



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 11:41 am BST

PDB ID : 5LZA / pdb_00005lza
EMDB ID : EMD-4121
Title : Structure of the 70S ribosome with SECIS-mRNA and P-site tRNA (Initial complex, IC)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

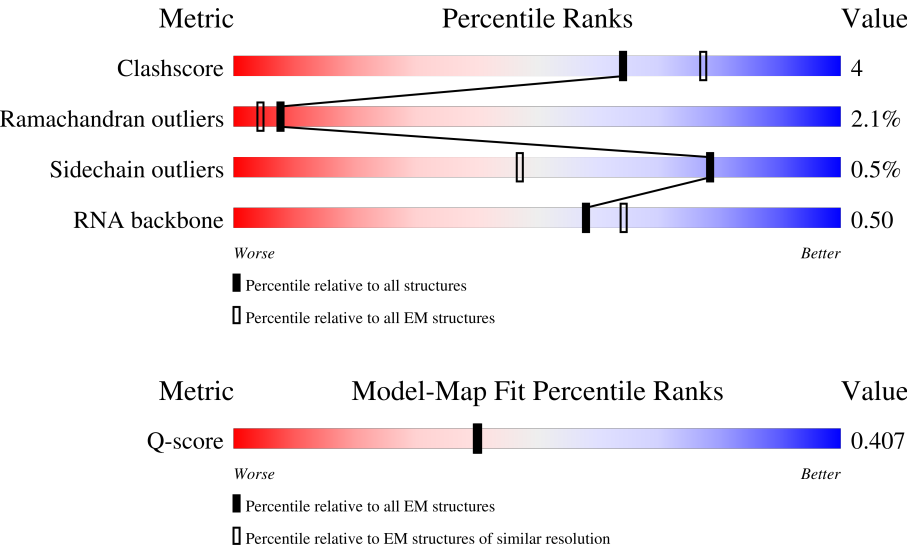
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	

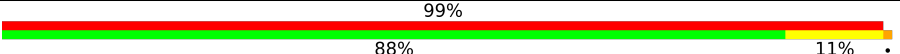
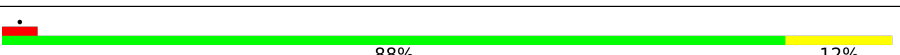
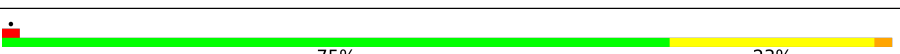
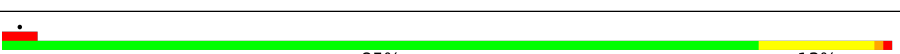
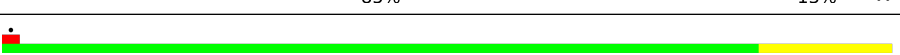
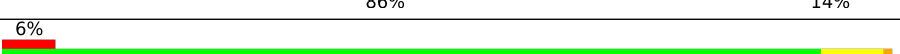
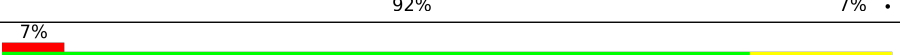
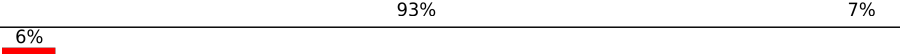
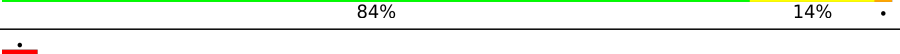
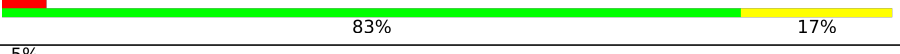
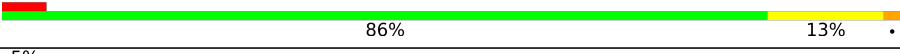
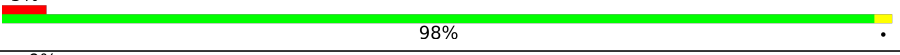
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Mol	Chain	Length	Quality of chain
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	100	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	v	77	
23	x	48	
24	A	2903	
25	B	120	
26	C	271	
27	D	209	
28	E	201	

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Mol	Chain	Length	Quality of chain
29	F	177	
30	G	176	
31	I	141	
32	H	149	
33	J	142	
34	K	122	
35	L	143	
36	M	136	
37	N	120	
38	O	116	
39	P	114	
40	Q	117	
41	R	103	
42	S	110	
43	T	93	
44	U	102	
45	V	94	
46	W	75	
47	X	77	
48	Y	63	
49	Z	58	
50	0	56	
51	1	50	
52	2	46	
53	3	64	

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Mol	Chain	Length	Quality of chain
54	4	38	 89% 8%
55	6	66	 38% 74% 24%

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
1	G7M	a	527	X	-	-	-
24	G7M	A	2069	X	-	-	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 146037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	4	0
			33119	14778	6072	10726	1543		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2900	Total	C	N	O	P	1	0
			62296	27797	11464	20134	2901		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

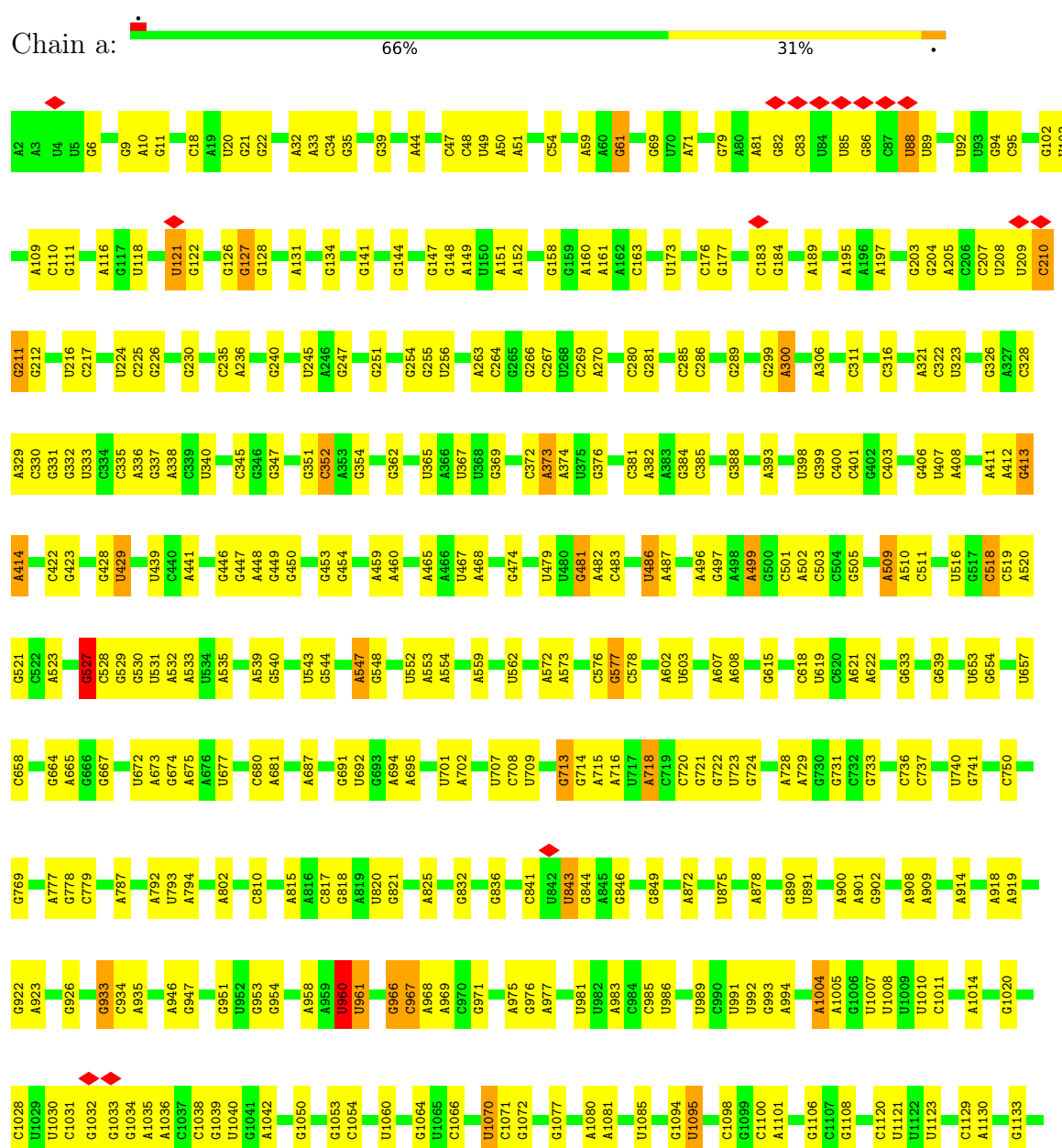
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

