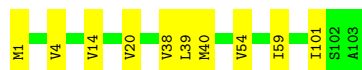
- Molecule 41: 50S ribosomal protein L20

Chain S:  94% 5% .

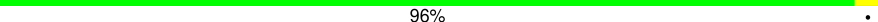


- Molecule 42: Ribosomal protein L21

Chain T:  90% 10%



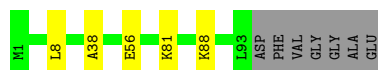
- Molecule 43: 50S ribosomal protein L22

Chain U:  96% ..



- Molecule 44: 50S ribosomal protein L23

Chain V:  88% 5% 7%



- Molecule 45: 50S ribosomal protein L24

Chain W:  91% 7% .

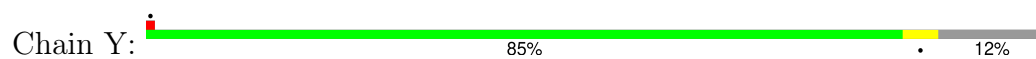


- Molecule 46: Large ribosomal subunit protein bL25

Chain X:  93% 7%



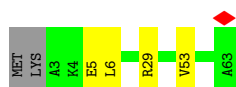
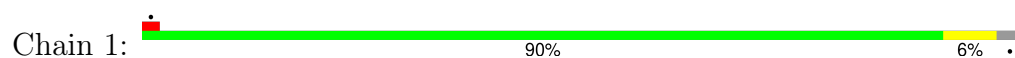
- Molecule 47: 50S ribosomal protein L27



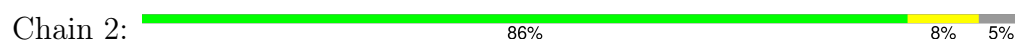
- Molecule 48: 50S ribosomal protein L28



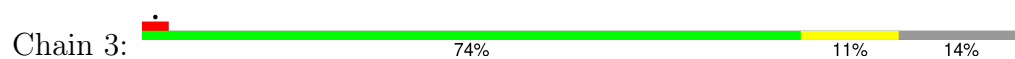
- Molecule 49: Large ribosomal subunit protein uL29



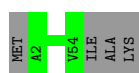
- Molecule 50: 50S ribosomal protein L30



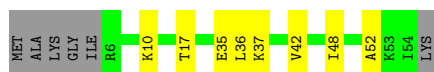
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S ribosomal protein L35

Chain 7:  95% . .



- Molecule 56: 50S ribosomal protein L36

Chain 8:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.299	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.852	Depositor
Minimum map value	-0.261	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	441.4976, 441.4976, 441.4976	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8623, 0.8623, 0.8623	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MG, G7M, FME, UR3, 5MU, 4SU, 3TD, OMU, 2MA, MEQ, MG, 4OC, PSU, IAS, OMC, 5MC, GCP, 6MZ, 4D4, D2T, H2U, MS6, ZN, 1MG, OMG

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	0.27	0/36303	0.33	0/56626
2	b	0.13	0/1102	0.29	0/1531
3	c	0.21	0/1561	0.40	0/2117
4	d	0.20	0/1659	0.35	0/2220
5	e	0.23	0/1157	0.39	0/1557
6	f	0.16	0/510	0.32	0/710
7	g	0.23	0/965	0.52	0/1310
8	h	0.23	0/982	0.43	0/1318
9	i	0.19	0/968	0.38	0/1297
10	j	0.19	0/672	0.38	0/925
11	k	0.21	0/860	0.39	0/1162
12	l	0.30	0/933	0.40	0/1255
13	m	0.18	0/867	0.40	0/1164
14	n	0.19	0/788	0.37	0/1053
15	o	0.22	0/647	0.41	0/875
16	p	0.22	0/639	0.39	0/860
17	q	0.26	0/633	0.44	0/849
18	r	0.13	0/326	0.24	0/453
19	s	0.19	0/645	0.38	0/876
20	t	0.24	0/676	0.45	0/895
21	u	0.12	0/318	0.22	0/443
22	w	0.20	0/97	0.27	0/149
23	v	0.36	1/1724 (0.1%)	0.48	3/2686 (0.1%)
24	x	0.24	0/4464	0.39	0/6040
25	y	0.23	0/584	0.41	0/783
26	A	0.42	0/67852	0.36	0/105848
27	B	0.28	0/2853	0.35	0/4449
28	C	0.36	0/2121	0.41	0/2852
29	D	0.36	0/1568	0.41	0/2109
30	E	0.33	0/1571	0.35	0/2113
31	F	0.21	0/1428	0.42	0/1919

