



Full wwPDB EM Validation Report ⓘ

Jul 28, 2026 – 05:55 PM EDT

PDB ID : 8VV4 / pdb_00008vv4
EMDB ID : EMD-43549
Title : E. coli 70S ribosome with unmodified Lys-tRNA^{Pro}(GGG) in the P/P conformation on a slippery CCC-C codon
Authors : Kimbrough, E.M.; Dunham, C.M.; Nguyen, H.A.
Deposited on : 2024-01-30
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

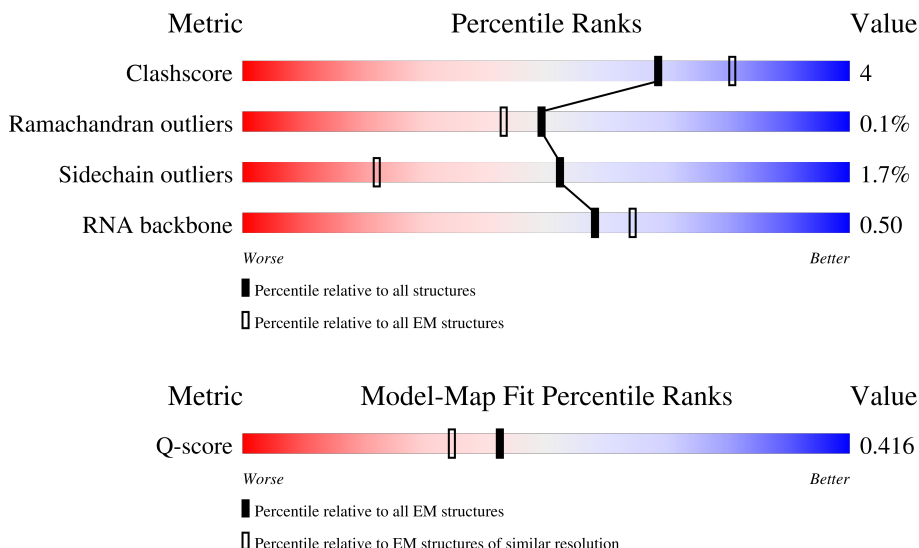
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.40 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.



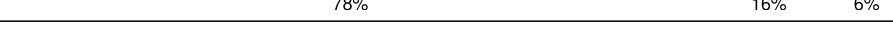
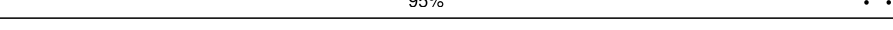
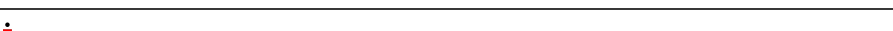
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	B	273	
2	C	209	
3	D	201	

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Mol	Chain	Length	Quality of chain
4	E	179	 76% 23% .
5	F	177	 91% 7% ..
6	G	149	 89% 11%
7	J	142	 89% 11%
8	K	123	 84% 16%
9	L	144	 5% 90% 10%
10	M	136	 88% 12% .
11	N	127	 83% 10% 6%
12	O	117	 84% 15% ..
13	P	115	 86% 12% ..
14	Q	118	 86% 13% .
15	R	103	 89% 11%
16	S	110	 91% 9%
17	T	100	 78% 16% 6%
18	U	104	 84% 15% .
19	V	94	 95% . .
20	W	84	 79% 11% 11%
21	X	78	 87% 12% .
22	Y	63	 79% 19% .
23	Z	59	 81% 17% .
24	1	2904	 70% 26% . .
25	2	1540	 69% 29% .
26	3	120	 64% 34% .
27	4	18	 6% 33% 6% 61%
28	5	77	 64% 29% 6% .

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Mol	Chain	Length	Quality of chain
29	a	70	
30	b	57	
31	c	55	
32	d	46	
33	e	65	
34	f	38	
35	g	241	
36	h	233	
37	i	206	
38	j	167	
39	k	135	
40	l	179	
41	m	130	
42	n	130	
43	o	103	
44	p	129	
45	q	124	
46	r	118	
47	s	101	
48	t	89	
49	u	82	
50	v	84	
51	w	75	
52	x	92	
53	y	87	

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Mol	Chain	Length	Quality of chain
54	z	71	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	2MG	2	1207	X	-	-	-
25	5MC	2	1407	X	-	-	-
25	2MG	2	1516	X	-	-	-
25	2MG	2	966	X	-	-	-
25	5MC	2	967	X	-	-	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 143506 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 6 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

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

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 13 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	2821	Total	C	N	O	P	0	0
			60570	27020	11157	19572	2821		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 2327815913
1	1847	G	A	conflict	GB 2327815913
1	2069	A	G	conflict	GB 2327815913

- Molecule 25 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	7	Total	C	N	O	P	0	0
			145	65	24	49	7		

- Molecule 28 is a RNA chain called tRNA^{Pro}L (GGG).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	77	Total	C	N	O	P	0	0
			1648	733	297	541	77		

- Molecule 29 is a protein called 50S ribosomal protein L31.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called Large ribosomal subunit protein bL33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

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

- Molecule 45 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

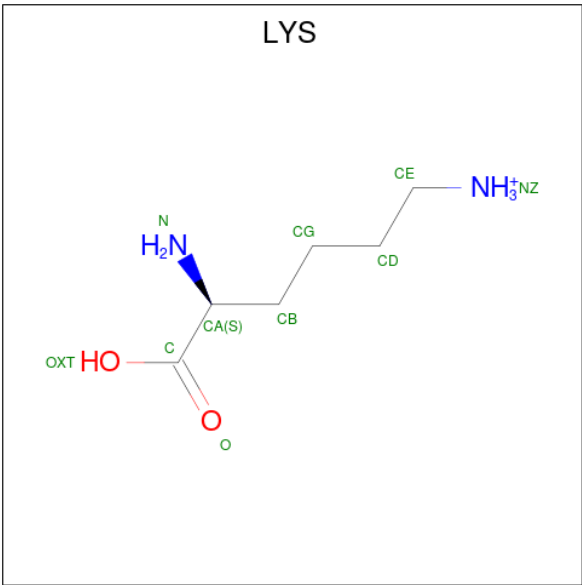
- Molecule 54 is a protein called 30S ribosomal protein S21.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	B	1	Total 1	Mg 1	0
55	C	1	Total 1	Mg 1	0
55	D	3	Total 3	Mg 3	0
55	F	1	Total 1	Mg 1	0
55	P	1	Total 1	Mg 1	0
55	Q	1	Total 1	Mg 1	0
55	R	1	Total 1	Mg 1	0
55	T	1	Total 1	Mg 1	0
55	X	1	Total 1	Mg 1	0
55	Z	1	Total 1	Mg 1	0
55	1	295	Total 295	Mg 295	0
55	2	104	Total 104	Mg 104	0
55	3	8	Total 8	Mg 8	0
55	b	1	Total 1	Mg 1	0
55	e	2	Total 2	Mg 2	0
55	z	2	Total 2	Mg 2	0

- Molecule 56 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
56	1	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	B	1	Total	O	0
			1	1	
57	C	6	Total	O	0
			6	6	
57	D	7	Total	O	0
			7	7	
57	E	8	Total	O	0
			8	8	
57	F	11	Total	O	0
			11	11	
57	G	20	Total	O	0
			20	20	
57	J	2	Total	O	0
			2	2	
57	K	5	Total	O	0
			5	5	
57	L	5	Total	O	0
			5	5	
57	M	3	Total	O	0
			3	3	
57	N	4	Total	O	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
57	O	4	Total 4	O 4	0
57	R	7	Total 7	O 7	0
57	S	3	Total 3	O 3	0
57	T	2	Total 2	O 2	0
57	U	1	Total 1	O 1	0
57	V	4	Total 4	O 4	0
57	W	1	Total 1	O 1	0
57	Y	4	Total 4	O 4	0
57	1	147	Total 147	O 147	0
57	2	106	Total 106	O 106	0
57	3	5	Total 5	O 5	0
57	4	1	Total 1	O 1	0
57	5	14	Total 14	O 14	0
57	a	30	Total 30	O 30	0
57	b	1	Total 1	O 1	0
57	c	2	Total 2	O 2	0
57	g	33	Total 33	O 33	0
57	h	12	Total 12	O 12	0
57	i	4	Total 4	O 4	0
57	j	7	Total 7	O 7	0
57	k	7	Total 7	O 7	0

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Mol	Chain	Residues	Atoms		AltConf
57	l	12	Total 12	O 12	0
57	m	9	Total 9	O 9	0
57	n	5	Total 5	O 5	0
57	o	11	Total 11	O 11	0
57	p	4	Total 4	O 4	0
57	q	5	Total 5	O 5	0
57	r	7	Total 7	O 7	0
57	s	5	Total 5	O 5	0
57	t	4	Total 4	O 4	0
57	u	5	Total 5	O 5	0
57	v	2	Total 2	O 2	0
57	w	9	Total 9	O 9	0
57	x	1	Total 1	O 1	0
57	y	1	Total 1	O 1	0
57	z	13	Total 13	O 13	0

Chain F:  91% 7% ..



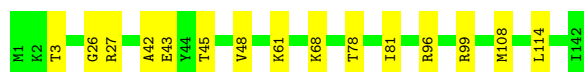
- Molecule 6: Large ribosomal subunit protein bL9

Chain G:  89% 11%



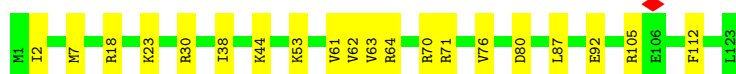
- Molecule 7: Large ribosomal subunit protein uL13

Chain J:  89% 11%



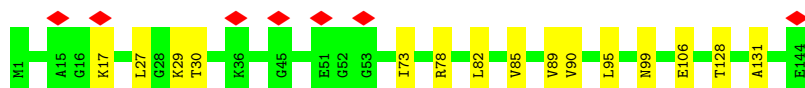
- Molecule 8: 50S ribosomal protein L14

Chain K:  84% 16%



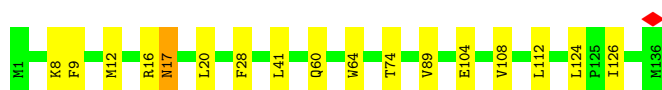
- Molecule 9: 50S ribosomal protein L15

Chain L:  5% 90% 10%



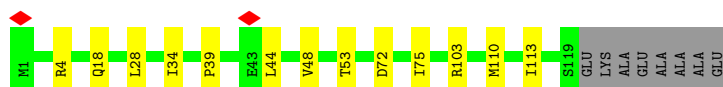
- Molecule 10: 50S ribosomal protein L16

Chain M:  88% 12%



- Molecule 11: Large ribosomal subunit protein bL17

Chain N:  83% 10% 6%



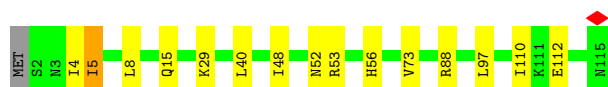
- Molecule 12: Large ribosomal subunit protein uL18

Chain O:  84% 15% ..



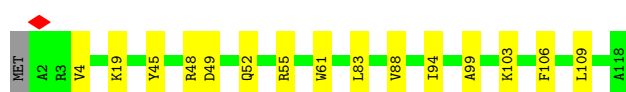
- Molecule 13: Large ribosomal subunit protein bL19

Chain P:  86% 12% ..



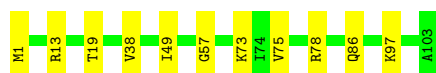
- Molecule 14: 50S ribosomal protein L20

Chain Q:  86% 13% .



- Molecule 15: 50S ribosomal protein L21

Chain R:  89% 11%



- Molecule 16: 50S ribosomal protein L22

Chain S:  91% 9%



- Molecule 17: 50S ribosomal protein L23

Chain T:  78% 16% 6%



- Molecule 18: 50S ribosomal protein L24

Chain U:  84% 15% .



- Molecule 19: Large ribosomal subunit protein bL25

Chain V: 95%



- Molecule 20: Large ribosomal subunit protein bL27

Chain W: 79% 11% 11%



- Molecule 21: 50S ribosomal protein L28

Chain X: 87% 12%



- Molecule 22: Large ribosomal subunit protein uL29

Chain Y: 79% 19%



- Molecule 23: 50S ribosomal protein L30

Chain Z: 81% 17%

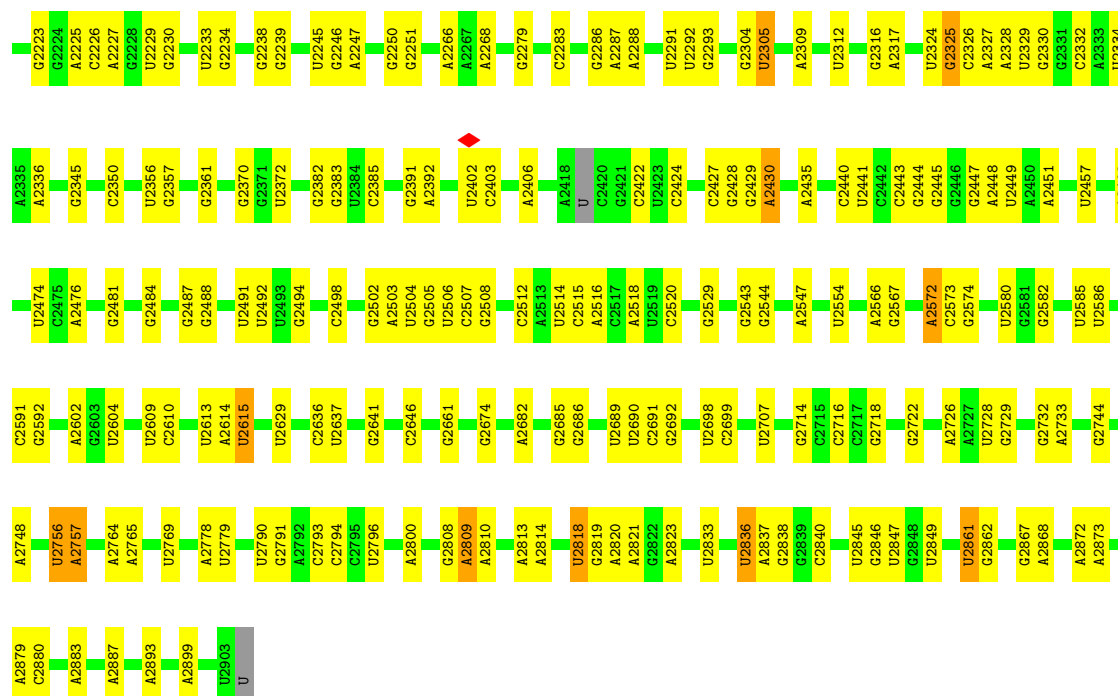


- Molecule 24: 23S ribosomal RNA

Chain 1: 70% 26%

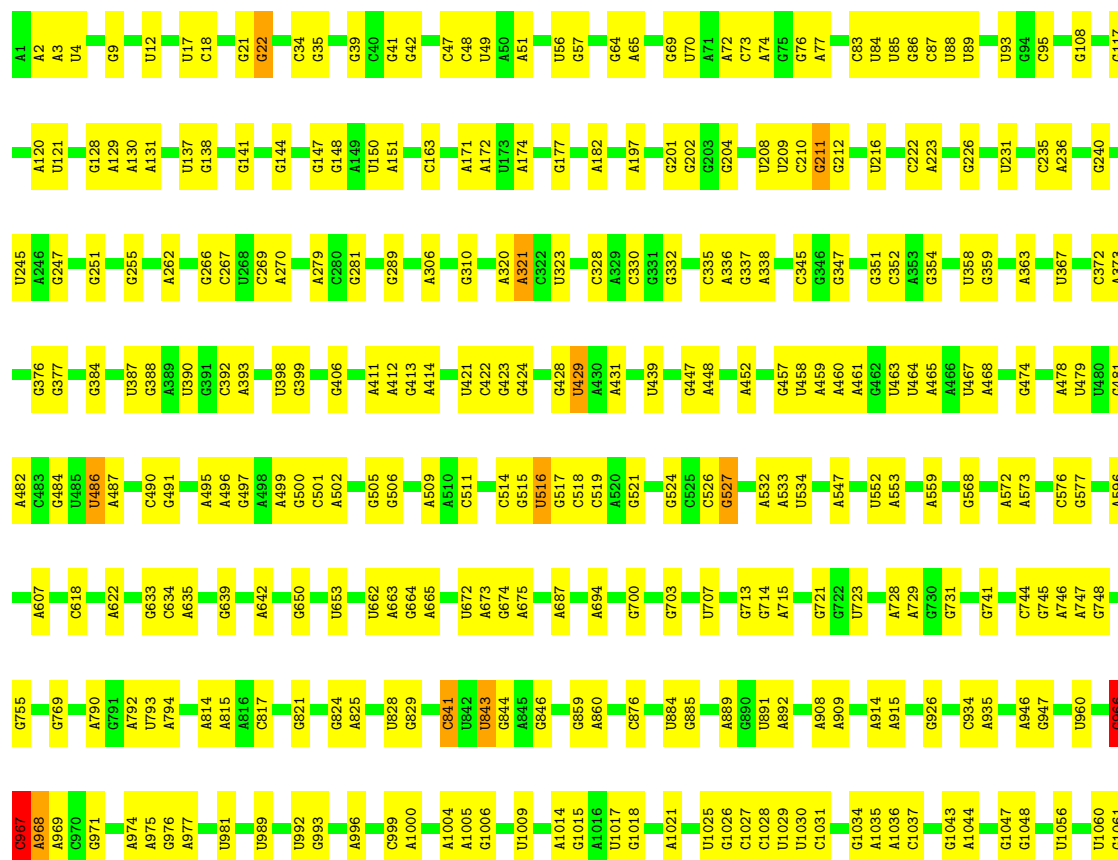


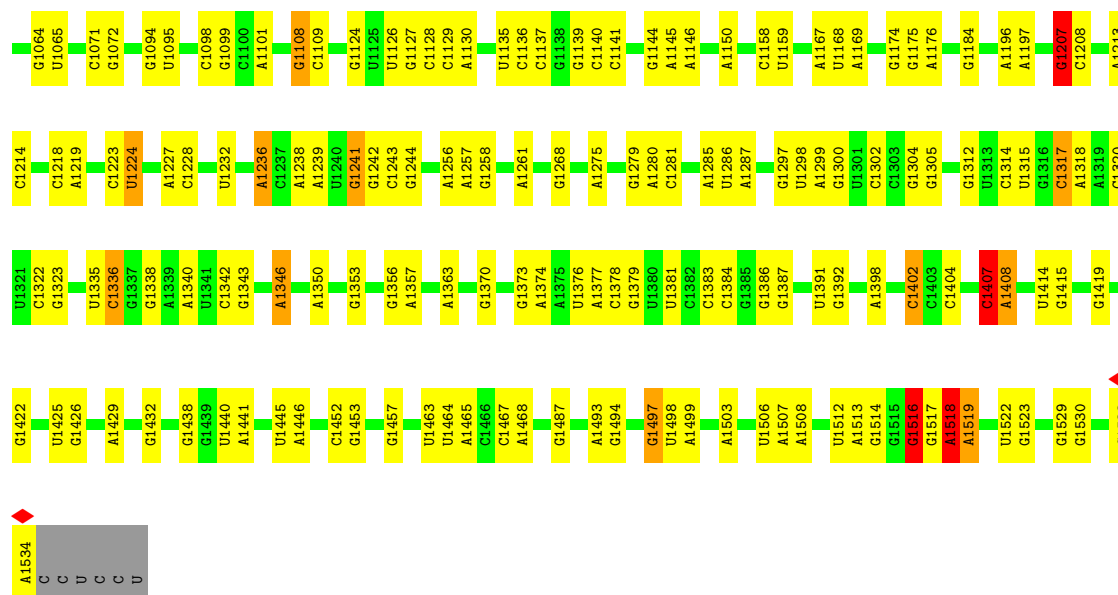
U	G2087	G1964	C1800	C1646	G1179	U1065	U955	A845	G696	A563	G424	U296
C	A2088	A1966	A1801	U1647	U1180	U1066	C961	U846	G704	A572	U846	G297
G		C1967	A1802	U1648	U1181	A1067	G962	U847	C345	A573	C435	A300
C	G2093	A1570	A1808	G1651	A1204	A1070	U970	A849	G711	A574	U448	A311
A	A2094	U1971	A1809	A1654	A1205	G1071	G971	G856	C717	A575	U576	
U	A2095	G1972	A1809	G1368	G1206	C1072	A972	G857	A721	U577	U451	C323
G	C2096	A1987	C1816	A1668	C1211	A1073	G974	G858	A722	C581	A454	
A	A2097	G1988	A1819	A1672	G1212	C1074	A979	G859	A726	A582	G458	G329
G	U2098	A1873	G1673	U1379	G1225	C1075						A330
C	U2099	G1674	U1513	A1383	G1235	C1076		G869	A730	A586	G467	
C	G2100	G1674	G1514	C1386	G1235	A1077	C982	G874	A738	U596	A471	C334
G	A2101	C1694	A1515	A1387	G1238	U1078	A983	G879	A743	G597		C335
A	G2102	G1695	G1524	U1397	G1245	C1079	C995	A996	A742	U598	G481	G338
C	C2103	G1695	G1529	U1408	A1246	A1084	A996	A996	A743	A599	A482	A345
C	U2104	G1695	A1532	U1409	A1247	A1085	G997	G879	A747	G600	A483	
U	U2105	A1698	C1533	U1410	G1248	A1086	C998	G882	G757	A603	G489	G350
G		G1699	U1534	G1410	A1247	A1087	C998	G883	G757	A614	C351	C351
A	A	G1709	U1534	G1410	G1248	A1088	C1005	U884	G757	U615	A491	A352
A	A	G1710	A1535	G1410	G1248	A1089	C1006	C885	A764	A616	G494	A353
A	A	G1711	C1536	G1410	G1248	A1090		A886	G765		G495	U355
A	A	U1712	U1542	G1416	G1256	G1093	A1009	U	C772	G622	G496	G356
C	A	U1713	U1548	C1428	A1265	U1094	U1012	C	C772	A627	G359	
C	A	G1715	A1549	G1429	A1265	A1095	U1013	G891	U774	U499	U360	U360
A	A	G1716	A1555	G1430	A1268	A1096	A1014	G892	G775	A505	G361	G361
A	A	U1717	G1555	A1431	A1269	U1097	U1019	A893	G776		A362	
A	A	G1718	C1558	A1432	A1270	A1098	A1020	U894	A782	A508	G367	
A	A	G1719	U1559	A1433	A1271	A1099	A1021	U895	A509	C509	A508	
A	A	G1720	G1560	A1434	A1272	G1099	G1022	A896	C510	G511	A371	A371
A	A	G1721	U1560	C1437	A1272	C1102	U1023	C897	U511		G372	
A	A	G1722	C1565	U1443	A1276	A1103	G1026	G907	A526	A526	G386	
A	A	G1723	U1569	U1443	A1276	C1104	U1033	A910	A529	A529	U387	
A	A	G1724	A1570	G1444	C1278	U105	U1033	A917	A529	G530	G388	
A	A	G1725	A1571	G1447	G1279	A1111	G1041	A917	A654	C531	U395	
A	A	G1726	A1572	G1448	A1301	G1112	G1042	A917	A655	A655	G396	
A	A	G1727	U1578	G1452	A1306	U1113	C1045	G924	G805	A659	U397	
A	A	G1728	C1585	A1453	C1306	C1114	G1047	A925	C812	G659	U403	
A	A	G1729	U1583	C1461	U1310	G1115	A1047	G926	C814	G664	A404	
A	A	G1730	C1585	C1461	G1311	U1130	C1052	A927	A819	G669	U405	
A	A	G1731	U1589	A1469	U1312	U1131	C1053	U931	A820	A670	G406	
A	A	G1732	A1591	A1470	U1132	A1133	A1054	C935	A827	A677	G411	
A	A	G1733	U1591	G1475	U1133	C1135	A1057	A936	U828	A677	U545	
A	A	G1734	A1597	G1478	A1321	G1139	U1058	A941	G831	C680	A547	
A	A	G1735	A1598	G1482	U1329	C1140	G1059	G941	U832	C680	C413	
A	A	G1736	A1608	A1490	C1330	U1414	U1060	C946	U832	G681	C414	
A	A	G1737	C1611	G1491	G1341	A1142	U1061	A947	A833	C550	A415	
A	A	G1738		G1491	G1341	A1155	G1062	G948	C854	U686	U416	
A	A	G1739		A1494	C1345	A1175	G1063	G949	G836	U694	C417	
A	A	G1740				U1176	C1064			G695	C421	



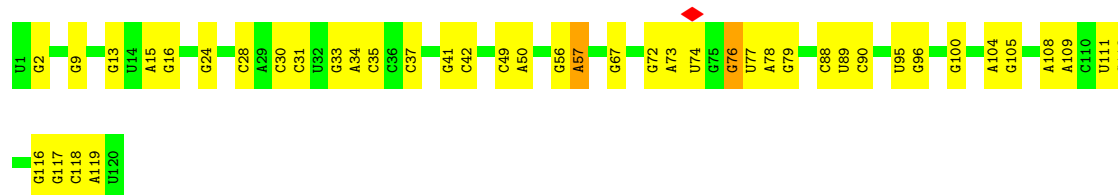
• Molecule 25: 16S ribosomal RNA

Chain 2: 69% 29% .