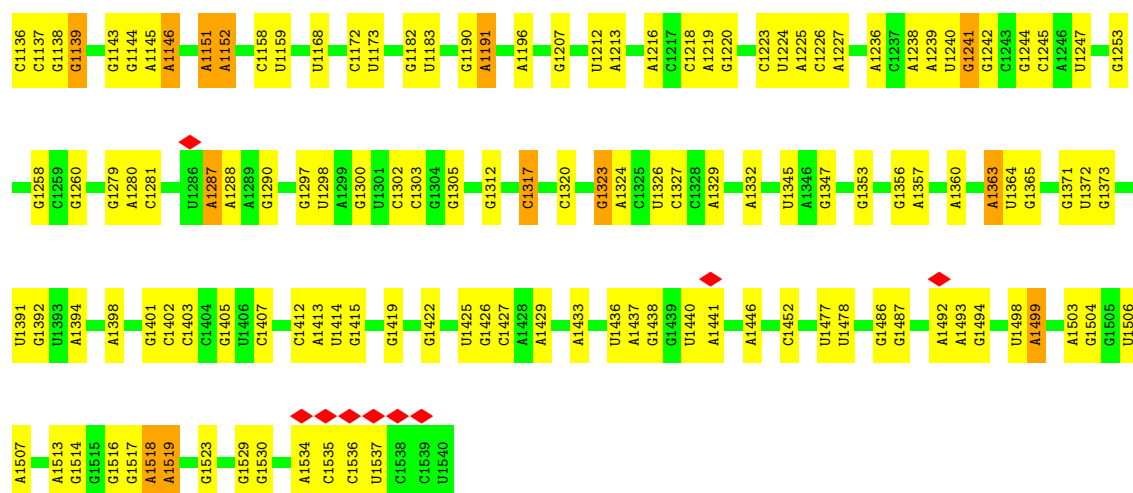
Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total 1	Zn 1	0
56	6	1	Total 1	Zn 1	0

3 Residue-property plots

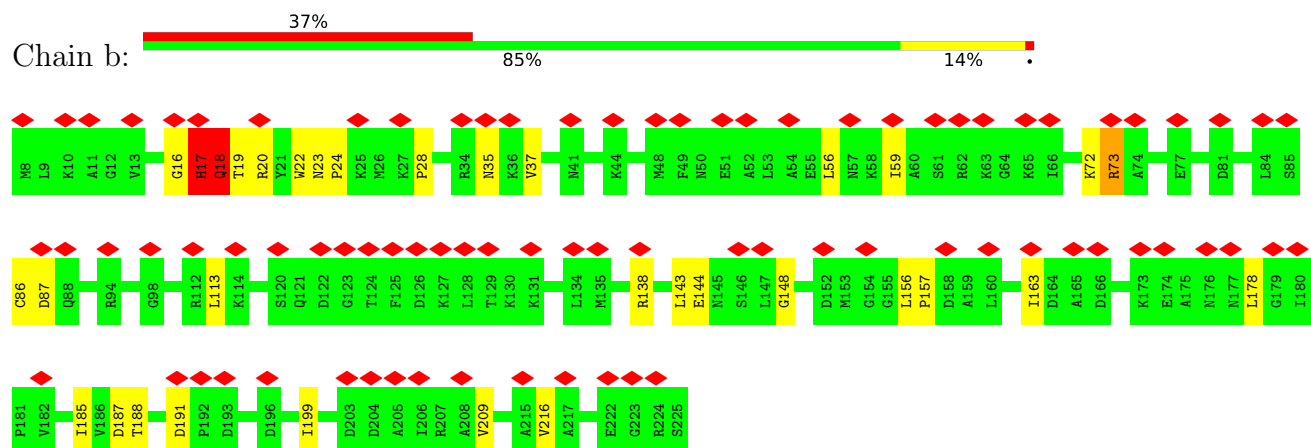
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

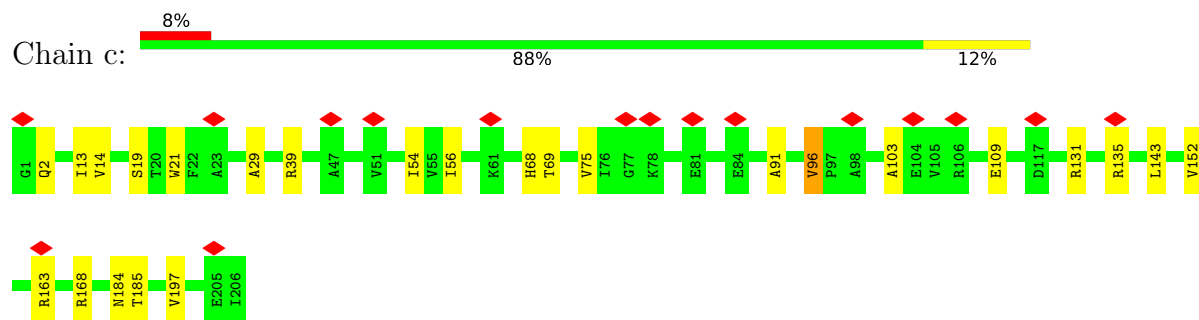




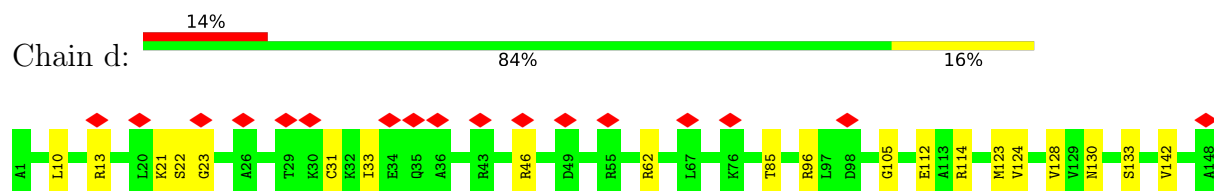
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



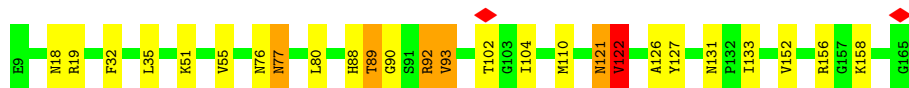
• Molecule 4: 30S ribosomal protein S4





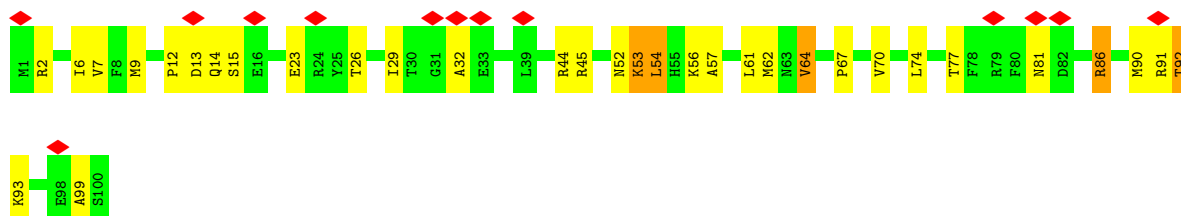
- Molecule 5: 30S ribosomal protein S5

Chain e: 83% 13%



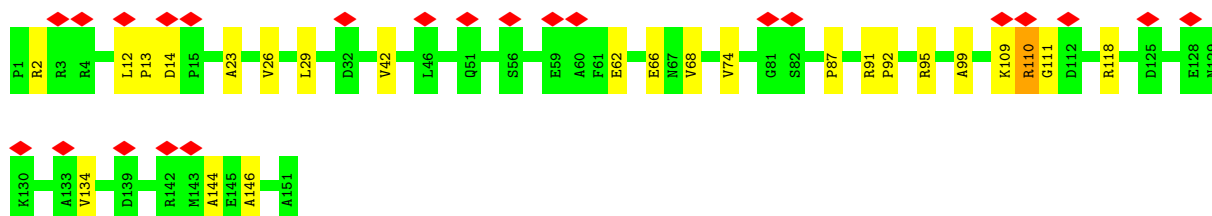
- Molecule 6: 30S ribosomal protein S6

Chain f: 13% 67% 28% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g: 15% 84% 15%