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	G	0.24	0/1324	0.41	0/1794
33	H	0.19	0/836	0.36	0/1151
34	L	0.35	0/1139	0.37	0/1535
35	M	0.37	0/955	0.40	0/1279
36	N	0.36	0/1061	0.37	0/1412
37	O	0.35	0/1073	0.38	0/1433
38	P	0.35	0/958	0.36	0/1281
39	Q	0.23	0/902	0.38	0/1209
40	R	0.29	0/916	0.35	0/1227
41	S	0.40	0/960	0.35	0/1278
42	T	0.32	0/829	0.37	0/1107
43	U	0.35	0/852	0.35	0/1142
44	V	0.31	0/741	0.35	0/991
45	W	0.27	0/779	0.38	0/1041
46	X	0.28	0/766	0.39	0/1025
47	Y	0.32	0/576	0.36	0/762
48	Z	0.34	0/635	0.34	0/848
49	1	0.26	0/493	0.35	0/656
50	2	0.32	0/439	0.35	0/587
51	3	0.18	0/438	0.35	0/587
52	4	0.39	0/423	0.43	0/566
53	5	0.26	0/412	0.36	0/549
54	6	0.44	0/380	0.35	0/498
55	7	0.37	0/513	0.40	0/676
56	8	0.36	0/303	0.37	0/397
All	All	0.34	1/156176 (0.0%)	0.36	3/233475 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	v	8	4SU	O3'-P	8.36	1.64	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	v	76	C	OP2-P-O3'	-10.25	77.26	108.00
23	v	7	G	C2'-C3'-O3'	9.99	124.49	109.50
23	v	77	A	O4'-C1'-N9	-5.05	98.40	108.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32672	0	16462	145	0
2	b	1103	0	520	2	0
3	c	1536	0	1543	9	0
4	d	1637	0	1691	17	0
5	e	1144	0	1185	14	0
6	f	511	0	234	2	0
7	g	961	0	804	7	0
8	h	972	0	1010	12	0
9	i	956	0	945	13	0
10	j	662	0	582	6	0
11	k	853	0	841	12	0
12	l	930	0	960	7	0
13	m	858	0	878	9	0
14	n	776	0	788	7	0
15	o	639	0	600	10	0
16	p	629	0	638	6	0
17	q	624	0	658	7	0
18	r	327	0	150	1	0
19	s	629	0	614	11	0
20	t	670	0	719	9	0
21	u	319	0	153	0	0
22	w	87	0	44	0	0
23	v	1624	0	828	4	0
24	x	4413	0	4387	29	0
25	y	577	0	598	6	0
26	A	61097	0	30753	117	0
27	B	2551	0	1291	8	0
28	C	2082	0	2154	22	0
29	D	1558	0	1606	5	0
30	E	1552	0	1619	6	0
31	F	1404	0	1433	25	0
32	G	1304	0	1345	16	0
33	H	833	0	595	9	0
34	L	1116	0	1147	7	0
35	M	946	0	1023	5	0
36	N	1052	0	1127	3	0
37	O	1075	0	1145	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	P	945	0	989	2	0
39	Q	892	0	923	5	0
40	R	904	0	945	2	0
41	S	947	0	1019	5	0
42	T	816	0	839	6	0
43	U	845	0	909	3	0
44	V	735	0	800	3	0
45	W	771	0	823	5	0
46	X	753	0	780	5	0
47	Y	569	0	581	2	0
48	Z	625	0	652	2	0
49	1	492	0	518	4	0
50	2	435	0	470	3	0
51	3	432	0	394	5	0
52	4	417	0	418	0	0
53	5	405	0	437	6	0
54	6	377	0	418	0	0
55	7	504	0	572	1	0
56	8	302	0	340	2	0
57	4	1	0	0	0	0
57	A	237	0	0	0	0
57	B	3	0	0	0	0
57	D	1	0	0	0	0
57	S	1	0	0	0	0
57	a	56	0	0	0	0
57	w	1	0	0	0	0
57	x	1	0	0	0	0
58	v	10	0	10	1	0
59	x	32	0	14	0	0
60	3	1	0	0	0	0
60	8	1	0	0	0	0
61	4	2	0	0	0	0
61	A	245	0	0	5	0
61	C	2	0	0	0	0
61	P	1	0	0	0	0
61	U	2	0	0	1	0
61	a	22	0	0	0	0
All	All	145464	0	95921	547	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:L:62:VAL:HG11	34:L:101:ILE:HD11	1.37	1.04
28:C:94:VAL:HG21	28:C:116:ILE:HD11	1.56	0.85
28:C:154:LEU:HD23	28:C:176:LEU:HD11	1.58	0.84
1:a:433:G:N2	24:x:299:PHE:O	2.11	0.83
31:F:140:GLU:OE1	51:3:26:SER:OG	1.98	0.81
1:a:138:G:O2'	1:a:139:A:OP1	1.97	0.81
45:W:10:GLU:OE2	45:W:22:ARG:NH1	2.14	0.81
26:A:1529:G:O6	26:A:1542:U:O2	1.99	0.79
26:A:100:U:O2	45:W:91:LYS:NZ	2.14	0.79
1:a:843:U:OP1	1:a:844:G:N2	2.17	0.78
46:X:51:GLN:OE1	46:X:57:TYR:OH	2.02	0.77
4:d:23:SER:O	4:d:165:ARG:NH2	2.18	0.76
24:x:602:GLU:OE1	24:x:632:SER:OG	2.05	0.75
14:n:39:GLU:OE2	14:n:43:ASN:ND2	2.20	0.75
44:V:8:LEU:O	49:1:29:ARG:NH2	2.20	0.74
50:2:6:LYS:NZ	50:2:37:GLU:OE1	2.15	0.74
1:a:99:C:O2	1:a:100:G:N2	2.20	0.74
25:y:6:ASN:ND2	25:y:57:LEU:O	2.20	0.74
1:a:407:U:OP1	4:d:3:ARG:NH1	2.21	0.74
26:A:895:U:O2'	26:A:897:C:N4	2.20	0.74
26:A:2130:U:O2'	26:A:2159:G:N2	2.21	0.74
26:A:1912:A:N6	26:A:1919:A:O5'	2.21	0.74
4:d:101:VAL:HG22	4:d:105:MET:HE3	1.69	0.73
1:a:226:G:O2'	1:a:227:G:O5'	2.07	0.73
26:A:781:A:OP1	28:C:217:ARG:NH2	2.21	0.73
10:j:57:VAL:HG12	10:j:58:ASN:H	1.54	0.73
27:B:2:G:O2'	27:B:3:C:OP1	2.07	0.73
1:a:405:U:O4	4:d:2:ALA:N	2.22	0.72
26:A:1715:G:N2	26:A:1744:A:OP2	2.22	0.72
15:o:49:ASP:OD2	15:o:52:SER:OG	2.07	0.72
36:N:141:LYS:NZ	36:N:143:GLU:OE1	2.23	0.72
14:n:30:ILE:O	14:n:41:ARG:NH2	2.22	0.72
1:a:261:U:OP2	20:t:74:ARG:NH2	2.22	0.71
26:A:1153:C:OP1	41:S:92:ARG:NH2	2.23	0.71
26:A:1126:A:N1	61:A:3304:HOH:O	2.23	0.71
1:a:1229:A:OP2	13:m:113:ARG:NH2	2.24	0.70
26:A:1315:C:O2'	26:A:1392:A:N3	2.23	0.70
1:a:662:U:O2'	1:a:836:G:OP1	2.08	0.70
26:A:275:C:O2	26:A:362:A:N6	2.24	0.70
1:a:811:C:O2'	1:a:901:A:N1	2.25	0.70
1:a:951:G:OP2	13:m:101:ARG:NH1	2.24	0.70
1:a:110:C:O2'	16:p:25:ARG:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2013:A:O2'	43:U:94:ASP:OD2	2.09	0.69
1:a:493:A:O2'	1:a:494:G:O4'	2.07	0.69
26:A:534:U:O2'	41:S:49:ASP:OD2	2.03	0.69
1:a:120:A:O2'	1:a:122:G:N7	2.20	0.69
1:a:1061:G:OP2	3:c:3:GLN:NE2	2.25	0.69
26:A:1417:C:O2'	26:A:1587:G:O2'	2.10	0.69
1:a:1003:G:N2	1:a:1005:A:OP1	2.26	0.69
26:A:1649:G:O2'	38:P:106:ASP:OD2	2.06	0.69
1:a:1379:G:N2	1:a:1381:U:O4	2.19	0.69
31:F:39:GLY:O	31:F:150:ARG:NH2	2.26	0.69
29:D:46:ARG:NH1	29:D:85:ALA:O	2.26	0.68
26:A:2163:A:OP2	26:A:2164:C:N4	2.25	0.68
1:a:790:A:OP1	23:v:39:A:O2'	2.10	0.68
26:A:2636:C:O2'	29:D:45:TYR:OH	2.12	0.68
1:a:1314:C:OP2	19:s:4:SER:OG	2.04	0.68
31:F:61:SER:O	31:F:95:ARG:NH2	2.25	0.68
28:C:2:ALA:N	28:C:20:VAL:O	2.27	0.67
1:a:1149:C:O2'	1:a:1280:A:N1	2.22	0.67
33:H:134:VAL:N	33:H:138:VAL:O	2.27	0.67
31:F:8:TYR:OH	31:F:29:PRO:O	2.13	0.67
26:A:1125:G:OP2	26:A:1126:A:O2'	2.11	0.67
33:H:116:ARG:N	33:H:131:SER:O	2.27	0.67
1:a:84:U:O2'	1:a:86:G:O5'	2.14	0.66
26:A:1607:C:N4	26:A:1622:G:OP2	2.29	0.66
51:3:42:PRO:O	51:3:46:GLY:N	2.28	0.66
26:A:989:G:OP2	50:2:12:SER:OG	2.13	0.66
1:a:861:G:HO2'	1:a:874:G:HO2'	1.41	0.66
31:F:38:MET:HE3	31:F:57:LEU:HD12	1.77	0.66
1:a:578:C:O2'	1:a:728:A:N3	2.26	0.65
1:a:1296:C:O4'	1:a:1302:C:N4	2.29	0.65
1:a:1064:G:O2'	1:a:1190:G:N2	2.30	0.65
17:q:77:ARG:NH2	17:q:79:VAL:HG12	2.11	0.65
26:A:2376:A:N3	39:Q:111:ARG:NH2	2.44	0.65
28:C:69:ARG:NH2	28:C:127:GLY:O	2.28	0.65
43:U:88:ARG:NE	61:U:201:HOH:O	2.29	0.65
35:M:71:ARG:NH2	35:M:123:LEU:O	2.30	0.64
1:a:214:C:H2'	1:a:215:C:C6	2.33	0.64
28:C:84:ASP:OD2	28:C:87:ARG:NE	2.30	0.64
26:A:1528:A:OP2	26:A:1543:G:N2	2.30	0.64
1:a:1497:G:H1'	1:a:1518:MA6:H2	1.78	0.64
26:A:1529:G:O6	26:A:1542:U:C2	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:58:VAL:HG23	17:q:79:VAL:HG23	1.80	0.64
19:s:12:ASP:OD2	19:s:35:SER:OG	2.15	0.64
26:A:1508:A:HO2'	26:A:1509:A:C1'	2.10	0.64
19:s:11:ILE:HD11	19:s:15:LEU:HD22	1.80	0.64
24:x:504:GLU:OE1	32:G:93:GLY:N	2.30	0.64
42:T:14:VAL:HG12	42:T:20:VAL:HG11	1.80	0.63
1:a:407:U:O2'	4:d:113:GLU:OE2	2.16	0.63
11:k:23:ILE:HD12	11:k:96:THR:HG21	1.79	0.63
8:h:52:GLU:N	8:h:52:GLU:OE1	2.32	0.63
26:A:27:G:O2'	26:A:28:A:OP2	2.17	0.63
53:5:17:THR:HG21	53:5:42:VAL:HB	1.80	0.63
41:S:48:ARG:NH1	41:S:49:ASP:OD1	2.31	0.63
15:o:88:ARG:NH1	26:A:714:U:OP2	2.32	0.62
31:F:134:GLU:HG3	31:F:136:ILE:HG22	1.81	0.62
4:d:99:ASP:OD1	4:d:100:ASN:N	2.32	0.62
24:x:513:GLU:OE1	24:x:516:GLN:NE2	2.33	0.61
9:i:106:ARG:NH1	9:i:107:ASP:O	2.32	0.61
26:A:279:A:OP2	26:A:361:G:N2	2.32	0.61
1:a:1493:A:O2'	25:y:20:THR:OG1	2.06	0.61
26:A:1508:A:O2'	26:A:1509:A:O4'	2.11	0.61
11:k:56:ARG:O	11:k:59:THR:HG22	2.00	0.61
20:t:35:VAL:HG22	20:t:50:ALA:HB1	1.82	0.61
1:a:1530:G:O2'	1:a:1531:A:OP2	2.16	0.61
26:A:1447:C:O2'	26:A:1544:A:N3	2.33	0.61
26:A:2162:G:OP1	26:A:2171:A:N6	2.33	0.61
48:Z:62:LYS:NZ	48:Z:70:GLU:OE1	2.34	0.61
13:m:107:ARG:O	13:m:111:GLY:N	2.34	0.61
26:A:320:A:N3	30:E:163:ASN:ND2	2.49	0.61
1:a:502:A:OP1	12:l:115:SER:OG	2.14	0.60
30:E:18:THR:HG23	30:E:200:LEU:HD11	1.82	0.60
1:a:436:C:O2'	1:a:437:U:OP2	2.14	0.60
26:A:2124:G:O6	26:A:2125:G:N2	2.35	0.60
1:a:979:C:O2	14:n:59:ARG:NH2	2.34	0.60
28:C:135:ILE:O	28:C:167:ARG:NH2	2.33	0.60
1:a:996:A:N6	1:a:1046:A:O2'	2.34	0.59
1:a:1006:G:O6	1:a:1023:U:O2'	2.18	0.59
26:A:2667:C:N3	32:G:110:SER:OG	2.29	0.59
31:F:4:LEU:O	31:F:8:TYR:N	2.35	0.59
1:a:875:U:O2'	8:h:15:ARG:NH1	2.34	0.59
30:E:46:GLN:O	30:E:88:ARG:NH2	2.36	0.59
1:a:993:G:O2'	1:a:994:A:N7	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2720:U:OP1	40:R:53:ARG:NH2	2.36	0.58
1:a:195:A:N3	1:a:222:C:O2'	2.32	0.58
4:d:105:MET:HG2	4:d:171:LEU:HD21	1.85	0.58
7:g:39:ALA:O	7:g:43:VAL:HG12	2.04	0.58
26:A:2306:C:N3	31:F:150:ARG:NH2	2.50	0.58
1:a:134:G:O6	16:p:25:ARG:NH1	2.36	0.58
5:e:114:VAL:HG11	5:e:140:THR:HG21	1.84	0.58
14:n:41:ARG:O	14:n:45:VAL:HG22	2.03	0.58
1:a:67:C:O2'	1:a:171:A:N3	2.36	0.58
5:e:13:GLU:OE2	5:e:68:ARG:NH2	2.35	0.58
31:F:46:ASP:OD1	31:F:47:LYS:N	2.36	0.58
5:e:45:ARG:NH1	5:e:73:ASN:OD1	2.36	0.58
1:a:28:A:O2'	1:a:296:U:OP1	2.21	0.58
8:h:11:LEU:HD12	8:h:75:ILE:HG13	1.86	0.58
1:a:923:A:O2'	1:a:1399:C:OP2	2.18	0.58
34:L:31:GLU:OE2	34:L:35:ARG:NH1	2.35	0.58
1:a:434:U:O4	1:a:435:A:N6	2.37	0.58
4:d:116:GLN:OE1	4:d:120:HIS:NE2	2.36	0.58
1:a:72:A:N1	1:a:98:A:O2'	2.36	0.57
4:d:88:GLU:N	4:d:88:GLU:OE1	2.37	0.57
11:k:36:ASP:OD1	11:k:40:ASN:N	2.36	0.57
32:G:35:ARG:HG2	32:G:75:MET:HE1	1.84	0.57
1:a:8:A:N6	4:d:202:GLU:O	2.37	0.57
1:a:1060:U:H5''	10:j:53:ILE:HD12	1.86	0.57
1:a:226:G:HO2'	1:a:227:G:C5'	2.16	0.57
39:Q:67:ASN:OD1	39:Q:70:ALA:N	2.35	0.57
7:g:126:ASP:O	7:g:130:ASN:N	2.37	0.57
1:a:1445:U:O2	1:a:1457:G:O6	2.23	0.57
4:d:128:ARG:NH1	4:d:129:VAL:O	2.37	0.57
26:A:629:G:N3	26:A:639:U:O2'	2.38	0.57
40:R:88:ARG:NH2	40:R:112:GLU:OE1	2.38	0.56
1:a:424:G:O2'	1:a:425:G:OP1	2.19	0.56
1:a:972:C:OP2	10:j:59:LYS:NZ	2.37	0.56
26:A:475:C:O2	26:A:479:A:N6	2.38	0.56
16:p:38:PHE:O	16:p:50:THR:OG1	2.17	0.56
24:x:435:THR:OG1	24:x:438:GLY:O	2.23	0.56
24:x:768:TYR:OH	24:x:777:GLU:OE1	2.19	0.56
1:a:177:G:OP2	1:a:177:G:N2	2.19	0.56
7:g:27:VAL:O	7:g:31:MET:N	2.38	0.56
26:A:1797:G:O2'	28:C:257:THR:OG1	2.23	0.56
1:a:1124:G:N2	1:a:1125:U:O4	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:17:MET:O	31:F:21:ASN:N	2.39	0.56
1:a:816:A:OP1	1:a:1526:G:O2'	2.23	0.56
26:A:1416:G:O2'	26:A:1417:C:OP2	2.17	0.56
30:E:200:LEU:O	30:E:200:LEU:HD12	2.06	0.56
33:H:41:LYS:O	33:H:45:GLU:N	2.38	0.56
1:a:652:U:O4	1:a:752:G:O2'	2.07	0.55
26:A:249:C:O2'	36:N:63:LYS:NZ	2.34	0.55
5:e:45:ARG:NH2	5:e:71:MET:SD	2.79	0.55
26:A:693:A:O2'	26:A:1353:A:N3	2.35	0.55
19:s:36:ARG:NH2	19:s:52:HIS:O	2.40	0.55
33:H:96:THR:O	33:H:100:ALA:N	2.39	0.55
1:a:1349:A:N3	1:a:1374:A:N6	2.54	0.55
3:c:113:ALA:HB3	3:c:185:ASN:HD22	1.71	0.55
26:A:700:G:O2'	26:A:1632:A:N3	2.35	0.55
5:e:154:ALA:CB	5:e:161:VAL:HG12	2.37	0.55
11:k:71:ALA:O	11:k:75:LYS:N	2.40	0.55
1:a:1316:G:N1	1:a:1319:A:OP2	2.38	0.55
47:Y:59:LEU:HD12	47:Y:80:ILE:HD12	1.89	0.55
24:x:748:VAL:O	24:x:749:ARG:NH1	2.39	0.55
31:F:49:LEU:HD12	31:F:50:LEU:N	2.22	0.55
27:B:48:U:OP1	39:Q:30:ARG:NH1	2.41	0.54
1:a:1346:A:N6	1:a:1375:A:N7	2.55	0.54
19:s:3:ARG:NE	19:s:8:GLY:O	2.38	0.54
26:A:2134:A:N6	26:A:2157:G:O4'	2.40	0.54
7:g:50:LEU:O	7:g:54:SER:OG	2.20	0.54
24:x:592:HIS:N	24:x:595:ASP:OD2	2.41	0.54
26:A:2528:U:O2'	26:A:2530:A:OP1	2.21	0.54
19:s:22:ALA:O	19:s:26:GLY:N	2.37	0.54
28:C:154:LEU:CD2	28:C:176:LEU:HD11	2.34	0.54
50:2:27:LEU:O	50:2:38:ARG:NH1	2.40	0.54
26:A:1797:G:OP2	28:C:271:ARG:NH2	2.41	0.54
26:A:1913:A:P	26:A:1915:3TD:H2'	2.48	0.54
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.89	0.54
3:c:140:ASN:OD1	3:c:143:ARG:NH2	2.41	0.53
1:a:362:G:N2	1:a:365:U:OP2	2.41	0.53
49:1:5:GLU:HG2	49:1:6:LEU:HD12	1.91	0.53
16:p:4:ILE:HG12	16:p:21:VAL:HG12	1.89	0.53
26:A:1715:G:O2'	26:A:1743:G:O6	2.26	0.53
26:A:2773:C:OP1	29:D:169:ARG:NH1	2.42	0.53
42:T:1:MET:HG3	42:T:101:ILE:HD11	1.89	0.53
42:T:4:VAL:HG22	42:T:40:MET:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:98:GLU:O	31:F:102:ARG:NE	2.38	0.53
1:a:483:C:O2	16:p:13:LYS:NZ	2.42	0.53
26:A:1378:A:O2'	26:A:1379:U:OP2	2.25	0.53
13:m:90:ARG:NE	13:m:96:PRO:O	2.40	0.53
26:A:1913:A:OP2	26:A:1915:3TD:H2'	2.09	0.53
12:l:68:GLY:O	12:l:99:ARG:NH1	2.42	0.52
17:q:13:VAL:HG11	17:q:24:ALA:HB2	1.90	0.52
25:y:46:ARG:O	25:y:70:ARG:NH1	2.42	0.52
1:a:297:G:N2	1:a:300:A:OP2	2.41	0.52
1:a:1181:G:O2'	1:a:1182:G:N7	2.41	0.52
3:c:50:ALA:O	3:c:70:THR:OG1	2.27	0.52
26:A:1954:G:O2'	26:A:1956:U:O4	2.25	0.52
1:a:224:U:OP1	20:t:69:LYS:NZ	2.40	0.52
26:A:2540:C:O2'	26:A:2740:A:N3	2.39	0.52
29:D:103:ASP:OD2	29:D:103:ASP:N	2.43	0.52
1:a:1268:G:N3	1:a:1326:U:O2'	2.41	0.52
32:G:80:THR:OG1	32:G:81:GLU:OE1	2.25	0.52
1:a:1347:G:O6	9:i:12:ARG:NH2	2.43	0.52
26:A:568:U:H1'	26:A:2030:6MZ:H9C1	1.92	0.52
1:a:253:A:O2'	17:q:17:MET:SD	2.68	0.52
5:e:55:GLU:N	5:e:55:GLU:OE1	2.43	0.52
9:i:30:ILE:HG21	9:i:38:TYR:CD2	2.45	0.52
26:A:1385:A:O2'	26:A:1396:U:O2	2.28	0.52
1:a:462:G:O2'	1:a:463:U:O5'	2.27	0.52
1:a:1111:A:H61	3:c:177:THR:HG22	1.74	0.52
5:e:96:MET:HE1	5:e:144:LEU:HD22	1.91	0.51
12:l:83:ARG:NH1	12:l:84:GLY:O	2.43	0.51
24:x:394:VAL:HG12	24:x:464:ILE:HB	1.92	0.51
1:a:130:A:O2'	1:a:131:A:O5'	2.28	0.51
26:A:2250:G:O2'	26:A:2496:C:OP1	2.17	0.51
46:X:30:ILE:HD11	46:X:40:ILE:HD13	1.92	0.51
31:F:35:THR:O	31:F:36:LEU:HD23	2.10	0.51
1:a:1118:U:O2'	1:a:1119:C:O5'	2.28	0.51
26:A:1837:C:O2'	26:A:1927:A:N3	2.40	0.51
31:F:5:HIS:O	31:F:9:LYS:N	2.44	0.51
42:T:38:VAL:HG23	42:T:54:VAL:HG22	1.92	0.51
51:3:35:ASP:OD1	51:3:36:VAL:N	2.43	0.51
28:C:78:VAL:HG11	28:C:110:LEU:HD21	1.92	0.51
11:k:13:ARG:O	11:k:15:GLN:NE2	2.42	0.51
26:A:84:A:O2'	45:W:7:ARG:NH2	2.44	0.51
1:a:1166:G:N2	1:a:1169:A:OP2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2291:U:OP1	26:A:2380:C:O2'	2.27	0.50
1:a:195:A:OP1	20:t:60:ARG:NH1	2.43	0.50
5:e:160:SER:OG	5:e:161:VAL:N	2.44	0.50
34:L:88:THR:HG23	34:L:91:GLU:H	1.76	0.50
26:A:1918:A:O2'	26:A:1920:C:N4	2.44	0.50
29:D:4:LEU:HD22	29:D:32:ASN:OD1	2.12	0.50
26:A:219:A:N3	26:A:234:U:O2'	2.32	0.50
1:a:1309:G:OP2	13:m:98:ARG:NH1	2.44	0.50
4:d:95:GLU:OE2	4:d:104:ARG:NE	2.40	0.50
11:k:25:ALA:O	11:k:90:GLY:N	2.43	0.50
15:o:79:THR:HA	15:o:82:ILE:HG22	1.94	0.50
24:x:506:ASP:OD1	24:x:506:ASP:N	2.43	0.50
31:F:134:GLU:CG	31:F:136:ILE:HG22	2.41	0.50
1:a:327:A:O2'	1:a:328:C:O4'	2.29	0.50
9:i:91:ASP:OD2	9:i:94:LEU:N	2.44	0.50
41:S:50:ARG:O	41:S:54:LYS:NZ	2.44	0.50
1:a:214:C:H2'	1:a:215:C:H6	1.74	0.49
1:a:664:G:H22	1:a:741:G:H1	1.58	0.49
1:a:1123:U:O2'	10:j:39:PRO:O	2.30	0.49
26:A:2157:G:O2'	26:A:2158:A:O4'	2.29	0.49
1:a:575:G:O2'	1:a:821:G:OP2	2.18	0.49
5:e:115:LEU:CD2	5:e:123:VAL:HG11	2.43	0.49
26:A:2726:A:O2'	26:A:2727:A:O5'	2.29	0.49
31:F:38:MET:CE	31:F:57:LEU:HD12	2.42	0.49
1:a:63:C:OP1	1:a:383:A:N6	2.45	0.49
1:a:409:U:O2'	24:x:297:GLN:O	2.27	0.49
12:l:76:GLU:OE1	12:l:77:HIS:ND1	2.45	0.49
14:n:42:TRP:HD1	14:n:46:LEU:HD23	1.77	0.49
1:a:1191:A:OP1	3:c:4:LYS:NZ	2.44	0.49
8:h:39:VAL:O	8:h:42:GLU:N	2.46	0.49
24:x:824:ARG:NH2	24:x:851:ASP:OD1	2.45	0.49
1:a:509:A:N3	1:a:543:U:O2'	2.37	0.49
19:s:69:HIS:ND1	19:s:73:GLU:OE2	2.46	0.49
26:A:2467:C:O2	37:O:123:LYS:NZ	2.44	0.49
28:C:107:PRO:HD2	28:C:110:LEU:HD22	1.95	0.49
9:i:26:GLY:N	9:i:62:ASP:OD1	2.46	0.49
23:v:77:A:N1	24:x:844:SER:OG	2.43	0.49
26:A:2144:G:H21	26:A:2148:G:H22	1.61	0.49
1:a:50:A:O2'	1:a:360:G:N2	2.45	0.49
12:l:102:LEU:O	24:x:662:ARG:NH2	2.38	0.49
15:o:27:VAL:O	15:o:31:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:F:6:ASP:O	31:F:10:ASP:N	2.46	0.49
1:a:81:A:HO2'	1:a:88:U:H3	1.54	0.49
33:H:63:ALA:O	33:H:67:ALA:N	2.45	0.49
1:a:1393:U:HO2'	1:a:1501:C:HO2'	1.61	0.48
4:d:140:ASN:N	4:d:182:PHE:O	2.46	0.48
26:A:1009:A:N3	26:A:1153:C:O2'	2.45	0.48
53:5:10:LYS:O	53:5:52:ALA:N	2.46	0.48
1:a:196:A:OP1	20:t:64:LYS:NZ	2.45	0.48
31:F:36:LEU:HD22	31:F:154:ILE:CD1	2.43	0.48
1:a:1287:A:N3	1:a:1353:G:O2'	2.45	0.48
31:F:57:LEU:HD22	31:F:65:PRO:HB3	1.95	0.48
26:A:2:G:N2	26:A:2903:U:O2	2.46	0.48
26:A:1884:G:O2'	26:A:1885:A:OP2	2.24	0.48
47:Y:43:THR:O	47:Y:43:THR:HG23	2.13	0.48
1:a:201:G:O6	1:a:217:C:N4	2.46	0.48
8:h:47:GLU:OE2	8:h:47:GLU:N	2.46	0.48
10:j:35:GLN:CB	10:j:77:VAL:O	2.61	0.48
1:a:604:G:H2'	1:a:605:U:O4'	2.14	0.48
13:m:11:ASP:OD1	13:m:46:SER:N	2.46	0.48
26:A:659:G:O2'	30:E:95:LYS:O	2.30	0.48
26:A:2508:G:O6	61:A:3301:HOH:O	2.20	0.48
28:C:141:VAL:CG1	28:C:190:ALA:HB1	2.44	0.48
26:A:1475:G:O2'	26:A:1514:G:O6	2.32	0.48
24:x:473:ASP:OD2	24:x:476:MET:HE3	2.14	0.47
31:F:66:LEU:HD23	31:F:88:LYS:HE3	1.96	0.47
1:a:72:A:H61	1:a:98:A:C2'	2.27	0.47
1:a:691:G:N7	11:k:28:ASN:ND2	2.61	0.47
7:g:47:LEU:HD22	7:g:58:GLU:OE1	2.14	0.47
37:O:77:PRO:HG2	37:O:80:VAL:HG21	1.97	0.47
20:t:35:VAL:HG11	20:t:79:LEU:HD21	1.96	0.47
26:A:411:G:OP2	26:A:2406:A:O2'	2.33	0.47
26:A:2375:G:N2	26:A:2378:A:OP2	2.37	0.47
28:C:133:ARG:NH1	28:C:187:ASP:OD1	2.47	0.47
32:G:104:ASN:ND2	32:G:114:ASP:OD1	2.45	0.47
44:V:38:ALA:O	44:V:81:LYS:NZ	2.43	0.47
5:e:115:LEU:HD23	5:e:123:VAL:HG11	1.97	0.47
5:e:140:THR:O	5:e:144:LEU:HD23	2.14	0.47
24:x:409:ASP:O	24:x:413:SER:N	2.47	0.47
26:A:1650:A:N6	61:A:3312:HOH:O	2.38	0.47
26:A:2304:G:H22	26:A:2312:U:H3	1.61	0.47
26:A:2307:G:O4'	26:A:2308:G:N2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E:125:SER:O	30:E:137:LYS:NZ	2.47	0.47
9:i:98:LEU:O	9:i:102:GLY:N	2.47	0.47
25:y:20:THR:O	25:y:20:THR:HG22	2.13	0.47
51:3:13:THR:N	51:3:31:ASP:OD1	2.46	0.47
1:a:492:C:H4'	1:a:493:A:OP1	2.15	0.46
8:h:74:SER:O	8:h:130:ALA:N	2.48	0.46
12:l:46:ASN:ND2	12:l:89:D2T:SB	2.88	0.46
17:q:68:SER:OG	17:q:69:LYS:N	2.48	0.46
25:y:12:THR:HG22	25:y:52:LYS:NZ	2.31	0.46
1:a:397:A:O2'	1:a:398:U:OP2	2.31	0.46
1:a:716:A:C2	11:k:119:IAS:HB2	2.50	0.46
35:M:41:ILE:HD11	35:M:86:LEU:HD22	1.96	0.46
5:e:15:LEU:HD13	5:e:60:ILE:CD1	2.45	0.46
23:v:19:G:N2	23:v:59:A:O4'	2.49	0.46
23:v:20:G:OP1	23:v:60:A:N6	2.48	0.46
24:x:602:GLU:OE1	24:x:633:GLY:N	2.48	0.46
24:x:828:ILE:HG21	24:x:842:LEU:HG	1.97	0.46
1:a:1518:MA6:H92	1:a:1519:MA6:C10	2.45	0.46
49:1:6:LEU:CD2	49:1:53:VAL:HG22	2.44	0.46
1:a:1000:A:N6	1:a:1041:G:O6	2.48	0.46
1:a:1375:A:O2'	1:a:1376:U:O4'	2.26	0.46
31:F:115:ARG:O	31:F:178:ARG:NH1	2.48	0.46
46:X:64:VAL:HG23	46:X:64:VAL:O	2.16	0.46
1:a:668:G:H21	15:o:46:HIS:HE1	1.63	0.46
2:b:32:PHE:N	2:b:40:ILE:O	2.46	0.46
32:G:80:THR:HG1	32:G:81:GLU:CD	2.23	0.46
32:G:94:TYR:OH	32:G:152:ARG:NH1	2.48	0.46
15:o:80:GLN:O	15:o:84:ARG:CB	2.64	0.45
13:m:21:SER:O	13:m:21:SER:OG	2.28	0.45
14:n:45:VAL:HG23	14:n:46:LEU:HD22	1.98	0.45
20:t:35:VAL:HG22	20:t:50:ALA:CB	2.45	0.45
26:A:1481:U:O2	26:A:1510:G:O6	2.33	0.45
28:C:146:MET:SD	28:C:154:LEU:HD11	2.56	0.45
24:x:744:VAL:HG11	24:x:774:LEU:HD11	1.99	0.45
26:A:1536:C:HO2'	26:A:1537:G:N2	2.15	0.45
37:O:34:LYS:NZ	46:X:81:PRO:O	2.44	0.45
53:5:35:GLU:C	53:5:36:LEU:HD22	2.41	0.45
1:a:1269:A:N1	1:a:1312:G:O2'	2.43	0.45
26:A:1113:U:OP1	32:G:3:ARG:NH1	2.43	0.45
26:A:1425:G:O6	61:A:3302:HOH:O	2.20	0.45
26:A:2031:A:N3	26:A:2455:G:O2'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:G:42:GLU:OE1	32:G:42:GLU:N	2.49	0.45
1:a:753:A:OP1	15:o:69:TYR:OH	2.32	0.45
6:f:76:THR:O	6:f:80:PHE:N	2.47	0.45
49:1:6:LEU:HD23	49:1:53:VAL:HG22	1.99	0.45
8:h:7:ILE:O	8:h:11:LEU:HD23	2.17	0.45
24:x:564:MET:HB3	24:x:643:VAL:HG23	1.99	0.45
26:A:2657:A:O2'	32:G:160:LYS:NZ	2.49	0.45
1:a:1151:A:O2'	1:a:1152:A:O5'	2.33	0.45
4:d:200:ILE:HD12	4:d:200:ILE:H	1.81	0.45
26:A:307:G:N1	26:A:310:A:OP2	2.45	0.45
26:A:2014:A:O2'	43:U:92:ARG:NH2	2.46	0.45
26:A:2307:G:C5'	26:A:2308:G:H21	2.30	0.45
26:A:2159:G:O2'	26:A:2160:C:O4'	2.19	0.45
34:L:32:LEU:HD22	34:L:54:ILE:HG21	1.99	0.45
35:M:4:GLU:OE1	35:M:4:GLU:N	2.47	0.45
1:a:1116:U:O4	1:a:1117:A:N6	2.51	0.44
1:a:1455:G:O2'	1:a:1456:A:O5'	2.29	0.44
19:s:41:PHE:H	19:s:44:MET:HE2	1.82	0.44
26:A:1779:U:OP2	26:A:1784:A:N6	2.42	0.44
53:5:37:LYS:HG3	53:5:48:ILE:HD13	1.98	0.44
1:a:1129:C:O2'	1:a:1130:A:OP2	2.25	0.44
8:h:120:GLY:C	8:h:121:LEU:HD22	2.43	0.44
2:b:68:LEU:O	2:b:162:PHE:N	2.49	0.44
17:q:58:VAL:HG23	17:q:79:VAL:CG2	2.47	0.44
24:x:409:ASP:OD1	24:x:416:VAL:HG12	2.17	0.44
32:G:52:PHE:HZ	32:G:72:LEU:HD23	1.82	0.44
39:Q:31:THR:O	39:Q:102:ARG:NH2	2.50	0.44
1:a:1519:MA6:N7	1:a:1519:MA6:H93	2.32	0.44
13:m:86:TYR:N	19:s:73:GLU:O	2.50	0.44
24:x:519:ILE:C	24:x:520:LEU:HD22	2.43	0.44
1:a:1319:A:O2'	1:a:1323:G:N7	2.45	0.44
26:A:2467:C:OP1	56:8:8:LYS:NZ	2.42	0.44
26:A:2646:C:OP2	26:A:2732:G:O2'	2.36	0.44
1:a:1296:C:C4'	1:a:1302:C:H41	2.31	0.44
24:x:459:ALA:O	24:x:462:THR:HG22	2.18	0.44
1:a:254:G:O2'	17:q:18:GLU:O	2.35	0.44
26:A:624:C:O2'	26:A:657:U:OP1	2.22	0.44
26:A:1582:C:O2'	26:A:1585:C:N3	2.49	0.44
53:5:17:THR:HG22	53:5:17:THR:O	2.18	0.44
1:a:1360:A:OP2	14:n:75:ARG:NH2	2.51	0.43
6:f:11:HIS:N	6:f:83:ALA:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:48:ARG:O	18:r:52:GLN:N	2.46	0.43
1:a:1346:A:OP1	9:i:122:ARG:NH1	2.44	0.43
15:o:42:HIS:O	15:o:45:GLU:N	2.50	0.43
1:a:686:U:O4	1:a:703:G:O2'	2.18	0.43
11:k:112:ASP:OD1	11:k:114:THR:HG23	2.17	0.43
26:A:2101:A:N6	26:A:2102:G:O6	2.51	0.43
26:A:2306:C:OP2	26:A:2307:G:O2'	2.34	0.43
26:A:2498:OMC:HM22	26:A:2499:C:H5'	2.00	0.43
34:L:44:TYR:O	41:S:64:ARG:NH2	2.51	0.43
11:k:64:GLN:HG2	11:k:99:ALA:HB2	2.01	0.43
31:F:35:THR:C	31:F:36:LEU:HD23	2.44	0.43
32:G:143:GLN:NE2	32:G:147:ASP:OD1	2.48	0.43
26:A:332:A:O2'	26:A:334:C:OP2	2.31	0.43
33:H:30:LEU:HD12	33:H:35:LYS:HB2	2.01	0.43
55:7:17:THR:HG21	55:7:49:MET:HE1	2.01	0.43
1:a:1077:G:N2	1:a:1080:A:OP2	2.38	0.43
28:C:76:ALA:HB1	28:C:94:VAL:HG22	1.99	0.43
1:a:109:A:O2'	1:a:326:G:N2	2.52	0.43
1:a:1407:5MC:H2'	1:a:1408:A:C8	2.54	0.43
1:a:1518:MA6:H92	1:a:1519:MA6:N6	2.34	0.43
26:A:245:G:O2'	26:A:384:A:N1	2.44	0.43
26:A:483:A:O2'	45:W:57:GLY:N	2.49	0.43
35:M:90:ASN:OD1	35:M:91:SER:N	2.52	0.43
24:x:409:ASP:OD2	24:x:416:VAL:N	2.52	0.43
26:A:1790:C:O2'	28:C:208:ALA:HB2	2.18	0.43
5:e:44:GLY:O	5:e:74:VAL:N	2.46	0.43
7:g:29:ILE:CD1	7:g:101:MET:HB3	2.49	0.43
4:d:188:ARG:NH1	4:d:192:SER:O	2.49	0.42
9:i:65:ILE:HG21	9:i:79:ILE:CD1	2.49	0.42
1:a:192:A:N3	20:t:55:GLN:NE2	2.67	0.42
1:a:1086:U:H5	1:a:1099:G:H22	1.66	0.42
9:i:8:GLY:O	9:i:19:VAL:HG12	2.19	0.42
1:a:967:5MC:H2'	1:a:968:A:C8	2.54	0.42
26:A:864:G:O2'	26:A:914:G:O6	2.38	0.42
26:A:2316:G:O2'	31:F:125:ARG:NH2	2.52	0.42
33:H:126:GLY:N	33:H:146:VAL:O	2.52	0.42
8:h:105:SER:O	8:h:105:SER:OG	2.33	0.42
26:A:546:U:OP2	26:A:548:G:N1	2.52	0.42
26:A:807:U:OP2	36:N:41:ARG:NH2	2.51	0.42
34:L:25:LEU:CD1	34:L:101:ILE:HD13	2.50	0.42
1:a:1312:G:H5'	19:s:5:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:2134:A:O2'	26:A:2159:G:N3	2.52	0.42
1:a:1239:A:H61	1:a:1296:C:H2'	1.85	0.42
24:x:440:ILE:CD1	24:x:548:ILE:HG21	2.49	0.42
38:P:95:THR:HG21	38:P:113:ILE:HD11	2.01	0.42
1:a:424:G:HO2'	1:a:425:G:P	2.40	0.42
8:h:18:GLN:HE21	8:h:72:VAL:HG22	1.84	0.42
1:a:145:G:N2	1:a:178:C:N3	2.68	0.42
24:x:448:HIS:O	24:x:455:ARG:NH2	2.51	0.42
24:x:608:ALA:HB3	24:x:629:LEU:HD12	2.01	0.42
35:M:113:MET:HA	35:M:116:ILE:HG22	2.01	0.42
33:H:51:ARG:O	33:H:55:GLU:N	2.52	0.42
1:a:1458:G:OP1	20:t:30:THR:OG1	2.26	0.42
15:o:5:THR:O	15:o:8:THR:OG1	2.26	0.42
26:A:2104:C:N4	26:A:2185:U:O4	2.52	0.42
26:A:2655:G:O2'	26:A:2664:G:O6	2.37	0.42
1:a:138:G:HO2'	1:a:139:A:P	2.31	0.41
1:a:606:G:N2	1:a:633:G:N7	2.68	0.41
4:d:27:ALA:O	4:d:30:THR:OG1	2.38	0.41
11:k:13:ARG:NH2	11:k:76:GLU:O	2.53	0.41
26:A:601:C:O2'	26:A:605:G:OP1	2.35	0.41
1:a:968:A:C8	1:a:1062:U:H4'	2.55	0.41
1:a:1233:G:OP1	9:i:119:ARG:NH1	2.45	0.41
26:A:2147:A:H62	26:A:2148:G:H21	1.67	0.41
39:Q:35:ILE:HD11	39:Q:102:ARG:HE	1.85	0.41
3:c:187:SER:OG	3:c:188:GLU:N	2.52	0.41
26:A:2111:U:O4'	26:A:2118:U:O2'	2.37	0.41
1:a:713:G:H21	1:a:777:A:H1'	1.84	0.41
13:m:76:SER:O	13:m:80:LEU:HD23	2.20	0.41
26:A:784:G:H5'	26:A:785:G:OP1	2.21	0.41
27:B:10:G:H2'	27:B:11:C:O4'	2.20	0.41
48:Z:39:TRP:NE1	48:Z:41:GLU:OE1	2.42	0.41
1:a:544:G:O2'	1:a:545:C:O5'	2.35	0.41
15:o:79:THR:O	15:o:83:GLU:OE1	2.39	0.41
27:B:31:C:O2'	27:B:53:A:N1	2.53	0.41
27:B:55:U:O4'	31:F:26:MET:HE1	2.19	0.41
5:e:72:ILE:HG21	5:e:145:GLU:OE2	2.20	0.41
58:v:101:FME:HE1	24:x:801:ARG:HB2	2.03	0.41
26:A:277:G:O2'	26:A:278:A:O5'	2.30	0.41
28:C:67:PHE:CE1	28:C:105:LEU:HD11	2.56	0.41
28:C:271:ARG:O	28:C:272:SER:OG	2.25	0.41
42:T:4:VAL:HG23	42:T:39:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:W:4:LYS:O	45:W:94:ARG:NH1	2.54	0.41
1:a:1088:G:N3	1:a:1167:A:N6	2.69	0.41
1:a:1356:G:H2'	1:a:1357:A:C8	2.56	0.41
26:A:1536:C:O2'	26:A:1537:G:N2	2.53	0.41
26:A:1948:G:O6	61:A:3303:HOH:O	2.21	0.41
1:a:94:G:N1	1:a:98:A:N1	2.68	0.41
3:c:87:LEU:O	3:c:91:VAL:HG22	2.21	0.41
26:A:569:U:O2'	26:A:983:A:N1	2.50	0.41
28:C:263:THR:O	28:C:263:THR:HG22	2.21	0.41
32:G:86:LYS:O	32:G:87:LEU:HD23	2.21	0.41
37:O:136:MET:O	46:X:79:ARG:NH1	2.50	0.41
1:a:62:U:O2'	1:a:63:C:O5'	2.39	0.41
1:a:83:C:O2'	1:a:85:U:OP2	2.28	0.41
1:a:562:U:O2'	12:l:13:ALA:O	2.31	0.41
1:a:976:G:OP2	1:a:1358:U:O2'	2.38	0.41
1:a:1368:A:OP1	10:j:64:GLN:NE2	2.54	0.41
4:d:62:ARG:O	4:d:66:GLY:N	2.51	0.41
7:g:57:SER:OG	7:g:58:GLU:N	2.52	0.41
16:p:19:VAL:HG12	16:p:37:GLY:C	2.46	0.41
26:A:2638:G:O2'	26:A:2775:G:N2	2.52	0.41
28:C:117:GLN:N	28:C:128:ASN:OD1	2.46	0.41
1:a:673:A:H2'	1:a:674:G:C8	2.56	0.41
8:h:11:LEU:HD12	8:h:75:ILE:CG1	2.49	0.41
9:i:21:ILE:HD11	9:i:61:LEU:HB3	2.02	0.41
9:i:30:ILE:HD13	9:i:65:ILE:HB	2.03	0.41
24:x:372:GLU:O	24:x:374:GLU:N	2.53	0.41
26:A:2564:A:OP1	26:A:2648:G:O2'	2.33	0.41
26:A:2640:G:OP1	34:L:95:ARG:NH1	2.54	0.41
26:A:2526:G:O2'	56:8:34:LYS:NZ	2.53	0.40
27:B:14:U:OP2	27:B:70:C:O2'	2.38	0.40
32:G:5:ALA:HB2	32:G:66:GLY:HA2	2.03	0.40
33:H:52:ALA:O	33:H:56:ALA:HB2	2.21	0.40
44:V:56:GLU:OE1	44:V:88:LYS:NZ	2.45	0.40
53:5:35:GLU:O	53:5:36:LEU:HD22	2.21	0.40
1:a:81:A:O2'	1:a:88:U:N3	2.44	0.40
27:B:2:G:HO2'	27:B:3:C:P	2.37	0.40
1:a:203:G:H21	1:a:465:A:N6	2.19	0.40
1:a:218:U:O2'	1:a:219:U:O5'	2.38	0.40
32:G:149:ARG:HA	32:G:162:VAL:HG13	2.04	0.40
42:T:59:ILE:HG12	42:T:101:ILE:HG22	2.03	0.40
1:a:745:G:O3'	1:a:836:G:N2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:21:THR:O	3:c:21:THR:HG23	2.21	0.40
9:i:59:GLU:OE1	9:i:59:GLU:N	2.54	0.40
26:A:2210:U:H3	26:A:2214:C:N4	2.20	0.40
27:B:42:C:OP2	51:3:2:LYS:NZ	2.53	0.40
28:C:141:VAL:HG11	28:C:190:ALA:HB1	2.03	0.40
1:a:126:G:OP1	1:a:605:U:O2'	2.29	0.40
1:a:927:G:N2	1:a:1532:U:OP1	2.51	0.40
1:a:1088:G:H21	1:a:1167:A:N6	2.20	0.40
8:h:75:ILE:O	8:h:75:ILE:HG23	2.22	0.40
11:k:64:GLN:NE2	11:k:68:GLU:OE2	2.53	0.40
25:y:53:VAL:HG21	25:y:67:ILE:HG12	2.03	0.40
31:F:8:TYR:HA	31:F:12:VAL:HG22	2.03	0.40
32:G:52:PHE:CZ	32:G:72:LEU:HD23	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/241 (92%)	206 (93%)	15 (7%)	1 (0%)	24	60
3	c	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
4	d	203/206 (98%)	193 (95%)	10 (5%)	0	100	100
5	e	153/167 (92%)	143 (94%)	9 (6%)	1 (1%)	18	53
6	f	101/131 (77%)	90 (89%)	11 (11%)	0	100	100
7	g	149/156 (96%)	139 (93%)	10 (7%)	0	100	100
8	h	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
9	i	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	j	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	12	45
11	k	112/129 (87%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
13	m	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	p	78/82 (95%)	71 (91%)	7 (9%)	0	100	100
17	q	75/84 (89%)	72 (96%)	3 (4%)	0	100	100
18	r	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
19	s	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
20	t	84/87 (97%)	84 (100%)	0	0	100	100
21	u	62/71 (87%)	61 (98%)	1 (2%)	0	100	100
24	x	593/890 (67%)	554 (93%)	38 (6%)	1 (0%)	43	76
25	y	70/72 (97%)	64 (91%)	6 (9%)	0	100	100
28	C	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
29	D	205/209 (98%)	195 (95%)	9 (4%)	1 (0%)	24	60
30	E	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
31	F	175/179 (98%)	152 (87%)	23 (13%)	0	100	100
32	G	172/177 (97%)	165 (96%)	7 (4%)	0	100	100
33	H	147/149 (99%)	130 (88%)	16 (11%)	1 (1%)	18	53
34	L	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
35	M	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
36	N	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
37	O	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
38	P	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
39	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
40	R	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
41	S	115/118 (98%)	115 (100%)	0	0	100	100
42	T	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
43	U	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
44	V	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
45	W	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
46	X	92/94 (98%)	88 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	Y	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
48	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
49	1	59/63 (94%)	59 (100%)	0	0	100	100
50	2	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
51	3	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
52	4	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
53	5	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
54	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
55	7	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
56	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	6222/6848 (91%)	5904 (95%)	312 (5%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	25	PRO
10	j	57	VAL
24	x	686	VAL
29	D	149	ASN
5	e	90	THR
33	H	122	LEU