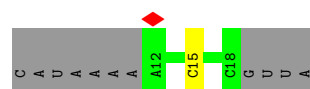




• Molecule 26: 5S ribosomal RNA



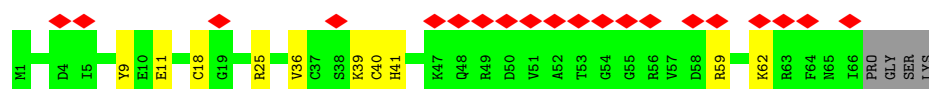
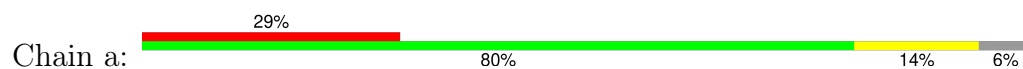
• Molecule 27: mRNA



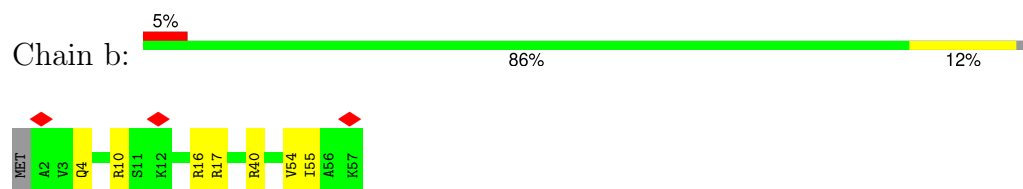
• Molecule 28: tRNA^{Pro}L (GGG)



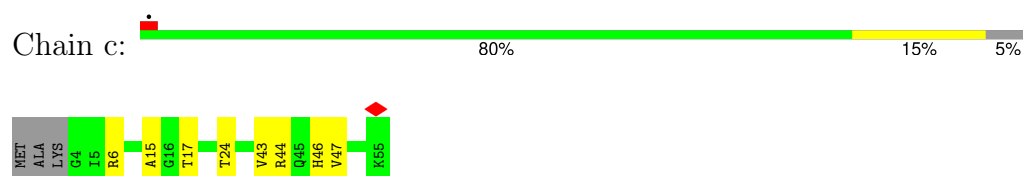
• Molecule 29: 50S ribosomal protein L31



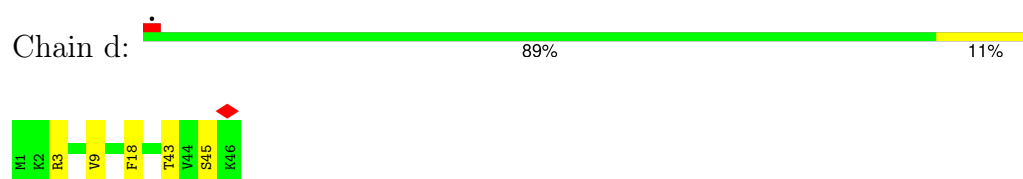
- Molecule 30: 50S ribosomal protein L32



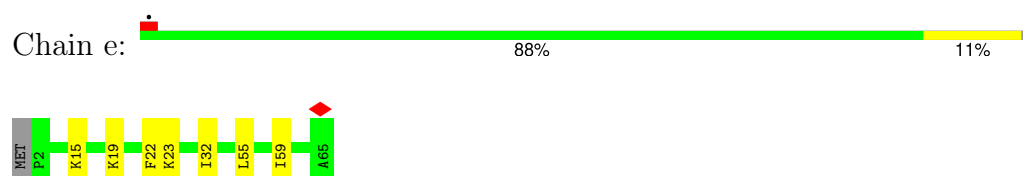
- Molecule 31: Large ribosomal subunit protein bL33



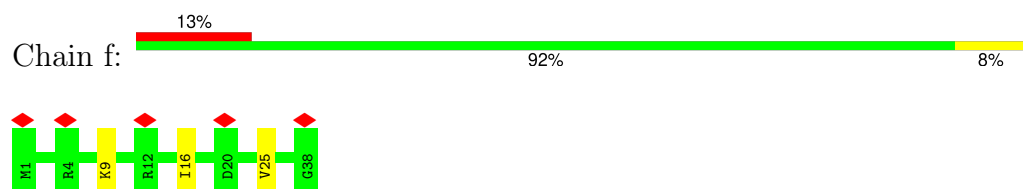
- Molecule 32: 50S ribosomal protein L34



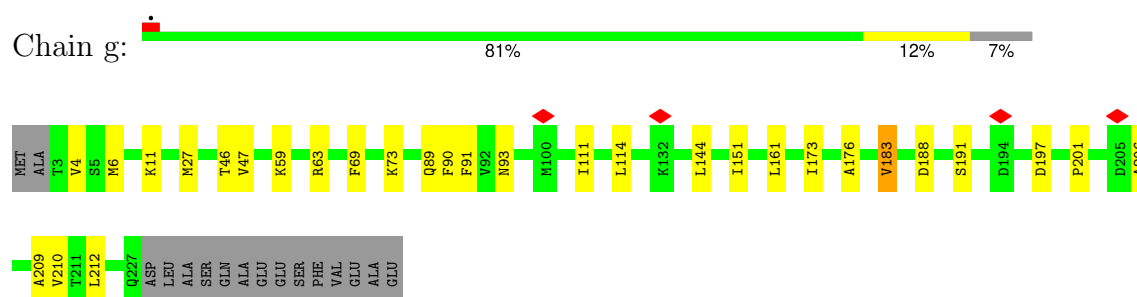
- Molecule 33: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L36

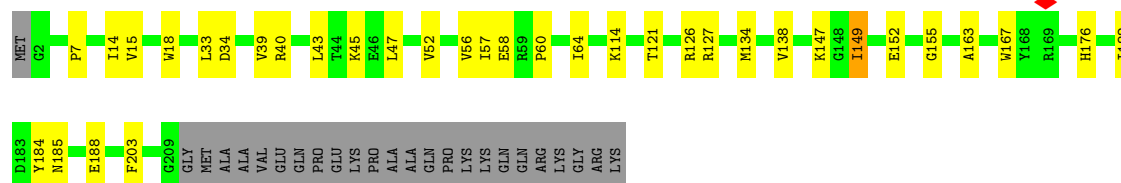


- Molecule 35: 30S ribosomal protein S2



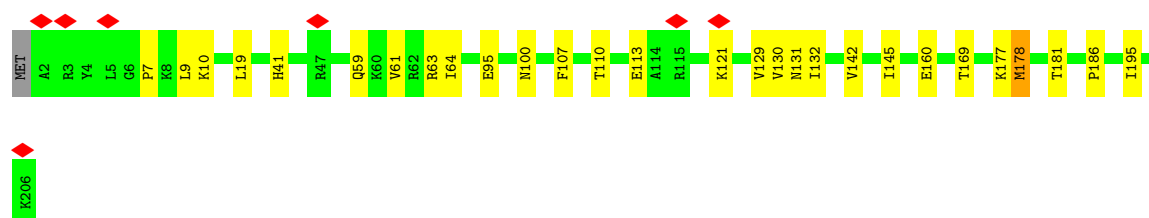
- Molecule 36: 30S ribosomal protein S3

Chain h: 



- Molecule 37: 30S ribosomal protein S4

Chain i: 



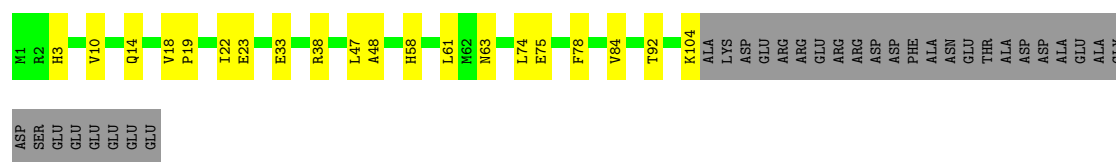
- Molecule 38: 30S ribosomal protein S5

Chain j: 



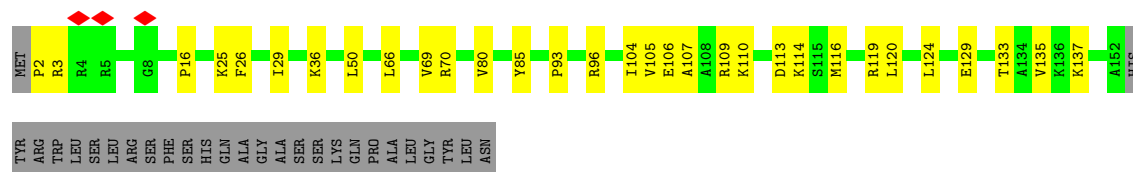
- Molecule 39: 30S ribosomal protein S6

Chain k: 



- Molecule 40: 30S ribosomal protein S7

Chain l: 

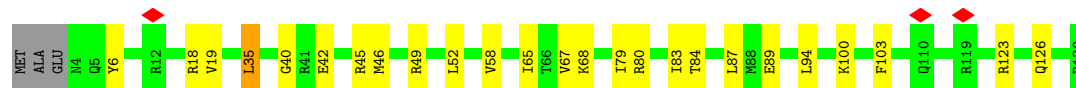
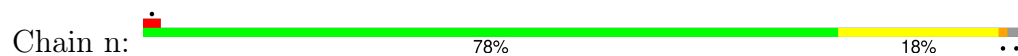


- Molecule 41: Small ribosomal subunit protein uS8

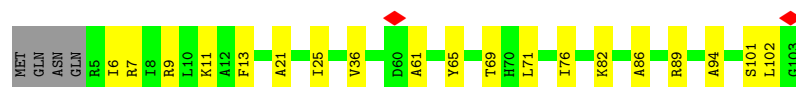
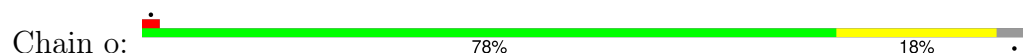
Chain m: 



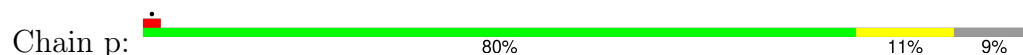
- Molecule 42: Small ribosomal subunit protein uS9



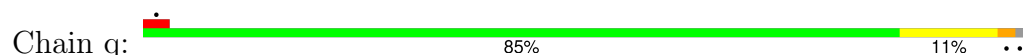
- Molecule 43: Small ribosomal subunit protein uS10



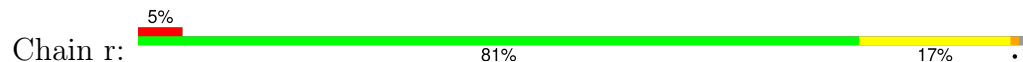
- Molecule 44: 30S ribosomal protein S11



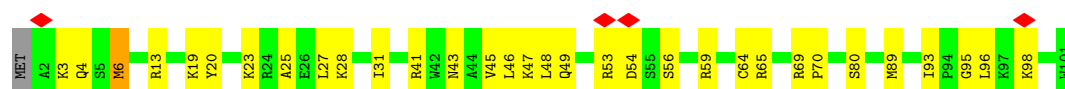
- Molecule 45: Small ribosomal subunit protein uS12



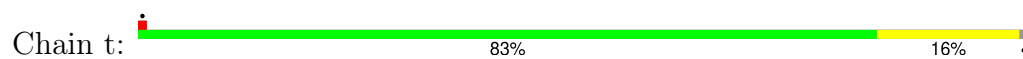
- Molecule 46: 30S ribosomal protein S13



- Molecule 47: Small ribosomal subunit protein uS14



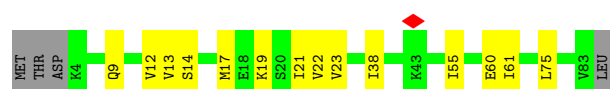
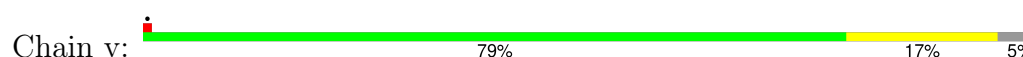
- Molecule 48: Small ribosomal subunit protein uS15



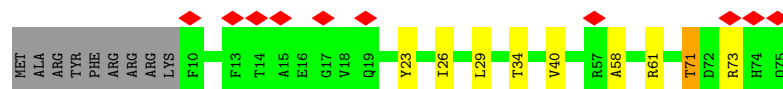
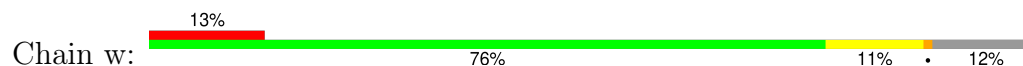
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: Small ribosomal subunit protein uS17



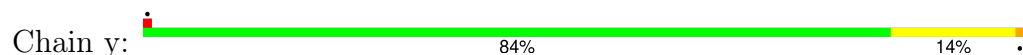
- Molecule 51: 30S ribosomal protein S18



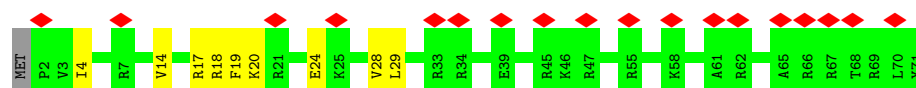
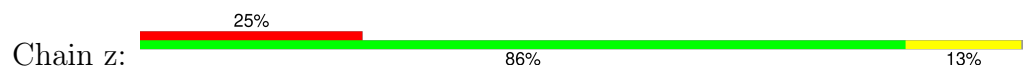
- Molecule 52: Small ribosomal subunit protein uS19



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.07	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00281	Depositor
Map size ($\text{\AA}$)	547.3792, 547.3792, 547.3792	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0691, 1.0691, 1.0691	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MA6, 2MG, UR3, 5MC, G7M, 0TD, MG, 4OC

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	B	0.30	0/2121	0.64	0/2852
2	C	0.30	0/1586	0.79	0/2134
3	D	0.31	0/1571	0.77	0/2113
4	E	0.34	0/1434	0.83	0/1926
5	F	0.23	0/1333	0.66	0/1805
6	G	0.31	0/1122	0.85	0/1515
7	J	0.29	0/1152	0.69	0/1551
8	K	0.30	0/955	0.76	1/1279 (0.1%)
9	L	0.30	0/1062	0.75	0/1413
10	M	0.32	0/1093	0.77	0/1460
11	N	0.33	0/964	0.70	0/1289
12	O	0.34	0/902	0.84	2/1209 (0.2%)
13	P	0.27	0/929	0.61	0/1242
14	Q	0.30	0/960	0.63	0/1278
15	R	0.31	0/829	0.79	1/1107 (0.1%)
16	S	0.27	0/864	0.60	0/1156
17	T	0.25	0/752	0.69	0/1005
18	U	0.31	0/796	0.79	0/1062
19	V	0.33	0/766	0.84	0/1025
20	W	0.29	0/582	0.69	0/769
21	X	0.28	0/635	0.63	0/848
22	Y	0.26	0/502	0.79	0/667
23	Z	0.26	0/452	0.65	0/605
24	1	0.23	0/67839	0.39	3/105827 (0.0%)
25	2	0.20	0/36590	0.35	0/57074
26	3	0.21	0/2872	0.38	0/4478
27	4	0.20	0/160	0.45	0/246
28	5	0.20	0/1841	0.46	2/2870 (0.1%)
29	a	0.28	0/531	0.82	1/709 (0.1%)
30	b	0.26	0/450	0.62	0/599
31	c	0.28	0/433	0.68	0/576
32	d	0.26	0/380	0.60	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.27	0/513	0.73	0/676
34	f	0.27	0/303	0.60	0/397
35	g	0.32	0/1791	0.86	2/2413 (0.1%)
36	h	0.29	0/1663	0.79	3/2241 (0.1%)
37	i	0.29	0/1665	0.76	1/2227 (0.0%)
38	j	0.33	0/1165	0.83	0/1568
39	k	0.33	0/867	0.90	2/1171 (0.2%)
40	l	0.25	0/1195	0.78	3/1602 (0.2%)
41	m	0.30	0/989	0.77	1/1326 (0.1%)
42	n	0.33	0/1034	0.82	1/1375 (0.1%)
43	o	0.30	0/800	0.73	0/1082
44	p	0.29	0/893	0.78	0/1205
45	q	0.28	0/960	0.64	0/1286
46	r	0.27	0/909	0.82	2/1215 (0.2%)
47	s	0.27	0/817	0.81	2/1088 (0.2%)
48	t	0.27	0/722	0.75	0/964
49	u	0.28	0/659	0.73	0/884
50	v	0.30	0/657	0.81	0/881
51	w	0.27	0/553	0.85	0/743
52	x	0.32	0/680	0.88	0/915
53	y	0.30	0/675	0.76	0/895
54	z	0.26	0/597	0.67	0/792
All	All	0.25	0/154565	0.51	27/231133 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
12	O	0	1
25	2	10	0
46	r	0	1
All	All	10	3

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	l	80	VAL	N-CA-C	-9.05	97.78	108.82
41	m	96	MET	CA-CB-CG	6.89	127.89	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	r	79	ARG	CG-CD-NE	-6.75	97.16	112.00
36	h	47	LEU	CA-CB-CG	6.74	139.87	116.30
35	g	11	LYS	CB-CG-CD	6.44	126.12	111.30
42	n	100	LYS	CA-CB-CG	6.25	126.59	114.10
47	s	6	MET	CB-CG-SD	5.85	130.24	112.70
29	a	59	ARG	CA-CB-CG	5.78	125.66	114.10
37	i	160	GLU	CA-CB-CG	5.70	125.49	114.10
12	O	63	LYS	CA-CB-CG	5.69	125.48	114.10
35	g	73	LYS	CA-C-O	-5.69	111.94	119.10
39	k	33	GLU	CB-CG-CD	5.58	122.08	112.60
47	s	89	MET	CB-CG-SD	5.46	129.09	112.70
40	l	129	GLU	CA-CB-CG	5.43	124.95	114.10
36	h	58	GLU	CA-CB-CG	5.39	124.89	114.10
24	1	1111	A	P-O3'-C3'	5.38	128.28	120.20
39	k	23	GLU	CA-CB-CG	5.30	124.69	114.10
15	R	1	MET	CB-CG-SD	5.29	128.58	112.70
12	O	61	GLN	CA-CB-CG	5.20	124.51	114.10
28	5	72	G	P-O3'-C3'	5.14	127.91	120.20
8	K	53	LYS	CB-CG-CD	5.13	123.10	111.30
40	l	80	VAL	CB-CA-C	5.13	118.52	111.34
36	h	45	LYS	CA-CB-CG	5.11	124.32	114.10
24	1	1022	G	P-O3'-C3'	5.09	127.83	120.20
24	1	1070	A	P-O3'-C3'	5.08	127.82	120.20
46	r	78	LYS	CA-CB-CG	5.07	124.24	114.10
28	5	2	G	P-O3'-C3'	5.03	127.75	120.20

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	2	966	2MG	C2',C1'
25	2	967	5MC	C4',C3'
25	2	1207	2MG	C4',C3'
25	2	1407	5MC	C4',C3'
25	2	1516	2MG	C4',C3'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	151	THR	Peptide
12	O	10	ARG	Sidechain
46	r	79	ARG	Sidechain

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	B	2082	0	2154	26	0
2	C	1565	0	1616	26	0
3	D	1552	0	1619	15	0
4	E	1410	0	1444	46	0
5	F	1313	0	1358	8	0
6	G	1111	0	1148	12	0
7	J	1129	0	1162	14	0
8	K	946	0	1023	17	0
9	L	1053	0	1129	7	0
10	M	1074	0	1157	13	0
11	N	951	0	994	8	0
12	O	892	0	923	9	0
13	P	917	0	962	7	0
14	Q	947	0	1019	11	0
15	R	816	0	839	7	0
16	S	857	0	922	6	0
17	T	746	0	811	13	0
18	U	788	0	844	10	0
19	V	753	0	780	3	0
20	W	575	0	592	5	0
21	X	625	0	652	6	0
22	Y	501	0	531	6	0
23	Z	448	0	488	5	0
24	1	60570	0	30467	210	0
25	2	32929	0	16581	138	0
26	3	2569	0	1301	16	0
27	4	145	0	77	0	0
28	5	1648	0	834	3	0
29	a	522	0	524	5	0
30	b	444	0	458	6	0
31	c	426	0	464	6	0
32	d	377	0	418	5	0
33	e	504	0	572	4	0
34	f	302	0	343	1	0
35	g	1760	0	1787	19	0
36	h	1636	0	1710	20	0
37	i	1643	0	1707	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	j	1152	0	1196	18	0
39	k	848	0	846	10	0
40	l	1181	0	1238	22	0
41	m	979	0	1031	17	0
42	n	1022	0	1070	18	0
43	o	790	0	831	25	0
44	p	877	0	887	10	0
45	q	957	0	1017	16	0
46	r	900	0	965	11	0
47	s	805	0	844	32	0
48	t	714	0	734	8	0
49	u	649	0	666	8	0
50	v	648	0	691	19	0
51	w	544	0	560	9	0
52	x	663	0	688	15	0
53	y	669	0	719	8	0
54	z	589	0	629	10	0
55	1	295	0	0	0	0
55	2	104	0	0	0	0
55	3	8	0	0	0	0
55	B	1	0	0	0	0
55	C	1	0	0	0	0
55	D	3	0	0	0	0
55	F	1	0	0	0	0
55	P	1	0	0	0	0
55	Q	1	0	0	0	0
55	R	1	0	0	0	0
55	T	1	0	0	0	0
55	X	1	0	0	0	0
55	Z	1	0	0	0	0
55	b	1	0	0	0	0
55	e	2	0	0	0	0
55	z	2	0	0	0	0
56	1	9	0	12	0	0
57	1	147	0	0	0	0
57	2	106	0	0	0	0
57	3	5	0	0	0	0
57	4	1	0	0	0	0
57	5	14	0	0	0	0
57	B	1	0	0	0	0
57	C	6	0	0	0	0
57	D	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	E	8	0	0	0	0
57	F	11	0	0	1	0
57	G	20	0	0	0	0
57	J	2	0	0	0	0
57	K	5	0	0	0	0
57	L	5	0	0	0	0
57	M	3	0	0	0	0
57	N	4	0	0	0	0
57	O	4	0	0	0	0
57	R	7	0	0	0	0
57	S	3	0	0	0	0
57	T	2	0	0	0	0
57	U	1	0	0	0	0
57	V	4	0	0	0	0
57	W	1	0	0	0	0
57	Y	4	0	0	0	0
57	a	30	0	0	0	0
57	b	1	0	0	0	0
57	c	2	0	0	0	0
57	g	33	0	0	0	0
57	h	12	0	0	0	0
57	i	4	0	0	0	0
57	j	7	0	0	0	0
57	k	7	0	0	0	0
57	l	12	0	0	0	0
57	m	9	0	0	0	0
57	n	5	0	0	0	0
57	o	11	0	0	0	0
57	p	4	0	0	0	0
57	q	5	0	0	0	0
57	r	7	0	0	0	0
57	s	5	0	0	0	0
57	t	4	0	0	0	0
57	u	5	0	0	0	0
57	v	2	0	0	0	0
57	w	9	0	0	0	0
57	x	1	0	0	0	0
57	y	1	0	0	0	0
57	z	13	0	0	0	0
All	All	143506	0	96034	885	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 4.