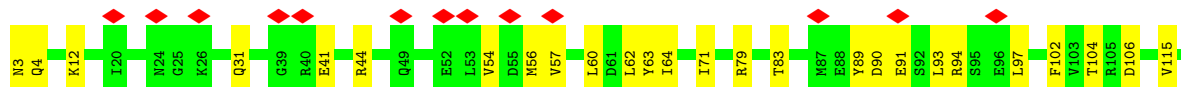
- Molecule 8: 30S ribosomal protein S8

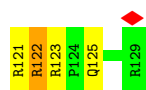
Chain h: 7% 83% 16%



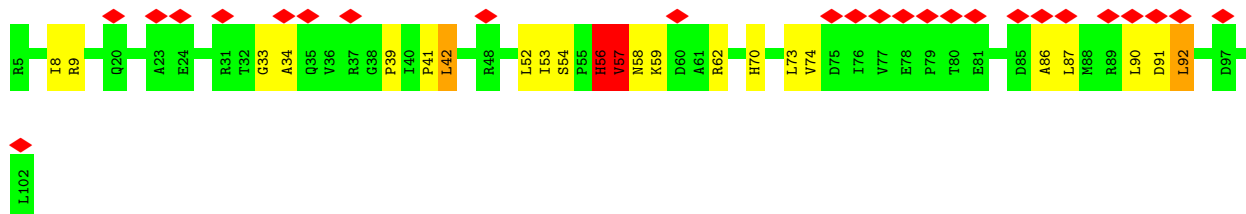
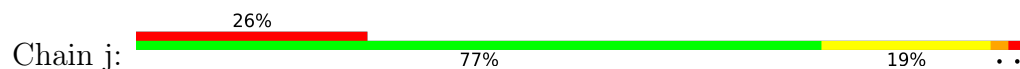
- Molecule 9: 30S ribosomal protein S9

Chain i: 11% 76% 23%

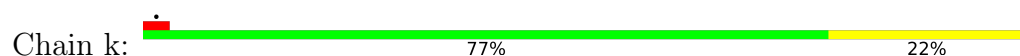




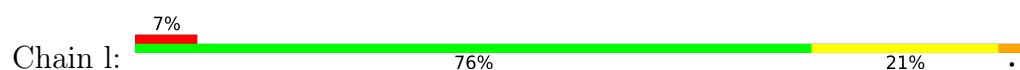
- Molecule 10: 30S ribosomal protein S10



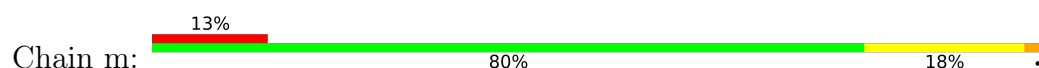
- Molecule 11: 30S ribosomal protein S11



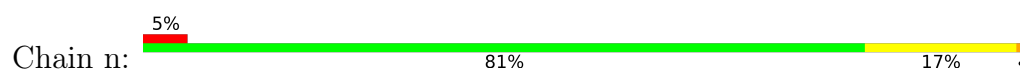
- Molecule 12: 30S ribosomal protein S12



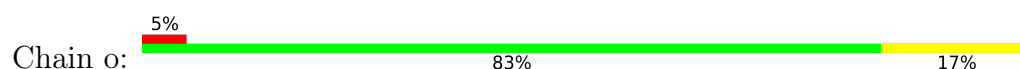
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

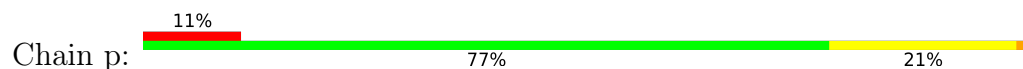


- Molecule 15: 30S ribosomal protein S15

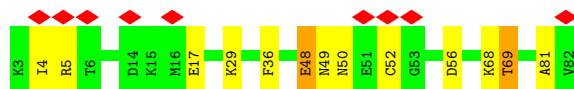
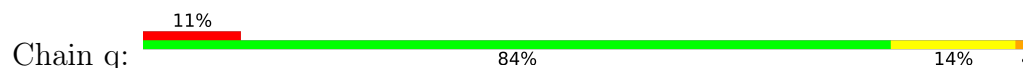




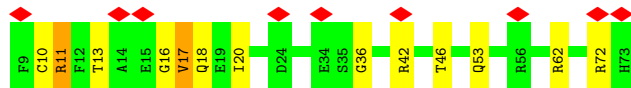
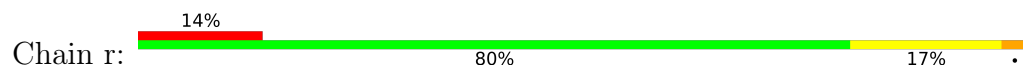
- Molecule 16: 30S ribosomal protein S16



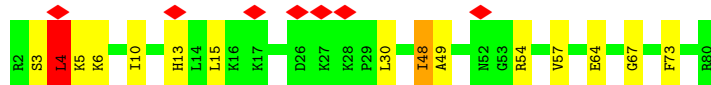
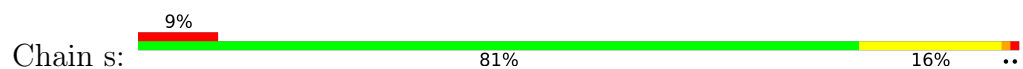
- Molecule 17: 30S ribosomal protein S17



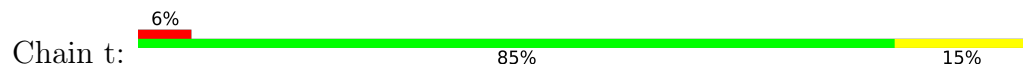
- Molecule 18: 30S ribosomal protein S18



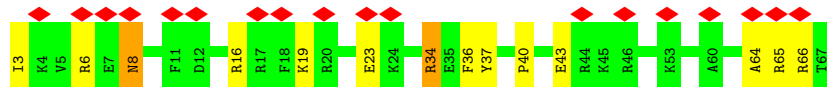
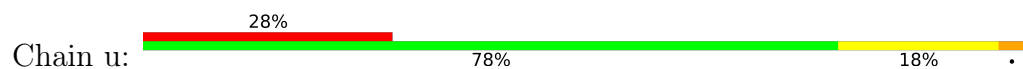
- Molecule 19: 30S ribosomal protein S19



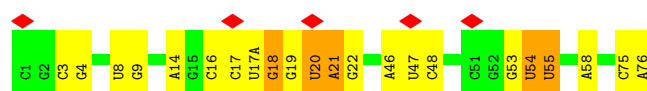
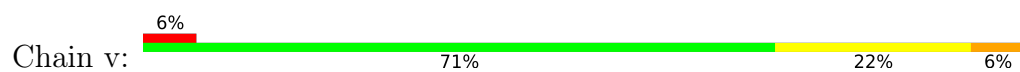
- Molecule 20: 30S ribosomal protein S20



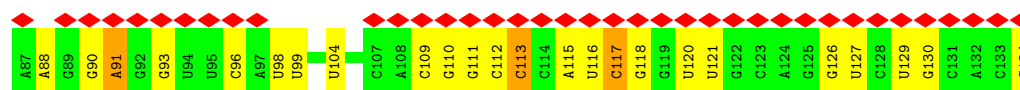
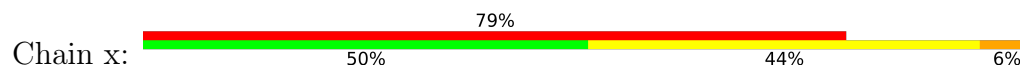
- Molecule 21: 30S ribosomal protein S21