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	150/190 (79%)	150 (100%)	0	100	100
4	d	170/173 (98%)	170 (100%)	0	100	100
5	e	118/126 (94%)	118 (100%)	0	100	100
7	g	63/129 (49%)	63 (100%)	0	100	100
8	h	101/105 (96%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	88/107 (82%)	88 (100%)	0	100	100
10	j	53/90 (59%)	53 (100%)	0	100	100
11	k	84/98 (86%)	84 (100%)	0	100	100
12	l	96/103 (93%)	96 (100%)	0	100	100
13	m	83/96 (86%)	83 (100%)	0	100	100
14	n	75/84 (89%)	75 (100%)	0	100	100
15	o	59/77 (77%)	59 (100%)	0	100	100
16	p	63/65 (97%)	63 (100%)	0	100	100
17	q	71/78 (91%)	71 (100%)	0	100	100
19	s	63/79 (80%)	63 (100%)	0	100	100
20	t	65/66 (98%)	65 (100%)	0	100	100
24	x	451/713 (63%)	450 (100%)	1 (0%)	87	92
25	y	65/65 (100%)	65 (100%)	0	100	100
28	C	216/218 (99%)	216 (100%)	0	100	100
29	D	162/163 (99%)	162 (100%)	0	100	100
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	147/150 (98%)	147 (100%)	0	100	100
32	G	135/138 (98%)	135 (100%)	0	100	100
33	H	31/114 (27%)	31 (100%)	0	100	100
34	L	114/116 (98%)	114 (100%)	0	100	100
35	M	104/104 (100%)	104 (100%)	0	100	100
36	N	103/103 (100%)	103 (100%)	0	100	100
37	O	107/107 (100%)	107 (100%)	0	100	100
38	P	98/103 (95%)	98 (100%)	0	100	100
39	Q	86/87 (99%)	86 (100%)	0	100	100
40	R	97/100 (97%)	97 (100%)	0	100	100
41	S	89/90 (99%)	89 (100%)	0	100	100
42	T	84/84 (100%)	84 (100%)	0	100	100
43	U	92/93 (99%)	92 (100%)	0	100	100
44	V	79/84 (94%)	79 (100%)	0	100	100
45	W	81/85 (95%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	X	78/78 (100%)	78 (100%)	0	100	100
47	Y	56/63 (89%)	56 (100%)	0	100	100
48	Z	67/68 (98%)	67 (100%)	0	100	100
49	1	53/55 (96%)	53 (100%)	0	100	100
50	2	47/49 (96%)	47 (100%)	0	100	100
51	3	44/62 (71%)	44 (100%)	0	100	100
52	4	44/48 (92%)	44 (100%)	0	100	100
53	5	45/49 (92%)	45 (100%)	0	100	100
54	6	38/38 (100%)	38 (100%)	0	100	100
55	7	51/52 (98%)	51 (100%)	0	100	100
56	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4465/5144 (87%)	4464 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
24	x	404	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	185	ASN
4	d	54	GLN
4	d	198	HIS
5	e	135	ASN
5	e	148	ASN
8	h	118	GLN
11	k	109	ASN
15	o	46	HIS
19	s	56	GLN
20	t	20	HIS
20	t	78	ASN
24	x	432	HIS
24	x	825	HIS
25	y	10	GLN
25	y	30	HIS
25	y	43	ASN