All (885) 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)
43:o:11:LYS:CE	43:o:71:LEU:HD21	1.64	1.27
43:o:11:LYS:HG2	43:o:71:LEU:CD2	1.74	1.18
48:t:3:LEU:HG	48:t:35:GLN:OE1	1.48	1.11
6:G:84:ALA:HB2	6:G:90:LEU:HD23	1.31	1.10
37:i:142:VAL:HG22	37:i:181:THR:HG22	1.27	1.09
36:h:39:VAL:O	36:h:43:LEU:HD13	1.49	1.09
54:z:4:ILE:HG23	54:z:18:ARG:NH1	1.68	1.09
43:o:11:LYS:HE2	43:o:71:LEU:HD21	1.29	1.06
43:o:11:LYS:HG2	43:o:71:LEU:HD23	1.11	1.05
43:o:11:LYS:CG	43:o:71:LEU:CD2	2.36	1.03
43:o:11:LYS:CG	43:o:71:LEU:HD23	1.89	1.02
40:l:50:LEU:HD11	40:l:124:LEU:HD23	1.45	0.97
14:Q:99:ALA:O	14:Q:103:LYS:NZ	1.97	0.96
17:T:29:THR:CG2	17:T:86:THR:HG22	1.95	0.96
51:w:34:THR:HG22	51:w:40:VAL:CG2	1.98	0.93
4:E:72:LYS:HG3	4:E:74:VAL:HG23	1.48	0.93
4:E:141:ILE:CG1	4:E:146:VAL:CG2	2.47	0.92
17:T:29:THR:HG22	17:T:86:THR:HG22	1.51	0.90
46:r:90:ARG:NH2	46:r:95:LEU:HD13	1.89	0.88
10:M:28:PHE:HB2	10:M:104:GLU:OE1	1.74	0.87
39:k:19:PRO:HA	39:k:22:ILE:HD12	1.57	0.86
43:o:11:LYS:HE2	43:o:71:LEU:CD2	2.07	0.85
54:z:4:ILE:HG23	54:z:18:ARG:HH12	1.39	0.84
4:E:167:ARG:NH1	4:E:177:PHE:CE1	2.46	0.82
45:q:8:VAL:HG21	50:v:38:ILE:HD11	1.61	0.82
4:E:167:ARG:HD2	4:E:177:PHE:CZ	2.14	0.81
43:o:11:LYS:CG	43:o:71:LEU:HD21	2.05	0.81
38:j:88:VAL:HG22	38:j:93:ARG:HG3	1.61	0.81
2:C:2:ILE:CD1	2:C:82:PHE:HB2	2.11	0.80
3:D:148:ILE:HG13	3:D:169:VAL:HG22	1.63	0.80
45:q:8:VAL:HG11	50:v:38:ILE:CD1	2.11	0.80
2:C:5:VAL:HG23	2:C:82:PHE:CZ	2.16	0.80
49:u:44:SER:O	49:u:47:GLU:OE2	2.00	0.80
2:C:5:VAL:HG23	2:C:82:PHE:HZ	1.47	0.80
47:s:56:SER:OG	47:s:59:ARG:HG2	1.83	0.79
51:w:34:THR:HG22	51:w:40:VAL:HG23	1.61	0.79
4:E:167:ARG:HD2	4:E:177:PHE:HZ	1.48	0.79
50:v:14:SER:OG	50:v:22:VAL:HG22	1.84	0.78
25:2:1445:U:H3	25:2:1457:G:H1	1.31	0.77
8:K:61:VAL:HG23	8:K:87:LEU:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:11:LYS:HE3	43:o:71:LEU:HD21	1.64	0.76
45:q:8:VAL:HG11	50:v:38:ILE:HD13	1.66	0.76
4:E:141:ILE:HG13	4:E:146:VAL:CG2	2.14	0.76
2:C:2:ILE:HD12	2:C:82:PHE:CB	2.16	0.75
38:j:33:PHE:CG	38:j:56:VAL:HG22	2.22	0.75
2:C:5:VAL:HG22	2:C:202:ILE:HG12	1.69	0.74
6:G:84:ALA:HB2	6:G:90:LEU:CD2	2.16	0.74
37:i:59:GLN:HB3	37:i:63:ARG:HE	1.51	0.74
43:o:11:LYS:CD	43:o:71:LEU:HD21	2.17	0.74
40:l:50:LEU:CD1	40:l:124:LEU:HD23	2.17	0.73
25:2:458:U:H3	25:2:474:G:H1	1.33	0.73
6:G:84:ALA:CB	6:G:90:LEU:HD23	2.15	0.73
24:1:2682:A:H61	24:1:2728:U:H1'	1.54	0.72
25:2:447:G:H21	25:2:487:A:H62	1.37	0.72
54:z:4:ILE:CG2	54:z:18:ARG:NH1	2.51	0.72
47:s:49:GLN:HE22	52:x:10:PHE:HZ	1.38	0.72
25:2:1312:G:H5'	52:x:5:LEU:HD11	1.71	0.71
39:k:18:VAL:O	39:k:22:ILE:HG13	1.90	0.71
37:i:145:ILE:HD12	37:i:178:MET:HB2	1.73	0.70
25:2:201:G:H1	25:2:216:U:H3	1.36	0.70
4:E:141:ILE:HG12	4:E:146:VAL:CG2	2.21	0.69
50:v:12:VAL:HG22	50:v:23:VAL:HG22	1.74	0.69
8:K:61:VAL:HG21	8:K:112:PHE:HE2	1.58	0.69
41:m:18:GLN:HE21	41:m:63:LEU:HD22	1.58	0.69
18:U:9:ASP:OD2	18:U:72:ILE:HD12	1.92	0.69
25:2:323:U:H5''	53:y:21:ASN:HD21	1.59	0.68
8:K:30:ARG:HD2	24:1:2674:G:H4'	1.76	0.68
2:C:186:LEU:HD21	13:P:4:ILE:HD11	1.75	0.68
25:2:1061:G:H5'	43:o:61:ALA:HB2	1.75	0.68
47:s:49:GLN:NE2	52:x:10:PHE:HZ	1.90	0.68
1:B:17:VAL:HG22	1:B:204:VAL:HG22	1.74	0.67
7:J:108:MET:HG2	24:1:1006:C:H1'	1.77	0.67
26:3:72:G:H21	26:3:104:A:H62	1.43	0.67
36:h:114:LYS:HD3	36:h:185:ASN:HD21	1.57	0.67
26:3:30:C:H1'	26:3:57:A:H61	1.58	0.67
51:w:34:THR:HG22	51:w:40:VAL:HG22	1.75	0.66
8:K:61:VAL:HG23	8:K:87:LEU:CD1	2.26	0.66
25:2:76:G:H1	25:2:93:U:H3	1.44	0.66
25:2:1438:G:H1	25:2:1463:U:H3	1.42	0.65
37:i:110:THR:HG23	37:i:113:GLU:H	1.61	0.65
7:J:3:THR:HG23	24:1:995:C:O2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:r:90:ARG:HH22	46:r:95:LEU:HD13	1.61	0.65
25:2:1497:G:H1'	25:2:1518:MA6:H2	1.79	0.65
54:z:4:ILE:HD12	54:z:19:PHE:HB2	1.79	0.65
50:v:12:VAL:HG22	50:v:23:VAL:CG2	2.28	0.64
17:T:29:THR:HG21	17:T:86:THR:HG22	1.79	0.64
25:2:841:C:H2'	25:2:843:U:H5'	1.80	0.64
35:g:111:ILE:HD11	35:g:151:ILE:HG22	1.80	0.64
31:c:17:THR:HG21	31:c:43:VAL:HG23	1.78	0.64
38:j:107:ALA:HB1	38:j:111:MET:HB3	1.79	0.64
3:D:138:LEU:HD11	3:D:167:VAL:HG11	1.78	0.64
43:o:9:ARG:NH2	43:o:11:LYS:HE3	2.13	0.64
49:u:45:GLU:O	49:u:47:GLU:OE1	2.16	0.63
4:E:141:ILE:HD11	4:E:146:VAL:CG2	2.28	0.63
10:M:74:THR:HG22	10:M:89:VAL:HG22	1.81	0.63
46:r:90:ARG:NH2	46:r:95:LEU:CD1	2.61	0.63
3:D:148:ILE:CG1	3:D:169:VAL:HG22	2.29	0.63
2:C:2:ILE:HD12	2:C:82:PHE:HB2	1.80	0.62
4:E:4:LEU:HD11	4:E:101:GLU:HB3	1.81	0.62
11:N:53:THR:HG21	24:1:2840:C:H5''	1.81	0.62
43:o:13:PHE:HE1	43:o:69:THR:HG1	1.47	0.62
45:q:50:ARG:HG3	45:q:90:LEU:HD11	1.81	0.62
8:K:61:VAL:HG21	8:K:112:PHE:CE2	2.35	0.62
15:R:78:ARG:HH22	24:1:974:G:H4'	1.65	0.62
35:g:183:VAL:HG13	35:g:197:ASP:H	1.65	0.62
4:E:167:ARG:CD	4:E:177:PHE:CZ	2.82	0.61
11:N:34:ILE:HD11	24:1:1278:C:H4'	1.82	0.61
25:2:310:G:H5''	49:u:31:ARG:HB2	1.83	0.61
25:2:429:U:H5'	37:i:9:LEU:HD11	1.83	0.61
45:q:8:VAL:CG1	50:v:38:ILE:CD1	2.78	0.61
2:C:2:ILE:HD12	2:C:82:PHE:HB3	1.83	0.61
2:C:5:VAL:CG2	2:C:82:PHE:HZ	2.13	0.61
43:o:21:ALA:O	43:o:25:ILE:HG13	2.01	0.61
1:B:95:LEU:HD21	24:1:1501:G:H4'	1.83	0.60
25:2:1223:C:H5''	25:2:1224:U:H5''	1.84	0.60
18:U:49:VAL:HG13	18:U:51:ALA:O	2.00	0.60
37:i:145:ILE:HD12	37:i:178:MET:HG3	1.84	0.60
2:C:55:LYS:HD2	2:C:77:ARG:HA	1.82	0.60
4:E:141:ILE:CG1	4:E:146:VAL:HG23	2.31	0.60
4:E:66:LEU:HD11	26:3:41:G:C8	2.37	0.59
4:E:122:PHE:HB3	4:E:163:ASP:HB2	1.83	0.59
24:1:2508:G:H1	24:1:2580:U:H5	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:91:PHE:HE1	35:g:93:ASN:HD22	1.51	0.59
31:c:6:ARG:HD2	31:c:24:THR:HB	1.84	0.59
43:o:86:ALA:HA	43:o:89:ARG:HE	1.68	0.59
4:E:141:ILE:HD11	4:E:146:VAL:HG23	1.85	0.59
49:u:44:SER:O	49:u:47:GLU:CD	2.45	0.59
14:Q:49:ASP:HA	14:Q:52:GLN:HB2	1.84	0.59
41:m:29:SER:HB3	41:m:59:LEU:HB2	1.85	0.59
45:q:8:VAL:CG1	50:v:38:ILE:HD13	2.33	0.59
4:E:141:ILE:HG13	4:E:146:VAL:HG23	1.84	0.59
24:1:281:C:H42	24:1:359:G:H1	1.49	0.59
4:E:131:GLY:HA3	24:1:2305:U:H5''	1.85	0.59
38:j:12:GLN:HG3	38:j:117:VAL:HG13	1.85	0.59
1:B:205:LEU:HD12	24:1:1791:A:H5''	1.84	0.58
4:E:141:ILE:CD1	4:E:146:VAL:CG2	2.81	0.58
5:F:84:THR:HG21	57:F:308:HOH:O	2.04	0.58
25:2:1128:C:H5''	42:n:68:LYS:NZ	2.19	0.58
39:k:3:HIS:HB3	39:k:92:THR:HG23	1.85	0.58
35:g:206:ALA:O	35:g:210:VAL:HG23	2.03	0.58
4:E:141:ILE:HG12	4:E:146:VAL:HG22	1.86	0.58
24:1:2324:U:H5''	24:1:2325:G:H5''	1.85	0.58
45:q:8:VAL:CG2	50:v:38:ILE:HD11	2.32	0.58
53:y:10:ARG:HA	53:y:13:GLN:HB2	1.84	0.58
10:M:8:LYS:HB2	10:M:9:PHE:HD1	1.69	0.58
45:q:8:VAL:HG11	50:v:38:ILE:HD11	1.83	0.58
54:z:4:ILE:HD11	54:z:19:PHE:HA	1.85	0.58
36:h:40:ARG:HH21	36:h:57:ILE:HG22	1.68	0.57
38:j:165:LEU:HB3	41:m:114:ARG:HH22	1.69	0.57
25:2:1522:U:H2'	25:2:1523:G:H8	1.69	0.57
38:j:33:PHE:CG	38:j:56:VAL:CG2	2.86	0.57
42:n:35:LEU:HD11	42:n:49:ARG:HH12	1.69	0.57
24:1:355:U:H2'	24:1:356:G:H8	1.69	0.57
40:l:93:PRO:HA	40:l:96:ARG:HG2	1.86	0.57
44:p:23:ILE:HG23	44:p:32:VAL:HG22	1.86	0.57
24:1:2229:U:H2'	24:1:2230:G:H8	1.69	0.57
15:R:75:VAL:HG23	15:R:86:GLN:HG3	1.87	0.57
4:E:141:ILE:CG1	4:E:146:VAL:HG22	2.33	0.57
25:2:967:5MC:H2'	25:2:968:A:C8	2.39	0.57
14:Q:55:ARG:HD3	24:1:1155:A:H5''	1.86	0.57
17:T:49:LYS:HG3	17:T:50:LEU:HD23	1.86	0.57
19:V:88:HIS:HE2	26:3:76:G:H1'	1.69	0.57
24:1:1936:A:H2	24:1:1943:U:H3	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:r:4:ILE:HG23	46:r:57:ARG:HG2	1.86	0.57
8:K:71:ARG:HH12	8:K:105:ARG:HB3	1.69	0.57
25:2:908:A:H2'	25:2:909:A:H8	1.69	0.57
42:n:19:VAL:HG12	42:n:65:ILE:HG12	1.86	0.57
37:i:107:PHE:CD2	37:i:145:ILE:HD11	2.40	0.56
1:B:120:VAL:CG2	1:B:134:ASN:ND2	2.68	0.56
2:C:5:VAL:CG2	2:C:82:PHE:CZ	2.87	0.56
24:1:1270:C:H5''	24:1:1271:G:H5'	1.88	0.56
40:l:105:VAL:HG22	40:l:109:ARG:HE	1.70	0.56
17:T:43:ILE:HG22	17:T:58:VAL:HG21	1.87	0.56
36:h:57:ILE:HD11	36:h:64:ILE:HD11	1.86	0.56
3:D:148:ILE:HB	3:D:169:VAL:HG22	1.88	0.56
11:N:28:LEU:HD23	11:N:48:VAL:HG21	1.87	0.56
24:1:1013:C:H2'	24:1:1014:A:H8	1.70	0.56
47:s:13:ARG:HD3	47:s:54:ASP:HB3	1.87	0.56
15:R:19:THR:HG22	15:R:97:LYS:HB2	1.87	0.56
25:2:1005:A:H3'	25:2:1006:G:H8	1.71	0.56
10:M:20:LEU:HD13	19:V:81:PRO:HG2	1.86	0.55
40:l:16:PRO:HB2	42:n:42:GLU:HG3	1.88	0.55
47:s:49:GLN:OE1	52:x:10:PHE:CE1	2.59	0.55
50:v:14:SER:OG	50:v:22:VAL:CG2	2.54	0.55
18:U:47:LYS:HD2	24:1:483:A:H5''	1.87	0.55
24:1:886:A:H1'	24:1:891:G:H22	1.72	0.55
37:i:19:LEU:HB3	37:i:64:ILE:HG12	1.87	0.55
24:1:1042:G:H1	24:1:1113:U:H3	1.54	0.55
25:2:21:G:H1'	25:2:915:A:H61	1.71	0.55
32:d:18:PHE:HB2	32:d:43:THR:HG21	1.89	0.55
41:m:105:SER:HB3	41:m:124:GLU:HG2	1.89	0.55
39:k:38:ARG:HB3	39:k:63:ASN:HB2	1.89	0.55
42:n:6:TYR:HD1	42:n:89:GLU:HG3	1.71	0.55
37:i:121:LYS:HG3	37:i:129:VAL:HG21	1.89	0.55
38:j:11:LEU:HD11	38:j:71:MET:HE1	1.87	0.55
9:L:78:ARG:HH22	24:1:627:A:H5''	1.71	0.55
53:y:30:THR:HA	53:y:33:LYS:HD3	1.88	0.55
7:J:81:ILE:HD13	24:1:2514:U:H4'	1.89	0.55
24:1:2861:U:H2'	24:1:2862:G:H8	1.71	0.55
25:2:1232:U:H5''	42:n:126:GLN:HB3	1.89	0.55
40:l:107:ALA:HB1	40:l:133:THR:OG1	2.07	0.55
17:T:34:VAL:HG21	17:T:43:ILE:HD11	1.90	0.54
25:2:1236:A:H4'	25:2:1304:G:H4'	1.89	0.54
4:E:66:LEU:CD1	26:3:41:G:C8	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:64:G:H4'	25:2:65:A:H3'	1.90	0.54
25:2:664:G:H22	25:2:741:G:H1	1.54	0.54
39:k:47:LEU:HD12	39:k:48:ALA:H	1.71	0.54
40:l:106:GLU:HA	40:l:109:ARG:HD2	1.90	0.54
24:1:1086:A:H1'	24:1:1103:A:H61	1.72	0.54
24:1:2245:U:H5''	24:1:2246:G:H5'	1.90	0.54
23:Z:9:GLN:HB2	23:Z:29:LEU:HD13	1.90	0.54
4:E:4:LEU:HA	4:E:7:TYR:HB3	1.90	0.54
30:b:54:VAL:O	30:b:55:ILE:HG13	2.08	0.54
2:C:109:VAL:HG22	2:C:203:VAL:HG12	1.90	0.53
9:L:82:LEU:HD12	9:L:90:VAL:HG11	1.90	0.53
4:E:141:ILE:CD1	4:E:146:VAL:HG23	2.38	0.53
6:G:54:LEU:HA	6:G:57:LYS:HG2	1.90	0.53
12:O:39:VAL:HG12	12:O:49:VAL:HG22	1.89	0.53
24:1:814:C:H1'	24:1:1225:G:H21	1.73	0.53
24:1:1478:G:H1	24:1:1513:U:H3	1.55	0.53
35:g:114:LEU:HD13	35:g:144:LEU:HB3	1.89	0.53
41:m:30:SER:H	41:m:33:LYS:HB2	1.73	0.53
54:z:4:ILE:CD1	54:z:19:PHE:HA	2.37	0.53
1:B:49:ILE:HD11	1:B:52:ARG:HA	1.90	0.53
7:J:26:GLY:HA3	24:1:1140:C:H5'	1.91	0.53
42:n:65:ILE:HG22	42:n:67:VAL:HG23	1.90	0.53
43:o:11:LYS:HE2	43:o:71:LEU:CG	2.38	0.53
4:E:72:LYS:CG	4:E:74:VAL:HG23	2.31	0.53
37:i:107:PHE:CG	37:i:145:ILE:HD11	2.43	0.53
24:1:2370:G:H4'	31:c:44:ARG:HH22	1.74	0.53
24:1:184:C:H2'	24:1:185:G:H8	1.74	0.53
35:g:4:VAL:HG11	35:g:212:LEU:HD21	1.91	0.53
35:g:59:LYS:HG2	35:g:63:ARG:HH22	1.74	0.53
20:W:37:ILE:HG22	20:W:38:VAL:HG13	1.91	0.53
36:h:14:ILE:HG22	36:h:15:VAL:HG13	1.91	0.53
6:G:81:ALA:HB1	6:G:149:GLU:HB2	1.90	0.53
24:1:970:U:H2'	24:1:971:G:H8	1.74	0.53
43:o:11:LYS:HG3	43:o:71:LEU:CD2	2.35	0.53
4:E:38:MET:HE2	4:E:53:ALA:HB1	1.91	0.53
17:T:73:ARG:HH11	24:1:65:U:H1'	1.74	0.53
51:w:34:THR:CG2	51:w:40:VAL:HG23	2.35	0.53
8:K:80:ASP:OD1	8:K:80:ASP:O	2.26	0.53
43:o:36:VAL:HG22	43:o:76:ILE:HG22	1.89	0.53
7:J:3:THR:HG21	14:Q:61:TRP:HE1	1.74	0.52
25:2:674:G:H2'	25:2:675:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:39:VAL:O	36:h:43:LEU:CD1	2.40	0.52
38:j:111:MET:HG3	38:j:140:THR:HG21	1.91	0.52
16:S:6:LYS:HB2	24:1:494:G:H4'	1.91	0.52
38:j:33:PHE:CD1	38:j:56:VAL:HG22	2.43	0.52
5:F:27:LYS:HD2	5:F:32:GLU:HG3	1.90	0.52
35:g:173:ILE:HG22	35:g:183:VAL:HG21	1.91	0.52
11:N:39:PRO:HG2	24:1:1651:G:H4'	1.91	0.52
45:q:83:ARG:HD3	45:q:98:VAL:HG12	1.92	0.52
36:h:34:ASP:HB2	47:s:65:ARG:HE	1.74	0.52
46:r:90:ARG:HB2	46:r:97:VAL:HG22	1.91	0.52
49:u:44:SER:N	49:u:47:GLU:OE2	2.43	0.52
1:B:5:LYS:HD2	1:B:17:VAL:HG12	1.92	0.52
12:O:31:THR:HG21	26:3:28:C:H5''	1.91	0.52
6:G:55:GLU:HA	6:G:58:LEU:HG	1.91	0.52
47:s:46:LEU:HB3	52:x:13:LEU:HD13	1.91	0.52
2:C:2:ILE:HD11	2:C:82:PHE:HB2	1.91	0.51
15:R:38:VAL:HG11	15:R:57:GLY:HA3	1.92	0.51
24:1:883:G:H22	24:1:893:C:H42	1.58	0.51
6:G:94:ILE:HG23	6:G:98:ASP:HB3	1.92	0.51
25:2:447:G:N2	25:2:487:A:H62	2.06	0.51
22:Y:21:LEU:HD21	22:Y:49:ASP:HB3	1.92	0.51
4:E:141:ILE:HG13	4:E:146:VAL:HG21	1.90	0.51
24:1:1310:G:H1'	24:1:1611:C:H5''	1.92	0.51
41:m:41:LYS:HG3	41:m:48:ASP:HA	1.92	0.51
4:E:101:GLU:HA	4:E:104:ILE:HG22	1.92	0.51
25:2:1071:C:H2'	25:2:1072:G:H8	1.75	0.51
29:a:18:CYS:HB2	29:a:40:CYS:HB3	1.93	0.51
34:f:16:ILE:HG22	34:f:25:VAL:HG22	1.93	0.51
47:s:49:GLN:NE2	52:x:10:PHE:CZ	2.75	0.51
48:t:67:LEU:HD13	48:t:78:TYR:HE1	1.76	0.51
1:B:209:GLY:HA3	24:1:764:A:H5''	1.91	0.51
44:p:65:VAL:HA	44:p:68:GLU:HG3	1.92	0.51
1:B:89:ALA:HB2	1:B:158:ALA:HA	1.92	0.51
6:G:30:LEU:HD13	6:G:36:ALA:HB3	1.91	0.51
47:s:19:LYS:HE3	47:s:20:TYR:HE1	1.75	0.51
3:D:148:ILE:CB	3:D:169:VAL:HG22	2.41	0.51
6:G:43:ASN:HA	6:G:46:PHE:HB3	1.91	0.51
7:J:42:ALA:HB3	14:Q:103:LYS:NZ	2.26	0.51
7:J:45:THR:HB	7:J:48:VAL:HG12	1.93	0.51
24:1:1278:C:H2'	24:1:1279:G:H8	1.75	0.51
25:2:1241:G:H2'	25:2:1242:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:52:LEU:HD12	42:n:58:VAL:HA	1.93	0.51
2:C:106:LYS:HD3	2:C:174:SER:HB2	1.93	0.51
33:e:22:PHE:HE2	33:e:59:ILE:HG13	1.76	0.51
43:o:11:LYS:HE2	43:o:71:LEU:HD11	1.92	0.51
52:x:52:HIS:CD2	52:x:54:GLY:H	2.29	0.51
31:c:15:ALA:HB2	31:c:47:VAL:HG11	1.92	0.50
8:K:63:VAL:HG23	8:K:64:ARG:HG3	1.92	0.50
35:g:46:THR:HB	35:g:201:PRO:HD2	1.93	0.50
46:r:25:VAL:HG22	46:r:29:ARG:HG2	1.93	0.50
25:2:1098:C:H2'	25:2:1099:G:C8	2.46	0.50
41:m:40:LEU:HD22	41:m:45:PHE:HB2	1.93	0.50
38:j:132:ASN:HB3	38:j:135:ASN:HB2	1.93	0.50
44:p:113:VAL:HG12	51:w:73:ARG:HG3	1.94	0.50
51:w:23:TYR:HA	51:w:58:ALA:HB1	1.93	0.50
53:y:20:HIS:O	53:y:23:SER:OG	2.25	0.50
37:i:130:VAL:HG12	37:i:132:ILE:H	1.76	0.50
39:k:75:GLU:HA	39:k:78:PHE:HB2	1.92	0.50
24:1:1278:C:H2'	24:1:1279:G:C8	2.46	0.50
2:C:156:PHE:HB3	7:J:81:ILE:HD11	1.93	0.50
47:s:54:ASP:HA	47:s:59:ARG:HG3	1.94	0.50
24:1:955:U:H5	24:1:962:G:H1	1.59	0.50
25:2:946:A:H2'	25:2:947:G:H8	1.75	0.50
39:k:10:VAL:HG13	39:k:58:HIS:HB3	1.93	0.50
54:z:28:VAL:HG23	54:z:29:LEU:HD12	1.94	0.50
1:B:67:PHE:HB3	1:B:152:GLY:H	1.77	0.49
5:F:105:LEU:HB3	5:F:107:LEU:HD13	1.94	0.49
24:1:820:A:H4'	24:1:836:G:H22	1.76	0.49
44:p:34:ILE:HD13	44:p:74:VAL:HG11	1.93	0.49
46:r:64:VAL:HG12	46:r:69:LEU:HB2	1.93	0.49
50:v:12:VAL:HG21	50:v:21:ILE:HD12	1.94	0.49
14:Q:94:ILE:HD12	15:R:13:ARG:HB2	1.94	0.49
4:E:141:ILE:CG1	4:E:146:VAL:HG21	2.36	0.49
7:J:27:ARG:HH22	24:1:1142:A:H4'	1.77	0.49
25:2:150:U:H2'	25:2:151:A:H8	1.76	0.49
25:2:1445:U:O4	25:2:1457:G:O6	2.30	0.49
42:n:87:LEU:HD23	42:n:94:LEU:HD11	1.94	0.49
2:C:179:ARG:HB3	2:C:188:LEU:HD12	1.95	0.49
22:Y:20:ASN:HA	22:Y:23:ARG:HE	1.77	0.49
25:2:946:A:H2'	25:2:947:G:C8	2.48	0.49
18:U:94:ARG:HB2	18:U:103:ILE:HG13	1.94	0.49
22:Y:28:LEU:HD13	22:Y:42:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:61:VAL:HG12	37:i:195:ILE:HD12	1.94	0.49
48:t:12:VAL:HG21	48:t:22:THR:HG22	1.94	0.49
52:x:77:THR:HG23	52:x:78:ARG:HD3	1.94	0.49
14:Q:83:LEU:HG	14:Q:88:VAL:HB	1.95	0.49
23:Z:41:THR:HG22	23:Z:43:ALA:H	1.78	0.49
39:k:10:VAL:HA	39:k:84:VAL:HA	1.94	0.49
10:M:64:TRP:HB2	10:M:104:GLU:HB2	1.95	0.49
24:1:2457:U:H5	24:1:2494:G:H1	1.60	0.49
42:n:84:THR:HG21	42:n:103:PHE:HB3	1.95	0.49
47:s:27:LEU:HD21	47:s:47:LYS:HG2	1.95	0.49
1:B:120:VAL:HG23	1:B:134:ASN:ND2	2.28	0.49
23:Z:6:LYS:HB2	23:Z:58:GLU:HB3	1.95	0.49
24:1:581:C:H2'	24:1:582:A:H8	1.78	0.49
24:1:935:C:H2'	24:1:936:A:H8	1.78	0.49
17:T:54:GLU:HB3	17:T:88:LYS:HE3	1.95	0.49
26:3:111:U:H2'	26:3:112:G:H8	1.77	0.49
29:a:11:GLU:HA	29:a:25:ARG:HA	1.95	0.49
2:C:128:ARG:HH21	24:1:1996:C:H5''	1.78	0.48
24:1:1386:C:H2'	24:1:1387:A:C8	2.48	0.48
24:1:2081:U:H2'	24:1:2082:A:H8	1.79	0.48
35:g:151:ILE:HG22	35:g:151:ILE:O	2.13	0.48
3:D:143:LEU:HD23	3:D:146:VAL:HG21	1.95	0.48
18:U:47:LYS:HE3	18:U:48:PRO:HD2	1.95	0.48
1:B:53:HIS:HA	1:B:217:ARG:HB2	1.94	0.48
14:Q:109:LEU:HD23	15:R:49:ILE:HD13	1.94	0.48
24:1:848:C:H2'	24:1:849:A:H8	1.78	0.48
25:2:1098:C:H2'	25:2:1099:G:H8	1.78	0.48
25:2:1464:U:H2'	25:2:1465:A:H8	1.78	0.48
24:1:1429:G:H2'	24:1:1430:G:H8	1.78	0.48
25:2:707:U:H4'	44:p:22:HIS:ND1	2.29	0.48
47:s:69:ARG:HD2	47:s:70:PRO:HD2	1.94	0.48
4:E:177:PHE:CD1	4:E:178:ARG:N	2.81	0.48
11:N:44:LEU:HD12	11:N:48:VAL:HG23	1.96	0.48
24:1:2087:G:H2'	24:1:2088:A:H8	1.79	0.48
25:2:1386:G:H2'	25:2:1387:G:H8	1.79	0.48
50:v:61:ILE:HA	50:v:75:LEU:HA	1.95	0.48
54:z:20:LYS:O	54:z:24:GLU:HG3	2.14	0.48
12:O:83:LEU:HD11	12:O:114:GLY:HA3	1.94	0.48
25:2:662:U:H2'	25:2:663:A:C8	2.49	0.48
25:2:1356:G:H2'	25:2:1357:A:C8	2.48	0.48
2:C:8:LYS:HG3	2:C:197:THR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:833:A:H2'	24:1:834:G:C8	2.49	0.48
25:2:12:U:H4'	25:2:526:C:H4'	1.96	0.48
30:b:17:ARG:H	30:b:17:ARG:HG2	1.51	0.48
38:j:153:VAL:HA	38:j:156:LYS:HB3	1.96	0.48
25:2:673:A:H2'	25:2:674:G:C8	2.48	0.48
1:B:205:LEU:HB2	24:1:1791:A:H4'	1.95	0.48
22:Y:37:LEU:HD12	22:Y:39:GLN:H	1.78	0.48
24:1:1432:G:H2'	24:1:1433:A:C8	2.49	0.48
31:c:17:THR:HG21	31:c:43:VAL:CG2	2.43	0.48
43:o:7:ARG:HB2	43:o:101:SER:HB3	1.94	0.48
24:1:1447:C:H2'	24:1:1448:G:H8	1.79	0.47
25:2:17:U:H2'	25:2:18:C:C6	2.49	0.47
25:2:501:C:H2'	25:2:502:A:C8	2.49	0.47
25:2:713:G:H2'	25:2:714:G:C8	2.49	0.47
26:3:72:G:N2	26:3:104:A:H62	2.09	0.47
36:h:60:PRO:HB3	43:o:94:ALA:HA	1.96	0.47
40:l:69:VAL:HG21	40:l:104:ILE:HD11	1.96	0.47
44:p:23:ILE:HD12	44:p:86:VAL:HB	1.96	0.47
44:p:87:LYS:HB2	44:p:113:VAL:HG23	1.96	0.47
13:P:29:LYS:HB3	13:P:40:LEU:HD12	1.95	0.47
17:T:55:VAL:HG22	17:T:87:LEU:HD13	1.96	0.47
22:Y:26:PHE:HD1	22:Y:29:ARG:HH21	1.61	0.47
24:1:125:A:H2	32:d:9:VAL:HG23	1.79	0.47
24:1:2291:U:H2'	24:1:2292:U:C6	2.49	0.47
25:2:335:C:H2'	25:2:336:A:H8	1.79	0.47
37:i:145:ILE:HD12	37:i:178:MET:CB	2.43	0.47
3:D:157:LEU:HG	3:D:169:VAL:HG11	1.95	0.47
12:O:18:LEU:HA	12:O:21:LEU:HB2	1.96	0.47
24:1:2047:C:H2'	24:1:2048:G:H8	1.79	0.47
1:B:120:VAL:HG23	1:B:134:ASN:HD22	1.78	0.47
3:D:21:ARG:HH21	3:D:106:LYS:HD3	1.79	0.47
24:1:2316:G:H2'	24:1:2317:A:C8	2.50	0.47
24:1:2515:C:H2'	24:1:2516:A:H8	1.79	0.47
24:1:2728:U:H2'	24:1:2729:G:H8	1.80	0.47
51:w:58:ALA:HA	51:w:61:ARG:HD2	1.95	0.47
4:E:38:MET:HG2	4:E:57:LEU:HD22	1.97	0.47
24:1:948:C:H2'	24:1:949:G:H8	1.79	0.47
24:1:2316:G:H2'	24:1:2317:A:H8	1.78	0.47
24:1:2615:U:C2	30:b:4:GLN:HA	2.50	0.47
25:2:744:C:H2'	25:2:745:G:H8	1.79	0.47
4:E:141:ILE:HD11	4:E:146:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:639:U:H2'	24:1:640:C:C6	2.49	0.47
25:2:618:C:O2	25:2:622:A:N6	2.48	0.47
3:D:149:ILE:HG21	3:D:175:ILE:HG12	1.96	0.47
24:1:1316:U:H2'	24:1:1317:G:H8	1.80	0.47
25:2:1317:C:H42	47:s:53:ARG:HE	1.62	0.47
24:1:284:U:H3	24:1:356:G:H1	1.63	0.47
50:v:13:VAL:HG23	50:v:22:VAL:HG23	1.97	0.47
1:B:120:VAL:CG2	1:B:134:ASN:HD22	2.28	0.47
2:C:5:VAL:HG23	2:C:82:PHE:CE2	2.50	0.47
3:D:188:MET:HE2	3:D:188:MET:HB3	1.88	0.47
7:J:78:THR:HB	24:1:2641:G:H5''	1.95	0.47
8:K:87:LEU:HD13	8:K:92:GLU:HG2	1.97	0.47
25:2:714:G:H2'	25:2:715:A:C8	2.50	0.47
25:2:1414:U:H2'	25:2:1415:G:H8	1.80	0.47
36:h:126:ARG:HA	36:h:127:ARG:HH11	1.80	0.47
41:m:64:LYS:HB3	41:m:71:VAL:HG11	1.97	0.47
1:B:3:VAL:HG22	1:B:19:VAL:HG12	1.97	0.46
5:F:87:LEU:HD23	5:F:164:TYR:HA	1.97	0.46
13:P:53:ARG:HB2	13:P:56:HIS:HB2	1.96	0.46
24:1:1589:U:H2'	24:1:1590:A:H8	1.80	0.46
24:1:1796:U:H2'	24:1:1797:G:H8	1.79	0.46
24:1:2451:A:H1'	28:5:76:A:H2'	1.97	0.46
3:D:175:ILE:HG21	3:D:180:LEU:HD11	1.96	0.46
24:1:1386:C:H2'	24:1:1387:A:H8	1.80	0.46
24:1:2691:C:H2'	24:1:2692:G:H8	1.81	0.46
25:2:514:C:H2'	25:2:515:G:H8	1.80	0.46
28:5:21:A:H62	28:5:47:U:H1'	1.80	0.46
33:e:15:LYS:HB2	33:e:23:LYS:HE2	1.96	0.46
46:r:101:ARG:HD3	46:r:103:LYS:HB3	1.96	0.46
21:X:59:ILE:HG23	21:X:64:ILE:HG22	1.97	0.46
25:2:150:U:H3	25:2:171:A:H62	1.63	0.46
48:t:29:VAL:HG21	48:t:67:LEU:HD23	1.97	0.46
24:1:414:C:H2'	24:1:415:A:H8	1.81	0.46
25:2:672:U:H2'	25:2:673:A:H8	1.81	0.46
35:g:161:LEU:HD22	35:g:176:ALA:HB2	1.97	0.46
40:l:66:LEU:HD23	40:l:70:ARG:HH21	1.81	0.46
40:l:110:LYS:HA	40:l:110:LYS:HD2	1.70	0.46
47:s:49:GLN:NE2	52:x:12:ASP:OD1	2.48	0.46
4:E:130:MET:HG3	4:E:154:ILE:HB	1.95	0.46
16:S:69:LEU:HD22	16:S:107:VAL:HG22	1.98	0.46
24:1:2692:G:H1'	24:1:2847:U:H1'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:1108:G:H5'	36:h:176:HIS:HD1	1.79	0.46
40:l:26:PHE:HZ	40:l:120:LEU:HD11	1.80	0.46
18:U:4:LYS:HZ2	18:U:85:PHE:HE1	1.63	0.46
24:1:1019:U:H3	24:1:1142:A:H62	1.63	0.46
25:2:1129:C:H4'	42:n:18:ARG:HH22	1.80	0.46
9:L:95:LEU:HD23	9:L:95:LEU:HA	1.79	0.46
25:2:891:U:H2'	25:2:892:A:H8	1.80	0.46
37:i:145:ILE:HD12	37:i:178:MET:CG	2.45	0.46
41:m:46:ILE:HG22	41:m:63:LEU:HD23	1.98	0.46
41:m:96:MET:HE2	41:m:99:LEU:HD22	1.97	0.46
1:B:132:MET:HE2	1:B:188:CYS:HB2	1.97	0.46
12:O:94:ARG:HH12	24:1:2293:G:H5''	1.80	0.46
25:2:1060:U:H2'	25:2:1061:G:H8	1.81	0.46
29:a:62:LYS:HE3	29:a:62:LYS:HB3	1.82	0.46
44:p:45:ALA:HB3	44:p:70:CYS:HB2	1.97	0.46
54:z:4:ILE:CG2	54:z:18:ARG:CZ	2.93	0.46
7:J:96:ARG:HG2	7:J:99:ARG:HG2	1.97	0.46
20:W:51:VAL:HG21	20:W:80:ILE:HG22	1.98	0.46
24:1:75:G:H22	24:1:111:A:H2	1.64	0.46
41:m:108:LYS:HA	41:m:108:LYS:HD3	1.75	0.46
4:E:35:THR:HG22	4:E:90:THR:HG23	1.98	0.46
4:E:38:MET:HB3	4:E:152:LEU:HB3	1.98	0.46
24:1:598:U:H2'	24:1:599:A:C8	2.51	0.46
39:k:19:PRO:CA	39:k:22:ILE:HD12	2.38	0.46
5:F:121:ILE:HG12	5:F:141:ILE:HG22	1.97	0.45
24:1:1857:G:H1'	24:1:1885:A:H62	1.81	0.45
47:s:93:ILE:HG21	47:s:96:LEU:HD22	1.98	0.45
1:B:160:THR:HG21	24:1:1819:A:H5''	1.98	0.45
24:1:2039:U:H2'	24:1:2040:G:C8	2.52	0.45
25:2:448:A:H62	25:2:486:U:H3	1.62	0.45
25:2:674:G:H2'	25:2:675:A:C8	2.50	0.45
13:P:48:ILE:HB	13:P:97:LEU:HB2	1.97	0.45
24:1:151:C:H2'	24:1:152:A:H8	1.81	0.45
25:2:1318:A:H4'	52:x:10:PHE:CG	2.52	0.45
24:1:414:C:H2'	24:1:415:A:C8	2.51	0.45
25:2:439:U:H5''	37:i:121:LYS:HD3	1.98	0.45
25:2:1342:C:H2'	25:2:1343:G:C8	2.51	0.45
1:B:78:VAL:HG21	1:B:110:LEU:HD12	1.97	0.45
25:2:269:C:H2'	25:2:270:A:C8	2.50	0.45
24:1:1571:A:H2'	24:1:1572:A:H8	1.82	0.45
37:i:7:PRO:HB2	37:i:10:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:ILE:HG12	2:C:24:VAL:HG21	1.98	0.45
4:E:95:ARG:HD3	4:E:98:GLU:OE2	2.16	0.45
6:G:6:LEU:HD11	6:G:37:VAL:HG23	1.97	0.45
24:1:171:U:H2'	24:1:172:A:H8	1.82	0.45