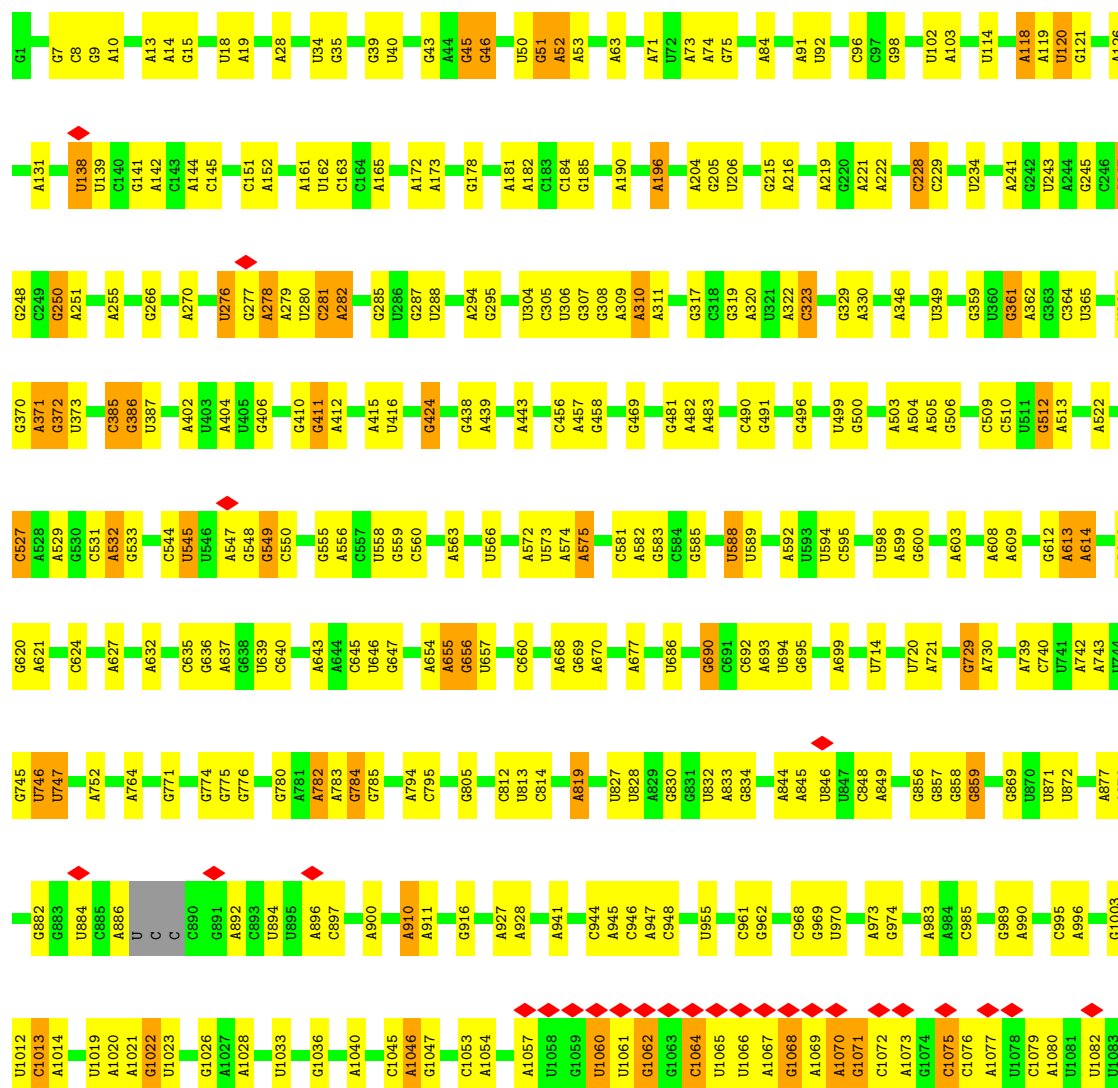
- Molecule 22: fMet-tRNA^{fMet}



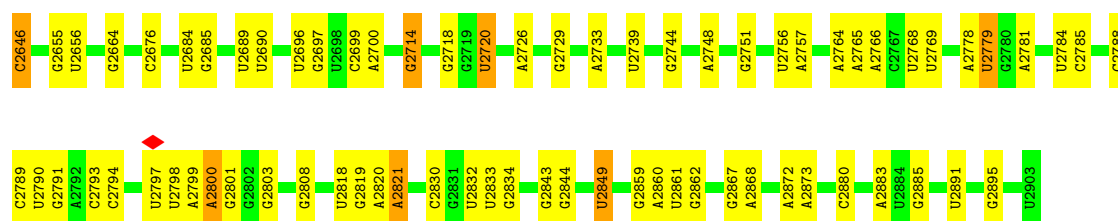
• Molecule 23: SECIS mRNA



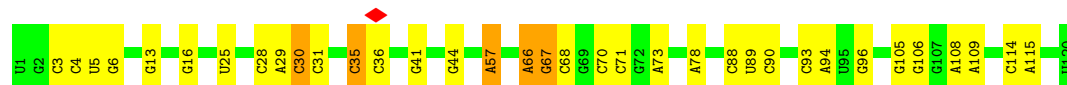
• Molecule 24: 23S ribosomal RNA



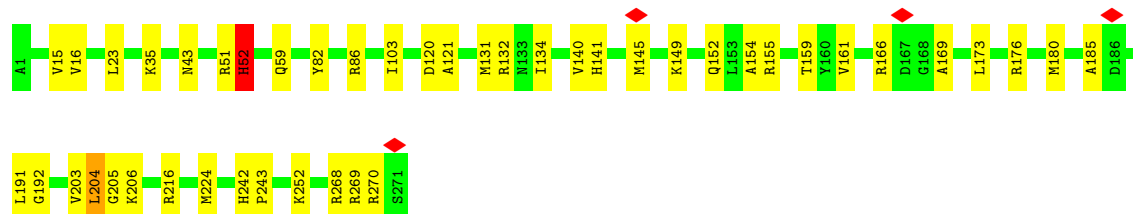
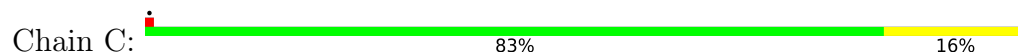




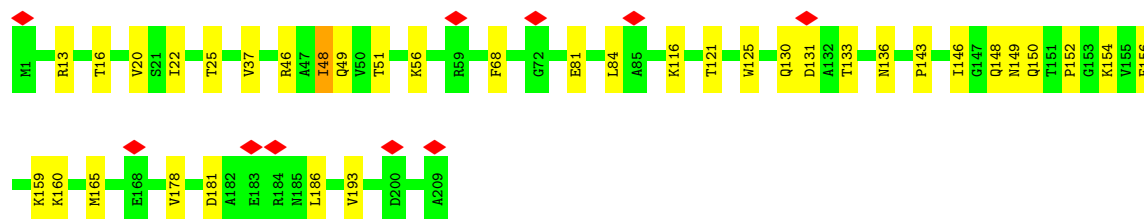
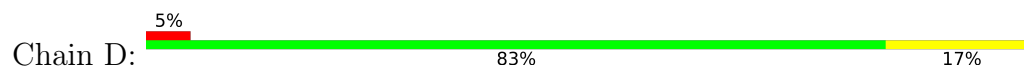
• Molecule 25: 5S ribosomal RNA



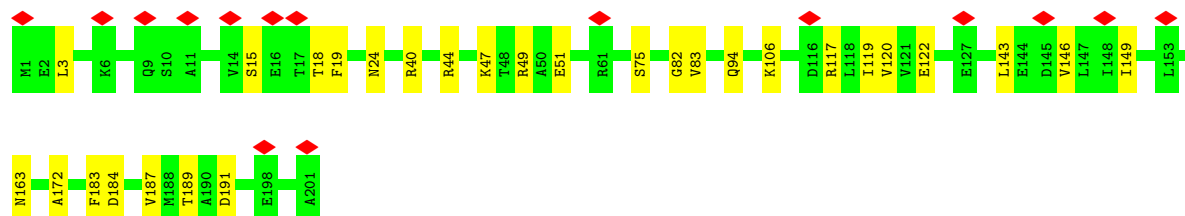
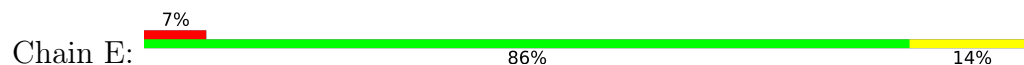
• Molecule 26: 50S ribosomal protein L2



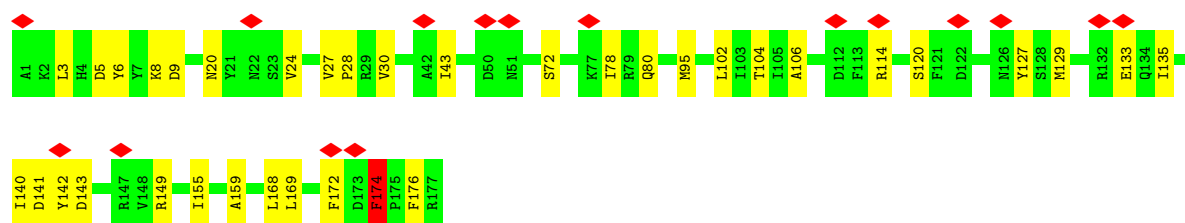
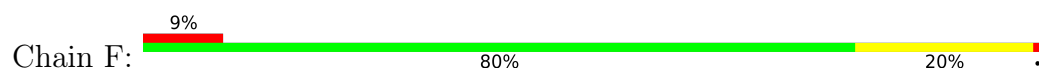
• Molecule 27: 50S ribosomal protein L3



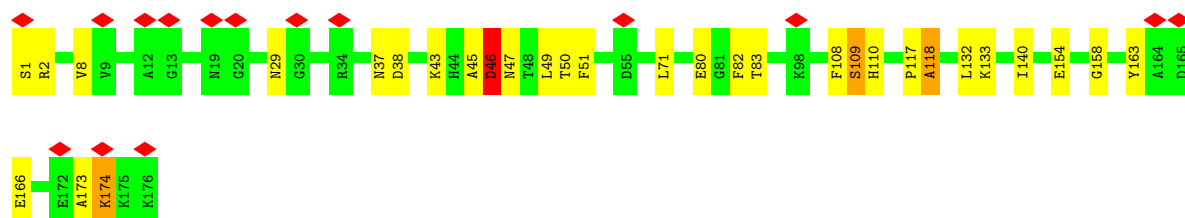
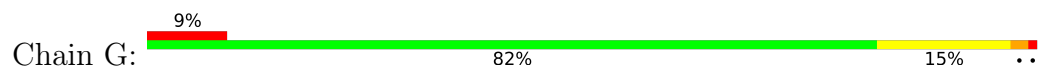
• Molecule 28: 50S ribosomal protein L4