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Mol	Chain	Res	Type
28	C	25	HIS
28	C	143	ASN
29	D	42	ASN
29	D	148	GLN
30	E	92	HIS
30	E	115	GLN
33	H	11	ASN
39	Q	116	GLN
40	R	75	GLN
41	S	20	GLN
42	T	12	HIS
42	T	82	HIS
42	T	86	GLN
43	U	9	HIS
46	X	5	ASN
46	X	24	ASN
46	X	75	GLN
47	Y	57	HIS
48	Z	36	HIS
49	1	36	GLN
53	5	19	HIS
56	8	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1520/1542 (98%)	279 (18%)	0
22	w	3/24 (12%)	0	0
23	v	75/77 (97%)	18 (24%)	0
26	A	2842/2904 (97%)	328 (11%)	10 (0%)
27	B	118/120 (98%)	15 (12%)	2 (1%)
All	All	4558/4667 (97%)	640 (14%)	12 (0%)

All (640) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	7	A
1	a	8	A
1	a	9	G
1	a	22	G

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Mol	Chain	Res	Type
1	a	31	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	52	C
1	a	63	C
1	a	64	G
1	a	66	A
1	a	68	G
1	a	71	A
1	a	76	G
1	a	80	A
1	a	81	A
1	a	82	G
1	a	83	C
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	91	U
1	a	94	G
1	a	95	C
1	a	98	A
1	a	99	C
1	a	101	A
1	a	109	A
1	a	116	A
1	a	120	A
1	a	121	U
1	a	127	G
1	a	131	A
1	a	139	A
1	a	140	U
1	a	141	G
1	a	144	G
1	a	164	G
1	a	174	A
1	a	182	A
1	a	219	U
1	a	226	G

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Mol	Chain	Res	Type
1	a	227	G
1	a	228	A
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	289	G
1	a	306	A
1	a	321	A
1	a	325	A
1	a	326	G
1	a	328	C
1	a	329	A
1	a	330	C
1	a	332	G
1	a	347	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	382	A
1	a	397	A
1	a	398	U
1	a	406	G
1	a	407	U
1	a	411	A
1	a	413	G
1	a	414	A
1	a	417	G
1	a	421	U
1	a	425	G
1	a	426	U
1	a	429	U
1	a	436	C
1	a	437	U
1	a	439	U
1	a	442	G
1	a	443	C
1	a	445	G
1	a	451	A

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Mol	Chain	Res	Type
1	a	458	U
1	a	461	A
1	a	462	G
1	a	463	U
1	a	467	U
1	a	468	A
1	a	479	U
1	a	484	G
1	a	486	U
1	a	491	G
1	a	492	C
1	a	493	A
1	a	495	A
1	a	497	G
1	a	511	C
1	a	517	G
1	a	518	C
1	a	519	C
1	a	521	G
1	a	524	G
1	a	527	G7M
1	a	529	G
1	a	530	G
1	a	531	U
1	a	533	A
1	a	545	C
1	a	547	A
1	a	548	G
1	a	559	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	584	G
1	a	595	A
1	a	607	A
1	a	612	C
1	a	618	C
1	a	633	G
1	a	650	G
1	a	653	U

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Mol	Chain	Res	Type
1	a	665	A
1	a	666	G
1	a	687	A
1	a	715	A
1	a	719	C
1	a	721	G
1	a	723	U
1	a	724	G
1	a	734	G
1	a	747	A
1	a	755	G
1	a	777	A
1	a	787	A
1	a	793	U
1	a	794	A
1	a	813	U
1	a	814	A
1	a	815	A
1	a	817	C
1	a	828	U
1	a	829	G
1	a	832	G
1	a	836	G
1	a	841	C
1	a	842	U
1	a	843	U
1	a	844	G
1	a	845	A
1	a	846	G
1	a	851	G
1	a	872	A
1	a	873	A
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	938	A
1	a	960	U
1	a	965	U
1	a	968	A
1	a	969	A
1	a	971	G

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Mol	Chain	Res	Type
1	a	975	A
1	a	976	G
1	a	977	A
1	a	982	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1000	A
1	a	1003	G
1	a	1004	A
1	a	1005	A
1	a	1006	G
1	a	1007	U
1	a	1008	U
1	a	1009	U
1	a	1019	A
1	a	1020	G
1	a	1021	A
1	a	1024	G
1	a	1025	U
1	a	1026	G
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1043	G
1	a	1045	C
1	a	1046	A
1	a	1065	U
1	a	1084	G
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1119	C
1	a	1125	U
1	a	1136	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1141	C

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Mol	Chain	Res	Type
1	a	1152	A
1	a	1157	A
1	a	1158	C
1	a	1159	U
1	a	1169	A
1	a	1174	G
1	a	1196	A
1	a	1197	A
1	a	1202	U
1	a	1213	A
1	a	1227	A
1	a	1238	A
1	a	1240	U
1	a	1248	A
1	a	1253	G
1	a	1260	G
1	a	1270	G
1	a	1280	A
1	a	1285	A
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1318	A
1	a	1320	C
1	a	1322	C
1	a	1332	A
1	a	1338	G
1	a	1363	A
1	a	1370	G
1	a	1375	A
1	a	1378	C
1	a	1379	G
1	a	1432	G
1	a	1441	A
1	a	1446	A
1	a	1448	C
1	a	1451	U

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Mol	Chain	Res	Type
1	a	1452	C
1	a	1453	G
1	a	1455	G
1	a	1456	A
1	a	1458	G
1	a	1459	G
1	a	1460	C
1	a	1461	G
1	a	1487	G
1	a	1491	G
1	a	1492	A
1	a	1494	G
1	a	1497	G
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1519	MA6
1	a	1529	G
1	a	1530	G
1	a	1531	A
1	a	1533	C
23	v	8	4SU
23	v	9	G
23	v	15	G
23	v	16	C
23	v	17	C
23	v	18	U
23	v	19	G
23	v	21	U
23	v	22	A
23	v	48	U
23	v	50	G
23	v	62	C
23	v	65	G
23	v	70	C
23	v	71	G
23	v	72	C
23	v	73	A
23	v	77	A
26	A	10	A
26	A	34	U

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Mol	Chain	Res	Type
26	A	71	A
26	A	74	A
26	A	75	G
26	A	84	A
26	A	101	A
26	A	102	U
26	A	118	A
26	A	119	A
26	A	120	U
26	A	125	A
26	A	139	U
26	A	142	A
26	A	149	A
26	A	163	C
26	A	181	A
26	A	196	A
26	A	199	A
26	A	215	G
26	A	216	A
26	A	221	A
26	A	222	A
26	A	223	A
26	A	233	A
26	A	248	G
26	A	266	G
26	A	272	A
26	A	276	U
26	A	278	A
26	A	279	A
26	A	281	C
26	A	311	A
26	A	329	G
26	A	330	A
26	A	362	A
26	A	385	C
26	A	386	G
26	A	396	G
26	A	404	A
26	A	405	U
26	A	411	G
26	A	412	A
26	A	481	G

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Mol	Chain	Res	Type
26	A	491	G
26	A	504	A
26	A	505	A
26	A	509	C
26	A	510	C
26	A	530	G
26	A	531	C
26	A	532	A
26	A	545	U
26	A	547	A
26	A	549	G
26	A	563	A
26	A	573	U
26	A	574	A
26	A	575	A
26	A	603	A
26	A	615	U
26	A	627	A
26	A	637	A
26	A	645	C
26	A	653	U
26	A	654	A
26	A	686	U
26	A	730	A
26	A	740	C
26	A	747	5MU
26	A	764	A
26	A	775	G
26	A	776	G
26	A	782	A
26	A	784	G
26	A	785	G
26	A	789	A
26	A	805	G
26	A	812	C
26	A	827	U
26	A	828	U
26	A	845	A
26	A	846	U
26	A	847	U
26	A	859	G
26	A	881	G

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Mol	Chain	Res	Type
26	A	884	U
26	A	890	C
26	A	895	U
26	A	896	A
26	A	897	C
26	A	907	G
26	A	910	A
26	A	931	U
26	A	934	U
26	A	945	A
26	A	946	C
26	A	958	U
26	A	961	C
26	A	973	A
26	A	974	G
26	A	983	A
26	A	996	A
26	A	1005	C
26	A	1012	U
26	A	1013	C
26	A	1027	A
26	A	1033	U
26	A	1044	C
26	A	1045	C
26	A	1046	A
26	A	1047	G
26	A	1051	G
26	A	1109	C
26	A	1110	G
26	A	1111	A
26	A	1112	G
26	A	1132	U
26	A	1133	A
26	A	1135	C
26	A	1136	G
26	A	1142	A
26	A	1187	G
26	A	1204	A
26	A	1210	G
26	A	1250	G
26	A	1253	A
26	A	1256	G

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Mol	Chain	Res	Type
26	A	1257	C
26	A	1268	A
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1300	G
26	A	1301	A
26	A	1359	A
26	A	1365	A
26	A	1379	U
26	A	1383	A
26	A	1387	A
26	A	1416	G
26	A	1417	C
26	A	1420	A
26	A	1428	C
26	A	1452	G
26	A	1455	G
26	A	1482	G
26	A	1483	G
26	A	1509	A
26	A	1515	A
26	A	1524	G
26	A	1529	G
26	A	1534	U
26	A	1535	A
26	A	1536	C
26	A	1569	A
26	A	1572	A
26	A	1584	U
26	A	1585	C
26	A	1586	A
26	A	1608	A
26	A	1647	U
26	A	1648	U
26	A	1649	G
26	A	1674	G
26	A	1675	C
26	A	1715	G
26	A	1729	U
26	A	1738	G
26	A	1744	A

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Mol	Chain	Res	Type
26	A	1764	C
26	A	1773	A
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1816	C
26	A	1829	A
26	A	1848	A
26	A	1858	A
26	A	1871	A
26	A	1906	G
26	A	1909	C
26	A	1912	A
26	A	1913	A
26	A	1914	C
26	A	1917	PSU
26	A	1918	A
26	A	1919	A
26	A	1923	U
26	A	1927	A
26	A	1929	G
26	A	1930	G
26	A	1936	A
26	A	1937	A
26	A	1955	U
26	A	1963	U
26	A	1964	G
26	A	1967	C
26	A	1970	A
26	A	1971	U
26	A	1972	G
26	A	1991	U
26	A	1993	U
26	A	2023	C
26	A	2031	A
26	A	2033	A
26	A	2043	C
26	A	2049	G
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G

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Mol	Chain	Res	Type
26	A	2062	A
26	A	2069	G7M
26	A	2093	G
26	A	2099	U
26	A	2104	C
26	A	2107	G
26	A	2110	G
26	A	2111	U
26	A	2112	G
26	A	2113	U
26	A	2114	A
26	A	2116	G
26	A	2117	A
26	A	2118	U
26	A	2121	G
26	A	2125	G
26	A	2126	A
26	A	2128	G
26	A	2132	U
26	A	2133	G
26	A	2135	A
26	A	2140	G
26	A	2145	C
26	A	2147	A
26	A	2157	G
26	A	2159	G
26	A	2160	C
26	A	2162	G
26	A	2164	C
26	A	2170	A
26	A	2171	A
26	A	2172	U
26	A	2173	A
26	A	2180	U
26	A	2182	U
26	A	2183	A
26	A	2186	G
26	A	2187	U
26	A	2188	U
26	A	2189	U
26	A	2190	G
26	A	2198	A

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Mol	Chain	Res	Type
26	A	2203	U
26	A	2204	G
26	A	2210	U
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2279	G
26	A	2283	C
26	A	2287	A
26	A	2288	A
26	A	2305	U
26	A	2306	C
26	A	2307	G
26	A	2308	G
26	A	2322	A
26	A	2325	G
26	A	2333	A
26	A	2347	C
26	A	2361	G
26	A	2379	G
26	A	2383	G
26	A	2385	C
26	A	2402	U
26	A	2403	C
26	A	2419	U
26	A	2425	A
26	A	2428	G
26	A	2429	G
26	A	2430	A
26	A	2435	A
26	A	2441	U
26	A	2448	A
26	A	2470	G
26	A	2474	U
26	A	2475	C
26	A	2498	OMC
26	A	2502	G
26	A	2505	G
26	A	2506	U
26	A	2513	A
26	A	2518	A
26	A	2547	A

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Mol	Chain	Res	Type
26	A	2566	A
26	A	2567	G
26	A	2586	U
26	A	2602	A
26	A	2609	U
26	A	2613	U
26	A	2615	U
26	A	2629	U
26	A	2630	G
26	A	2661	G
26	A	2663	G
26	A	2689	U
26	A	2690	U
26	A	2714	G
26	A	2723	C
26	A	2724	U
26	A	2726	A
26	A	2727	A
26	A	2744	G
26	A	2748	A
26	A	2765	A
26	A	2778	A
26	A	2793	C
26	A	2797	U
26	A	2798	U
26	A	2801	G
26	A	2820	A
26	A	2833	U
26	A	2861	U
26	A	2873	A
26	A	2880	C
26	A	2884	U
27	B	2	G
27	B	3	C
27	B	7	G
27	B	13	G
27	B	25	U
27	B	35	C
27	B	37	C
27	B	41	G
27	B	44	G
27	B	56	G

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Mol	Chain	Res	Type
27	B	67	G
27	B	89	U
27	B	90	C
27	B	99	A
27	B	109	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	277	G
26	A	404	A
26	A	406	G
26	A	424	G
26	A	425	G
26	A	547	A
26	A	784	G
26	A	1358	G
26	A	2182	U
26	A	2189	U
27	B	2	G
27	B	6	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	2MG	a	1516	1	23,26,27	1.28	4 (17%)	33,38,41	2.20	7 (21%)
26	2MA	A	2503	26,57	22,25,26	1.42	5 (22%)	32,37,40	2.30	8 (25%)
26	PSU	A	2604	26	18,21,22	1.51	4 (22%)	21,30,33	2.12	4 (19%)
26	PSU	A	955	26	18,21,22	1.50	4 (22%)	21,30,33	2.19	3 (14%)
23	5MC	v	33	23	19,22,23	1.50	3 (15%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PSU	A	2580	26	18,21,22	1.60	5 (27%)	21,30,33	2.18	4 (19%)
26	5MU	A	1939	26	19,22,23	1.41	4 (21%)	27,32,35	2.09	7 (25%)
26	PSU	A	2457	26	18,21,22	1.59	5 (27%)	21,30,33	2.18	3 (14%)
26	PSU	A	2605	26	18,21,22	1.56	4 (22%)	21,30,33	2.17	4 (19%)
26	H2U	A	2449	26	18,21,22	1.35	3 (16%)	19,30,33	1.06	1 (5%)
23	PSU	v	56	23	18,21,22	1.41	2 (11%)	21,30,33	1.99	4 (19%)
1	PSU	a	516	1	18,21,22	1.41	3 (16%)	21,30,33	2.25	5 (23%)
11	IAS	k	119	11	6,7,8	0.99	0	3,8,10	1.59	1 (33%)
12	D2T	l	89	12	8,9,10	2.49	1 (12%)	6,11,13	2.44	2 (33%)
26	1MG	A	745	26	23,26,27	1.11	3 (13%)	33,39,42	1.84	6 (18%)
1	5MC	a	967	1	19,22,23	1.51	3 (15%)	26,32,35	1.36	4 (15%)
26	PSU	A	1911	26	18,21,22	1.39	3 (16%)	21,30,33	1.97	3 (14%)
1	5MC	a	1407	1	19,22,23	1.47	3 (15%)	26,32,35	1.21	3 (11%)
37	4D4	O	81	37	9,11,12	2.56	2 (22%)	7,13,15	0.79	0
26	PSU	A	746	26,57	18,21,22	1.53	4 (22%)	21,30,33	2.01	4 (19%)
1	G7M	a	527	1	23,26,27	1.59	4 (17%)	34,39,42	1.72	5 (14%)
26	OMU	A	2552	26	19,22,23	1.36	4 (21%)	25,31,34	1.83	4 (16%)
26	OMG	A	2251	26	23,26,27	1.26	3 (13%)	32,38,41	2.10	8 (25%)
26	6MZ	A	2030	26	22,25,26	1.44	5 (22%)	29,36,39	2.43	10 (34%)
26	6MZ	A	1618	26	22,25,26	1.41	5 (22%)	29,36,39	2.50	9 (31%)
26	PSU	A	2504	26	18,21,22	1.52	4 (22%)	21,30,33	2.10	4 (19%)
1	2MG	a	1207	57,1	23,26,27	1.27	4 (17%)	33,38,41	2.32	11 (33%)
26	2MG	A	2445	26	23,26,27	1.34	4 (17%)	33,38,41	2.22	7 (21%)
26	OMC	A	2498	26,57	19,22,23	0.89	2 (10%)	25,31,34	0.94	2 (8%)
23	4SU	v	8	23	18,21,22	1.96	5 (27%)	25,30,33	2.53	8 (32%)
1	MA6	a	1519	1	23,26,27	1.43	5 (21%)	33,38,41	2.44	14 (42%)
23	5MU	v	55	23	19,22,23	1.40	5 (26%)	27,32,35	2.17	6 (22%)
1	2MG	a	966	1	23,26,27	1.26	3 (13%)	33,38,41	2.36	11 (33%)
26	5MU	A	747	26	19,22,23	1.42	4 (21%)	27,32,35	2.13	6 (22%)
26	2MG	A	1835	26	23,26,27	1.28	3 (13%)	33,38,41	2.27	11 (33%)
26	PSU	A	1917	26	18,21,22	1.33	2 (11%)	21,30,33	1.90	3 (14%)
26	G7M	A	2069	26	23,26,27	1.63	4 (17%)	34,39,42	1.66	5 (14%)
37	MS6	O	82	37	5,7,8	0.74	0	2,7,9	1.31	0
26	3TD	A	1915	26	19,22,23	4.38	7 (36%)	23,32,35	1.85	3 (13%)
26	5MC	A	1962	26	19,22,23	1.18	2 (10%)	26,32,35	1.14	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MEQ	D	150	29	8,9,10	0.46	0	5,10,12	0.48	0
1	UR3	a	1498	1	19,22,23	0.97	0	26,32,35	1.85	3 (11%)
1	4OC	a	1402	1	20,23,24	0.83	0	25,32,35	1.12	3 (12%)
1	MA6	a	1518	1	23,26,27	1.50	6 (26%)	33,38,41	2.43	14 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
26	2MA	A	2503	26,57	-	0/7/25/26	0/3/3/3
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
23	5MC	v	33	23	-	0/7/25/26	0/2/2/2
26	PSU	A	2580	26	-	2/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
23	PSU	v	56	23	-	0/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
11	IAS	k	119	11	-	1/7/7/8	-
12	D2T	l	89	12	-	2/7/12/14	-
26	1MG	A	745	26	-	0/7/25/26	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
37	4D4	O	81	37	-	4/11/12/14	-
26	PSU	A	746	26,57	-	2/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
26	OMU	A	2552	26	-	0/9/27/28	0/2/2/2
26	OMG	A	2251	26	-	0/9/27/28	0/3/3/3
26	6MZ	A	2030	26	-	2/9/27/28	0/3/3/3
26	6MZ	A	1618	26	-	0/9/27/28	0/3/3/3
26	PSU	A	2504	26	-	1/7/25/26	0/2/2/2
1	2MG	a	1207	57,1	-	0/9/27/28	0/3/3/3
26	2MG	A	2445	26	-	0/9/27/28	0/3/3/3
26	OMC	A	2498	26,57	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	4SU	v	8	23	-	2/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/11/29/30	0/3/3/3
23	5MU	v	55	23	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
26	2MG	A	1835	26	-	0/9/27/28	0/3/3/3
26	PSU	A	1917	26	-	2/7/25/26	0/2/2/2
26	G7M	A	2069	26	-	0/7/25/26	0/3/3/3
37	MS6	O	82	37	-	1/4/6/8	-
26	3TD	A	1915	26	-	1/7/25/26	0/2/2/2
26	5MC	A	1962	26	-	0/7/25/26	0/2/2/2
29	MEQ	D	150	29	-	2/8/9/11	-
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	1/9/29/30	0/2/2/2
1	MA6	a	1518	1	-	4/11/29/30	0/3/3/3