28:5:72:G:H1'	28:5:73:A:H5'	1.99	0.45
12:O:102:ARG:H	12:O:102:ARG:HG3	1.56	0.45
21:X:3:ARG:HE	21:X:30:LEU:HD22	1.81	0.45
24:1:1447:C:H2'	24:1:1448:G:C8	2.52	0.45
49:u:44:SER:C	49:u:47:GLU:OE2	2.58	0.45
1:B:74:ILE:HD13	1:B:74:ILE:HA	1.87	0.45
9:L:29:LYS:HG3	9:L:30:THR:HG23	1.98	0.45
24:1:2246:G:H2'	24:1:2247:A:H8	1.80	0.45
36:h:33:LEU:HD21	47:s:93:ILE:HD11	1.98	0.45
1:B:107:PRO:HD2	1:B:110:LEU:HG	1.98	0.45
8:K:38:ILE:HG13	8:K:61:VAL:HG22	1.99	0.45
9:L:128:THR:HG23	9:L:131:ALA:H	1.81	0.45
24:1:351:C:H2'	24:1:352:A:H8	1.82	0.45
24:1:721:A:H2'	24:1:722:A:C8	2.52	0.45
25:2:1129:C:H5'	42:n:18:ARG:HH12	1.82	0.45
52:x:50:ALA:HB1	52:x:57:HIS:HB3	1.98	0.45
4:E:29:PRO:HB2	4:E:169:LEU:HD12	1.98	0.44
11:N:72:ASP:HB3	11:N:75:ILE:HG12	1.99	0.44
15:R:73:LYS:HE3	15:R:73:LYS:HB3	1.72	0.44
18:U:11:VAL:HA	18:U:73:PHE:H	1.81	0.44
24:1:145:C:H2'	24:1:146:A:C8	2.52	0.44
24:1:572:A:H61	24:1:2029:G:H21	1.65	0.44
24:1:832:U:H2'	24:1:833:A:H8	1.82	0.44
24:1:2023:C:H2'	24:1:2024:G:H8	1.82	0.44
25:2:376:G:H2'	25:2:377:G:H8	1.81	0.44
29:a:36:VAL:HG21	29:a:41:HIS:HD2	1.82	0.44
30:b:54:VAL:C	30:b:55:ILE:HG13	2.41	0.44
4:E:70:ALA:HB3	4:E:82:GLY:H	1.82	0.44
10:M:74:THR:CG2	10:M:89:VAL:HG22	2.46	0.44
25:2:337:G:H2'	25:2:338:A:H8	1.80	0.44
25:2:501:C:H2'	25:2:502:A:H8	1.83	0.44
37:i:95:GLU:HG2	37:i:186:PRO:HG3	1.98	0.44
42:n:80:ARG:HG2	42:n:80:ARG:HH11	1.82	0.44
8:K:23:LYS:HD3	8:K:23:LYS:HA	1.72	0.44
8:K:38:ILE:HD11	8:K:112:PHE:HZ	1.83	0.44
25:2:56:U:H2'	25:2:57:G:H8	1.83	0.44
10:M:60:GLN:OE1	10:M:108:VAL:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:596:U:H2'	24:1:597:G:H8	1.82	0.44
24:1:1590:A:H2'	24:1:1591:A:C8	2.53	0.44
24:1:2036:C:H2'	24:1:2037:A:H8	1.83	0.44
25:2:335:C:H2'	25:2:336:A:C8	2.52	0.44
50:v:12:VAL:CG2	50:v:23:VAL:HG22	2.46	0.44
51:w:71:THR:HG21	51:w:73:ARG:HH21	1.83	0.44
4:E:141:ILE:CD1	4:E:146:VAL:HG22	2.48	0.44
10:M:12:MET:HE3	10:M:12:MET:HB2	1.83	0.44
17:T:58:VAL:HG12	17:T:59:ASN:N	2.31	0.44
20:W:47:ALA:HB2	20:W:59:LEU:HD22	2.00	0.44
20:W:78:LYS:HB3	20:W:78:LYS:HE2	1.81	0.44
24:1:1105:U:H2'	24:1:1106:G:C8	2.52	0.44
24:1:1509:A:H2'	24:1:1510:G:C8	2.52	0.44
24:1:2329:U:H2'	24:1:2330:G:C8	2.53	0.44
25:2:552:U:H2'	25:2:553:A:C8	2.53	0.44
45:q:3:THR:HG22	45:q:5:ASN:H	1.83	0.44
49:u:39:PHE:HB2	49:u:74:LEU:HD11	1.99	0.44
2:C:24:VAL:HG12	2:C:178:VAL:HG21	2.00	0.44
24:1:511:U:H4'	24:1:1235:G:H4'	2.00	0.44
24:1:581:C:H2'	24:1:582:A:C8	2.52	0.44
24:1:882:G:H22	24:1:895:U:H1'	1.83	0.44
24:1:1045:C:H4'	24:1:1047:G:H1'	1.99	0.44
24:1:1509:A:H2'	24:1:1510:G:H8	1.81	0.44
25:2:171:A:H2'	25:2:172:A:C8	2.53	0.44
25:2:634:C:H2'	25:2:635:A:H8	1.83	0.44
25:2:1127:G:H22	25:2:1145:A:H61	1.66	0.44
25:2:1407:5MC:H2'	25:2:1408:A:H8	1.81	0.44
32:d:43:THR:CG2	32:d:45:SER:OG	2.66	0.44
35:g:6:MET:HE1	35:g:47:VAL:HG11	2.00	0.44
41:m:18:GLN:HG3	41:m:72:VAL:HG22	1.99	0.44
41:m:81:PRO:HA	41:m:84:ARG:HH11	1.83	0.44
51:w:26:ILE:HA	51:w:29:LEU:HB2	2.00	0.44
7:J:68:LYS:HB2	7:J:68:LYS:HE3	1.73	0.44
25:2:21:G:H2'	25:2:22:G:C8	2.53	0.44
25:2:769:G:H4'	25:2:1513:A:H4'	2.00	0.44
25:2:1513:A:H2'	25:2:1514:G:C8	2.52	0.44
36:h:138:VAL:HG23	36:h:149:ILE:HG23	1.99	0.44
36:h:155:GLY:HA2	36:h:163:ALA:HB1	1.99	0.44
48:t:3:LEU:HG	48:t:35:GLN:CD	2.34	0.44
10:M:17:ASN:O	10:M:17:ASN:ND2	2.46	0.44
25:2:459:A:H2'	25:2:460:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:79:ILE:O	42:n:83:ILE:HD12	2.17	0.44
45:q:3:THR:HB	45:q:6:GLN:HG3	1.98	0.44
24:1:1469:A:H2'	24:1:1470:A:H8	1.83	0.44
25:2:34:C:H2'	25:2:35:G:H8	1.82	0.44
25:2:674:G:H21	44:p:118:HIS:HB2	1.83	0.44
25:2:1014:A:H2'	25:2:1015:G:C4	2.53	0.44
25:2:1144:G:H21	25:2:1146:A:H62	1.65	0.44
25:2:1218:C:H2'	25:2:1219:A:C8	2.52	0.44
25:2:1507:A:H2'	25:2:1508:A:C8	2.52	0.44
41:m:105:SER:HA	41:m:110:VAL:HG22	2.00	0.44
1:B:141:VAL:HG12	1:B:192:LEU:HD13	1.99	0.43
1:B:199:GLU:H	1:B:199:GLU:HG2	1.62	0.43
8:K:70:ARG:HA	8:K:76:VAL:HG12	1.99	0.43
19:V:30:ILE:HD11	19:V:63:ILE:HG21	1.99	0.43
24:1:873:C:H2'	24:1:874:G:H8	1.83	0.43
24:1:1570:A:H2'	24:1:1571:A:C8	2.52	0.43
24:1:2487:G:H2'	24:1:2488:G:H8	1.82	0.43
35:g:151:ILE:O	35:g:151:ILE:CG2	2.66	0.43
9:L:17:LYS:HD3	9:L:27:LEU:HD21	2.00	0.43
11:N:103:ARG:HD3	11:N:110:MET:HE2	2.00	0.43
16:S:42:LYS:HB3	24:1:2010:G:H5''	2.01	0.43
26:3:49:C:H2'	26:3:50:A:H8	1.83	0.43
36:h:18:TRP:NE1	47:s:95:GLY:H	2.16	0.43
40:l:50:LEU:HD21	40:l:124:LEU:HB3	2.00	0.43
46:r:27:LYS:HE3	46:r:27:LYS:HB2	1.68	0.43
47:s:27:LEU:HD23	47:s:48:LEU:HB2	2.00	0.43
7:J:61:LYS:HE2	7:J:61:LYS:HB2	1.74	0.43
24:1:184:C:H2'	24:1:185:G:C8	2.53	0.43
24:1:2443:C:H2'	24:1:2444:G:H8	1.83	0.43
12:O:67:ASN:HD22	12:O:70:ALA:H	1.65	0.43
24:1:2304:G:H22	24:1:2312:U:H3	1.67	0.43
25:2:210:C:H4'	25:2:211:G:H5''	2.00	0.43
25:2:269:C:H2'	25:2:270:A:H8	1.82	0.43
9:L:73:ILE:HD12	9:L:106:GLU:HG2	1.99	0.43
21:X:33:LEU:HD12	21:X:50:ARG:HG2	1.99	0.43
25:2:235:C:H2'	25:2:236:A:C8	2.53	0.43
25:2:1048:G:H4'	47:s:3:LYS:HE3	2.01	0.43
26:3:95:U:H2'	26:3:96:G:C8	2.53	0.43
38:j:106:ILE:HD13	38:j:106:ILE:HA	1.77	0.43
52:x:11:ILE:HD11	52:x:15:LEU:HD23	2.00	0.43
2:C:157:LYS:HD2	2:C:157:LYS:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:27:LEU:HD23	24:1:600:G:H5'	2.00	0.43
14:Q:45:TYR:HD2	14:Q:48:ARG:HH21	1.65	0.43
24:1:1597:A:H5''	24:1:1598:A:H5'	2.00	0.43
24:1:1709:U:H2'	24:1:1710:G:H8	1.83	0.43
24:1:2186:G:H2'	24:1:2187:U:H4'	2.00	0.43
24:1:2809:A:H2'	24:1:2810:A:C8	2.53	0.43
24:1:2836:U:H2'	24:1:2837:A:C8	2.54	0.43
25:2:999:C:H2'	25:2:1000:A:C8	2.54	0.43
25:2:1243:C:H2'	25:2:1244:G:H8	1.84	0.43
24:1:1744:A:H3'	24:1:1745:A:H8	1.83	0.43
24:1:2215:C:H2'	24:1:2216:G:H8	1.84	0.43
24:1:2685:G:H2'	24:1:2686:G:H8	1.82	0.43
24:1:2845:U:H2'	24:1:2846:G:C8	2.53	0.43
25:2:459:A:H2'	25:2:460:A:C8	2.53	0.43
38:j:33:PHE:CD1	38:j:56:VAL:CG2	3.01	0.43
52:x:49:ILE:HD13	52:x:49:ILE:HA	1.87	0.43
3:D:84:THR:HG21	24:1:586:A:H5'	2.00	0.43
39:k:104:LYS:HB2	39:k:104:LYS:HE2	1.86	0.43
54:z:14:VAL:HA	54:z:17:ARG:HB2	2.01	0.43
5:F:33:LEU:HD23	5:F:33:LEU:HA	1.88	0.43
10:M:41:LEU:HD13	10:M:124:LEU:HD22	2.01	0.43
24:1:20:C:H2'	24:1:21:A:H8	1.83	0.43
24:1:576:U:H2'	24:1:577:G:C8	2.53	0.43
24:1:1105:U:H2'	24:1:1106:G:H8	1.82	0.43
24:1:1796:U:H2'	24:1:1797:G:C8	2.52	0.43
24:1:2698:U:H2'	24:1:2699:C:C6	2.54	0.43
25:2:147:G:H2'	25:2:148:G:C8	2.54	0.43
25:2:1373:G:H5'	40:l:36:LYS:HB2	2.01	0.43
1:B:93:LEU:HB2	1:B:103:TYR:HE1	1.82	0.43
25:2:358:U:H2'	25:2:359:G:H8	1.84	0.43
25:2:1047:G:H5''	47:s:4:GLN:HG3	2.01	0.43
50:v:9:GLN:HG2	50:v:60:GLU:HB3	2.01	0.43
10:M:16:ARG:HA	10:M:16:ARG:HD3	1.79	0.42
17:T:80:TRP:HZ3	17:T:82:LYS:HB2	1.83	0.42
24:1:355:U:H2'	24:1:356:G:C8	2.52	0.42
24:1:645:C:H2'	24:1:647:G:C8	2.52	0.42
24:1:2291:U:H2'	24:1:2292:U:H6	1.84	0.42
24:1:2818:U:H2'	24:1:2819:G:C8	2.54	0.42
25:2:745:G:H2'	25:2:746:A:H8	1.83	0.42
47:s:41:ARG:HH22	52:x:6:LYS:HB2	1.84	0.42
7:J:96:ARG:NE	7:J:99:ARG:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:3:LYS:HD2	23:Z:3:LYS:HA	1.79	0.42
24:1:1987:A:H2'	24:1:1988:G:H8	1.83	0.42
24:1:2514:U:H2'	24:1:2515:C:H6	1.85	0.42
25:2:76:G:H2'	25:2:77:A:H8	1.84	0.42
38:j:101:GLU:HA	38:j:122:ASN:ND2	2.34	0.42
53:y:32:ILE:HG23	53:y:79:LEU:HD21	2.01	0.42
4:E:117:LEU:HD23	4:E:117:LEU:HA	1.90	0.42
22:Y:4:LYS:HE2	22:Y:4:LYS:HB3	1.89	0.42
24:1:742:A:H2'	24:1:743:A:C8	2.55	0.42
24:1:1316:U:H2'	24:1:1317:G:C8	2.55	0.42
25:2:824:G:H2'	25:2:825:A:H8	1.84	0.42
25:2:1356:G:H2'	25:2:1357:A:H8	1.84	0.42
30:b:40:ARG:HA	30:b:40:ARG:HD2	1.86	0.42
36:h:152:GLU:HB2	36:h:167:TRP:HB3	2.01	0.42
40:l:2:PRO:HB2	40:l:3:ARG:H	1.66	0.42
47:s:3:LYS:HE2	47:s:3:LYS:HB3	1.80	0.42
3:D:147:LEU:HB3	3:D:186:VAL:HG23	2.02	0.42
16:S:76:VAL:HG22	16:S:103:ILE:HG23	2.00	0.42
17:T:58:VAL:HG22	17:T:85:VAL:HG13	2.01	0.42
24:1:1668:A:H62	24:1:1991:U:H3	1.66	0.42
25:2:235:C:H2'	25:2:236:A:H8	1.84	0.42
25:2:376:G:H2'	25:2:377:G:C8	2.55	0.42
25:2:1376:U:H2'	25:2:1377:A:C8	2.53	0.42
45:q:73:ASN:HD22	45:q:73:ASN:C	2.28	0.42
47:s:23:LYS:HD2	47:s:27:LEU:HD13	2.01	0.42
53:y:36:TYR:HA	53:y:39:ILE:HD12	2.00	0.42
8:K:7:MET:HG3	8:K:18:ARG:HH21	1.84	0.42
24:1:926:G:H2'	24:1:927:A:C8	2.55	0.42
24:1:2097:A:H2'	24:1:2098:U:C2	2.54	0.42
24:1:2487:G:H2'	24:1:2488:G:C8	2.54	0.42
25:2:137:U:H2'	25:2:138:G:H8	1.84	0.42
25:2:634:C:H2'	25:2:635:A:C8	2.54	0.42
31:c:43:VAL:HG12	31:c:43:VAL:O	2.19	0.42
40:l:124:LEU:HD12	40:l:124:LEU:HA	1.88	0.42
42:n:40:GLY:HA2	42:n:45:ARG:HH12	1.84	0.42
47:s:43:ASN:HA	47:s:46:LEU:HD12	2.02	0.42
48:t:35:GLN:HG2	48:t:59:MET:HE1	2.01	0.42
12:O:27:VAL:HA	12:O:93:ASP:HB3	2.01	0.42
24:1:45:G:H5''	24:1:46:G:H5'	2.00	0.42
24:1:680:C:H2'	24:1:681:G:C8	2.55	0.42
41:m:6:PRO:HB2	41:m:33:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:y:29:ARG:O	53:y:33:LYS:HG3	2.20	0.42
17:T:55:VAL:HG13	17:T:86:THR:O	2.19	0.42
18:U:43:LYS:HZ3	24:1:499:U:H5''	1.83	0.42
24:1:598:U:H2'	24:1:599:A:H8	1.84	0.42
24:1:833:A:H2'	24:1:834:G:H8	1.83	0.42
24:1:2233:U:H2'	24:1:2234:G:H8	1.84	0.42
24:1:2246:G:H2'	24:1:2247:A:C8	2.54	0.42
24:1:2861:U:H2'	24:1:2862:G:C8	2.53	0.42
25:2:1335:U:H5''	25:2:1336:C:H5'	2.01	0.42
25:2:1512:U:H2'	25:2:1513:A:C8	2.54	0.42
26:3:95:U:H2'	26:3:96:G:H8	1.85	0.42
29:a:39:LYS:H	29:a:39:LYS:HG2	1.73	0.42
35:g:206:ALA:HB3	35:g:209:ALA:HB3	2.02	0.42
38:j:81:LEU:HD11	38:j:120:VAL:HG11	2.02	0.42
40:l:116:MET:HA	40:l:119:ARG:HB2	2.00	0.42
40:l:137:LYS:HB2	40:l:137:LYS:HE2	1.78	0.42
47:s:59:ARG:HD2	47:s:59:ARG:HA	1.66	0.42
49:u:5:ARG:HH12	49:u:22:ALA:HB3	1.84	0.42
24:1:2100:G:H2'	24:1:2101:A:C8	2.54	0.42
24:1:2756:U:H1'	24:1:2757:A:H5''	2.00	0.42
25:2:1402:4OC:H1'	25:2:1402:4OC:HM23	1.76	0.42
47:s:19:LYS:HE3	47:s:20:TYR:CE1	2.54	0.42
1:B:261:LYS:HD2	24:1:2227:A:H5''	2.01	0.42
4:E:175:PHE:HA	4:E:176:PRO:HD3	1.86	0.42
6:G:32:PRO:HA	21:X:39:TRP:CD1	2.55	0.42
16:S:82:MET:HB2	16:S:82:MET:HE3	1.82	0.42
24:1:2233:U:H2'	24:1:2234:G:C8	2.55	0.42
25:2:377:G:C6	25:2:387:U:N3	2.88	0.42
25:2:1391:U:H2'	25:2:1392:G:C8	2.55	0.42
26:3:33:G:H2'	26:3:34:A:C8	2.54	0.42
35:g:59:LYS:HG3	35:g:63:ARG:HH12	1.85	0.42
40:l:25:LYS:HD2	40:l:25:LYS:HA	1.76	0.42
40:l:113:ASP:HB2	40:l:119:ARG:HG3	2.02	0.42
48:t:33:THR:HG21	48:t:85:LEU:HD11	2.01	0.42
2:C:128:ARG:HG2	24:1:2512:C:P	2.60	0.42
10:M:108:VAL:HG11	10:M:112:LEU:HD22	2.02	0.42
21:X:32:ASN:HB2	24:1:397:U:H5''	2.00	0.42
21:X:62:LYS:HE2	21:X:62:LYS:HB2	1.70	0.42
24:1:18:U:H2'	24:1:19:A:C8	2.55	0.42
24:1:848:C:H2'	24:1:849:A:C8	2.55	0.42
24:1:2837:A:H2'	24:1:2838:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:460:A:H2'	25:2:461:A:H8	1.85	0.42
41:m:96:MET:HB3	41:m:100:GLY:H	1.85	0.42
45:q:99:ARG:HD2	45:q:104:CYS:SG	2.59	0.42
47:s:3:LYS:HB2	47:s:6:MET:HG2	2.02	0.42
2:C:128:ARG:NH2	24:1:1996:C:H5''	2.35	0.41
4:E:66:LEU:HD22	26:3:42:C:C5	2.55	0.41
5:F:117:LEU:HD21	5:F:121:ILE:HB	2.02	0.41
24:1:1443:U:H2'	24:1:1444:G:H8	1.85	0.41
25:2:363:A:H5'	45:q:31:ARG:HB2	2.02	0.41
25:2:447:G:H21	25:2:487:A:N6	2.13	0.41
25:2:1467:C:H2'	25:2:1468:A:H8	1.85	0.41
43:o:82:LYS:HE3	43:o:82:LYS:HB3	1.96	0.41
53:y:21:ASN:HB2	53:y:66:LEU:HD11	2.02	0.41
25:2:41:G:H2'	25:2:42:G:H8	1.85	0.41
25:2:222:C:H2'	25:2:223:A:H8	1.85	0.41
38:j:106:ILE:HB	38:j:124:LEU:HA	2.02	0.41
40:l:29:ILE:H	40:l:29:ILE:HG13	1.69	0.41
46:r:10:PRO:HG2	46:r:13:LYS:HD2	2.02	0.41
2:C:14:ILE:HD13	2:C:14:ILE:HA	1.91	0.41
23:Z:16:ARG:HG3	23:Z:54:MET:HE1	2.02	0.41
24:1:534:U:H2'	24:1:535:G:H8	1.85	0.41
24:1:917:A:H5''	24:1:2268:A:H61	1.86	0.41
25:2:76:G:H2'	25:2:77:A:C8	2.55	0.41
46:r:86:TYR:CZ	46:r:90:ARG:HD3	2.55	0.41
24:1:979:A:H2'	24:1:982:C:H42	1.85	0.41
24:1:1409:U:H2'	24:1:1410:G:H8	1.85	0.41
24:1:2215:C:H2'	24:1:2216:G:C8	2.54	0.41
25:2:514:C:H2'	25:2:515:G:C8	2.55	0.41
26:3:49:C:H2'	26:3:50:A:C8	2.55	0.41
32:d:3:ARG:HD3	32:d:3:ARG:HA	1.79	0.41
45:q:8:VAL:CG1	50:v:38:ILE:HD11	2.46	0.41
2:C:37:VAL:HG22	2:C:48:ILE:HG22	2.02	0.41
14:Q:19:LYS:HB3	14:Q:19:LYS:HE2	1.90	0.41
16:S:81:SER:HB3	16:S:99:ARG:HA	2.03	0.41
24:1:351:C:H2'	24:1:352:A:C8	2.56	0.41
24:1:813:U:H2'	24:1:814:C:H6	1.84	0.41
24:1:2036:C:H2'	24:1:2037:A:C8	2.55	0.41
24:1:2216:G:H2'	24:1:2217:G:H8	1.85	0.41
24:1:2514:U:H2'	24:1:2515:C:C6	2.55	0.41
25:2:728:A:H2'	25:2:729:A:C8	2.55	0.41
33:e:55:LEU:HD23	33:e:55:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:i:142:VAL:CG2	37:i:181:THR:HG22	2.20	0.41
40:l:16:PRO:HA	42:n:46:MET:SD	2.61	0.41
43:o:65:TYR:HB3	47:s:96:LEU:HG	2.02	0.41
48:t:71:LYS:O	48:t:75:VAL:HG22	2.20	0.41
8:K:7:MET:HE1	8:K:44:LYS:HG3	2.02	0.41
24:1:2229:U:H2'	24:1:2230:G:C8	2.52	0.41
35:g:27:MET:HE3	35:g:27:MET:HB3	1.85	0.41
36:h:134:MET:HE2	36:h:134:MET:HB3	1.84	0.41
4:E:47:LYS:HE2	4:E:47:LYS:HB2	1.90	0.41
18:U:43:LYS:NZ	24:1:499:U:H5''	2.35	0.41
24:1:596:U:H2'	24:1:597:G:C8	2.56	0.41
24:1:924:G:H2'	24:1:925:A:H8	1.86	0.41
24:1:2087:G:H2'	24:1:2088:A:C8	2.56	0.41
25:2:398:U:H2'	25:2:399:G:H8	1.86	0.41
43:o:71:LEU:HD23	43:o:71:LEU:HA	1.93	0.41
45:q:51:LYS:HA	45:q:51:LYS:HD3	1.95	0.41
47:s:25:ALA:HA	47:s:28:LYS:HD3	2.01	0.41
47:s:31:ILE:HD12	47:s:45:VAL:HG12	2.02	0.41
4:E:78:LYS:HA	4:E:78:LYS:HD3	1.80	0.41
6:G:84:ALA:HA	6:G:90:LEU:HA	2.03	0.41
24:1:296:U:H2'	24:1:297:G:C8	2.55	0.41
24:1:832:U:H2'	24:1:833:A:C8	2.56	0.41
24:1:1443:U:H2'	24:1:1444:G:C8	2.56	0.41
24:1:1709:U:H2'	24:1:1710:G:C8	2.55	0.41
24:1:2189:U:H2'	24:1:2190:G:C8	2.56	0.41
25:2:320:A:H2'	25:2:321:A:C8	2.56	0.41
26:3:111:U:H2'	26:3:112:G:C8	2.55	0.41
47:s:98:LYS:HE2	47:s:98:LYS:HB3	1.95	0.41
50:v:55:ILE:HD12	50:v:55:ILE:HA	1.96	0.41
1:B:36:LYS:HB3	24:1:1570:A:H5'	2.03	0.41
3:D:148:ILE:HB	3:D:169:VAL:HA	2.03	0.41
4:E:44:ILE:HG21	4:E:79:ILE:HG22	2.02	0.41
4:E:117:LEU:HB2	4:E:177:PHE:HA	2.03	0.41
8:K:2:ILE:HD13	8:K:2:ILE:HA	1.90	0.41
20:W:20:ARG:HG3	24:1:2356:U:H4'	2.02	0.41
24:1:161:A:H3'	24:1:162:U:H5''	2.03	0.41
24:1:191:A:H2'	24:1:192:C:H6	1.85	0.41
24:1:197:A:H62	24:1:2430:A:H2'	1.86	0.41
24:1:290:U:H2'	24:1:291:G:C8	2.56	0.41
24:1:639:U:H2'	24:1:640:C:H6	1.85	0.41
24:1:2037:A:H2'	24:1:2038:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:2591:C:H2'	24:1:2592:G:H8	1.86	0.41
25:2:255:G:H4'	50:v:19:LYS:HE2	2.02	0.41
25:2:505:G:H2'	25:2:506:G:C8	2.55	0.41
25:2:825:A:H2	41:m:12:THR:HG21	1.85	0.41
25:2:1108:G:H5'	36:h:176:HIS:ND1	2.35	0.41
25:2:1425:U:H2'	25:2:1426:G:H8	1.85	0.41
25:2:1518:MA6:OP2	25:2:1518:MA6:H8	2.20	0.41
35:g:6:MET:HE1	35:g:47:VAL:HG21	2.02	0.41
37:i:121:LYS:HD2	37:i:131:ASN:HD21	1.86	0.41
47:s:64:CYS:HB2	47:s:80:SER:HB3	2.03	0.41
4:E:74:VAL:HG12	4:E:76:GLY:H	1.86	0.41
24:1:171:U:H2'	24:1:172:A:C8	2.55	0.41
24:1:296:U:H2'	24:1:297:G:H8	1.86	0.41
24:1:1808:A:H3'	24:1:1809:A:C8	2.56	0.41
25:2:490:C:H2'	25:2:491:G:H8	1.86	0.41
25:2:908:A:H2'	25:2:909:A:C8	2.54	0.41
25:2:1298:U:H5	40:l:114:LYS:HA	1.85	0.41
25:2:1342:C:H2'	25:2:1343:G:H8	1.86	0.41
25:2:1350:A:P	42:n:123:ARG:HD2	2.61	0.41
35:g:188:ASP:H	35:g:191:SER:HB2	1.85	0.41
36:h:147:LYS:HB2	36:h:203:PHE:CD1	2.56	0.41
42:n:35:LEU:HD11	42:n:45:ARG:HG2	2.02	0.41
5:F:105:LEU:HB2	5:F:113:VAL:HB	2.03	0.40
8:K:76:VAL:H	13:P:73:VAL:HG23	1.86	0.40
11:N:4:ARG:HA	11:N:4:ARG:HD3	1.88	0.40
24:1:18:U:H2'	24:1:19:A:H8	1.86	0.40
24:1:1548:A:H2'	24:1:1549:A:C8	2.56	0.40
24:1:2813:A:H2'	24:1:2814:A:H8	1.86	0.40
1:B:116:ILE:HD13	1:B:116:ILE:HA	1.93	0.40
13:P:5:ILE:HD13	13:P:5:ILE:HA	1.81	0.40
14:Q:106:PHE:HA	14:Q:109:LEU:HB2	2.03	0.40
18:U:46:GLN:HE22	18:U:54:GLN:HG2	1.85	0.40
24:1:1265:A:H3'	30:b:16:ARG:HH22	1.85	0.40
24:1:1710:G:H2'	24:1:1711:A:C8	2.56	0.40
24:1:1915:U:H3'	24:1:1916:A:H8	1.86	0.40
25:2:694:A:H5''	44:p:55:SER:HB3	2.02	0.40
25:2:1314:C:H2'	25:2:1315:U:C6	2.57	0.40
36:h:7:PRO:HD2	36:h:184:TYR:CD2	2.57	0.40
43:o:11:LYS:HE2	43:o:71:LEU:CD1	2.51	0.40
4:E:26:MET:HE1	4:E:30:ARG:HH12	1.86	0.40
10:M:41:LEU:HD21	10:M:126:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:68:LYS:HE3	26:3:49:C:H5''	2.02	0.40
24:1:290:U:H2'	24:1:291:G:H8	1.87	0.40
24:1:558:U:H2'	24:1:559:G:H8	1.86	0.40
24:1:813:U:H2'	24:1:814:C:C6	2.56	0.40
24:1:2636:C:H2'	24:1:2637:U:H6	1.86	0.40
25:2:41:G:H2'	25:2:42:G:C8	2.57	0.40
25:2:490:C:H2'	25:2:491:G:C8	2.57	0.40
25:2:884:U:H4'	25:2:885:G:H5''	2.04	0.40
25:2:1346:A:H61	25:2:1374:A:H5''	1.86	0.40
35:g:69:PHE:HD1	35:g:90:PHE:O	2.05	0.40
38:j:76:LEU:HD12	38:j:76:LEU:HA	1.93	0.40
38:j:115:LEU:O	38:j:120:VAL:HG22	2.21	0.40
24:1:1590:A:H2'	24:1:1591:A:H8	1.86	0.40
24:1:2328:A:H2'	24:1:2329:U:C6	2.56	0.40
24:1:2572:A:H5''	24:1:2574:G:H4'	2.03	0.40
25:2:859:G:H2'	25:2:860:A:H8	1.87	0.40
36:h:147:LYS:HB2	36:h:203:PHE:HD1	1.86	0.40
37:i:177:LYS:HE3	37:i:177:LYS:HB2	1.79	0.40
52:x:63:THR:HG23	52:x:66:MET:HE3	2.02	0.40
13:P:88:ARG:HH12	13:P:112:GLU:HB2	1.87	0.40
24:1:151:C:H2'	24:1:152:A:C8	2.56	0.40
24:1:1114:C:H2'	24:1:1115:G:C8	2.56	0.40
24:1:2543:G:H2'	24:1:2544:G:C8	2.57	0.40
32:d:43:THR:HG21	32:d:45:SER:OG	2.21	0.40
33:e:19:LYS:HE3	33:e:19:LYS:HB2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	269/273 (98%)	260 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
3	D	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
4	E	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
5	F	173/177 (98%)	167 (96%)	6 (4%)	0	100	100
6	G	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
7	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
8	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
9	L	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
10	M	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
11	N	117/127 (92%)	111 (95%)	6 (5%)	0	100	100
12	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
13	P	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
14	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
15	R	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
16	S	108/110 (98%)	108 (100%)	0	0	100	100
17	T	92/100 (92%)	88 (96%)	4 (4%)	0	100	100
18	U	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
19	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
20	W	73/84 (87%)	71 (97%)	2 (3%)	0	100	100
21	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
22	Y	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
23	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
29	a	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
30	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
31	c	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	44 (100%)	0	0	100	100
33	e	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7	29
34	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
35	g	223/241 (92%)	203 (91%)	20 (9%)	0	100	100
36	h	206/233 (88%)	196 (95%)	10 (5%)	0	100	100
37	i	203/206 (98%)	199 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
39	k	102/135 (76%)	97 (95%)	5 (5%)	0	100	100
40	l	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
41	m	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
42	n	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
43	o	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
44	p	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
45	q	120/124 (97%)	109 (91%)	10 (8%)	1 (1%)	16	44
46	r	114/118 (97%)	112 (98%)	1 (1%)	1 (1%)	14	42
47	s	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
48	t	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
49	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
50	v	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
51	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
52	x	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
53	y	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
54	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5607/5912 (95%)	5349 (95%)	255 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	r	66	GLU
45	q	102	LEU
33	e	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/218 (99%)	215 (100%)	1 (0%)	81	81
2	C	164/164 (100%)	162 (99%)	2 (1%)	63	72
3	D	165/165 (100%)	162 (98%)	3 (2%)	51	67
4	E	148/150 (99%)	146 (99%)	2 (1%)	59	70
5	F	136/138 (99%)	132 (97%)	4 (3%)	37	60
6	G	114/114 (100%)	114 (100%)	0	100	100
7	J	116/116 (100%)	114 (98%)	2 (2%)	53	67
8	K	104/104 (100%)	103 (99%)	1 (1%)	68	75
9	L	103/103 (100%)	100 (97%)	3 (3%)	37	60
10	M	109/109 (100%)	108 (99%)	1 (1%)	70	76
11	N	99/103 (96%)	97 (98%)	2 (2%)	48	65
12	O	86/87 (99%)	84 (98%)	2 (2%)	44	63
13	P	99/100 (99%)	94 (95%)	5 (5%)	21	48
14	Q	89/90 (99%)	88 (99%)	1 (1%)	65	74
15	R	84/84 (100%)	84 (100%)	0	100	100
16	S	93/93 (100%)	92 (99%)	1 (1%)	65	74
17	T	81/84 (96%)	81 (100%)	0	100	100
18	U	84/85 (99%)	83 (99%)	1 (1%)	63	72
19	V	78/78 (100%)	76 (97%)	2 (3%)	40	61
20	W	57/62 (92%)	56 (98%)	1 (2%)	51	67
21	X	67/68 (98%)	67 (100%)	0	100	100
22	Y	54/55 (98%)	53 (98%)	1 (2%)	50	66
23	Z	48/49 (98%)	47 (98%)	1 (2%)	47	64
29	a	59/62 (95%)	58 (98%)	1 (2%)	53	67
30	b	47/48 (98%)	46 (98%)	1 (2%)	47	64
31	c	47/49 (96%)	46 (98%)	1 (2%)	47	64
32	d	38/38 (100%)	38 (100%)	0	100	100
33	e	51/52 (98%)	51 (100%)	0	100	100
34	f	34/34 (100%)	33 (97%)	1 (3%)	37	60
35	g	187/199 (94%)	185 (99%)	2 (1%)	65	74
36	h	171/190 (90%)	165 (96%)	6 (4%)	32	56
37	i	172/173 (99%)	168 (98%)	4 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	119/126 (94%)	117 (98%)	2 (2%)	53	67
39	k	91/116 (78%)	88 (97%)	3 (3%)	33	57
40	l	124/147 (84%)	122 (98%)	2 (2%)	55	68
41	m	104/105 (99%)	102 (98%)	2 (2%)	50	66
42	n	105/107 (98%)	104 (99%)	1 (1%)	68	75
43	o	86/90 (96%)	84 (98%)	2 (2%)	44	63
44	p	90/99 (91%)	90 (100%)	0	100	100
45	q	102/103 (99%)	97 (95%)	5 (5%)	22	49
46	r	94/96 (98%)	91 (97%)	3 (3%)	34	58
47	s	83/84 (99%)	83 (100%)	0	100	100
48	t	76/77 (99%)	74 (97%)	2 (3%)	40	61
49	u	65/65 (100%)	65 (100%)	0	100	100
50	v	74/78 (95%)	73 (99%)	1 (1%)	59	70
51	w	57/65 (88%)	56 (98%)	1 (2%)	51	67
52	x	72/79 (91%)	69 (96%)	3 (4%)	26	52
53	y	65/66 (98%)	64 (98%)	1 (2%)	57	69
54	z	60/61 (98%)	60 (100%)	0	100	100
All	All	4667/4828 (97%)	4587 (98%)	80 (2%)	52	67