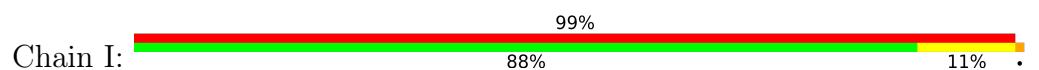
• Molecule 29: 50S ribosomal protein L5



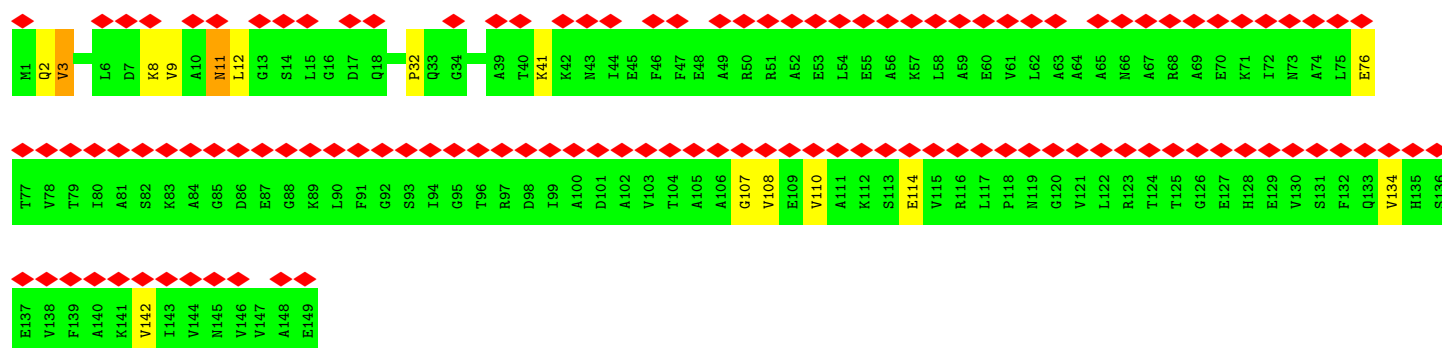
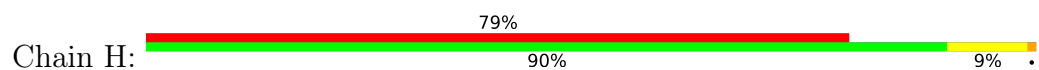
- Molecule 30: 50S ribosomal protein L6



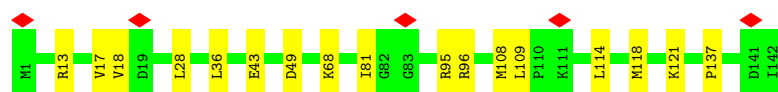
- Molecule 31: 50S ribosomal protein L11



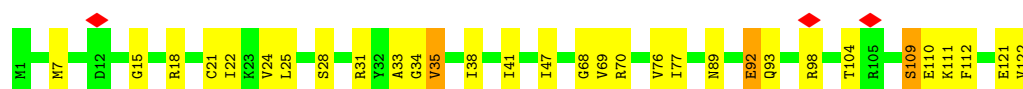
- Molecule 32: 50S ribosomal protein L9



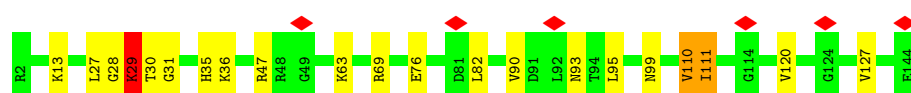
• Molecule 33: 50S ribosomal protein L13

Chain J:  88% 12%

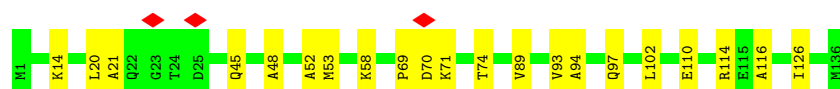
• Molecule 34: 50S ribosomal protein L14

Chain K:  75% 23%

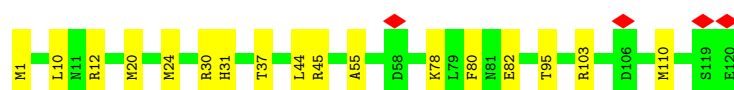
• Molecule 35: 50S ribosomal protein L15

Chain L:  85% 13%

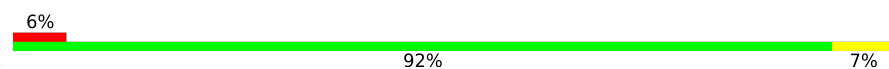
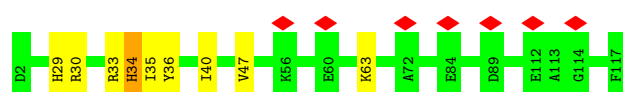
• Molecule 36: 50S ribosomal protein L16

Chain M:  85% 15%

• Molecule 37: 50S ribosomal protein L17

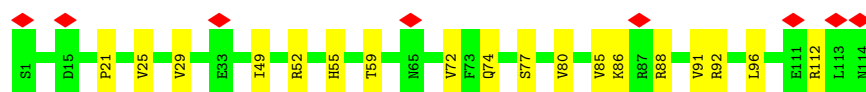
Chain N:  86% 14%

• Molecule 38: 50S ribosomal protein L18

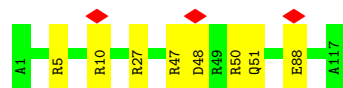
Chain O:  6% 92% 7%

• Molecule 39: 50S ribosomal protein L19

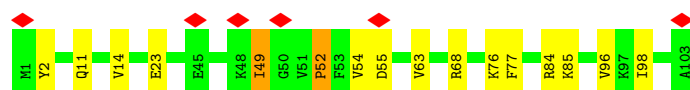
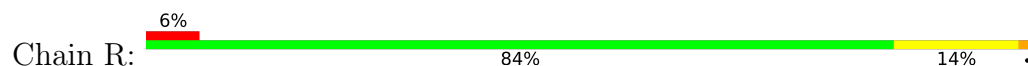
Chain P:  7% 84% 16%



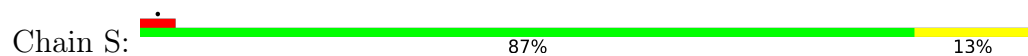
- Molecule 40: 50S ribosomal protein L20



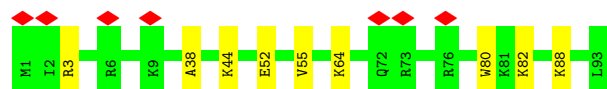
- Molecule 41: 50S ribosomal protein L21



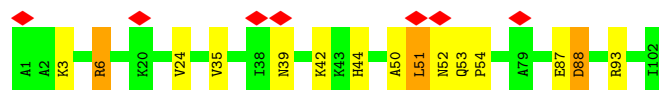
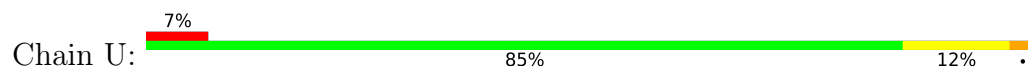
- Molecule 42: 50S ribosomal protein L22



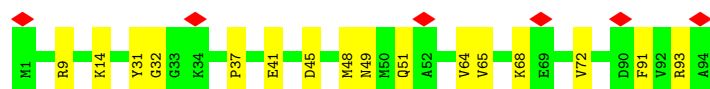
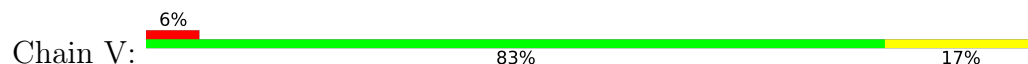
- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L27

Chain W:  83% 17%



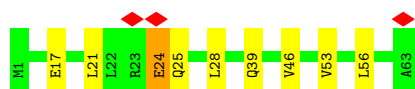
- Molecule 47: 50S ribosomal protein L28

Chain X:  5% 83% 17%



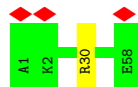
- Molecule 48: 50S ribosomal protein L29

Chain Y:  5% 86% 13%



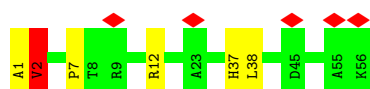
- Molecule 49: 50S ribosomal protein L30

Chain Z:  5% 98%



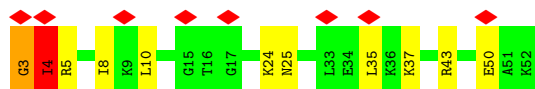
- Molecule 50: 50S ribosomal protein L32

Chain 0:  9% 89% 9%



- Molecule 51: 50S ribosomal protein L33

Chain 1:  16% 78% 18%



- Molecule 52: 50S ribosomal protein L34

Chain 2:  83% 17%



- Molecule 53: 50S ribosomal protein L35

Chain 3:  88% 11% .