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C6-C5	12.91	1.49	1.35
26	A	1915	3TD	C2-N1	10.39	1.50	1.37
12	l	89	D2T	CB-CA	-6.46	1.52	1.54
37	O	81	4D4	CZ-NE	6.35	1.45	1.33
26	A	1915	3TD	C6-N1	6.16	1.46	1.36
26	A	2069	G7M	C5-N7	-5.66	1.32	1.39
1	a	527	G7M	C5-N7	-5.45	1.32	1.39
26	A	1915	3TD	C2-N3	5.30	1.49	1.38
1	a	967	5MC	C5-C4	5.17	1.48	1.44
23	v	33	5MC	C5-C4	5.15	1.48	1.44
1	a	1407	5MC	C5-C4	5.03	1.47	1.44
23	v	8	4SU	C4-S4	-5.00	1.59	1.68
1	a	1518	MA6	C5-C4	4.37	1.46	1.39
1	a	1519	MA6	C5-C4	4.08	1.46	1.39
26	A	1618	6MZ	C5-C4	3.90	1.46	1.39
26	A	2503	2MA	C5-C4	3.80	1.45	1.39
26	A	1962	5MC	C5-C4	3.68	1.46	1.44
26	A	1917	PSU	C6-C5	3.63	1.39	1.35
26	A	2030	6MZ	C5-C4	3.55	1.45	1.39
23	v	8	4SU	C4-N3	-3.51	1.34	1.37
26	A	2605	PSU	C4-N3	-3.45	1.32	1.38
23	v	56	PSU	C6-C5	3.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2457	PSU	C4-N3	-3.40	1.32	1.38
26	A	746	PSU	C4-N3	-3.33	1.32	1.38
26	A	2580	PSU	C4-N3	-3.33	1.32	1.38
26	A	2449	H2U	C4-N3	-3.33	1.32	1.37
26	A	2504	PSU	C4-N3	-3.28	1.32	1.38
26	A	1939	5MU	C4-N3	-3.26	1.32	1.38
26	A	2445	2MG	C6-N1	-3.26	1.32	1.38
26	A	2552	OMU	C4-N3	-3.25	1.33	1.38
26	A	955	PSU	C4-N3	-3.24	1.32	1.38
26	A	747	5MU	C4-N3	-3.19	1.32	1.38
26	A	2604	PSU	C4-N3	-3.18	1.32	1.38
26	A	2449	H2U	C2-N3	-3.13	1.32	1.38
26	A	1911	PSU	C6-C5	3.08	1.38	1.35
37	O	81	4D4	CZ-NH1	3.08	1.45	1.34
26	A	2030	6MZ	C5-N7	-3.06	1.33	1.39
26	A	2069	G7M	C6-N1	-3.04	1.33	1.38
26	A	1835	2MG	C6-N1	-2.98	1.33	1.38
26	A	2580	PSU	C2-N1	-2.98	1.32	1.36
26	A	2552	OMU	C2-N3	-2.97	1.32	1.38
26	A	2605	PSU	C2-N1	-2.92	1.32	1.36
1	a	516	PSU	C4-N3	-2.91	1.33	1.38
26	A	2251	OMG	C6-N1	-2.90	1.33	1.38
1	a	1516	2MG	C5-C4	2.90	1.46	1.38
1	a	1207	2MG	C5-C4	2.87	1.46	1.38
1	a	966	2MG	C5-C4	2.86	1.46	1.38
1	a	516	PSU	C6-C5	2.86	1.38	1.35
26	A	2503	2MA	C5-N7	-2.86	1.33	1.39
26	A	2457	PSU	C2-N1	-2.85	1.32	1.36
1	a	527	G7M	C5-C4	2.85	1.45	1.38
26	A	2504	PSU	C2-N3	-2.84	1.32	1.37
26	A	747	5MU	C6-N1	-2.83	1.33	1.38
26	A	2457	PSU	C2-N3	-2.80	1.32	1.37
26	A	1911	PSU	C4-N3	-2.78	1.33	1.38
26	A	2605	PSU	C2-N3	-2.77	1.32	1.37
26	A	1939	5MU	C2-N3	-2.77	1.33	1.38
26	A	1618	6MZ	C5-N7	-2.77	1.34	1.39
26	A	1962	5MC	C6-N1	-2.76	1.33	1.38
26	A	747	5MU	C2-N3	-2.76	1.33	1.38
26	A	1835	2MG	C5-C4	2.75	1.46	1.38
26	A	2504	PSU	C2-N1	-2.75	1.33	1.36
26	A	2445	2MG	C5-N7	-2.74	1.33	1.39
1	a	527	G7M	C6-N1	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1516	2MG	C6-N1	-2.73	1.33	1.38
23	v	8	4SU	C5-C4	-2.72	1.39	1.42
26	A	955	PSU	C2-N3	-2.72	1.33	1.37
23	v	56	PSU	C4-N3	-2.71	1.33	1.38
26	A	2251	OMG	C5-C4	2.71	1.46	1.38
26	A	746	PSU	C2-N3	-2.70	1.33	1.37
23	v	55	5MU	C6-C5	2.70	1.39	1.34
23	v	33	5MC	C6-N1	-2.69	1.33	1.38
26	A	1915	3TD	C4-N3	2.67	1.46	1.40
26	A	2604	PSU	C2-N3	-2.66	1.33	1.37
26	A	2604	PSU	C2-N1	-2.64	1.33	1.36
26	A	2251	OMG	C5-N7	-2.64	1.33	1.39
1	a	1207	2MG	C6-N1	-2.64	1.33	1.38
26	A	1939	5MU	C6-N1	-2.63	1.33	1.38
26	A	747	5MU	C6-C5	2.60	1.38	1.34
1	a	966	2MG	C6-N1	-2.59	1.34	1.38
26	A	2449	H2U	C2-N1	-2.58	1.32	1.35
1	a	1518	MA6	C5-N7	-2.57	1.34	1.39
1	a	1518	MA6	C5-C6	2.57	1.48	1.41
26	A	2580	PSU	O4'-C1'	-2.57	1.40	1.43
23	v	55	5MU	C4-N3	-2.57	1.34	1.38
26	A	955	PSU	C2-N1	-2.57	1.33	1.36
26	A	745	1MG	C5-C4	2.57	1.45	1.38
1	a	967	5MC	C6-N1	-2.56	1.33	1.38
26	A	2580	PSU	C2-N3	-2.55	1.33	1.37
26	A	1915	3TD	O2-C2	-2.54	1.18	1.23
26	A	2069	G7M	C5-C4	2.52	1.44	1.38
26	A	2552	OMU	C5-C4	-2.51	1.38	1.43
26	A	1835	2MG	C5-N7	-2.48	1.34	1.39
1	a	1519	MA6	C5-N7	-2.47	1.34	1.39
23	v	33	5MC	C6-C5	2.45	1.38	1.34
26	A	2030	6MZ	C4-N9	-2.45	1.32	1.37
26	A	2445	2MG	C5-C4	2.44	1.45	1.38
26	A	2030	6MZ	C5-C6	2.44	1.47	1.41
1	a	1407	5MC	C6-N1	-2.42	1.33	1.38
1	a	1519	MA6	C5-C6	2.41	1.47	1.41
26	A	746	PSU	C2-N1	-2.40	1.33	1.36
26	A	746	PSU	C6-C5	2.38	1.37	1.35
26	A	2069	G7M	C4-N9	-2.38	1.32	1.38
1	a	1519	MA6	C4-N9	-2.38	1.32	1.37
23	v	55	5MU	C4-C5	2.37	1.48	1.44
26	A	1917	PSU	C4-N3	-2.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1518	MA6	C4-N9	-2.37	1.32	1.37
26	A	1618	6MZ	C5-C6	2.36	1.47	1.41
26	A	2498	OMC	C6-N1	-2.36	1.32	1.38
26	A	1939	5MU	C6-C5	2.35	1.38	1.34
26	A	745	1MG	C5-N7	-2.34	1.34	1.39
26	A	2503	2MA	C5-C6	2.34	1.47	1.41
26	A	1618	6MZ	C4-N9	-2.34	1.32	1.37
23	v	8	4SU	O3'-C3'	2.34	1.48	1.43
23	v	55	5MU	C2-N1	2.30	1.42	1.38
26	A	2030	6MZ	C8-N9	-2.29	1.33	1.37
1	a	967	5MC	C6-C5	2.29	1.38	1.34
1	a	1407	5MC	C6-C5	2.27	1.38	1.34
26	A	745	1MG	C4-N9	-2.27	1.32	1.38
26	A	2503	2MA	C4-N9	-2.26	1.33	1.37
23	v	55	5MU	C6-N1	-2.25	1.34	1.38
26	A	2457	PSU	O4'-C1'	-2.25	1.40	1.43
26	A	955	PSU	C6-C5	2.24	1.37	1.35
26	A	2552	OMU	C6-N1	-2.22	1.32	1.38
1	a	966	2MG	C5-N7	-2.20	1.34	1.39
26	A	2457	PSU	C6-N1	-2.15	1.32	1.36
1	a	1516	2MG	C5-N7	-2.15	1.34	1.39
26	A	2498	OMC	C5-C4	-2.14	1.37	1.42
26	A	2445	2MG	C4-N9	-2.14	1.32	1.38
1	a	1207	2MG	C5-N7	-2.14	1.34	1.39
26	A	2580	PSU	C6-N1	-2.13	1.32	1.36
26	A	2604	PSU	C6-C5	2.12	1.37	1.35
26	A	2503	2MA	C8-N9	-2.11	1.34	1.37
1	a	527	G7M	C4-N9	-2.11	1.32	1.38
23	v	8	4SU	C2-N3	-2.11	1.34	1.38
26	A	2605	PSU	C6-C5	2.10	1.37	1.35
26	A	1911	PSU	C2-N3	-2.09	1.34	1.37
26	A	1618	6MZ	C8-N9	-2.09	1.34	1.37
1	a	516	PSU	C2-N3	-2.09	1.34	1.37
1	a	1519	MA6	C8-N7	2.08	1.35	1.31
26	A	1915	3TD	O4-C4	-2.08	1.18	1.23
26	A	2504	PSU	C6-C5	2.05	1.37	1.35
1	a	1518	MA6	C8-N7	2.04	1.35	1.31
1	a	1516	2MG	C4-N9	-2.03	1.32	1.38
1	a	1207	2MG	C4-N9	-2.02	1.32	1.38
1	a	1518	MA6	C8-N9	-2.02	1.34	1.37