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	201	MET
2	C	128	ARG
2	C	187	LEU
3	D	43	THR
3	D	52	VAL
3	D	146	VAL
4	E	103	LEU
4	E	155	THR
5	F	79	VAL
5	F	107	LEU
5	F	121	ILE
5	F	168	VAL
7	J	43	GLU
7	J	114	LEU

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Mol	Chain	Res	Type
8	K	62	VAL
9	L	85	VAL
9	L	89	VAL
9	L	99	ASN
10	M	17	ASN
11	N	18	GLN
11	N	113	ILE
12	O	67	ASN
12	O	100	HIS
13	P	5	ILE
13	P	8	LEU
13	P	15	GLN
13	P	52	ASN
13	P	110	ILE
14	Q	4	VAL
16	S	74	ILE
18	U	97	LYS
19	V	5	ASN
19	V	88	HIS
20	W	67	VAL
22	Y	54	LYS
23	Z	27	LEU
29	a	9	TYR
30	b	10	ARG
31	c	46	HIS
34	f	9	LYS
35	g	89	GLN
35	g	183	VAL
36	h	52	VAL
36	h	56	VAL
36	h	121	THR
36	h	149	ILE
36	h	182	ILE
36	h	188	GLU
37	i	41	HIS
37	i	100	ASN
37	i	169	THR
37	i	178	MET
38	j	135	ASN
38	j	144	LEU
39	k	14	GLN
39	k	61	LEU

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Mol	Chain	Res	Type
39	k	74	LEU
40	l	85	TYR
40	l	135	VAL
41	m	89	LYS
41	m	106	THR
42	n	35	LEU
43	o	6	ILE
43	o	102	LEU
45	q	5	ASN
45	q	16	VAL
45	q	73	ASN
45	q	102	LEU
45	q	103	ASP
46	r	65	VAL
46	r	76	SER
46	r	89	LEU
48	t	17	ARG
48	t	26	GLU
50	v	17	MET
51	w	71	THR
52	x	16	LEU
52	x	43	ASN
52	x	60	VAL
53	y	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	70	ASN
1	B	117	GLN
1	B	134	ASN
1	B	197	ASN
1	B	251	GLN
5	F	64	GLN
5	F	116	GLN
6	G	18	GLN
8	K	89	ASN
10	M	97	GLN
12	O	38	GLN
12	O	67	ASN
14	Q	71	GLN
15	R	12	HIS

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Mol	Chain	Res	Type
16	S	15	GLN
17	T	72	GLN
20	W	50	ASN
29	a	20	ASN
35	g	122	GLN
35	g	203	ASN
36	h	185	ASN
37	i	59	GLN
37	i	74	ASN
37	i	131	ASN
38	j	135	ASN
38	j	146	ASN
39	k	63	ASN
39	k	68	GLN
42	n	5	GLN
42	n	25	ASN
43	o	58	ASN
44	p	38	GLN
45	q	5	ASN
49	u	9	HIS
53	y	21	ASN
53	y	84	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	1	2817/2904 (97%)	542 (19%)	14 (0%)
25	2	1532/1540 (99%)	291 (18%)	10 (0%)
26	3	119/120 (99%)	29 (24%)	0
27	4	6/18 (33%)	1 (16%)	0
28	5	76/77 (98%)	27 (35%)	2 (2%)
All	All	4550/4659 (97%)	890 (19%)	26 (0%)

All (890) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	1	10	A
24	1	15	G
24	1	27	G
24	1	34	U
24	1	35	G

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Mol	Chain	Res	Type
24	1	36	G
24	1	46	G
24	1	50	U
24	1	51	G
24	1	52	A
24	1	62	U
24	1	63	A
24	1	71	A
24	1	72	U
24	1	74	A
24	1	75	G
24	1	84	A
24	1	98	G
24	1	118	A
24	1	119	A
24	1	120	U
24	1	125	A
24	1	139	U
24	1	140	C
24	1	141	G
24	1	142	A
24	1	155	A
24	1	162	U
24	1	163	C
24	1	181	A
24	1	196	A
24	1	199	A
24	1	215	G
24	1	216	A
24	1	219	A
24	1	221	A
24	1	222	A
24	1	225	C
24	1	229	C
24	1	233	A
24	1	241	A
24	1	242	G
24	1	243	U
24	1	248	G
24	1	255	A
24	1	261	G
24	1	265	A

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Mol	Chain	Res	Type
24	1	267	C
24	1	276	U
24	1	278	A
24	1	279	A
24	1	281	C
24	1	285	G
24	1	300	A
24	1	311	A
24	1	323	C
24	1	329	G
24	1	330	A
24	1	334	C
24	1	335	C
24	1	338	G
24	1	345	A
24	1	350	G
24	1	353	C
24	1	361	G
24	1	362	A
24	1	367	G
24	1	371	A
24	1	372	G
24	1	386	G
24	1	387	U
24	1	388	G
24	1	395	U
24	1	396	G
24	1	403	U
24	1	404	A
24	1	406	G
24	1	411	G
24	1	412	A
24	1	417	C
24	1	421	C
24	1	424	G
24	1	435	C
24	1	448	U
24	1	451	U
24	1	454	A
24	1	458	G
24	1	467	G
24	1	471	A

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Mol	Chain	Res	Type
24	1	481	G
24	1	489	G
24	1	491	G
24	1	496	G
24	1	505	A
24	1	508	A
24	1	509	C
24	1	526	A
24	1	529	A
24	1	530	G
24	1	531	C
24	1	532	A
24	1	543	G
24	1	545	U
24	1	546	U
24	1	547	A
24	1	548	G
24	1	550	C
24	1	563	A
24	1	572	A
24	1	573	U
24	1	575	A
24	1	603	A
24	1	614	A
24	1	615	U
24	1	616	A
24	1	622	G
24	1	627	A
24	1	634	C
24	1	637	A
24	1	645	C
24	1	646	U
24	1	654	A
24	1	655	A
24	1	659	G
24	1	664	G
24	1	669	G
24	1	670	A
24	1	677	A
24	1	686	U
24	1	694	U
24	1	695	G

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Mol	Chain	Res	Type
24	1	696	G
24	1	704	G
24	1	711	G
24	1	717	C
24	1	726	G
24	1	730	A
24	1	738	G
24	1	747	C
24	1	757	G
24	1	765	C
24	1	772	C
24	1	774	G
24	1	775	G
24	1	776	G
24	1	782	A
24	1	783	A
24	1	784	G
24	1	785	G
24	1	791	C
24	1	800	A
24	1	805	G
24	1	812	C
24	1	819	A
24	1	827	U
24	1	828	U
24	1	831	G
24	1	845	A
24	1	846	U
24	1	847	U
24	1	856	G
24	1	858	G
24	1	859	G
24	1	869	G
24	1	878	A
24	1	879	G
24	1	885	C
24	1	886	A
24	1	896	A
24	1	897	C
24	1	907	G
24	1	910	A
24	1	931	U