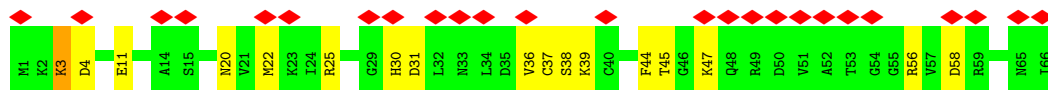
- Molecule 54: 50S ribosomal protein L36

Chain 4:  89% 8% .



- Molecule 55: 50S ribosomal protein L31

Chain 6:  38% 74% 24% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.934	Depositor
Minimum map value	-2.060	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.265	Depositor
Recommended contour level	0.52	Depositor
Map size ($\text{\AA}$)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.34	1/36803 (0.0%)	0.49	3/57406 (0.0%)
2	b	0.43	0/1736	0.86	3/2338 (0.1%)
3	c	0.40	0/1652	0.79	0/2225
4	d	0.41	0/1665	0.84	2/2227 (0.1%)
5	e	0.46	0/1170	1.04	7/1573 (0.4%)
6	f	0.52	0/836	1.07	3/1128 (0.3%)
7	g	0.42	0/1196	0.88	2/1602 (0.1%)
8	h	0.40	0/989	0.83	0/1326
9	i	0.43	0/1034	0.92	2/1375 (0.1%)
10	j	0.40	0/797	0.91	3/1077 (0.3%)
11	k	0.41	0/886	0.89	0/1195
12	l	0.44	0/969	0.96	1/1300 (0.1%)
13	m	0.47	0/893	0.98	2/1193 (0.2%)
14	n	0.49	0/806	0.94	2/1074 (0.2%)
15	o	0.46	0/722	0.84	0/964
16	p	0.43	0/659	0.88	1/884 (0.1%)
17	q	0.44	0/658	0.97	2/881 (0.2%)
18	r	0.45	0/512	0.92	0/689
19	s	0.41	0/653	0.86	1/877 (0.1%)
20	t	0.51	0/671	0.87	0/888
21	u	0.54	0/501	1.10	0/668
22	v	0.30	0/1747	0.45	0/2721
23	x	0.28	0/1145	0.40	0/1781
24	A	0.37	0/69196	0.52	8/107943 (0.0%)
25	B	0.32	0/2873	0.48	0/4478
26	C	0.46	0/2122	0.89	2/2852 (0.1%)
27	D	0.42	0/1586	0.81	0/2134
28	E	0.41	0/1571	0.79	0/2113
29	F	0.44	0/1435	0.89	3/1926 (0.2%)
30	G	0.39	0/1343	0.84	4/1816 (0.2%)
31	I	0.37	0/1046	0.79	0/1410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	H	0.40	0/1122	0.88	2/1515 (0.1%)
33	J	0.43	0/1152	0.79	0/1551
34	K	0.46	0/948	0.89	0/1268
35	L	0.45	0/1054	0.96	1/1403 (0.1%)
36	M	0.44	0/1093	0.88	0/1460
37	N	0.47	0/974	0.83	0/1301
38	O	0.43	0/902	0.80	0/1209
39	P	0.43	0/929	0.80	0/1242
40	Q	0.47	0/960	0.81	0/1278
41	R	0.43	0/829	0.93	2/1107 (0.2%)
42	S	0.43	0/864	0.81	2/1156 (0.2%)
43	T	0.39	0/745	0.80	0/994
44	U	0.42	0/788	0.95	3/1051 (0.3%)
45	V	0.36	0/766	0.76	0/1025
46	W	0.34	0/582	0.72	0/769
47	X	0.38	0/635	0.70	0/848
48	Y	0.48	0/510	0.86	0/677
49	Z	0.44	0/453	0.78	0/605
50	0	0.42	0/450	0.92	2/599 (0.3%)
51	1	0.43	0/417	1.02	2/554 (0.4%)
52	2	0.43	0/380	0.86	0/498
53	3	0.49	0/513	0.89	1/676 (0.1%)
54	4	0.50	0/303	0.93	0/397
55	6	0.40	0/532	0.75	0/709
All	All	0.38	1/157773 (0.0%)	0.62	66/235956 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
2	b	0	4
5	e	0	4
6	f	0	1
7	g	0	2
8	h	0	1
9	i	0	1
10	j	0	5
12	l	0	1
13	m	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
16	p	0	1
17	q	0	2
18	r	0	3
19	s	0	1
21	u	0	1
24	A	2	0
26	C	0	1
28	E	0	1
30	G	0	3
32	H	0	2
34	K	0	3
35	L	0	4
42	S	0	1
44	U	0	3
48	Y	0	1
50	0	0	2
51	1	0	1
53	3	0	1
All	All	4	51

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	G7M	O3'-P	6.38	1.62	1.56

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	77	ASN	N-CA-CB	-11.08	91.77	110.49
13	m	65	GLU	N-CA-CB	-10.30	93.08	110.49
44	U	51	LEU	N-CA-CB	-9.70	94.11	110.49
12	l	101	LEU	N-CA-CB	-9.13	95.06	110.49
2	b	73	ARG	N-CA-CB	-8.79	95.64	110.49
17	q	69	THR	N-CA-CB	-8.77	95.68	110.49
7	g	110	ARG	N-CA-CB	-8.07	96.85	110.49
29	F	172	PHE	CA-C-N	7.88	136.59	121.54
29	F	172	PHE	C-N-CA	7.88	136.59	121.54
6	f	53	LYS	N-CA-CB	7.87	123.78	110.49
5	e	122	VAL	N-CA-CB	-7.86	98.26	111.23
24	A	2069	G7M	P-O3'-C3'	7.78	129.03	119.70
30	G	46	ASP	N-CA-CB	-7.68	97.51	110.49
16	p	44	SER	N-CA-CB	-7.64	97.58	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	33	VAL	CA-C-N	7.23	135.36	121.54
14	n	33	VAL	C-N-CA	7.23	135.36	121.54
30	G	174	LYS	N-CA-C	-7.17	95.52	110.80
30	G	46	ASP	N-CA-C	7.16	126.04	110.80
24	A	2447	G	P-O3'-C3'	7.12	130.89	120.20
19	s	4	LEU	CA-CB-CG	6.94	140.57	116.30
5	e	122	VAL	N-CA-C	6.88	123.66	109.34
1	a	527	G7M	P-O3'-C3'	6.80	127.86	119.70
7	g	110	ARG	N-CA-C	6.78	125.24	110.80
2	b	17	HIS	N-CA-CB	-6.75	99.07	110.49
30	G	174	LYS	N-CA-CB	6.39	121.29	110.49
9	i	89	TYR	CA-C-N	6.22	133.43	121.54
9	i	89	TYR	C-N-CA	6.22	133.43	121.54
5	e	93	VAL	N-CA-C	6.02	121.85	109.34
53	3	31	ILE	N-CA-CB	-6.01	101.31	111.23
35	L	29	LYS	N-CA-CB	-5.95	100.43	110.49
32	H	107	GLY	N-CA-C	5.95	117.14	111.67
51	1	4	ILE	N-CA-C	5.85	121.50	109.34
44	U	88	ASP	N-CA-CB	-5.82	100.66	110.49
42	S	63	GLY	CA-C-N	5.81	132.64	121.54
42	S	63	GLY	C-N-CA	5.81	132.64	121.54
6	f	54	LEU	N-CA-C	5.79	123.13	110.80
6	f	53	LYS	N-CA-C	-5.78	98.49	110.80
4	d	190	LEU	CA-C-N	5.72	132.47	121.54
4	d	190	LEU	C-N-CA	5.72	132.47	121.54
10	j	57	VAL	N-CA-CB	-5.72	101.80	111.23
24	A	2447	G	C4'-C3'-O3'	5.72	117.97	109.40
50	0	2	VAL	N-CA-CB	-5.70	101.83	111.23
51	1	4	ILE	N-CA-CB	-5.62	101.96	111.23
13	m	4	ALA	N-CA-CB	-5.58	101.05	110.49
5	e	121	ASN	CA-C-N	5.50	131.86	121.97
5	e	121	ASN	C-N-CA	5.50	131.86	121.97
2	b	18	GLN	N-CA-CB	-5.44	101.30	110.49
41	R	49	ILE	N-CA-C	5.43	116.28	106.61
32	H	3	VAL	N-CA-CB	-5.42	102.29	111.23
24	A	385	C	OP2-P-O3'	5.37	124.11	108.00
24	A	2610	C	P-O3'-C3'	5.29	128.14	120.20
26	C	204	LEU	N-CA-CB	-5.28	101.58	110.49
17	q	48	GLU	N-CA-C	-5.25	101.90	110.20
24	A	1212	G	P-O3'-C3'	5.24	128.06	120.20
24	A	228	C	P-O3'-C3'	5.18	127.97	120.20
26	C	52	HIS	N-CA-C	5.17	121.82	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	R	52	PRO	N-CA-C	-5.13	103.71	111.41
1	a	960	U	P-O3'-C3'	5.12	127.87	120.20
44	U	6	ARG	N-CA-C	5.11	121.68	110.80
1	a	1297	G	P-O3'-C3'	5.10	127.85	120.20
5	e	93	VAL	N-CA-CB	-5.10	102.82	111.23
29	F	174	PHE	N-CA-C	5.09	121.07	109.81
10	j	56	HIS	CA-C-N	5.02	131.01	121.97
10	j	56	HIS	C-N-CA	5.02	131.01	121.97
24	A	2610	C	C4'-C3'-O3'	5.01	116.92	109.40
50	0	2	VAL	N-CA-C	5.00	119.75	109.34