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2503	2MA	C5-C4-N3	-8.35	118.39	127.18
26	A	2445	2MG	C2-N3-C4	7.34	121.18	112.00
26	A	1835	2MG	C2-N3-C4	7.34	121.18	112.00
1	a	966	2MG	C2-N3-C4	7.20	121.01	112.00
23	v	8	4SU	C4-N3-C2	-7.14	120.47	127.31
1	a	1498	UR3	C4-N3-C2	-7.13	118.84	124.58
1	a	1207	2MG	C2-N3-C4	7.12	120.91	112.00
1	a	1516	2MG	C2-N3-C4	6.92	120.66	112.00
26	A	2251	OMG	C5-C4-N3	-6.89	117.43	128.39
26	A	2457	PSU	N1-C2-N3	6.87	122.41	115.17
26	A	955	PSU	N1-C2-N3	6.86	122.41	115.17
26	A	2580	PSU	N1-C2-N3	6.76	122.30	115.17
1	a	516	PSU	N1-C2-N3	6.68	122.22	115.17
26	A	2605	PSU	N1-C2-N3	6.59	122.12	115.17
26	A	2604	PSU	N1-C2-N3	6.51	122.04	115.17
26	A	1618	6MZ	C9-N6-C6	-6.50	116.82	122.85
26	A	2030	6MZ	C5-C4-N3	-6.34	117.99	126.72
26	A	1835	2MG	C5-C4-N3	-6.33	118.31	128.39
26	A	2504	PSU	N1-C2-N3	6.33	121.85	115.17
26	A	1618	6MZ	C5-C4-N3	-6.31	118.03	126.72
26	A	2503	2MA	N3-C4-N9	6.31	134.99	126.99
26	A	2445	2MG	C5-C4-N3	-6.16	118.59	128.39
26	A	1911	PSU	N1-C2-N3	6.12	121.62	115.17
23	v	56	PSU	N1-C2-N3	6.12	121.62	115.17
1	a	966	2MG	C5-C4-N3	-6.01	118.83	128.39
1	a	1207	2MG	C5-C4-N3	-6.00	118.83	128.39
26	A	746	PSU	N1-C2-N3	5.98	121.48	115.17
26	A	1917	PSU	N1-C2-N3	5.85	121.34	115.17
26	A	1915	3TD	N1-C2-N3	5.84	120.38	116.13
1	a	1516	2MG	C5-C4-N3	-5.83	119.12	128.39
1	a	1518	MA6	C5-C4-N3	-5.64	118.94	126.72
26	A	745	1MG	C5-C4-N3	-5.44	119.73	128.39
26	A	2251	OMG	C2-N3-C4	5.42	121.64	112.30
1	a	1519	MA6	C5-C4-N3	-5.42	119.25	126.72
23	v	8	4SU	C5-C4-N3	5.42	119.79	114.75
26	A	747	5MU	N3-C2-N1	5.29	121.77	114.89
26	A	747	5MU	C4-N3-C2	-5.26	120.44	127.34
1	a	527	G7M	N9-C4-N3	5.26	136.47	125.95
26	A	2030	6MZ	C9-N6-C6	-5.25	117.98	122.85
23	v	55	5MU	C4-N3-C2	-5.25	120.46	127.34
26	A	1939	5MU	N3-C2-N1	5.24	121.72	114.89
1	a	527	G7M	C5-C4-N3	-5.21	118.31	128.15
23	v	55	5MU	N3-C2-N1	5.03	121.44	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1518	MA6	N1-C6-N6	4.99	122.93	116.86
26	A	1618	6MZ	N3-C4-N9	4.98	135.64	127.17
26	A	747	5MU	C5-C4-N3	4.96	119.64	115.32
23	v	8	4SU	N3-C2-N1	4.91	121.29	114.89
26	A	2552	OMU	C4-N3-C2	-4.91	120.52	126.61
26	A	1939	5MU	C4-N3-C2	-4.90	120.92	127.34
26	A	2069	G7M	N9-C4-N3	4.86	135.67	125.95
26	A	2251	OMG	N9-C4-N3	4.82	135.59	125.95
26	A	2069	G7M	C5-C4-N3	-4.75	119.18	128.15
26	A	2030	6MZ	N3-C4-N9	4.71	135.18	127.17
1	a	527	G7M	C2-N3-C4	4.68	120.35	112.30
26	A	1835	2MG	N9-C4-N3	4.60	135.16	125.95
26	A	1915	3TD	C4-N3-C2	-4.59	119.75	124.61
26	A	2069	G7M	C2-N3-C4	4.54	120.11	112.30
26	A	2445	2MG	N9-C4-N3	4.53	135.02	125.95
23	v	55	5MU	C5-C4-N3	4.53	119.26	115.32
26	A	745	1MG	C2-N3-C4	4.44	121.96	111.98
26	A	1939	5MU	C5-C4-N3	4.43	119.17	115.32
26	A	2605	PSU	C4-N3-C2	-4.42	120.28	126.37
12	l	89	D2T	CB1-SB-CB	4.42	110.31	102.36
1	a	516	PSU	C4-N3-C2	-4.40	120.31	126.37
1	a	966	2MG	N9-C4-N3	4.39	134.72	125.95
1	a	1519	MA6	N1-C6-N6	4.36	122.17	116.86
26	A	2457	PSU	C4-N3-C2	-4.36	120.36	126.37
26	A	2552	OMU	N3-C2-N1	4.36	120.57	114.89
26	A	2504	PSU	C4-N3-C2	-4.30	120.45	126.37
1	a	1518	MA6	N3-C4-N9	4.29	134.47	127.17
26	A	2580	PSU	C4-N3-C2	-4.28	120.47	126.37
1	a	1519	MA6	C2-N1-C6	4.28	122.28	111.83
26	A	746	PSU	C4-N3-C2	-4.26	120.50	126.37
26	A	955	PSU	C4-N3-C2	-4.26	120.51	126.37
1	a	1519	MA6	N3-C4-N9	4.22	134.35	127.17
26	A	2604	PSU	C4-N3-C2	-4.22	120.56	126.37
23	v	55	5MU	O4-C4-C5	-4.21	120.10	124.92
1	a	1519	MA6	C9-N6-C6	-4.19	109.87	120.52
1	a	1207	2MG	N9-C4-N3	4.18	134.32	125.95
23	v	56	PSU	C4-N3-C2	-4.17	120.63	126.37
1	a	1516	2MG	N9-C4-N3	4.17	134.28	125.95
26	A	1618	6MZ	C2-N3-C4	4.11	121.87	111.83
1	a	1518	MA6	C2-N1-C6	4.07	121.77	111.83
26	A	2030	6MZ	C4-C5-N7	-4.06	105.94	110.58
26	A	1939	5MU	O4-C4-C5	-4.02	120.32	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2552	OMU	C5-C4-N3	4.00	120.40	114.80
26	A	2580	PSU	O2-C2-N1	-4.00	118.66	122.79
23	v	8	4SU	C5-C4-S4	-3.98	119.76	124.31
26	A	745	1MG	N9-C4-N3	3.96	133.87	125.95
26	A	1911	PSU	C4-N3-C2	-3.93	120.96	126.37
1	a	516	PSU	O2-C2-N1	-3.84	118.82	122.79
26	A	2457	PSU	O2-C2-N1	-3.84	118.82	122.79
1	a	1518	MA6	C4-C5-N7	-3.77	106.28	110.58
26	A	747	5MU	O4-C4-C5	-3.75	120.62	124.92
26	A	1917	PSU	C4-N3-C2	-3.73	121.23	126.37
1	a	967	5MC	C5-C6-N1	-3.72	119.28	123.31
26	A	955	PSU	O2-C2-N1	-3.71	118.96	122.79
26	A	2030	6MZ	C2-N3-C4	3.67	120.78	111.83
26	A	2504	PSU	O2-C2-N1	-3.64	119.03	122.79
26	A	2604	PSU	O2-C2-N1	-3.64	119.03	122.79
1	a	1519	MA6	C2-N3-C4	3.62	120.67	111.83
1	a	1498	UR3	C5-C4-N3	3.61	119.79	115.04
1	a	1518	MA6	C9-N6-C6	-3.57	111.45	120.52
1	a	1518	MA6	C10-N6-C6	-3.54	111.52	120.52
1	a	1207	2MG	C6-C5-N7	3.54	136.73	130.29
1	a	1519	MA6	C4-C5-N7	-3.52	106.56	110.58
26	A	746	PSU	O2-C2-N1	-3.51	119.17	122.79
1	a	1519	MA6	N1-C2-N3	-3.49	123.30	128.58
1	a	1516	2MG	C6-C5-N7	3.47	136.61	130.29
26	A	1618	6MZ	N1-C2-N3	-3.46	123.35	128.58
23	v	55	5MU	C5-C6-N1	-3.46	119.56	123.31
26	A	2030	6MZ	C6-C5-N7	3.44	136.18	132.43
1	a	966	2MG	C6-C5-N7	3.42	136.51	130.29
23	v	33	5MC	C5-C6-N1	-3.39	119.64	123.31
26	A	2503	2MA	C4-C5-N7	-3.38	106.72	110.58
26	A	1917	PSU	O2-C2-N1	-3.38	119.30	122.79
26	A	1911	PSU	O2-C2-N1	-3.35	119.33	122.79
26	A	747	5MU	O2-C2-N1	-3.33	118.47	122.80
26	A	1618	6MZ	C6-C5-N7	3.30	136.02	132.43
1	a	1518	MA6	C2-N3-C4	3.29	119.88	111.83
26	A	2445	2MG	C6-C5-N7	3.27	136.25	130.29
26	A	2605	PSU	O2-C2-N1	-3.25	119.43	122.79
1	a	516	PSU	C3'-C2'-C1'	3.23	105.50	101.69
23	v	56	PSU	O2-C2-N1	-3.21	119.47	122.79
26	A	1618	6MZ	C4-C5-N7	-3.17	106.96	110.58
26	A	1835	2MG	C6-C5-N7	3.15	136.03	130.29
26	A	1915	3TD	C6-C5-C4	3.15	120.31	118.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1518	MA6	C5-C6-N6	-3.14	120.37	125.33
1	a	1519	MA6	C5-C6-N6	-3.12	120.39	125.33
26	A	747	5MU	C5-C6-N1	-3.12	119.92	123.31
26	A	2030	6MZ	C5-N7-C8	3.09	108.30	103.45
1	a	1519	MA6	C10-N6-C6	-3.08	112.69	120.52
1	a	1407	5MC	C5-C6-N1	-3.05	120.00	123.31
26	A	2552	OMU	O4-C4-C5	-3.05	119.90	125.16
12	l	89	D2T	OD2-CG-CB	3.01	119.65	113.15
23	v	8	4SU	O3'-C3'-C4'	2.99	119.68	111.08
26	A	2251	OMG	C6-C5-N7	2.99	135.73	130.29
1	a	1518	MA6	C10-N6-C9	-2.99	106.58	116.18
23	v	8	4SU	C3'-C2'-C1'	2.98	107.10	101.46
26	A	746	PSU	C6-C5-C4	-2.97	116.17	118.17
1	a	1519	MA6	C4-N9-C8	2.93	108.81	105.74
1	a	966	2MG	N1-C2-N2	2.90	119.52	116.56
26	A	745	1MG	C6-C5-N7	2.89	135.78	129.36
26	A	1939	5MU	C5-C6-N1	-2.88	120.19	123.31
23	v	33	5MC	C5-C4-N3	-2.80	118.89	121.75
26	A	2503	2MA	N6-C6-N1	2.77	120.76	117.03
1	a	1207	2MG	C4-C5-N7	-2.76	106.29	110.67
26	A	1962	5MC	O2-C2-N3	-2.75	117.99	122.33
26	A	745	1MG	C4-C5-N7	-2.73	106.35	110.67
23	v	55	5MU	O2-C2-N1	-2.72	119.26	122.80
26	A	2030	6MZ	C4-N9-C8	2.69	108.56	105.74
11	k	119	IAS	OD1-CG-CB	-2.67	117.61	125.38
1	a	1407	5MC	C5-C4-N3	-2.66	119.02	121.75
1	a	1519	MA6	C10-N6-C9	-2.65	107.67	116.18
1	a	1518	MA6	C4-N9-C8	2.63	108.50	105.74
26	A	1962	5MC	C5-C4-N3	-2.62	119.06	121.75
1	a	966	2MG	C4-C5-N7	-2.60	106.55	110.67
26	A	2251	OMG	C4-C5-N7	-2.59	106.56	110.67
1	a	1402	4OC	O2-C2-N3	-2.59	118.25	122.33
1	a	1207	2MG	N1-C2-N2	2.59	119.20	116.56
1	a	1516	2MG	C4-C5-N7	-2.58	106.58	110.67
1	a	966	2MG	C2'-C1'-N9	-2.58	106.08	113.25
26	A	2449	H2U	C5-C6-N1	-2.57	103.75	111.52
1	a	1518	MA6	N1-C2-N3	-2.56	124.70	128.58
1	a	1207	2MG	C2'-C1'-N9	-2.56	106.14	113.25
1	a	1518	MA6	C5-N7-C8	2.56	107.47	103.45
26	A	2445	2MG	C4-C5-N7	-2.55	106.63	110.67
1	a	527	G7M	O6-C6-C5	-2.53	122.36	128.01
26	A	2030	6MZ	N9-C8-N7	-2.52	110.36	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2030	6MZ	N1-C2-N3	-2.50	124.79	128.58
1	a	1519	MA6	C5-N7-C8	2.49	107.36	103.45
26	A	2069	G7M	O6-C6-C5	-2.47	122.50	128.01
26	A	1618	6MZ	C4-N9-C8	2.46	108.32	105.74
23	v	8	4SU	O2-C2-N1	-2.45	119.60	122.80
26	A	2503	2MA	C2-N1-C6	2.45	121.86	118.10
1	a	966	2MG	N2-C2-N3	-2.44	117.40	120.51
1	a	967	5MC	C5-C4-N3	-2.41	119.28	121.75
26	A	1835	2MG	C4-C5-N7	-2.41	106.86	110.67
26	A	2503	2MA	C5-N7-C8	2.38	107.18	103.45
26	A	1835	2MG	C2-N1-C6	-2.37	121.68	124.55
1	a	1516	2MG	C2'-C1'-N9	-2.36	106.69	113.25
26	A	2069	G7M	C5-C6-N1	2.35	116.70	111.84
1	a	966	2MG	CM2-N2-C2	-2.35	118.60	123.65
26	A	2498	OMC	O4'-C4'-C5'	2.34	116.85	109.33
1	a	1207	2MG	N2-C2-N3	-2.33	117.54	120.51
1	a	1407	5MC	C2'-C1'-N1	-2.32	106.80	113.25
26	A	1835	2MG	CM2-N2-C2	-2.31	118.68	123.65
1	a	967	5MC	C3'-C2'-C1'	2.31	105.82	101.46
26	A	2580	PSU	O4'-C1'-C2'	2.30	108.34	105.15
26	A	2498	OMC	C5'-C4'-C3'	2.30	123.49	115.21
1	a	516	PSU	C5-C6-N1	-2.29	118.96	122.14
26	A	1835	2MG	N1-C2-N2	2.29	118.90	116.56
26	A	2503	2MA	C6-C5-N7	2.29	136.50	132.09
1	a	527	G7M	C5-C6-N1	2.29	116.57	111.84
26	A	1835	2MG	O6-C6-C5	-2.28	120.51	126.53
26	A	2445	2MG	O6-C6-C5	-2.28	120.51	126.53
26	A	2251	OMG	O6-C6-C5	-2.28	120.52	126.53
1	a	1207	2MG	CM2-N2-C2	-2.26	118.80	123.65
1	a	1207	2MG	C2-N1-C6	-2.26	121.82	124.55
26	A	745	1MG	CM1-N1-C6	2.22	121.09	117.64
1	a	966	2MG	O6-C6-C5	-2.21	120.69	126.53
26	A	1618	6MZ	C5-N7-C8	2.21	106.93	103.45
26	A	2503	2MA	C4-N9-C8	2.21	108.06	105.74
1	a	1498	UR3	C3U-N3-C4	2.20	120.92	117.87
1	a	966	2MG	C2-N1-C6	-2.19	121.91	124.55
1	a	1519	MA6	N9-C8-N7	-2.17	110.86	113.94
1	a	1402	4OC	C6-C5-C4	2.16	119.60	117.00
26	A	1939	5MU	O2-C2-N1	-2.16	119.98	122.80
26	A	1939	5MU	C5M-C5-C4	2.12	121.05	118.78
26	A	2251	OMG	C2-N1-C6	-2.11	121.28	125.11
26	A	2605	PSU	O4-C4-C5	-2.10	118.80	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1516	2MG	O6-C6-C5	-2.09	121.00	126.53
26	A	2504	PSU	C6-C5-C4	-2.09	116.77	118.17
23	v	56	PSU	C5-C6-N1	-2.07	119.26	122.14
26	A	1835	2MG	C5-C6-N1	2.07	118.52	113.25
1	a	1207	2MG	O6-C6-C5	-2.07	121.07	126.53
1	a	1402	4OC	C2'-C1'-N1	-2.06	110.32	114.24
1	a	1518	MA6	C4-C5-C6	2.06	118.03	115.91
26	A	2251	OMG	C5-C6-N1	2.05	118.47	113.25
26	A	2445	2MG	N1-C2-N2	2.05	118.65	116.56
1	a	967	5MC	O2-C2-N3	-2.04	119.11	122.33
26	A	1835	2MG	N2-C2-N3	-2.04	117.92	120.51
23	v	8	4SU	C6-N1-C2	-2.03	118.53	121.00
26	A	1962	5MC	CM5-C5-C6	-2.01	120.14	122.85
26	A	2604	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	527	G7M	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10
1	a	1518	MA6	N1-C6-N6-C9
23	v	8	4SU	O4'-C4'-C5'-O5'
26	A	746	PSU	O4'-C1'-C5-C6
1	a	1519	MA6	O4'-C4'-C5'-O5'
23	v	8	4SU	C3'-C4'-C5'-O5'
1	a	1518	MA6	N1-C6-N6-C10
26	A	2580	PSU	O4'-C4'-C5'-O5'
1	a	1519	MA6	C3'-C4'-C5'-O5'
26	A	2504	PSU	O4'-C4'-C5'-O5'
26	A	2030	6MZ	O4'-C4'-C5'-O5'
37	O	82	MS6	CB-CG-SD-CE
29	D	150	MEQ	OE1-CD-CG-CB
29	D	150	MEQ	NE2-CD-CG-CB
26	A	2030	6MZ	C3'-C4'-C5'-O5'
26	A	2498	OMC	C3'-C4'-C5'-O5'
37	O	81	4D4	OB-CB-CG-CD
37	O	81	4D4	CA-CB-CG-CD
37	O	81	4D4	NE-CD-CG-CB
11	k	119	IAS	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
26	A	1917	PSU	O4'-C4'-C5'-O5'
26	A	1915	3TD	O4'-C1'-C5-C4
1	a	1519	MA6	C5-C6-N6-C9
26	A	2498	OMC	C4'-C5'-O5'-P
26	A	1917	PSU	C4'-C5'-O5'-P
12	l	89	D2T	CA-CB-CG-OD2
12	l	89	D2T	CG-CB-SB-CB1
26	A	746	PSU	C2'-C1'-C5-C6
26	A	2580	PSU	C3'-C4'-C5'-O5'
37	O	81	4D4	O-C-CA-CB
1	a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	k	119	IAS	1	0
12	l	89	D2T	1	0
1	a	967	5MC	1	0
1	a	1407	5MC	1	0
26	A	2030	6MZ	1	0
26	A	2498	OMC	1	0
1	a	1519	MA6	3	0
26	A	1915	3TD	2	0
1	a	1518	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 303 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GCP	x	902	57	32,34,34	0.76	1 (3%)	49,54,54	0.58	1 (2%)
58	FME	v	101	23	8,9,10	0.33	0	8,9,11	1.22	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GCP	x	902	57	-	0/19/38/38	0/3/3/3
58	FME	v	101	23	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	902	GCP	PB-O2B	-2.31	1.50	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	v	101	FME	O1-CN-N	-2.14	119.79	125.32
59	x	902	GCP	O1G-PG-C3B	-2.13	106.74	111.37

There are no chirality outliers.

There are no torsion outliers.

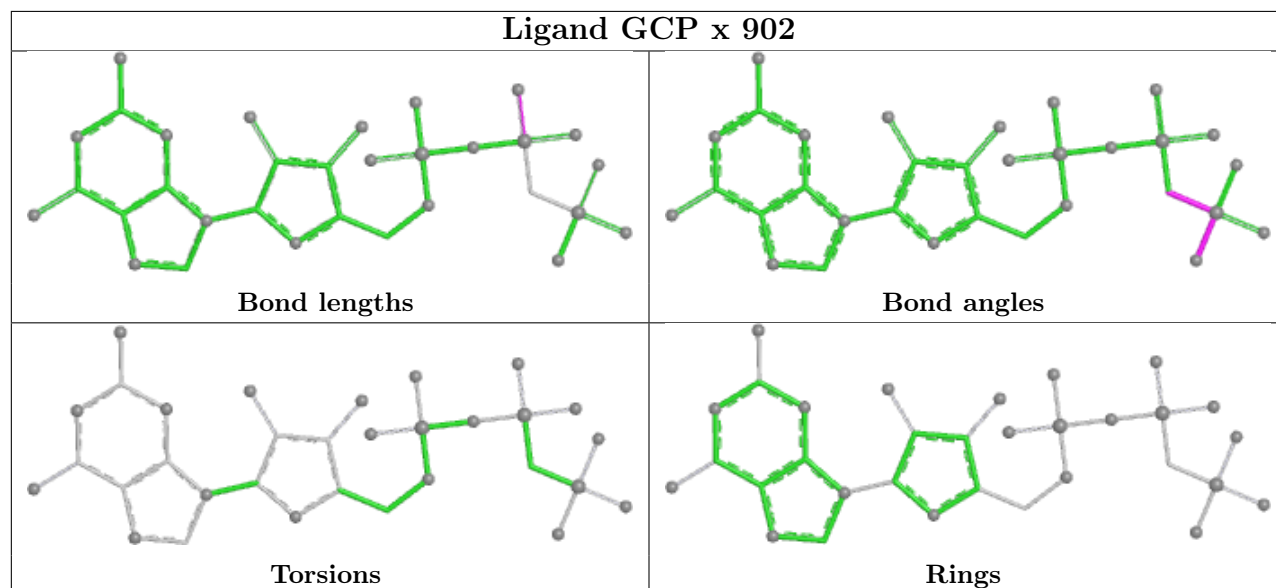
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	v	101	FME	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

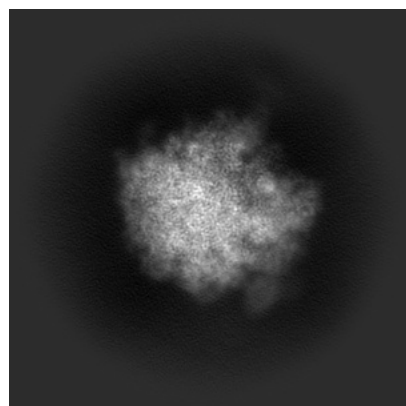
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74431. These allow visual inspection of the internal detail of the map and identification of artifacts.

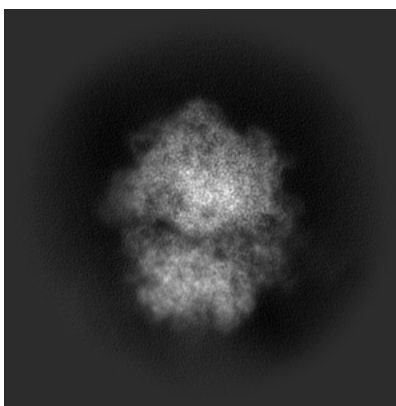
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

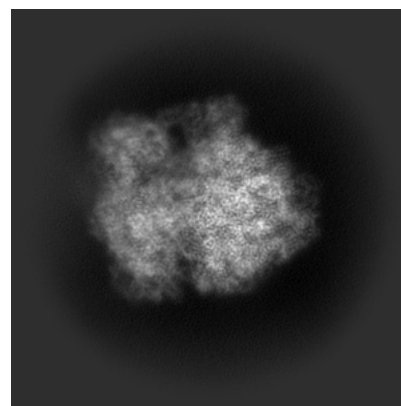
6.1.1 Primary map



X

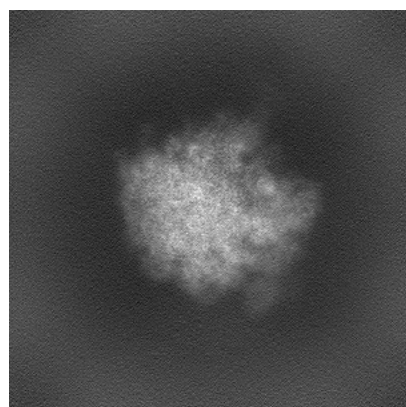


Y

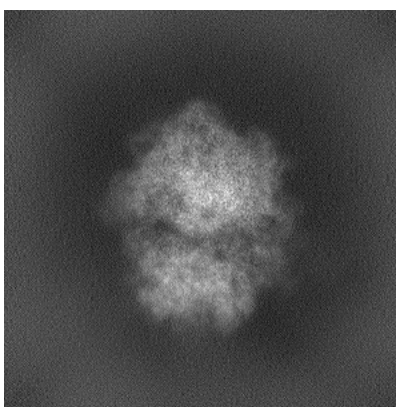


Z

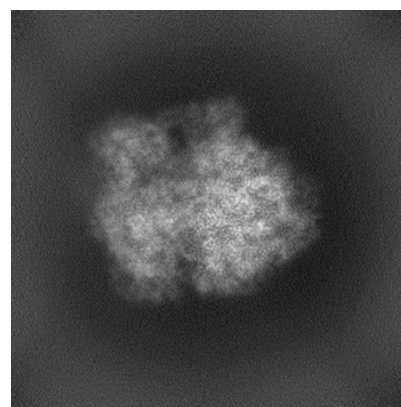
6.1.2 Raw map



X



Y

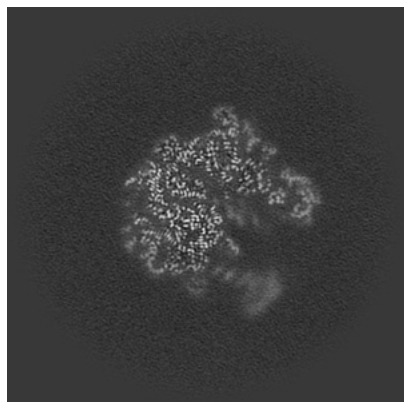


Z

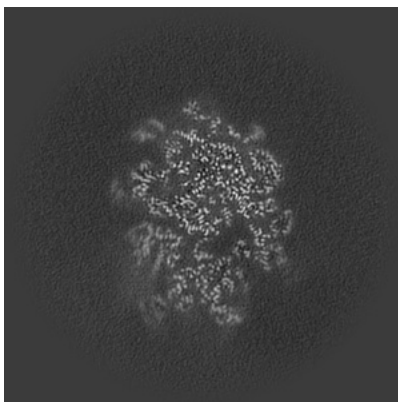
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