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Mol	Chain	Res	Type
24	1	941	A
24	1	946	C
24	1	961	C
24	1	973	A
24	1	974	G
24	1	983	A
24	1	995	C
24	1	996	A
24	1	997	G
24	1	999	U
24	1	1005	C
24	1	1009	A
24	1	1012	U
24	1	1013	C
24	1	1021	A
24	1	1023	U
24	1	1026	G
24	1	1033	U
24	1	1041	G
24	1	1045	C
24	1	1046	A
24	1	1047	G
24	1	1052	C
24	1	1054	A
24	1	1057	A
24	1	1059	G
24	1	1060	U
24	1	1061	U
24	1	1062	G
24	1	1063	G
24	1	1064	C
24	1	1065	U
24	1	1066	U
24	1	1067	A
24	1	1070	A
24	1	1071	G
24	1	1072	C
24	1	1073	A
24	1	1076	C
24	1	1078	U
24	1	1079	C
24	1	1084	A

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Mol	Chain	Res	Type
24	1	1085	A
24	1	1087	G
24	1	1088	A
24	1	1089	A
24	1	1090	A
24	1	1094	U
24	1	1097	U
24	1	1098	A
24	1	1099	G
24	1	1102	C
24	1	1103	A
24	1	1104	C
24	1	1106	G
24	1	1111	A
24	1	1112	G
24	1	1130	U
24	1	1131	G
24	1	1132	U
24	1	1133	A
24	1	1135	C
24	1	1139	G
24	1	1142	A
24	1	1175	A
24	1	1176	U
24	1	1180	U
24	1	1181	U
24	1	1204	A
24	1	1205	A
24	1	1206	G
24	1	1211	C
24	1	1212	G
24	1	1238	G
24	1	1245	G
24	1	1247	A
24	1	1248	G
24	1	1252	G
24	1	1253	A
24	1	1256	G
24	1	1265	A
24	1	1268	A
24	1	1271	G
24	1	1272	A

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Mol	Chain	Res	Type
24	1	1275	A
24	1	1300	G
24	1	1301	A
24	1	1306	C
24	1	1312	U
24	1	1321	A
24	1	1329	U
24	1	1330	C
24	1	1341	G
24	1	1345	C
24	1	1352	U
24	1	1359	A
24	1	1365	A
24	1	1368	G
24	1	1378	A
24	1	1379	U
24	1	1383	A
24	1	1396	U
24	1	1397	U
24	1	1408	G
24	1	1416	G
24	1	1428	C
24	1	1434	A
24	1	1437	C
24	1	1452	G
24	1	1453	A
24	1	1461	C
24	1	1475	G
24	1	1482	G
24	1	1490	A
24	1	1491	G
24	1	1494	A
24	1	1497	U
24	1	1504	A
24	1	1508	A
24	1	1509	A
24	1	1515	A
24	1	1524	G
24	1	1529	G
24	1	1532	A
24	1	1534	U
24	1	1535	A

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Mol	Chain	Res	Type
24	1	1536	C
24	1	1542	U
24	1	1555	G
24	1	1558	C
24	1	1559	U
24	1	1560	G
24	1	1565	C
24	1	1569	A
24	1	1578	U
24	1	1583	A
24	1	1584	U
24	1	1585	C
24	1	1608	A
24	1	1611	C
24	1	1646	C
24	1	1647	U
24	1	1648	U
24	1	1651	G
24	1	1654	A
24	1	1672	A
24	1	1674	G
24	1	1694	C
24	1	1695	G
24	1	1698	A
24	1	1699	G
24	1	1713	A
24	1	1715	G
24	1	1729	U
24	1	1730	C
24	1	1732	C
24	1	1733	G
24	1	1738	G
24	1	1756	G
24	1	1758	U
24	1	1759	A
24	1	1764	C
24	1	1773	A
24	1	1776	G
24	1	1780	A
24	1	1782	U
24	1	1787	A
24	1	1800	C

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Mol	Chain	Res	Type
24	1	1801	A
24	1	1802	A
24	1	1808	A
24	1	1816	C
24	1	1829	A
24	1	1833	C
24	1	1847	G
24	1	1866	A
24	1	1869	G
24	1	1870	C
24	1	1871	A
24	1	1873	G
24	1	1884	G
24	1	1896	G
24	1	1901	A
24	1	1906	G
24	1	1913	A
24	1	1914	C
24	1	1915	U
24	1	1927	A
24	1	1929	G
24	1	1930	G
24	1	1931	U
24	1	1937	A
24	1	1938	A
24	1	1940	U
24	1	1941	C
24	1	1944	U
24	1	1955	U
24	1	1964	G
24	1	1966	A
24	1	1967	C
24	1	1970	A
24	1	1971	U
24	1	1972	G
24	1	1991	U
24	1	1992	G
24	1	1997	C
24	1	2004	G
24	1	2020	A
24	1	2022	U
24	1	2023	C

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Mol	Chain	Res	Type
24	1	2030	A
24	1	2031	A
24	1	2033	A
24	1	2043	C
24	1	2052	A
24	1	2055	C
24	1	2056	G
24	1	2060	A
24	1	2061	G
24	1	2062	A
24	1	2069	A
24	1	2072	C
24	1	2093	G
24	1	2094	A
24	1	2095	A
24	1	2096	C
24	1	2097	A
24	1	2101	A
24	1	2103	C
24	1	2104	U
24	1	2105	U
24	1	2187	U
24	1	2188	U
24	1	2189	U
24	1	2190	G
24	1	2191	A
24	1	2193	G
24	1	2198	A
24	1	2199	A
24	1	2204	G
24	1	2211	A
24	1	2212	A
24	1	2213	U
24	1	2214	C
24	1	2219	U
24	1	2223	G
24	1	2225	A
24	1	2226	C
24	1	2238	G
24	1	2239	G
24	1	2250	G
24	1	2251	G

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Mol	Chain	Res	Type
24	1	2266	A
24	1	2279	G
24	1	2283	C
24	1	2287	A
24	1	2288	A
24	1	2305	U
24	1	2309	A
24	1	2325	G
24	1	2327	A
24	1	2332	C
24	1	2334	U
24	1	2336	A
24	1	2345	G
24	1	2350	C
24	1	2357	G
24	1	2361	G
24	1	2372	U
24	1	2382	G
24	1	2383	G
24	1	2385	C
24	1	2392	A
24	1	2402	U
24	1	2403	C
24	1	2406	A
24	1	2422	C
24	1	2424	C
24	1	2427	C
24	1	2428	G
24	1	2429	G
24	1	2430	A
24	1	2435	A
24	1	2440	C
24	1	2441	U
24	1	2445	G
24	1	2447	G
24	1	2448	A
24	1	2449	U
24	1	2469	A
24	1	2474	U
24	1	2476	A
24	1	2481	G
24	1	2484	G

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Mol	Chain	Res	Type
24	1	2491	U
24	1	2492	U
24	1	2498	C
24	1	2502	G
24	1	2503	A
24	1	2504	U
24	1	2505	G
24	1	2506	U
24	1	2507	C
24	1	2518	A
24	1	2520	C
24	1	2529	G
24	1	2547	A
24	1	2554	U
24	1	2566	A
24	1	2567	G
24	1	2572	A
24	1	2573	C
24	1	2582	G
24	1	2585	U
24	1	2586	U
24	1	2602	A
24	1	2604	U
24	1	2609	U
24	1	2610	C
24	1	2613	U
24	1	2614	A
24	1	2615	U
24	1	2629	U
24	1	2646	C
24	1	2661	G
24	1	2689	U
24	1	2690	U
24	1	2707	U
24	1	2714	G
24	1	2716	C
24	1	2718	G
24	1	2722	G
24	1	2726	A
24	1	2732	G
24	1	2733	A
24	1	2744	G

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Mol	Chain	Res	Type
24	1	2748	A
24	1	2757	A
24	1	2764	A
24	1	2765	A
24	1	2769	U
24	1	2778	A
24	1	2779	U
24	1	2790	U
24	1	2791	G
24	1	2793	C
24	1	2794	C
24	1	2796	U
24	1	2800	A
24	1	2808	G
24	1	2809	A
24	1	2818	U
24	1	2820	A
24	1	2821	A
24	1	2823	A
24	1	2833	U
24	1	2836	U
24	1	2849	U
24	1	2861	U
24	1	2867	G
24	1	2868	A
24	1	2872	A
24	1	2873	A
24	1	2879	A
24	1	2880	C
24	1	2883	A
24	1	2887	A
24	1	2893	A
24	1	2899	A
25	2	2	A
25	2	3	A
25	2	4	U
25	2	9	G
25	2	22	G
25	2	39	G
25	2	47	C
25	2	48	C
25	2	49	U

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Mol	Chain	Res	Type
25	2	51	A
25	2	69	G
25	2	70	U
25	2	72	A
25	2	73	C
25	2	74	A
25	2	83	C
25	2	84	U
25	2	85	U
25	2	86	G
25	2	87	C
25	2	88	U
25	2	89	U
25	2	95	C
25	2	108	G
25	2	117	G
25	2	120	A
25	2	121	U
25	2	128	G
25	2	129	A
25	2	130	A
25	2	131	A
25	2	141	G
25	2	144	G
25	2	163	C
25	2	174	A
25	2	177	G
25	2	182	A
25	2	197	A
25	2	202	G
25	2	204	G
25	2	208	U
25	2	209	U
25	2	211	G
25	2	212	G
25	2	226	G
25	2	231	U
25	2	240	G
25	2	245	U
25	2	247	G
25	2	251	G
25	2	262	A

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Mol	Chain	Res	Type
25	2	266	G
25	2	267	C
25	2	279	A
25	2	281	G
25	2	289	G
25	2	306	A
25	2	321	A
25	2	328	C
25	2	330	C
25	2	332	G
25	2	345	C
25	2	347	G
25	2	351	G
25	2	352	C
25	2	354	G
25	2	367	U
25	2	372	C
25	2	373	A
25	2	384	G
25	2	388	G
25	2	390	U
25	2	392	C
25	2	393	A
25	2	406	G
25	2	411	A
25	2	412	A
25	2	413	G
25	2	414	A
25	2	421	U
25	2	422	C
25	2	423	G
25	2	424	G
25	2	428	G
25	2	429	U
25	2	431	A
25	2	452	A
25	2	457	G
25	2	463	U
25	2	464	U
25	2	465	A
25	2	467	U
25	2	468	A

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Mol	Chain	Res	Type
25	2	478	A
25	2	479	U
25	2	481	G
25	2	482	A
25	2	484	G
25	2	486	U
25	2	495	A
25	2	496	A
25	2	497	G
25	2	499	A
25	2	500	G
25	2	509	A
25	2	511	C
25	2	517	G
25	2	518	C
25	2	519	C
25	2	521	G
25	2	524	G
25	2	527	G7M
25	2	532	A
25	2	533	A
25	2	534	U
25	2	547	A
25	2	559	A
25	2	568	G
25	2	572	A
25	2	573	A
25	2	576	C
25	2	577	G
25	2	596	A
25	2	607	A
25	2	633	G
25	2	639	G
25	2	642	A
25	2	650	G
25	2	653	U
25	2	665	A
25	2	687	A
25	2	700	G
25	2	703	G
25	2	721	G
25	2	723	U

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Mol	Chain	Res	Type
25	2	731	G
25	2	747	A
25	2	748	G
25	2	755	G
25	2	790	A
25	2	792	A
25	2	793	U
25	2	794	A
25	2	814	A
25	2	815	A
25	2	817	C
25	2	821	G
25	2	828	U
25	2	829	G
25	2	841	C
25	2	843	U
25	2	844	G
25	2	846	G
25	2	876	C
25	2	889	A
25	2	914	A
25	2	926	G
25	2	934	C
25	2	935	A
25	2	960	U
25	2	966	2MG
25	2	967	5MC
25	2	968	A
25	2	969	A
25	2	971	G
25	2	974	A
25	2	975	A
25	2	976	G
25	2	977	A
25	2	981	U
25	2	989	U
25	2	992	U
25	2	993	G
25	2	996	A
25	2	1004	A
25	2	1009	U
25	2	1017	U

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Mol	Chain	Res	Type
25	2	1018	G
25	2	1021	A
25	2	1025	U
25	2	1026	G
25	2	1027	C
25	2	1028	C
25	2	1029	U
25	2	1030	U
25	2	1031	C
25	2	1034	G
25	2	1035	A
25	2	1036	A
25	2	1037	C
25	2	1043	G
25	2	1044	A
25	2	1056	U
25	2	1064	G
25	2	1065	U
25	2	1094	G
25	2	1095	U
25	2	1101	A
25	2	1108	G
25	2	1124	G
25	2	1126	U
25	2	1130	A
25	2	1135	U
25	2	1136	C
25	2	1137	C
25	2	1139	G
25	2	1140	C
25	2	1141	C
25	2	1150	A
25	2	1158	C
25	2	1159	U
25	2	1167	A
25	2	1168	U
25	2	1169	A
25	2	1174	G
25	2	1175	G
25	2	1176	A
25	2	1184	G
25	2	1196	A

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Mol	Chain	Res	Type
25	2	1197	A
25	2	1207	2MG
25	2	1208	C
25	2	1213	A
25	2	1214	C
25	2	1224	U
25	2	1227	A
25	2	1228	C
25	2	1236	A
25	2	1238	A
25	2	1239	A
25	2	1241	G
25	2	1256	A
25	2	1257	A
25	2	1258	G
25	2	1261	A
25	2	1268	G
25	2	1275	A
25	2	1279	G
25	2	1280	A
25	2	1281	C
25	2	1285	A
25	2	1286	U
25	2	1287	A
25	2	1297	G
25	2	1299	A
25	2	1300	G
25	2	1302	C
25	2	1305	G
25	2	1317	C
25	2	1320	C
25	2	1322	C
25	2	1323	G
25	2	1336	C
25	2	1338	G
25	2	1340	A
25	2	1346	A
25	2	1353	G
25	2	1363	A
25	2	1370	G
25	2	1378	C
25	2	1379	G

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Mol	Chain	Res	Type
25	2	1381	U
25	2	1384	C
25	2	1398	A
25	2	1404	C
25	2	1407	5MC
25	2	1408	A
25	2	1419	G
25	2	1422	G
25	2	1429	A
25	2	1432	G
25	2	1440	U
25	2	1441	A
25	2	1446	A
25	2	1452	C
25	2	1453	G
25	2	1487	G
25	2	1493	A
25	2	1494	G
25	2	1497	G
25	2	1499	A
25	2	1503	A
25	2	1506	U
25	2	1516	2MG
25	2	1517	G
25	2	1518	MA6
25	2	1519	MA6
25	2	1529	G
25	2	1530	G
25	2	1533	C
25	2	1534	A
26	3	2	G
26	3	9	G
26	3	13	G
26	3	15	A
26	3	16	G
26	3	24	G
26	3	31	C
26	3	35	C
26	3	37	C
26	3	56	G
26	3	57	A
26	3	67	G

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Mol	Chain	Res	Type
26	3	73	A
26	3	74	U
26	3	76	G
26	3	77	U
26	3	78	A
26	3	79	G
26	3	88	C
26	3	89	U
26	3	90	C
26	3	100	G
26	3	105	G
26	3	108	A
26	3	109	A
26	3	116	G
26	3	117	G
26	3	118	C
26	3	119	A
27	4	15	C
28	5	2	G
28	5	3	G
28	5	4	C
28	5	5	A
28	5	6	C
28	5	8	U
28	5	10	G
28	5	14	A
28	5	15	G
28	5	16	C
28	5	17	C
28	5	18	G
28	5	20	U
28	5	21	A
28	5	22	G
28	5	28	C
28	5	40	U
28	5	46	G
28	5	47	U
28	5	48	C
28	5	54	U
28	5	56	C
28	5	60	U
28	5	66	C

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Mol	Chain	Res	Type
28	5	73	A
28	5	74	C
28	5	76	A

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	1	51	G
24	1	242	G
24	1	1020	A
24	1	1022	G
24	1	1070	A
24	1	1111	A
24	1	1930	G
24	1	1940	U
24	1	2190	G
24	1	2286	G
24	1	2326	C
24	1	2391	G
24	1	2756	U
24	1	2808	G
25	2	428	G
25	2	496	A
25	2	516	PSU
25	2	966	2MG
25	2	967	5MC
25	2	1109	C
25	2	1207	2MG
25	2	1383	C
25	2	1407	5MC
25	2	1516	2MG
28	5	2	G
28	5	72	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MC	2	967	25	19,22,23	3.92	8 (42%)	26,32,35	2.38	10 (38%)
25	4OC	2	1402	25	20,23,24	3.45	8 (40%)	25,32,35	1.26	3 (12%)
25	UR3	2	1498	25	19,22,23	2.71	8 (42%)	26,32,35	1.58	3 (11%)
25	MA6	2	1519	25	23,26,27	1.37	3 (13%)	33,38,41	3.21	13 (39%)
25	2MG	2	966	25	23,26,27	2.99	7 (30%)	33,38,41	3.70	22 (66%)
45	0TD	q	89	45	8,9,10	1.56	1 (12%)	6,11,13	1.65	2 (33%)
25	MA6	2	1518	25	23,26,27	1.37	4 (17%)	33,38,41	3.11	12 (36%)
25	2MG	2	1207	25	23,26,27	2.92	8 (34%)	33,38,41	3.45	21 (63%)
25	2MG	2	1516	25	23,26,27	2.91	8 (34%)	33,38,41	3.57	21 (63%)
25	5MC	2	1407	25	19,22,23	3.80	8 (42%)	26,32,35	2.38	12 (46%)
25	PSU	2	516	25	18,21,22	1.05	1 (5%)	21,30,33	1.79	4 (19%)
25	G7M	2	527	25	23,26,27	2.74	7 (30%)	34,39,42	2.26	10 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5MC	2	967	25	2/2/5/5	2/7/25/26	0/2/2/2
25	4OC	2	1402	25	-	1/9/29/30	0/2/2/2
25	UR3	2	1498	25	-	0/7/25/26	0/2/2/2
25	MA6	2	1519	25	-	3/11/29/30	0/3/3/3
25	2MG	2	966	25	2/2/5/6	3/9/27/28	0/3/3/3
45	0TD	q	89	45	-	2/7/12/14	-
25	MA6	2	1518	25	-	4/11/29/30	0/3/3/3
25	2MG	2	1207	25	2/2/5/6	2/9/27/28	0/3/3/3
25	2MG	2	1516	25	2/2/5/6	2/9/27/28	0/3/3/3
25	5MC	2	1407	25	2/2/5/5	3/7/25/26	0/2/2/2
25	PSU	2	516	25	-	3/7/25/26	0/2/2/2
25	G7M	2	527	25	-	3/7/25/26	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	967	5MC	C6-C5	9.09	1.49	1.34
25	2	1407	5MC	C6-C5	8.68	1.48	1.34
25	2	966	2MG	C4-N3	8.58	1.53	1.34
25	2	1207	2MG	C4-N3	8.37	1.53	1.34
25	2	1516	2MG	C4-N3	8.28	1.53	1.34
25	2	527	G7M	C4-N3	7.87	1.52	1.34
25	2	967	5MC	C5-C4	7.08	1.49	1.44
25	2	966	2MG	C2-N3	6.96	1.45	1.32
25	2	1498	UR3	C2-N1	6.93	1.48	1.38
25	2	1407	5MC	C4-N3	6.87	1.45	1.34
25	2	967	5MC	C4-N3	6.83	1.45	1.34
25	2	1207	2MG	C2-N3	6.71	1.44	1.32
25	2	1516	2MG	C2-N3	6.68	1.44	1.32
25	2	1402	4OC	C6-C5	6.58	1.50	1.35
25	2	1402	4OC	C2-N3	6.52	1.49	1.36
25	2	1407	5MC	C5-C4	6.48	1.49	1.44
25	2	1402	4OC	C4-N3	6.48	1.43	1.32
25	2	967	5MC	C2-N3	6.34	1.48	1.36
25	2	1402	4OC	C4-N4	6.31	1.49	1.36
25	2	1407	5MC	C2-N3	6.30	1.48	1.36
25	2	1498	UR3	C6-C5	6.14	1.49	1.35
25	2	527	G7M	C2-N3	5.27	1.46	1.33
25	2	1402	4OC	O2-C2	-5.20	1.14	1.23
25	2	966	2MG	C6-N1	5.05	1.48	1.38
25	2	1516	2MG	C6-N1	4.93	1.48	1.38
25	2	1207	2MG	C6-N1	4.91	1.48	1.38
25	2	1498	UR3	C2-N3	4.88	1.48	1.39
25	2	527	G7M	C5-C6	4.69	1.56	1.43
25	2	967	5MC	C6-N1	4.57	1.45	1.38
25	2	967	5MC	C4-N4	4.53	1.45	1.34
25	2	1407	5MC	C4-N4	4.50	1.45	1.34
25	2	966	2MG	C2-N2	4.43	1.42	1.33
25	2	527	G7M	C5-N7	-4.41	1.34	1.39
25	2	1207	2MG	C2-N2	4.40	1.42	1.33
25	2	1516	2MG	C2-N2	4.38	1.42	1.33
25	2	1407	5MC	C6-N1	4.38	1.45	1.38
25	2	967	5MC	C2-N1	4.32	1.49	1.40
25	2	1407	5MC	C2-N1	4.27	1.49	1.40
25	2	1402	4OC	C5-C4	4.02	1.49	1.41
25	2	1402	4OC	C2-N1	4.01	1.48	1.40
25	2	1518	MA6	C6-N6	3.85	1.47	1.36
25	2	1519	MA6	C6-N6	3.80	1.47	1.36
25	2	516	PSU	C6-C5	3.62	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	966	2MG	C2-N1	3.39	1.42	1.36
25	2	1207	2MG	C2-N1	3.37	1.42	1.36
25	2	1516	2MG	C2-N1	3.34	1.42	1.36
25	2	527	G7M	C2-N2	3.16	1.41	1.34
25	2	1402	4OC	C6-N1	3.04	1.45	1.38
25	2	527	G7M	O6-C6	-3.01	1.17	1.23
25	2	527	G7M	C2-N1	2.97	1.44	1.37
25	2	1498	UR3	C6-N1	2.85	1.44	1.38
25	2	1407	5MC	O2-C2	-2.80	1.18	1.23
25	2	967	5MC	O2-C2	-2.72	1.18	1.23
25	2	1516	2MG	C5-N7	-2.71	1.33	1.39
25	2	1207	2MG	C5-N7	-2.61	1.33	1.39
25	2	966	2MG	C5-N7	-2.57	1.33	1.39
25	2	1498	UR3	O4-C4	-2.34	1.18	1.23
25	2	1519	MA6	C10-N6	2.26	1.50	1.45
25	2	1518	MA6	C5-C6	-2.23	1.35	1.41
25	2	1498	UR3	O2-C2	-2.22	1.18	1.22
25	2	1498	UR3	C4-N3	2.20	1.45	1.40
25	2	1518	MA6	C10-N6	2.19	1.50	1.45
25	2	1498	UR3	C5-C4	2.18	1.49	1.43
25	2	966	2MG	C4-N9	-2.11	1.32	1.38
25	2	1207	2MG	C4-N9	-2.09	1.32	1.38
25	2	1516	2MG	C4-N9	-2.07	1.32	1.38
25	2	1519	MA6	C5-C6	-2.07	1.36	1.41
45	q	89	0TD	CSB-SB	-2.04	1.75	1.79
25	2	1516	2MG	C5-C6	2.03	1.52	1.44
25	2	1518	MA6	C5-N7	-2.02	1.35	1.39
25	2	1207	2MG	C5-C6	2.00	1.51	1.44