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3',C4'
24	A	2069	G7M	C3',C4'

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	0	1	ALA	Peptide,Mainchain
51	1	3	GLY	Mainchain
53	3	30	HIS	Peptide
26	C	120	ASP	Peptide
28	E	82	GLY	Peptide
30	G	117	PRO	Mainchain
30	G	118	ALA	Mainchain
30	G	173	ALA	Mainchain
32	H	2	GLN	Peptide
32	H	8	LYS	Peptide
34	K	34	GLY	Peptide
34	K	89	ASN	Mainchain
34	K	92	GLU	Mainchain
35	L	110	VAL	Mainchain
35	L	28	GLY	Mainchain
35	L	29	LYS	Mainchain
35	L	35	HIS	Mainchain
42	S	64	ALA	Mainchain
44	U	50	ALA	Peptide
44	U	87	GLU	Peptide,Mainchain
48	Y	24	GLU	Mainchain
2	b	16	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	b	17	HIS	Peptide,Mainchain
2	b	72	LYS	Peptide
5	e	121	ASN	Peptide
5	e	76	ASN	Peptide
5	e	88	HIS	Peptide
5	e	92	ARG	Peptide
6	f	52	ASN	Mainchain
7	g	109	LYS	Peptide,Mainchain
8	h	46	GLU	Mainchain
9	i	56	MET	Peptide
10	j	33	GLY	Peptide
10	j	56	HIS	Mainchain
10	j	57	VAL	Mainchain
10	j	91	ASP	Mainchain
10	j	92	LEU	Mainchain
12	l	100	ALA	Peptide
13	m	3	ILE	Peptide
16	p	43	ALA	Peptide
17	q	48	GLU	Mainchain
17	q	68	LYS	Peptide
18	r	10	CYS	Peptide
18	r	11	ARG	Mainchain
18	r	16	GLY	Peptide
19	s	3	SER	Peptide
21	u	8	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33119	0	16685	208	0
2	b	1705	0	1732	15	0
3	c	1625	0	1699	17	0
4	d	1643	0	1710	20	0
5	e	1157	0	1199	15	0
6	f	818	0	808	17	0
7	g	1182	0	1240	12	0
8	h	979	0	1034	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	i	1022	0	1070	15	0
10	j	787	0	828	16	0
11	k	870	0	878	22	0
12	l	955	0	1019	13	0
13	m	884	0	944	12	0
14	n	794	0	836	15	0
15	o	714	0	737	9	0
16	p	649	0	666	11	0
17	q	649	0	691	5	0
18	r	505	0	502	5	0
19	s	638	0	665	9	0
20	t	665	0	714	12	0
21	u	496	0	486	10	0
22	v	1644	0	840	5	0
23	x	1025	0	518	6	0
24	A	62296	0	31354	324	0
25	B	2570	0	1301	11	0
26	C	2083	0	2157	29	0
27	D	1565	0	1616	26	0
28	E	1552	0	1619	18	0
29	F	1411	0	1447	21	0
30	G	1323	0	1374	13	0
31	I	1032	0	1088	8	0
32	H	1111	0	1148	5	0
33	J	1129	0	1162	12	0
34	K	939	0	1012	17	0
35	L	1045	0	1117	17	0
36	M	1074	0	1157	9	0
37	N	961	0	1000	11	0
38	O	892	0	923	4	0
39	P	917	0	965	11	0
40	Q	947	0	1022	8	0
41	R	816	0	839	11	0
42	S	857	0	922	7	0
43	T	739	0	807	4	0
44	U	780	0	834	5	0
45	V	753	0	780	9	0
46	W	575	0	592	8	0
47	X	625	0	655	10	0
48	Y	509	0	543	6	0
49	Z	449	0	491	1	0
50	0	444	0	461	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1	410	0	440	9	0
52	2	377	0	418	6	0
53	3	504	0	574	5	0
54	4	302	0	341	3	0
55	6	523	0	522	13	0
56	4	1	0	0	0	0
56	6	1	0	0	0	0
All	All	146037	0	98182	963	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 (963) 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)
18:r:13:THR:O	18:r:17:VAL:HA	1.68	0.94
1:a:664:G:H22	1:a:741:G:H1	1.26	0.83
30:G:83:THR:HA	30:G:132:LEU:O	1.83	0.79
39:P:88:ARG:HE	39:P:112:ARG:HH21	1.32	0.76
30:G:132:LEU:HB3	30:G:140:ILE:HD11	1.69	0.74
24:A:243:U:OP2	53:3:7:ARG:NH1	2.20	0.73
1:a:1405:G:H21	1:a:1518:MA6:H8	1.53	0.73
1:a:692:U:H5''	11:k:126:ARG:HH22	1.53	0.73
1:a:323:U:OP1	20:t:20:ASN:ND2	2.20	0.73
39:P:59:THR:HG22	39:P:72:VAL:HG12	1.70	0.72
24:A:1646:C:H5'	24:A:1647:U:H5''	1.70	0.72
24:A:2406:A:N3	35:L:69:ARG:NH2	2.38	0.72
1:a:1106:G:O2'	3:c:168:ARG:NH1	2.24	0.71
24:A:1466:U:HO2'	24:A:1546:G:HO2'	1.37	0.70
26:C:86:ARG:HH12	26:C:155:ARG:HH21	1.40	0.69
1:a:110:C:O2'	16:p:25:ARG:O	2.10	0.69
14:n:26:LEU:HA	14:n:30:ILE:HD12	1.75	0.69
24:A:660:C:O2'	35:L:13:LYS:NZ	2.26	0.69
24:A:1312:U:H4'	24:A:1313:U:H5'	1.75	0.69
24:A:1601:G:OP1	43:T:64:LYS:NZ	2.25	0.69
55:6:11:GLU:HA	55:6:25:ARG:HA	1.75	0.69
1:a:875:U:O2'	8:h:14:ARG:NH1	2.27	0.68
1:a:1493[C]:A:O2'	24:A:1913[C]:A:N7	2.26	0.68
24:A:585:G:N7	40:Q:5:ARG:NH1	2.42	0.68
24:A:1568:G:H5'	26:C:59:GLN:HA	1.76	0.67
52:2:12:ARG:HE	52:2:44:VAL:HG21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:127:G:O2'	17:q:5:ARG:NH2	2.27	0.67
29:F:104:THR:HG21	55:6:22:MET:HE1	1.77	0.67
41:R:14:VAL:HG21	41:R:98:ILE:HG13	1.77	0.67
16:p:4:ILE:HG12	16:p:21:VAL:HG22	1.77	0.66
24:A:621:A:OP2	35:L:99:ASN:ND2	2.29	0.66
19:s:10:ILE:HD13	19:s:15:LEU:HB2	1.78	0.66
26:C:141:HIS:ND1	26:C:192:GLY:O	2.24	0.66
24:A:28:A:O2'	40:Q:10:ARG:NH2	2.28	0.65
45:V:48:MET:SD	45:V:51:GLN:NE2	2.69	0.65
10:j:59:LYS:HE2	10:j:62:ARG:HH21	1.60	0.65
1:a:951:G:OP2	13:m:100:ARG:NH2	2.29	0.65
1:a:1143:G:H2'	1:a:1144:G:H8	1.60	0.65
24:A:2478:A:OP2	54:4:2:LYS:NZ	2.30	0.65
2:b:35:ASN:HB3	2:b:37:VAL:HG12	1.78	0.65
27:D:148:GLN:HB2	27:D:152:PRO:HG2	1.77	0.65
10:j:42:LEU:HD11	10:j:73:LEU:HG	1.80	0.64
30:G:82:PHE:O	30:G:133:LYS:HA	1.97	0.64