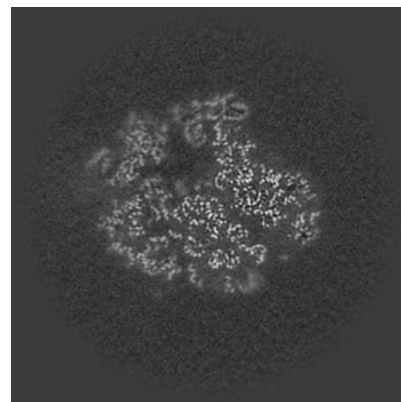
6.2.1 Primary map



X Index: 256

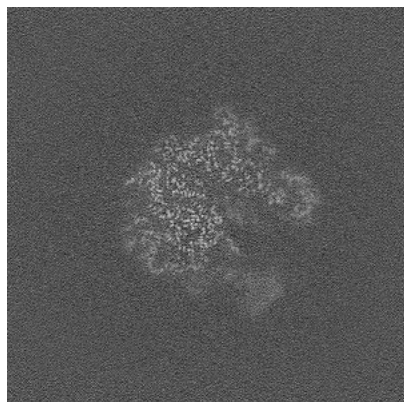


Y Index: 256

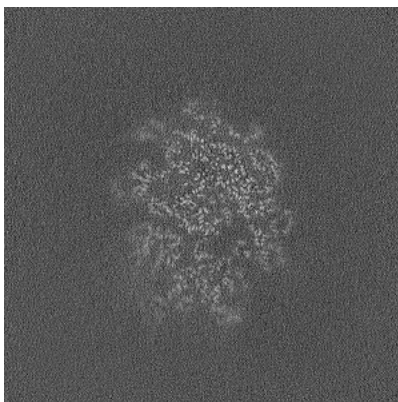


Z Index: 256

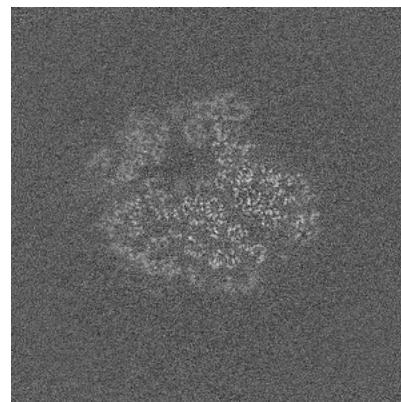
6.2.2 Raw map



X Index: 256



Y Index: 256

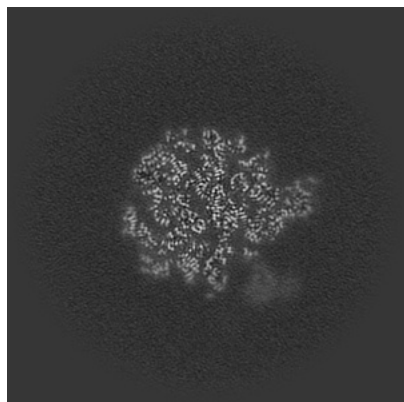


Z Index: 256

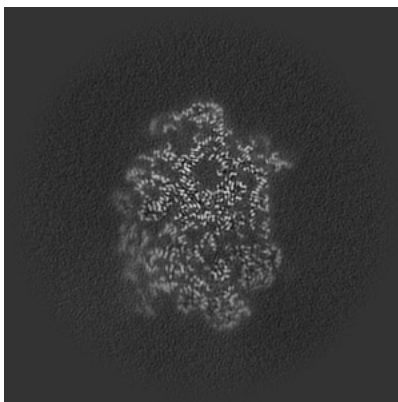
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

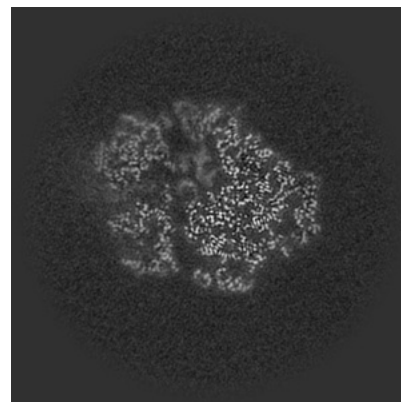
6.3.1 Primary map



X Index: 289

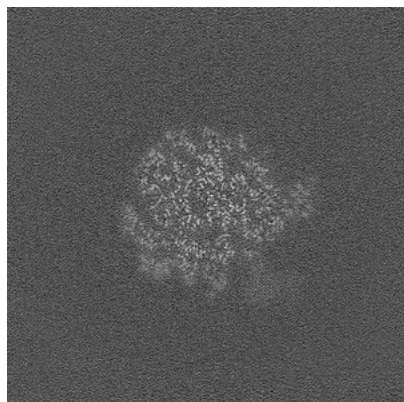


Y Index: 238

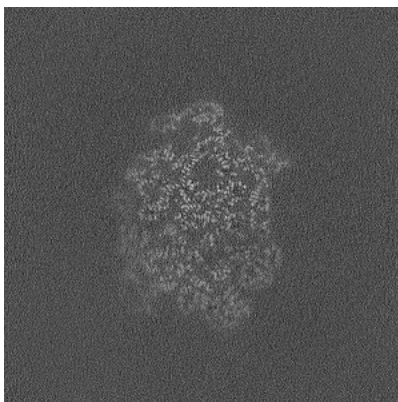


Z Index: 243

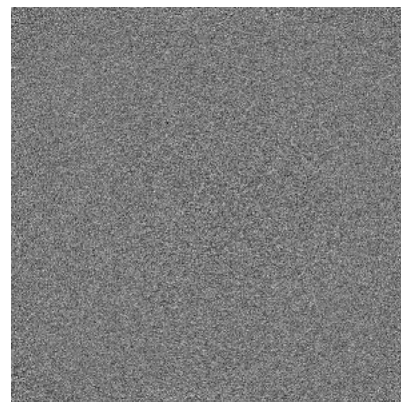
6.3.2 Raw map



X Index: 291



Y Index: 237

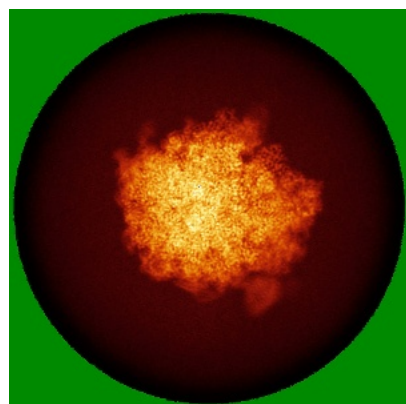


Z Index: 0

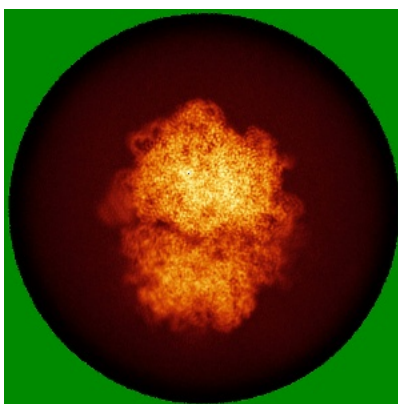
The images above show the largest variance slices of the map in three orthogonal directions.

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

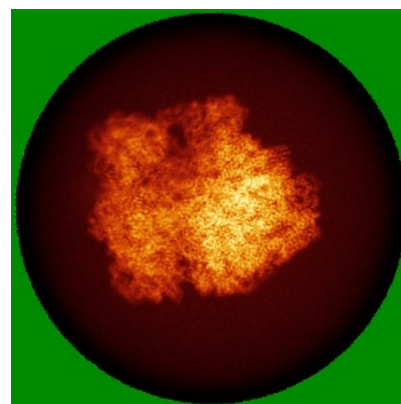
6.4.1 Primary map



X

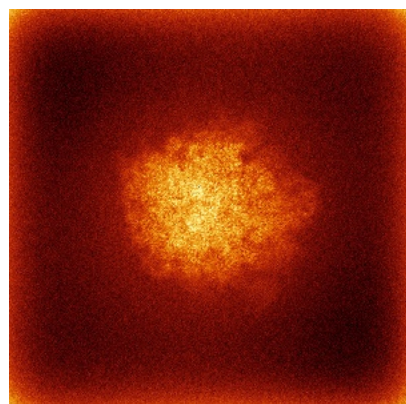


Y

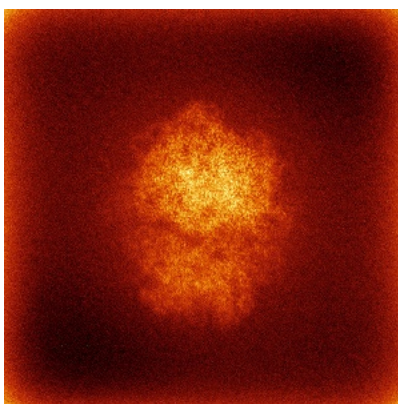


Z

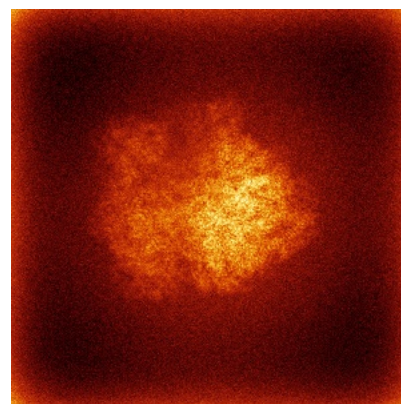
6.4.2 Raw map



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



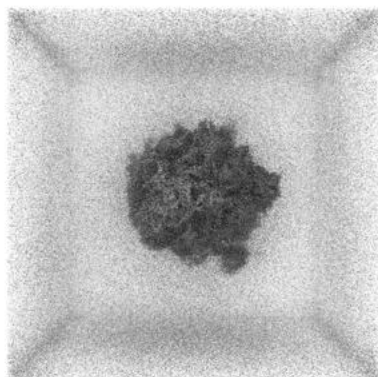
Y



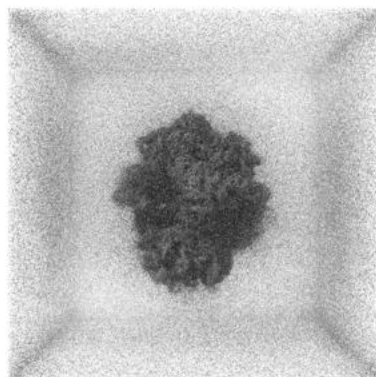
Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

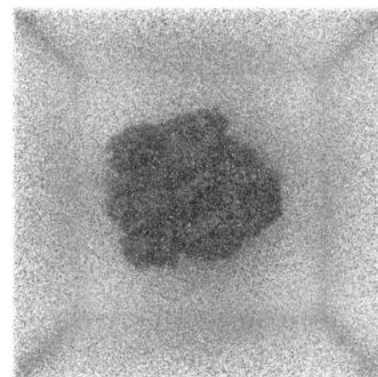
6.5.2 Raw map



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.

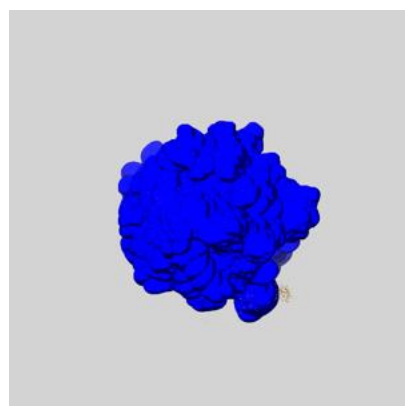
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

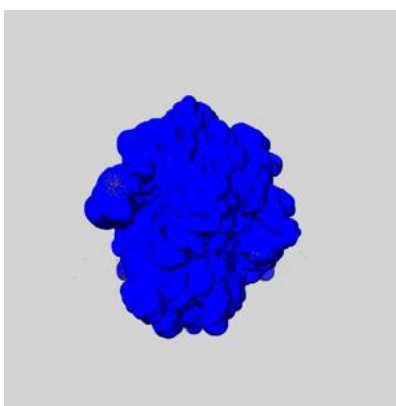
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

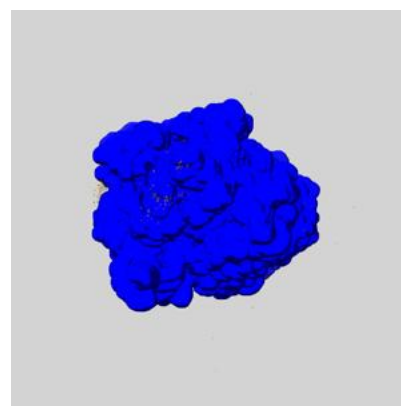
6.6.1 emd_74431_msk_1.map [i](#)



X



Y

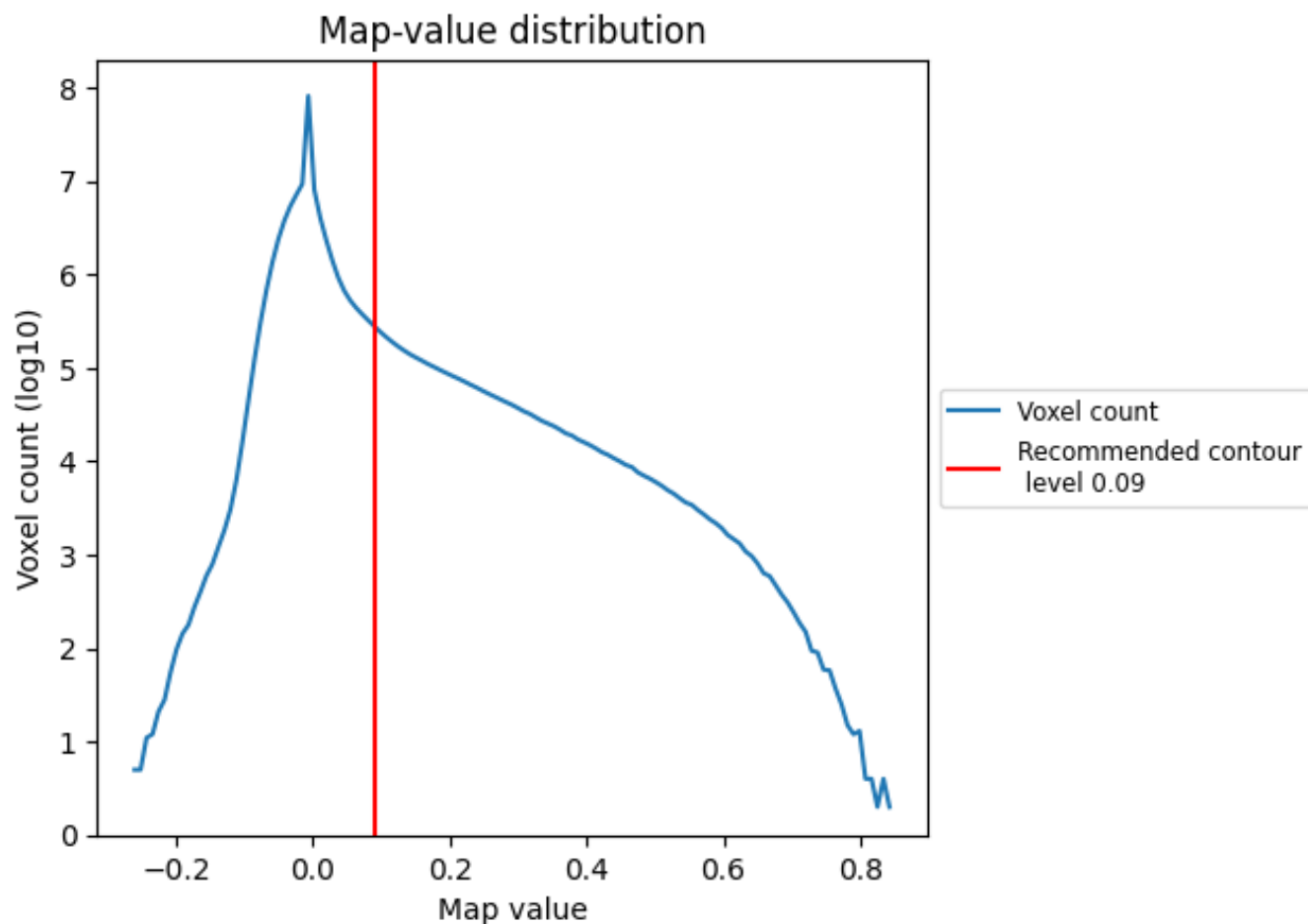


Z

7 Map analysis [i](#)

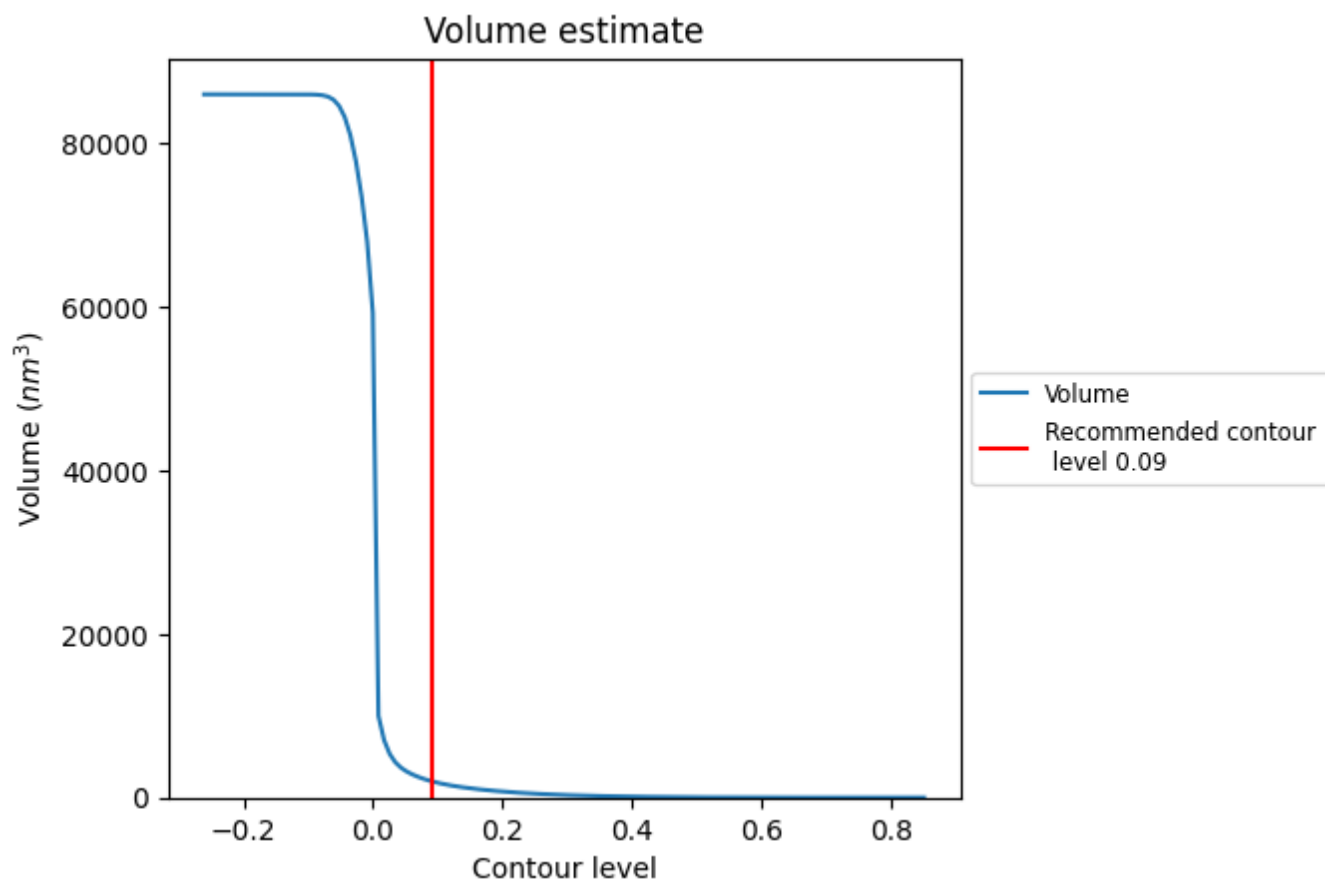
This section contains the results of statistical analysis of the map.