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	1519	MA6	N1-C6-N6	-11.39	102.97	116.86
25	2	1518	MA6	N1-C6-N6	-10.78	103.72	116.86
25	2	966	2MG	C1'-N9-C8	-9.86	98.72	126.73
25	2	1516	2MG	C1'-N9-C8	-9.73	99.08	126.73
25	2	1207	2MG	C1'-N9-C8	-9.45	99.89	126.73
25	2	1516	2MG	C1'-N9-C4	8.50	151.59	126.49
25	2	966	2MG	C1'-N9-C4	8.21	150.74	126.49
25	2	1207	2MG	C1'-N9-C4	8.01	150.13	126.49
25	2	1519	MA6	C5-C6-N6	7.81	137.70	125.33
25	2	1518	MA6	C5-C6-N6	7.41	137.06	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	1516	2MG	C2-N3-C4	6.37	119.97	112.00
25	2	966	2MG	O4'-C1'-N9	6.21	122.42	108.36
25	2	527	G7M	CN7-N7-C5	6.11	134.41	126.80
25	2	966	2MG	C2-N3-C4	6.05	119.57	112.00
25	2	1519	MA6	N1-C2-N3	-5.87	119.70	128.58
25	2	1207	2MG	C2-N3-C4	5.73	119.17	112.00
25	2	1518	MA6	N1-C2-N3	-5.55	120.17	128.58
25	2	1498	UR3	C4-N3-C2	-5.51	120.15	124.58
25	2	1516	2MG	O4'-C1'-N9	5.27	120.31	108.36
25	2	527	G7M	CN7-N7-C8	-5.07	117.11	124.79
25	2	1207	2MG	O4'-C1'-N9	5.00	119.69	108.36
25	2	1518	MA6	C5-C4-N3	-4.77	120.14	126.72
25	2	967	5MC	O4'-C1'-N1	4.74	119.09	108.36
25	2	1519	MA6	C5-C4-N3	-4.72	120.22	126.72
25	2	1516	2MG	C5-C4-N3	-4.54	121.16	128.39
25	2	967	5MC	O3'-C3'-C4'	4.46	123.89	111.08
25	2	966	2MG	C2'-C1'-N9	4.39	125.48	113.25
25	2	516	PSU	N1-C2-N3	4.39	119.80	115.17
25	2	516	PSU	C4-N3-C2	-4.31	120.43	126.37
25	2	966	2MG	C5-C4-N3	-4.31	121.53	128.39
25	2	527	G7M	C2-N3-C4	4.29	119.69	112.30
25	2	1207	2MG	N1-C2-N2	4.28	120.93	116.56
25	2	966	2MG	C2-N1-C6	-4.27	119.39	124.55
25	2	1407	5MC	O4'-C1'-N1	4.25	117.98	108.36
25	2	1518	MA6	C4-C5-C6	4.20	120.25	115.91
25	2	966	2MG	O2'-C2'-C3'	4.18	125.23	111.82
25	2	527	G7M	C5-C6-N1	4.10	120.31	111.84
25	2	1207	2MG	C5-C4-N3	-4.08	121.90	128.39
25	2	1207	2MG	O3'-C3'-C4'	4.05	122.72	111.08
25	2	1519	MA6	N9-C8-N7	-4.05	108.19	113.94
25	2	966	2MG	O3'-C3'-C4'	4.04	122.70	111.08
25	2	967	5MC	C2'-C1'-N1	3.97	124.29	113.25
25	2	1516	2MG	O3'-C3'-C4'	3.96	122.45	111.08
25	2	1516	2MG	N1-C2-N2	3.96	120.60	116.56
25	2	1518	MA6	N9-C8-N7	-3.93	108.36	113.94
25	2	1407	5MC	O3'-C3'-C4'	3.91	122.33	111.08
25	2	527	G7M	C5-C4-N3	-3.91	120.75	128.15
25	2	966	2MG	N9-C8-N7	-3.90	106.17	113.40
25	2	1519	MA6	C4-C5-C6	3.80	119.84	115.91
25	2	1516	2MG	C2-N1-C6	-3.75	120.02	124.55
25	2	1407	5MC	C1'-N1-C6	-3.71	115.04	121.15
25	2	967	5MC	C5'-C4'-C3'	3.70	128.53	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	1407	5MC	O4'-C4'-C5'	3.68	121.12	109.33
25	2	1207	2MG	N9-C8-N7	-3.68	106.58	113.40
25	2	1516	2MG	O4'-C4'-C5'	3.67	121.08	109.33
25	2	1402	4OC	C1'-N1-C6	3.66	128.61	120.78
25	2	1519	MA6	C2-N1-C6	3.65	120.74	111.83
25	2	1207	2MG	O4'-C4'-C5'	3.62	120.93	109.33
25	2	1498	UR3	C5-C4-N3	3.60	119.78	115.04
25	2	966	2MG	N1-C2-N2	3.57	120.20	116.56
25	2	1207	2MG	C5'-C4'-C3'	3.56	128.03	115.21
25	2	967	5MC	O4'-C4'-C5'	3.56	120.74	109.33
25	2	1407	5MC	C2'-C1'-N1	3.56	123.16	113.25
25	2	1407	5MC	C5'-C4'-C3'	3.55	127.98	115.21
25	2	967	5MC	O3'-C3'-C2'	3.54	123.15	111.82
25	2	1518	MA6	C2-N1-C6	3.53	120.45	111.83
25	2	1516	2MG	C5'-C4'-C3'	3.53	127.91	115.21
25	2	1519	MA6	C2-N3-C4	3.42	120.18	111.83
25	2	527	G7M	O6-C6-C5	-3.40	120.42	128.01
25	2	1516	2MG	N9-C8-N7	-3.39	107.12	113.40
25	2	1407	5MC	O3'-C3'-C2'	3.38	122.64	111.82
25	2	1516	2MG	O3'-C3'-C2'	3.37	122.63	111.82
25	2	966	2MG	O4'-C4'-C5'	3.37	120.13	109.33
25	2	967	5MC	O2'-C2'-C3'	3.35	122.56	111.82
25	2	1207	2MG	O3'-C3'-C2'	3.32	122.47	111.82
25	2	1516	2MG	O2'-C2'-C3'	3.31	122.42	111.82
25	2	966	2MG	O2'-C2'-C1'	3.31	121.49	110.10
25	2	527	G7M	C1'-N9-C4	-3.30	116.74	126.49
25	2	1207	2MG	C2-N1-C6	-3.28	120.58	124.55
25	2	1518	MA6	C2-N3-C4	3.24	119.75	111.83
25	2	1207	2MG	O2'-C2'-C3'	3.22	122.14	111.82
25	2	527	G7M	N9-C4-N3	3.20	132.36	125.95
25	2	966	2MG	C5'-C4'-C3'	3.18	126.66	115.21
25	2	967	5MC	O2'-C2'-C1'	3.12	120.84	110.10
25	2	1407	5MC	O2'-C2'-C3'	3.02	121.49	111.82
25	2	966	2MG	C5-C6-N1	3.00	120.88	113.25
25	2	966	2MG	O6-C6-C5	-2.99	118.63	126.53
25	2	1407	5MC	C1'-N1-C2	2.98	125.03	118.44
25	2	967	5MC	C5-C6-N1	-2.97	120.08	123.31
25	2	1407	5MC	O2'-C2'-C1'	2.95	120.25	110.10
25	2	1518	MA6	N3-C4-N9	2.94	132.16	127.17
25	2	527	G7M	C2-N1-C6	-2.93	119.80	125.11
25	2	1207	2MG	O2'-C2'-C1'	2.85	119.93	110.10
25	2	966	2MG	O3'-C3'-C2'	2.82	120.85	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	1519	MA6	C5-N7-C8	2.78	107.82	103.45
25	2	966	2MG	N9-C4-N3	2.76	131.48	125.95
25	2	1516	2MG	O2'-C2'-C1'	2.72	119.46	110.10
25	2	1518	MA6	C5-N7-C8	2.71	107.71	103.45
25	2	1516	2MG	C2'-C1'-N9	2.68	120.70	113.25
25	2	1519	MA6	N3-C4-N9	2.66	131.69	127.17
25	2	1516	2MG	C5-C6-N1	2.66	120.01	113.25
45	q	89	0TD	OD2-CG-CB	2.64	118.86	113.15
25	2	516	PSU	C6-N1-C2	-2.64	120.24	122.69
25	2	1207	2MG	C2'-C1'-N9	2.50	120.20	113.25
25	2	1402	4OC	C1'-N1-C2	-2.49	112.93	118.44
25	2	1516	2MG	O6-C6-C5	-2.47	120.03	126.53
25	2	1207	2MG	C5-C6-N1	2.46	119.51	113.25
25	2	527	G7M	N9-C8-N7	-2.43	106.58	112.48
25	2	1516	2MG	N9-C4-N3	2.38	130.72	125.95
25	2	1207	2MG	O6-C6-C5	-2.38	120.24	126.53
25	2	1407	5MC	C5-C6-N1	-2.37	120.74	123.31
45	q	89	0TD	O-C-CA	-2.37	118.68	124.77
25	2	1516	2MG	N1-C2-N3	-2.37	119.69	123.68
25	2	1516	2MG	CM2-N2-C2	-2.36	118.57	123.65
25	2	1519	MA6	C4-C5-N7	-2.36	107.89	110.58
25	2	1207	2MG	N1-C2-N3	-2.32	119.77	123.68
25	2	966	2MG	C8-N9-C4	2.26	110.27	106.03
25	2	1498	UR3	C6-N1-C2	-2.26	119.95	121.80
25	2	1518	MA6	C4-N9-C8	2.24	108.08	105.74
25	2	966	2MG	N1-C2-N3	-2.21	119.95	123.68
25	2	967	5MC	CM5-C5-C6	-2.19	119.88	122.85
25	2	516	PSU	O2-C2-N1	-2.19	120.53	122.79
25	2	1207	2MG	C8-N7-C5	2.18	108.15	104.26
25	2	1207	2MG	N9-C4-N3	2.17	130.29	125.95
25	2	1519	MA6	C4-N9-C8	2.16	108.01	105.74
25	2	966	2MG	C8-N7-C5	2.13	108.06	104.26
25	2	1518	MA6	C4-C5-N7	-2.13	108.14	110.58
25	2	1407	5MC	CM5-C5-C6	-2.12	119.98	122.85
25	2	966	2MG	CM2-N2-C2	-2.10	119.14	123.65
25	2	1519	MA6	C5-C4-N9	2.09	108.09	105.81
25	2	1402	4OC	C6-C5-C4	2.05	119.47	117.00
25	2	1516	2MG	C8-N7-C5	2.04	107.90	104.26
25	2	1207	2MG	CM2-N2-C2	-2.04	119.26	123.65

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	2	966	2MG	C2'
25	2	966	2MG	C1'
25	2	967	5MC	C4'
25	2	967	5MC	C3'
25	2	1207	2MG	C4'
25	2	1207	2MG	C3'
25	2	1407	5MC	C4'
25	2	1407	5MC	C3'
25	2	1516	2MG	C4'
25	2	1516	2MG	C3'

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	2	516	PSU	C2'-C1'-C5-C4
25	2	516	PSU	O4'-C1'-C5-C4
25	2	516	PSU	O4'-C1'-C5-C6
25	2	527	G7M	C3'-C4'-C5'-O5'
25	2	966	2MG	O4'-C4'-C5'-O5'
25	2	967	5MC	O4'-C4'-C5'-O5'
25	2	1402	4OC	C1'-C2'-O2'-CM2
25	2	1407	5MC	C3'-C4'-C5'-O5'
25	2	1519	MA6	O4'-C4'-C5'-O5'
25	2	967	5MC	C3'-C4'-C5'-O5'
25	2	1207	2MG	C3'-C4'-C5'-O5'
25	2	1516	2MG	C3'-C4'-C5'-O5'
25	2	527	G7M	O4'-C4'-C5'-O5'
25	2	966	2MG	C3'-C4'-C5'-O5'
25	2	1407	5MC	C4'-C5'-O5'-P
25	2	1519	MA6	C3'-C4'-C5'-O5'
25	2	1518	MA6	C5-C6-N6-C10
25	2	1519	MA6	C5-C6-N6-C10
45	q	89	0TD	CG-CB-SB-CSB
25	2	1518	MA6	C3'-C4'-C5'-O5'
45	q	89	0TD	SB-CB-CG-OD1
25	2	1516	2MG	C4'-C5'-O5'-P
25	2	1207	2MG	C4'-C5'-O5'-P
25	2	1518	MA6	O4'-C4'-C5'-O5'
25	2	1518	MA6	N1-C6-N6-C10
25	2	527	G7M	C4'-C5'-O5'-P
25	2	966	2MG	C4'-C5'-O5'-P
25	2	1407	5MC	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2	967	5MC	1	0
25	2	1402	4OC	1	0
25	2	1518	MA6	2	0
25	2	1407	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 425 ligands modelled in this entry, 424 are monoatomic - leaving 1 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	$\# Z > 2$
56	LYS	1	3296	-	7,8,9	0.46	0	3,8,10	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	LYS	1	3296	-	-	1/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1	3296	LYS	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

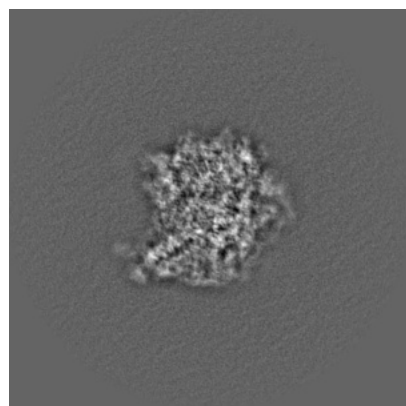
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43549. These allow visual inspection of the internal detail of the map and identification of artifacts.

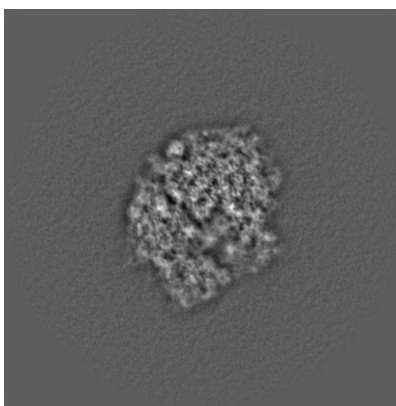
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

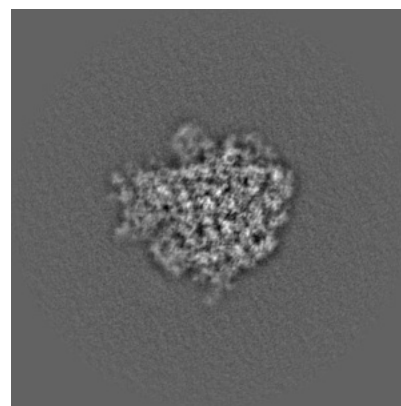
6.1.1 Primary map



X

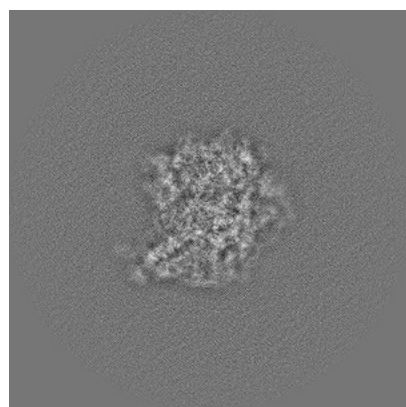


Y

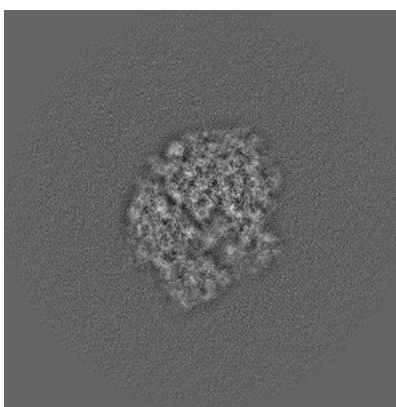


Z

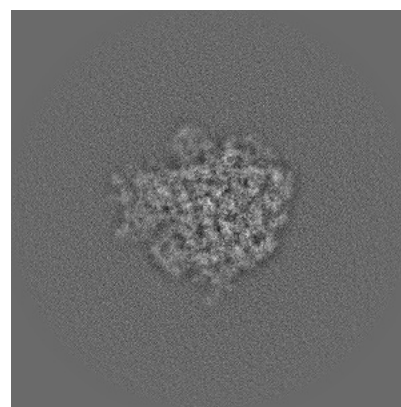
6.1.2 Raw map



X



Y

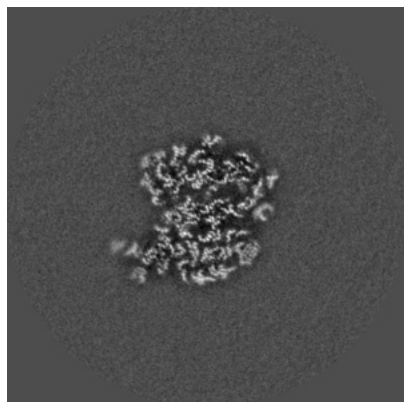


Z

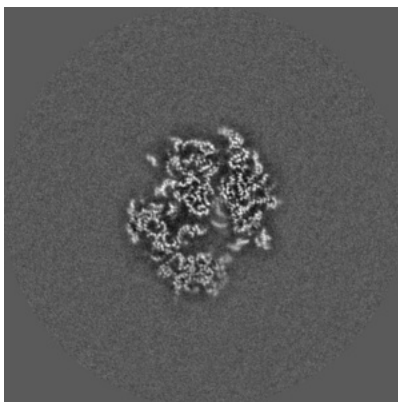
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

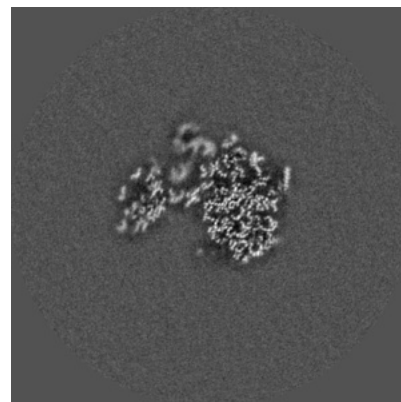
6.2.1 Primary map



X Index: 256

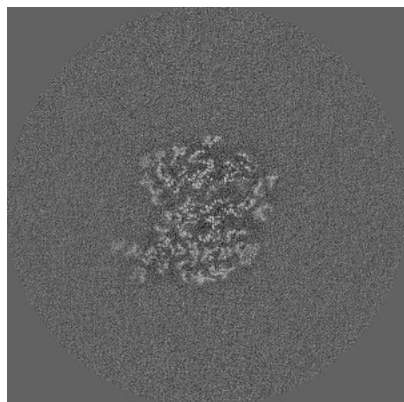


Y Index: 256

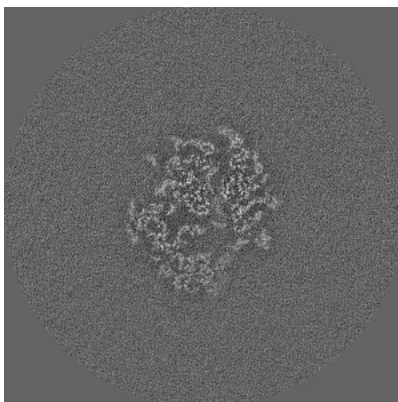


Z Index: 256

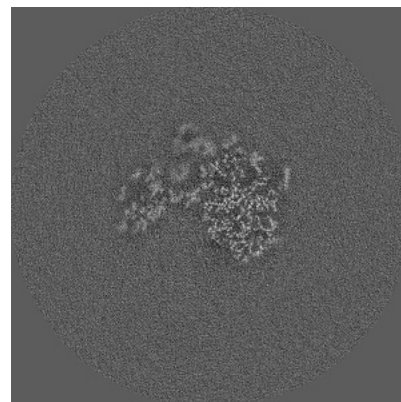
6.2.2 Raw map



X Index: 256



Y Index: 256

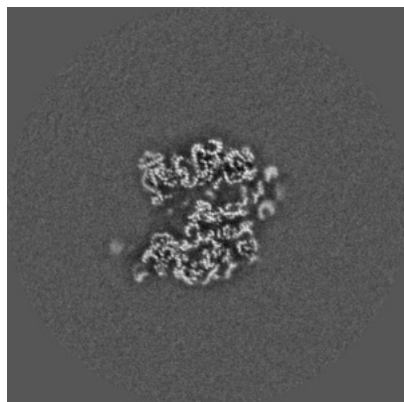


Z Index: 256

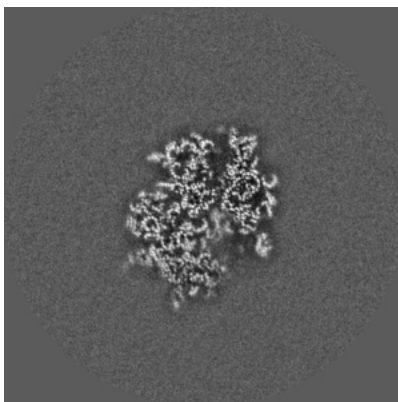
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

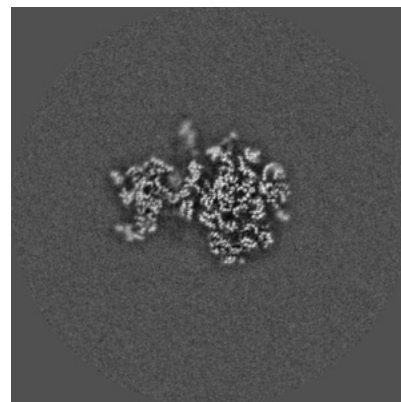
6.3.1 Primary map



X Index: 250

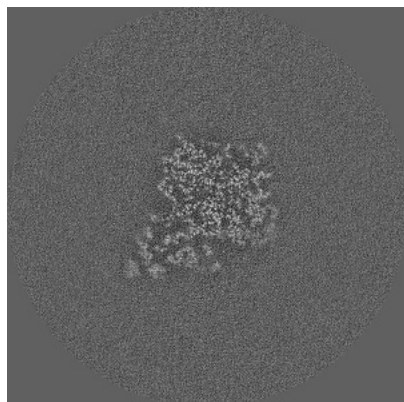


Y Index: 263

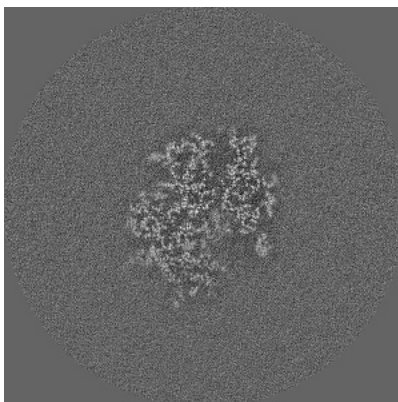


Z Index: 241

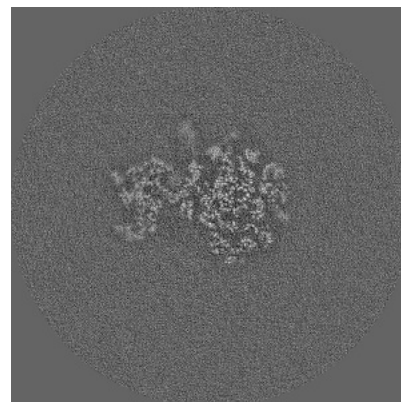
6.3.2 Raw map



X Index: 275



Y Index: 263

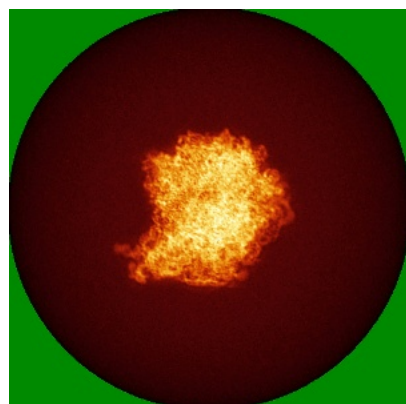


Z Index: 241

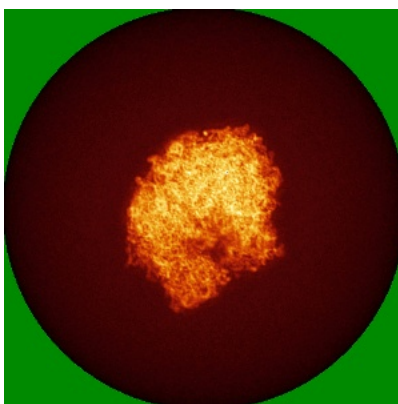
The images above show the largest variance slices of the map in three orthogonal directions.

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

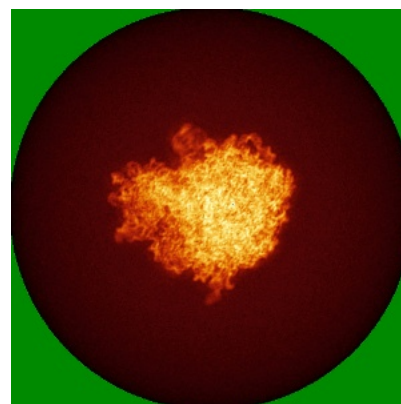
6.4.1 Primary map



X

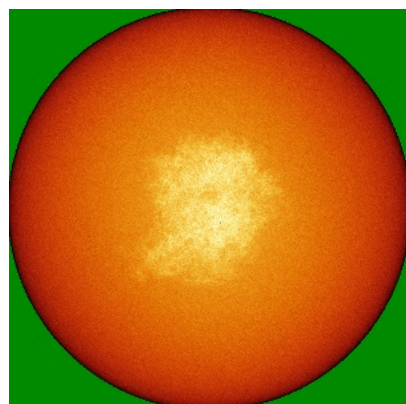


Y

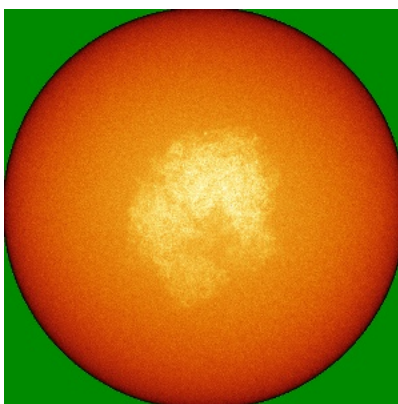


Z

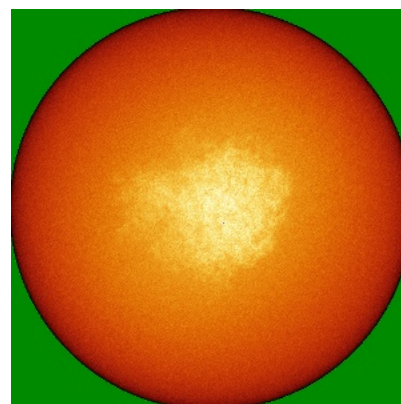
6.4.2 Raw map



X



Y

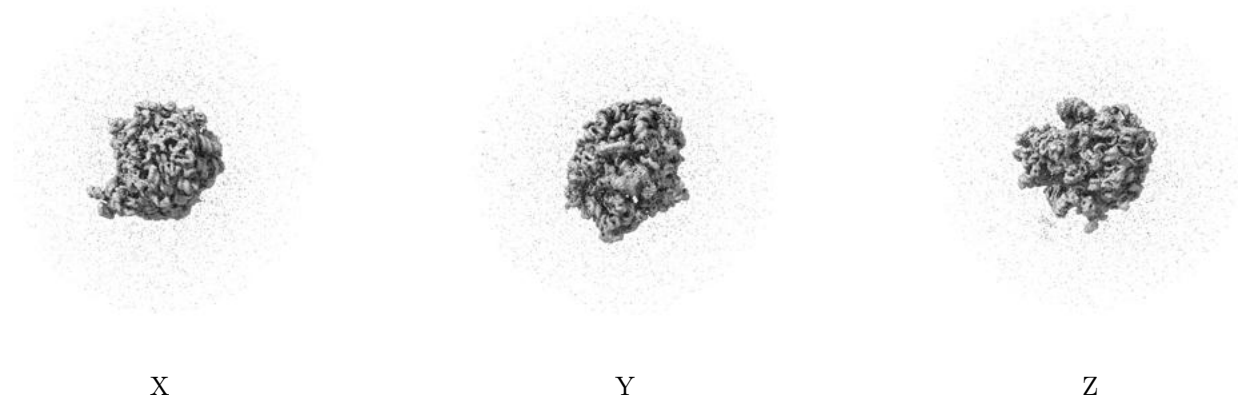


Z

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

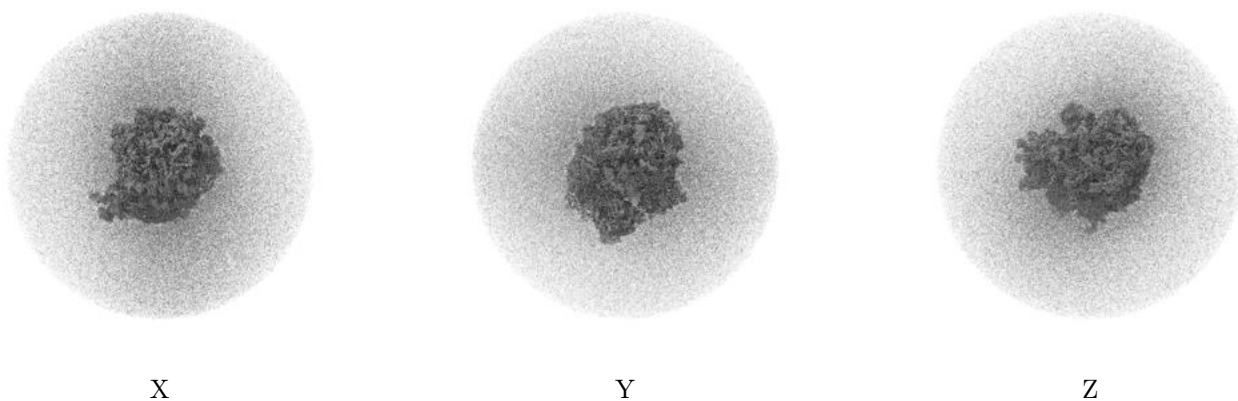
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00281. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

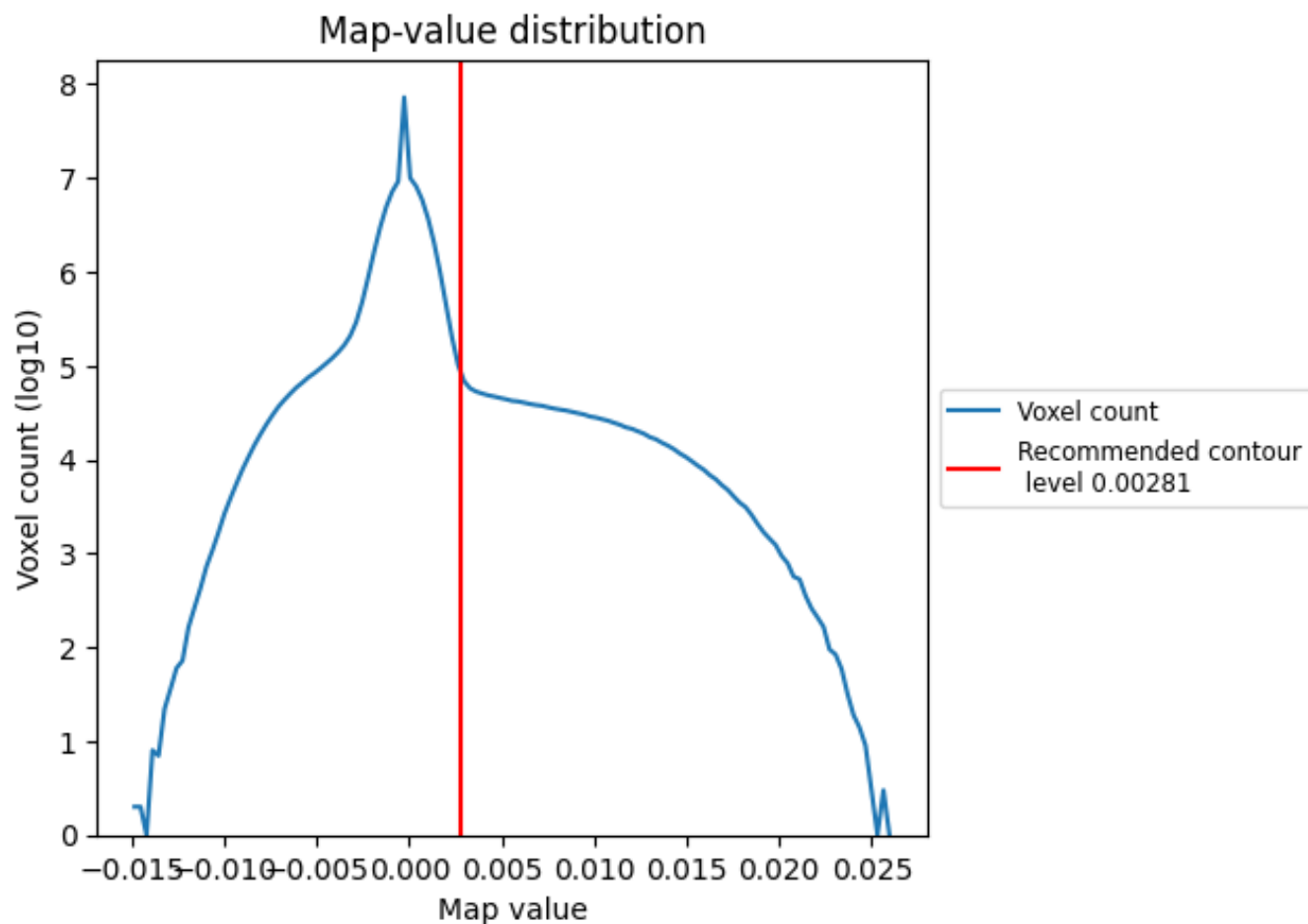
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

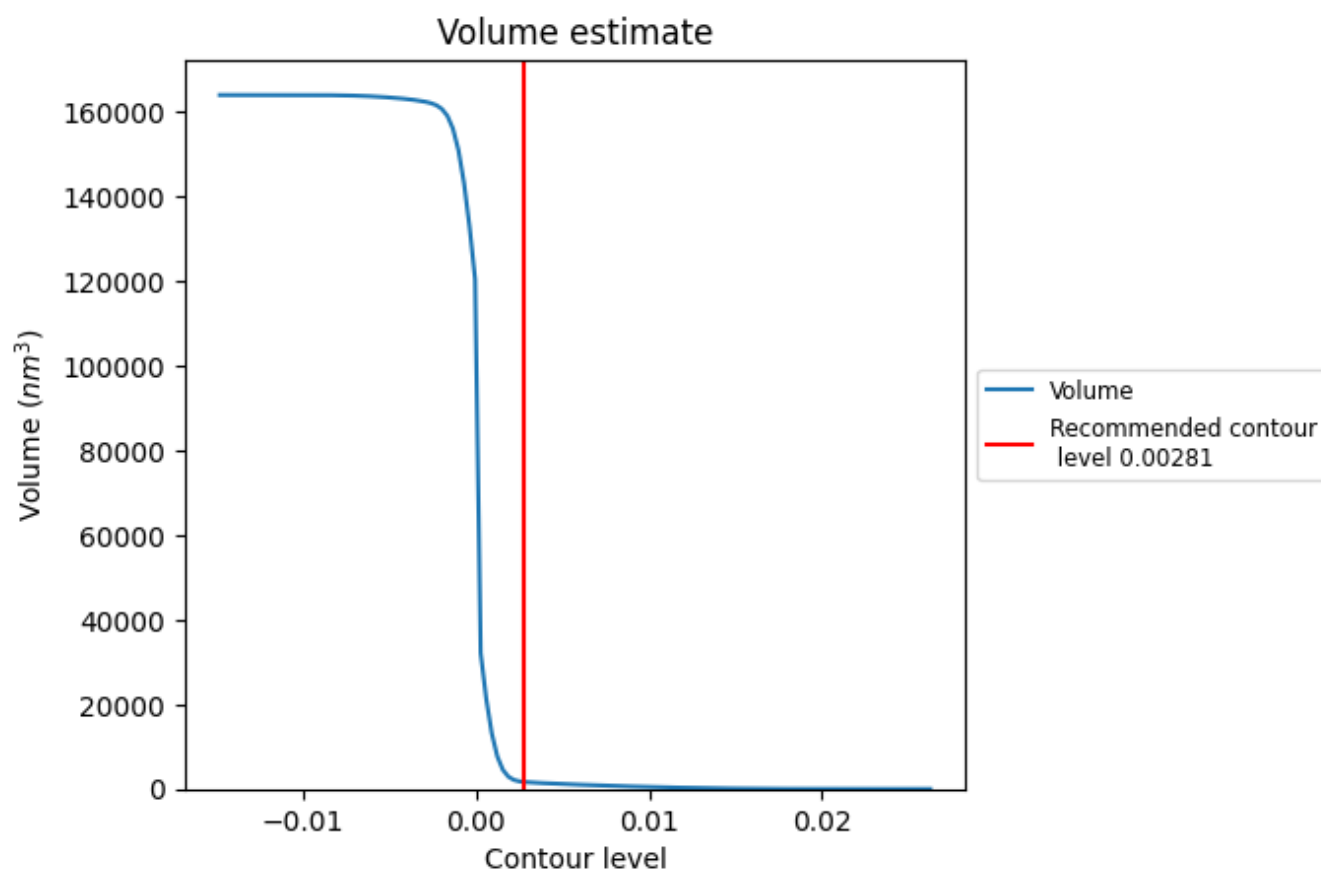
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

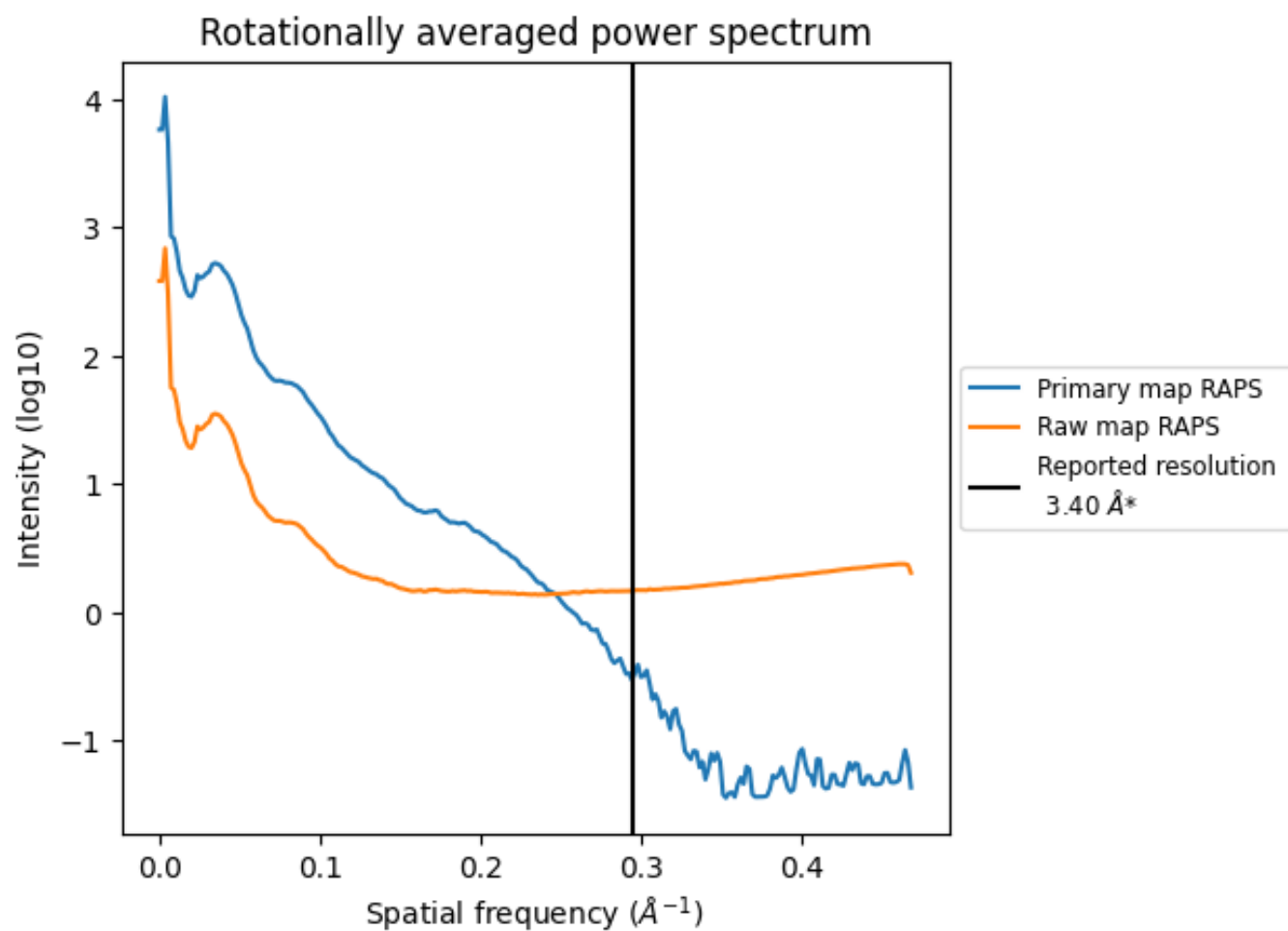
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1643 nm^3 ; this corresponds to an approximate mass of 1485 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 [i](#)

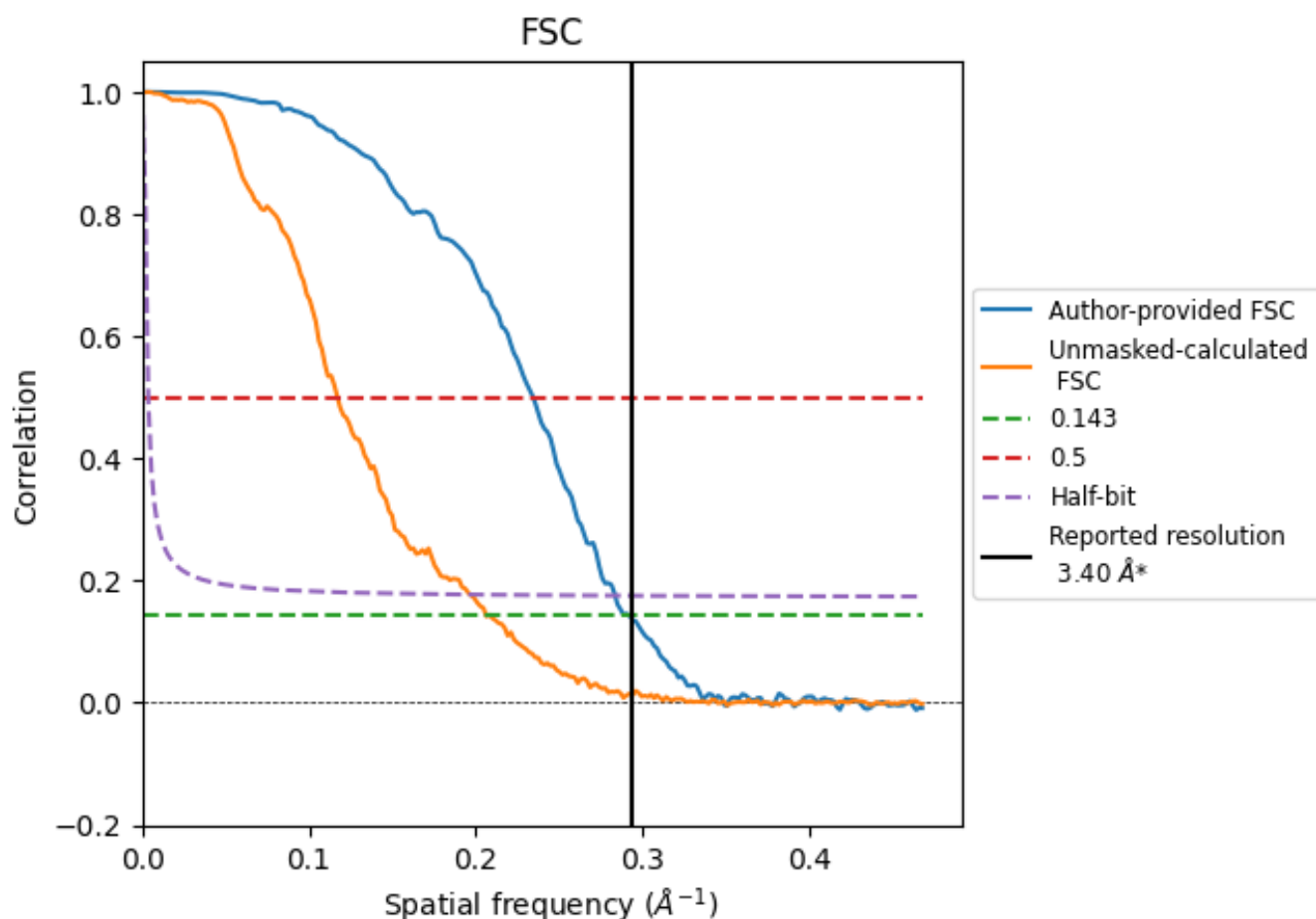


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

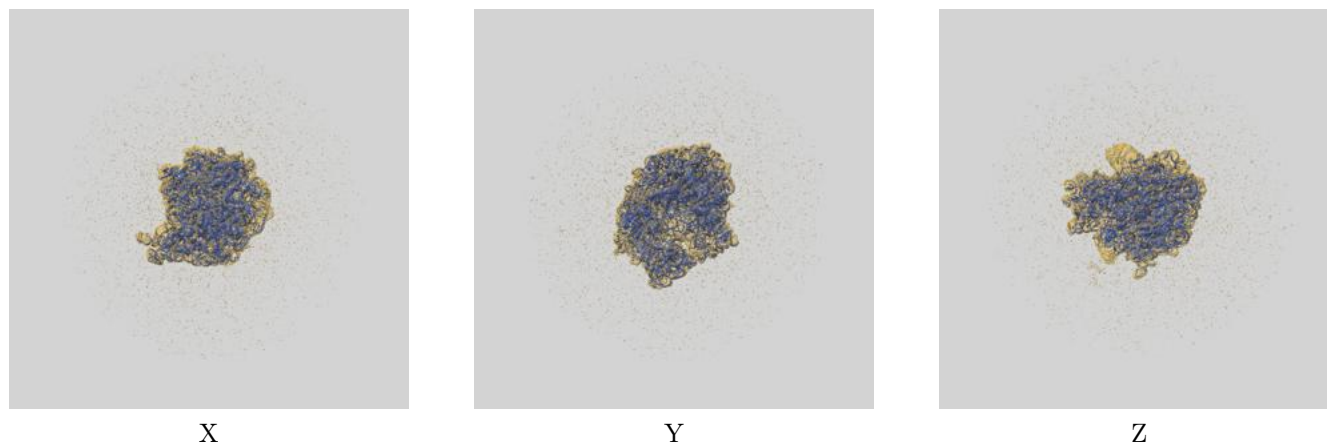
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.27	3.53
Unmasked-calculated*	4.85	8.54	5.08

*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 4.85 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

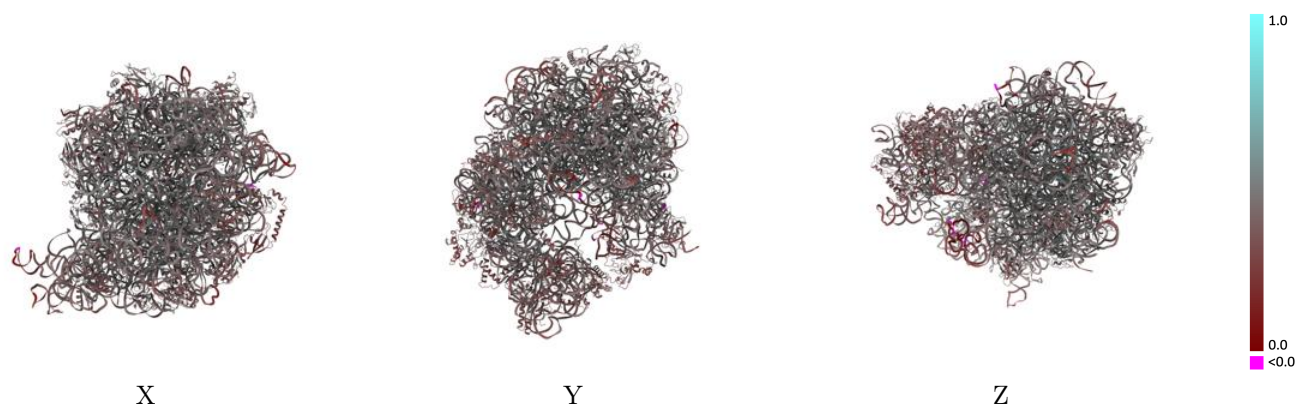
This section contains information regarding the fit between EMDB map EMD-43549 and PDB model 8VV4. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



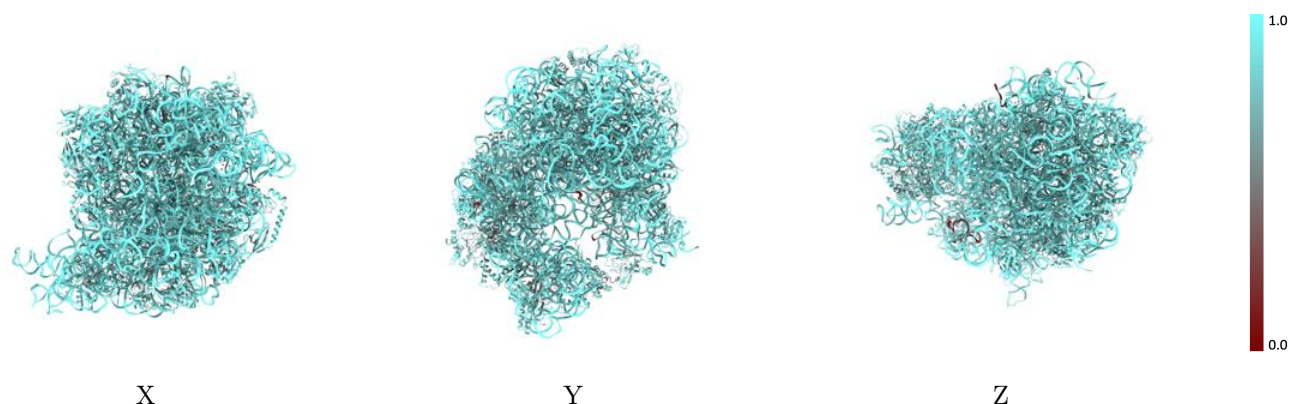
The images above show the 3D surface view of the map at the recommended contour level 0.00281 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



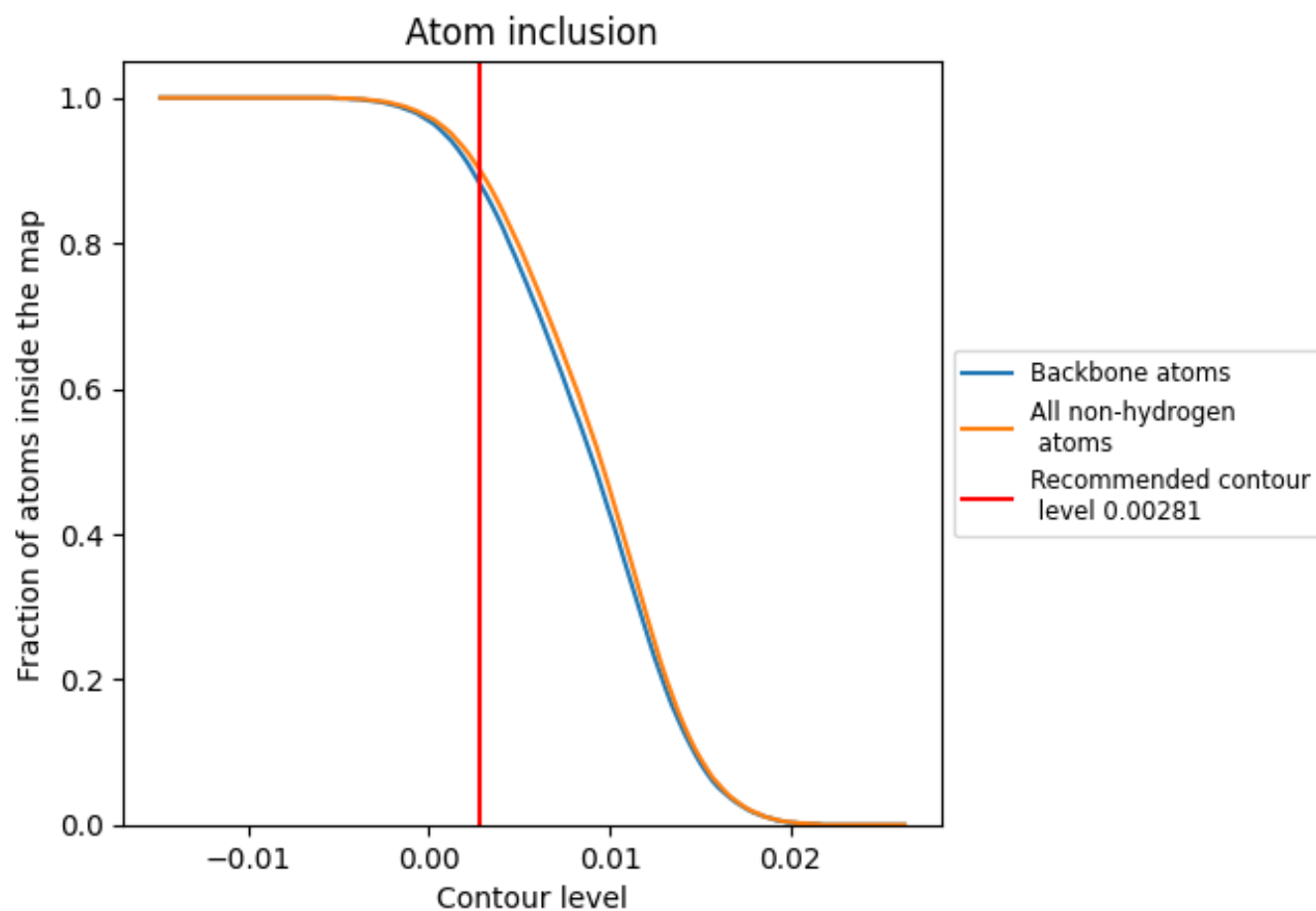
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00281).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00281) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.4160
1	 0.9520	 0.4310
2	 0.9540	 0.4120
3	 0.9620	 0.4000
4	 0.7380	 0.3990
5	 0.9230	 0.3720
B	 0.8000	 0.4610
C	 0.8150	 0.4470
D	 0.8270	 0.4200
E	 0.8190	 0.3420
F	 0.8720	 0.3930
G	 0.8390	 0.3160
J	 0.8250	 0.4370
K	 0.8020	 0.4510
L	 0.7960	 0.4390
M	 0.7990	 0.4400
N	 0.8000	 0.4460
O	 0.8250	 0.3930
P	 0.8380	 0.4440
Q	 0.7740	 0.4180
R	 0.8620	 0.4450
S	 0.8160	 0.4450
T	 0.7620	 0.4210
U	 0.8580	 0.4110
V	 0.8670	 0.4050
W	 0.7870	 0.4450
X	 0.7920	 0.4300
Y	 0.8280	 0.3610
Z	 0.8400	 0.4340
a	 0.5560	 0.3040
b	 0.7970	 0.4340
c	 0.8450	 0.4210
d	 0.7750	 0.4540
e	 0.7240	 0.4540
f	 0.6780	 0.4280



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Chain	Atom inclusion	Q-score
g	 0.7650	 0.3410
h	 0.8190	 0.3940
i	 0.7500	 0.3740
j	 0.8130	 0.4090
k	 0.8660	 0.3710
l	 0.7970	 0.3620
m	 0.8170	 0.4120
n	 0.7810	 0.3700
o	 0.7540	 0.3720
p	 0.8160	 0.4060
q	 0.8010	 0.4170
r	 0.7830	 0.3580
s	 0.7290	 0.3790
t	 0.8250	 0.3830
u	 0.7780	 0.4190
v	 0.8020	 0.3860
w	 0.6580	 0.3300
x	 0.7940	 0.3550
y	 0.7360	 0.3430
z	 0.5920	 0.3050