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.

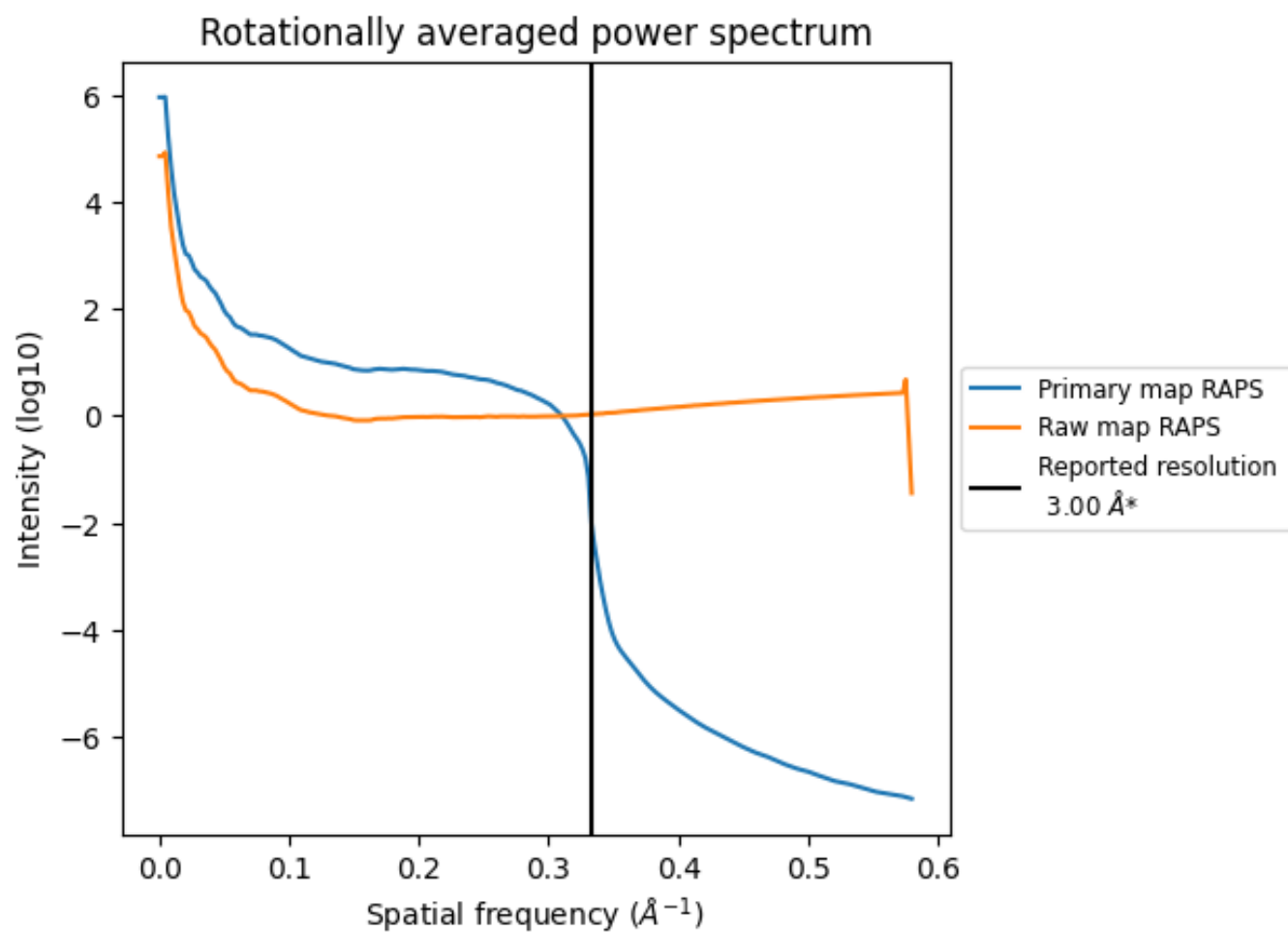
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2016 nm^3 ; this corresponds to an approximate mass of 1821 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

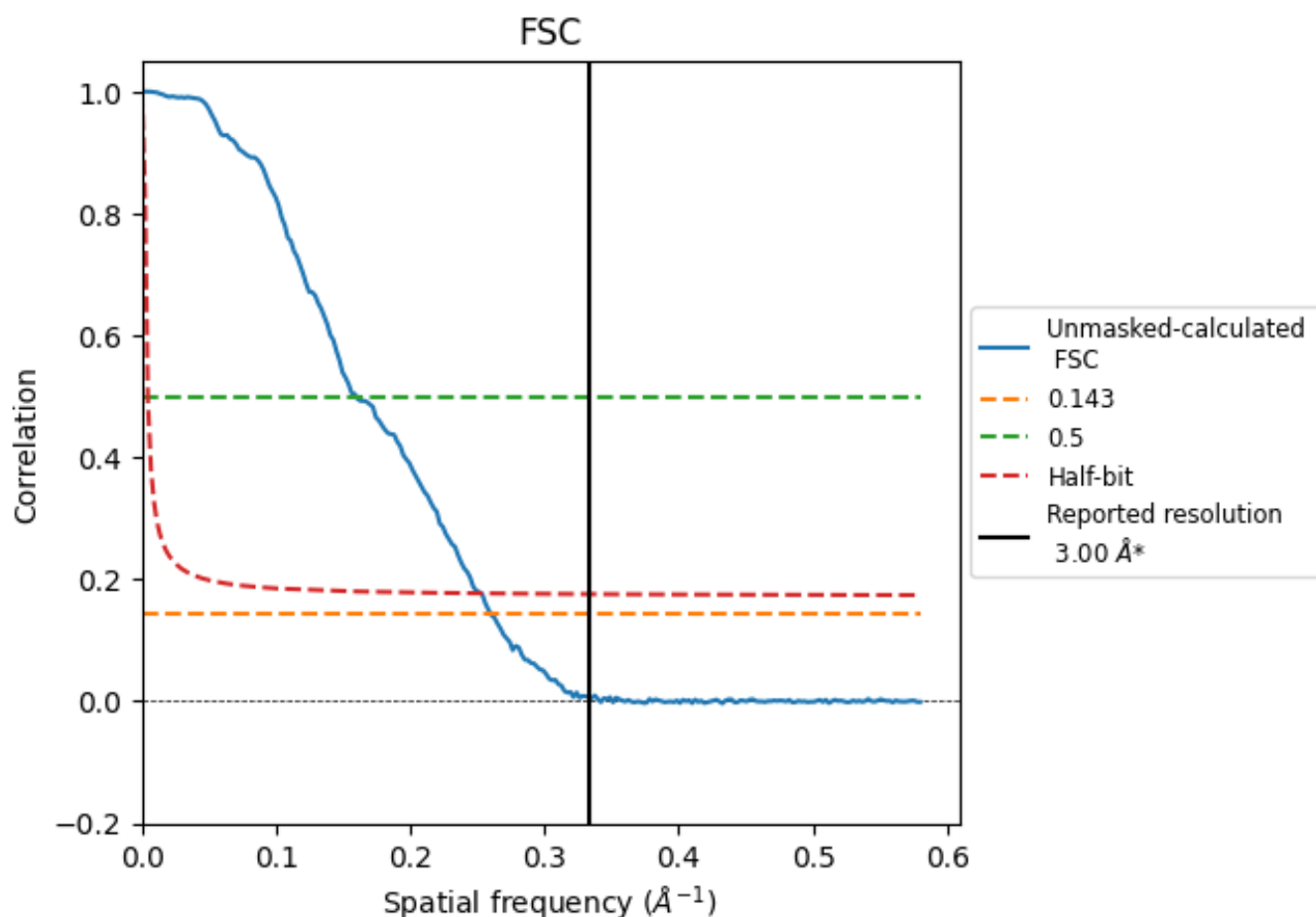


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

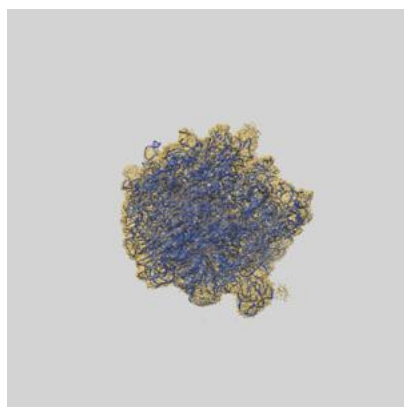
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	6.27	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.0 by more than 10 %

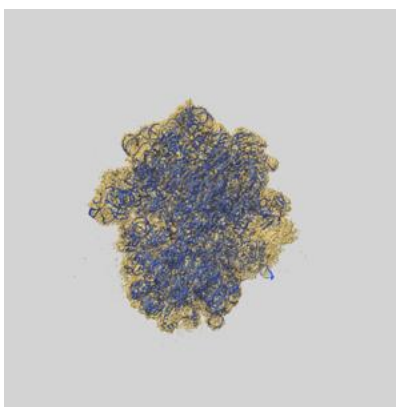
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74431 and PDB model 9ZN2. Per-residue inclusion information can be found in section [3](#) on page [17](#).

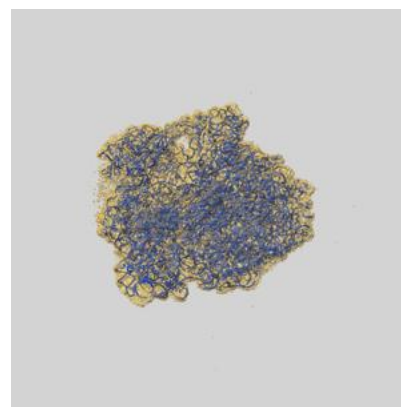
9.1 Map-model overlay [i](#)



X



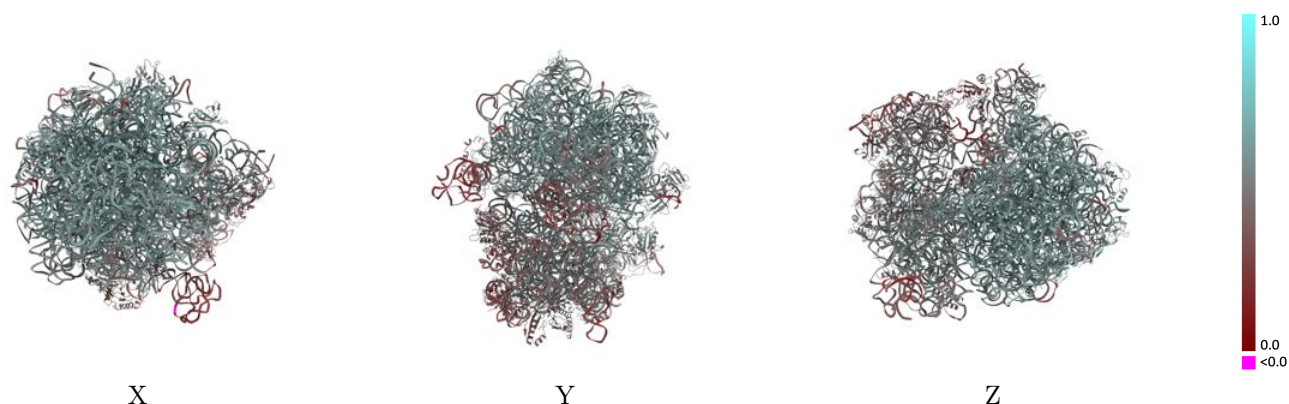
Y



Z

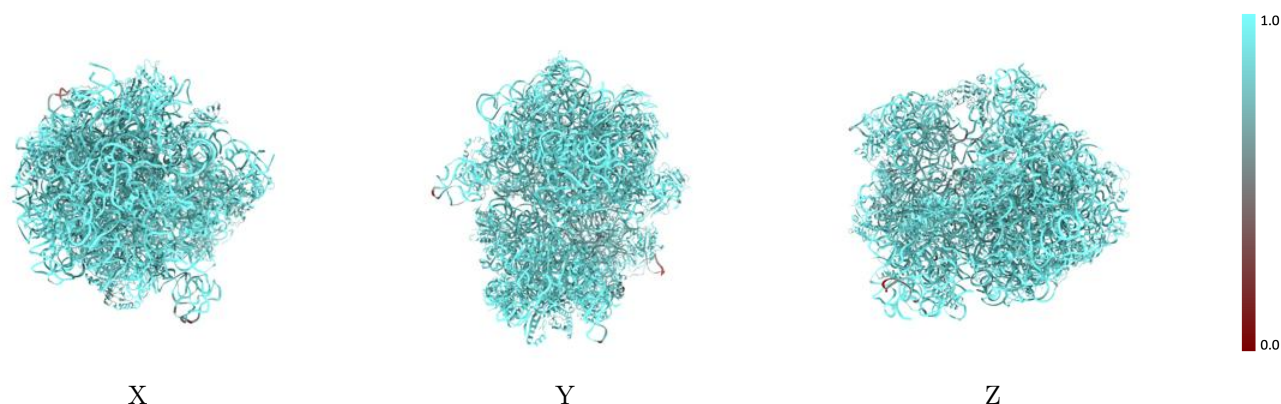
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



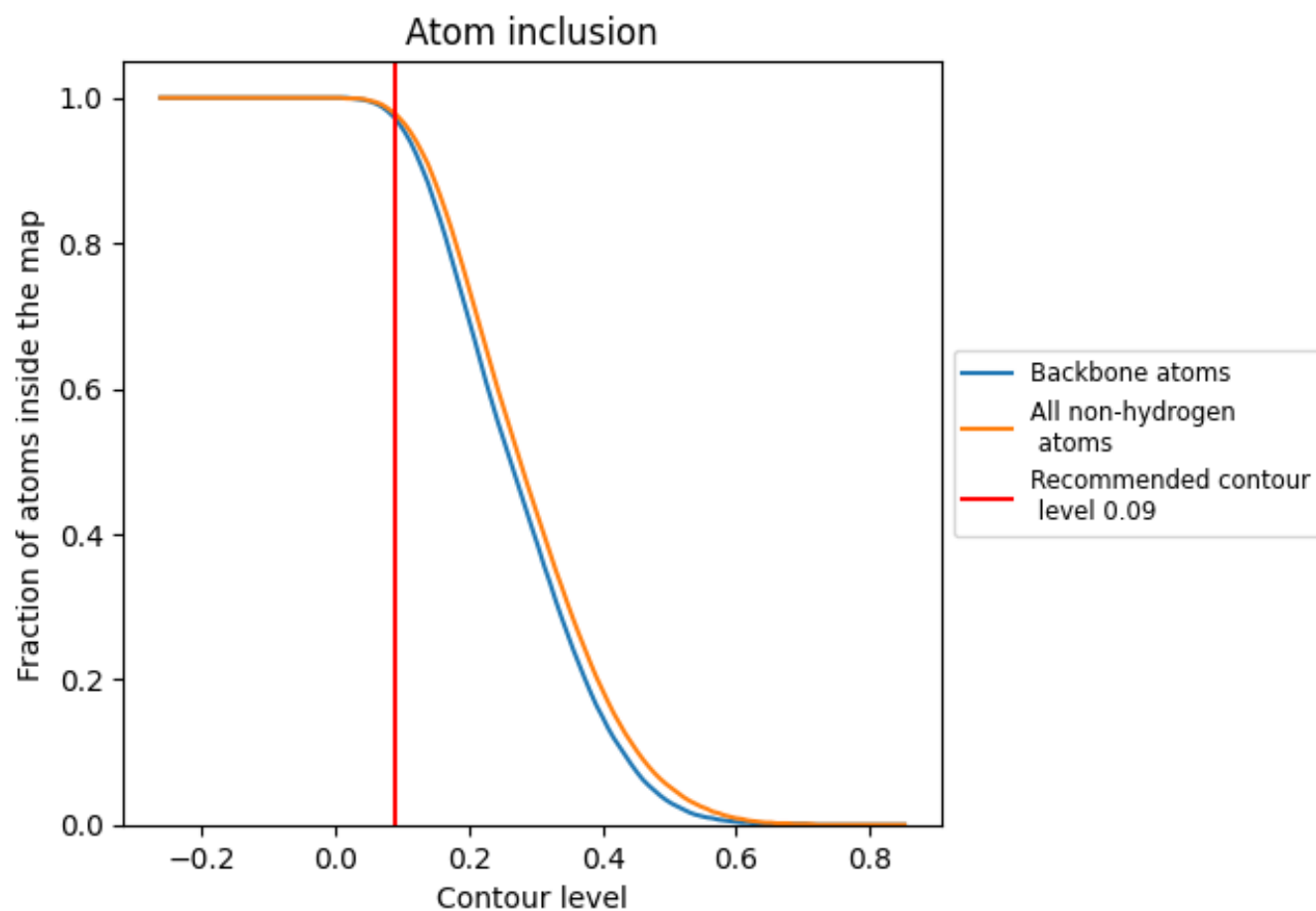
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9780	 0.5150
1	 0.9710	 0.5170
2	 0.9720	 0.5690
3	 0.8300	 0.2810
4	 0.9980	 0.5810
5	 0.9550	 0.5510
6	 0.9920	 0.6020
7	 0.9980	 0.5980
8	 0.9800	 0.5730
A	 0.9900	 0.5490
B	 0.9930	 0.4800
C	 0.9870	 0.5820
D	 0.9860	 0.5810
E	 0.9730	 0.5620
F	 0.8750	 0.3770
G	 0.9520	 0.5170
H	 0.8830	 0.4320
L	 0.9940	 0.5760
M	 0.9740	 0.5830
N	 0.9790	 0.5720
O	 0.9870	 0.5730
P	 0.9960	 0.5850
Q	 0.9680	 0.4930
R	 0.9710	 0.5740
S	 0.9930	 0.5840
T	 0.9770	 0.5700
U	 0.9830	 0.5790
V	 0.9830	 0.5600
W	 0.9760	 0.5390
X	 0.9420	 0.5360
Y	 0.9780	 0.5840
Z	 0.9880	 0.5740
a	 0.9880	 0.4730
b	 0.8780	 0.3770
c	 0.9650	 0.4670



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Chain	Atom inclusion	Q-score
d	 0.9700	 0.4940
e	 0.9720	 0.5080
f	 0.9770	 0.3960
g	 0.9440	 0.3880
h	 0.9640	 0.4850
i	 0.9680	 0.3860
j	 0.9740	 0.4250
k	 0.9210	 0.4220
l	 0.9710	 0.5600
m	 0.9340	 0.4090
n	 0.9730	 0.4490
o	 0.9630	 0.4480
p	 0.9590	 0.4970
q	 0.9670	 0.5250
r	 0.9880	 0.4390
s	 0.9350	 0.4250
t	 0.9650	 0.4830
u	 0.9690	 0.4100
v	 0.9740	 0.3720
w	 0.9430	 0.5130
x	 0.9000	 0.4960
y	 0.8920	 0.4800