3:c:29:ALA:HB1	14:n:64:ARG:HH22	1.62	0.64
1:a:1123:U:O2'	10:j:39:PRO:O	2.15	0.64
2:b:23:ASN:ND2	2:b:191:ASP:OD1	2.30	0.64
6:f:7:VAL:HG22	6:f:61:LEU:HG	1.80	0.64
51:1:3:GLY:O	51:1:5:ARG:N	2.29	0.64
16:p:6:LEU:HB3	16:p:17:TYR:HB3	1.79	0.63
21:u:36:PHE:HB3	21:u:40:PRO:HD3	1.79	0.63
24:A:1386:C:H2'	24:A:1387:A:C8	2.33	0.63
6:f:32:ALA:HB1	6:f:67:PRO:HD2	1.80	0.63
32:H:76:GLU:HB3	32:H:142:VAL:HG22	1.81	0.62
24:A:1064:C:O2'	24:A:1075:C:O2	2.16	0.62
24:A:2635:A:O2'	27:D:49:GLN:NE2	2.31	0.62
26:C:169:ALA:O	26:C:185:ALA:N	2.30	0.62
10:j:54:SER:OG	10:j:56:HIS:O	2.14	0.62
5:e:80:LEU:HG	5:e:122:VAL:HG21	1.83	0.61
1:a:958:A:N7	19:s:54:ARG:NH1	2.49	0.61
5:e:89:THR:OG1	5:e:90:GLY:N	2.32	0.61
5:e:35:LEU:HD11	5:e:133:ILE:HG12	1.81	0.61
11:k:125:LYS:O	21:u:34:ARG:NH1	2.31	0.61
24:A:2512:C:O2'	27:D:159:LYS:NZ	2.32	0.61
1:a:407:U:O2'	4:d:112:GLU:OE1	2.16	0.61
1:a:1081:A:OP2	5:e:51:LYS:NZ	2.34	0.61
45:V:45:ASP:O	45:V:49:ASN:ND2	2.33	0.60
1:a:981:U:H4'	14:n:60:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:877:A:O2'	24:A:900:A:N6	2.34	0.60
5:e:156:ARG:NH1	8:h:42:GLU:OE2	2.34	0.60
1:a:118:U:O2'	1:a:121:U:O4	2.18	0.60
24:A:1273:U:O2'	24:A:1275:A:OP1	2.19	0.60
2:b:18:GLN:NE2	2:b:187:ASP:OD2	2.35	0.60
16:p:7:ALA:O	16:p:29:ASN:ND2	2.34	0.60
21:u:16:ARG:HB2	21:u:19:LYS:HD3	1.83	0.60
26:C:140:VAL:HG12	26:C:191:LEU:HD23	1.83	0.60
1:a:750:C:O2'	15:o:20:ASP:OD1	2.19	0.59
1:a:618:C:O2'	16:p:14:ARG:NH1	2.35	0.59
24:A:1817:G:OP1	26:C:86:ARG:NH2	2.35	0.59
24:A:2333:A:OP2	46:W:73:ARG:NH2	2.33	0.59
30:G:46:ASP:OD1	30:G:47:ASN:N	2.29	0.59
24:A:45:G:H5'	24:A:46:G:H5'	1.83	0.59
10:j:52:LEU:HD21	10:j:59:LYS:HD2	1.84	0.59
24:A:219:A:N3	24:A:234:U:O2'	2.35	0.59
8:h:11:THR:O	8:h:15:ASN:ND2	2.34	0.59
1:a:674:G:H2'	1:a:675:A:C8	2.38	0.59
35:L:110:VAL:HG21	35:L:127:VAL:HG22	1.85	0.58
11:k:124:LYS:O	21:u:34:ARG:NH1	2.36	0.58
11:k:19:VAL:HG13	11:k:82:GLU:HB2	1.86	0.58
24:A:2566:A:H61	34:K:28:SER:HB2	1.68	0.58
1:a:235:C:H2'	1:a:236:A:C8	2.37	0.58
1:a:674:G:H2'	1:a:675:A:H8	1.68	0.58
24:A:1342:A:O2'	24:A:1344:U:OP2	2.20	0.58
4:d:46:ARG:O	23:x:113:C:N4	2.31	0.58
1:a:1218:C:H2'	1:a:1219:A:C8	2.39	0.58
30:G:8:VAL:HB	30:G:49:LEU:HB2	1.84	0.58
16:p:14:ARG:HE	16:p:42:ILE:HD12	1.68	0.58
24:A:2676:C:OP1	34:K:31:ARG:NH2	2.37	0.58
8:h:24:VAL:O	8:h:59:GLU:HA	2.04	0.57
24:A:833:A:H2'	24:A:834:G:C8	2.40	0.57
4:d:96:ARG:HH21	4:d:114:ARG:HH21	1.53	0.57
9:i:79:ARG:HD2	9:i:102:PHE:HD1	1.69	0.57
24:A:1140:C:OP2	33:J:68:LYS:NZ	2.37	0.57
31:I:98:GLY:HA3	31:I:137:LEU:HD22	1.86	0.57
34:K:121:GLU:HG2	34:K:122:VAL:HG23	1.86	0.57
1:a:1493[A]:A:H2'	24:A:1913[A]:A:N6	2.19	0.57
30:G:29:ASN:ND2	30:G:80:GLU:O	2.38	0.57
1:a:481:G:O2'	1:a:483:C:N4	2.38	0.57
24:A:320:A:N3	28:E:163:ASN:ND2	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:769:G:H4'	1:a:1513:A:H4'	1.85	0.57
24:A:1801:A:OP2	26:C:149:LYS:NZ	2.38	0.57
24:A:270:A:N1	24:A:369:U:O2'	2.36	0.57
1:a:333:U:OP1	20:t:2:ASN:N	2.38	0.57
1:a:673:A:H5''	6:f:86:ARG:HH21	1.69	0.57
28:E:119:ILE:O	28:E:187:VAL:HA	2.05	0.57
6:f:45:ARG:O	6:f:56:LYS:HA	2.05	0.57
24:A:547:A:O2'	24:A:548:G:N7	2.38	0.57
24:A:1019:U:H3	24:A:1142:A:H62	1.53	0.57
47:X:5:GLN:O	47:X:73:ARG:NH2	2.38	0.56
1:a:1412:C:H2'	1:a:1413:A:C8	2.40	0.56
1:a:946:A:H2'	1:a:947:G:C8	2.41	0.56
1:a:1143:G:H2'	1:a:1144:G:C8	2.39	0.56
3:c:13:ILE:HG22	3:c:14:VAL:HG13	1.86	0.56
24:A:600:G:OP1	28:E:24:ASN:ND2	2.37	0.56
24:A:2720:U:OP1	39:P:52:ARG:NH2	2.38	0.56
35:L:29:LYS:HG2	35:L:30:THR:HG23	1.88	0.56
35:L:82:LEU:HD11	35:L:90:VAL:HG21	1.86	0.56
1:a:692:U:OP1	11:k:126:ARG:NH2	2.39	0.56
24:A:1068:G:O2'	24:A:1070:A:N6	2.38	0.56
24:A:2140:G:H2'	24:A:2141:G:C8	2.41	0.56
24:A:1432:G:H2'	24:A:1433:A:C8	2.41	0.56
35:L:93:ASN:O	35:L:95:LEU:N	2.39	0.56
24:A:281:C:H2'	24:A:282:A:H8	1.71	0.56
24:A:668:A:H2'	24:A:670:A:H62	1.71	0.56
26:C:159:THR:HG23	26:C:176:ARG:HG2	1.87	0.56
34:K:7:MET:HE3	34:K:18:ARG:HG2	1.88	0.56
24:A:1796:U:H2'	24:A:1797:G:H8	1.70	0.56
24:A:1124:G:O2'	54:4:37:GLN:OE1	2.23	0.55
1:a:501:C:H2'	1:a:502:A:C8	2.41	0.55
1:a:691:G:O6	11:k:56:LYS:NZ	2.39	0.55
21:u:40:PRO:HA	21:u:43:GLU:HG2	1.88	0.55
24:A:2394:C:H5''	35:L:63:LYS:HE3	1.87	0.55
27:D:181:ASP:HB2	27:D:186:LEU:HB2	1.88	0.55
47:X:37:PHE:O	47:X:45:PHE:HA	2.07	0.55
1:a:18:C:OP1	5:e:131:ASN:ND2	2.38	0.55
6:f:6:ILE:HB	6:f:62:MET:HB2	1.87	0.55
24:A:819:A:OP2	24:A:1187:G:N2	2.37	0.55
24:A:833:A:H2'	24:A:834:G:H8	1.71	0.55
26:C:23:LEU:HD21	26:C:82:TYR:HB2	1.89	0.55
34:K:21:CYS:HA	34:K:41:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2327:A:H2'	24:A:2328:A:C8	2.41	0.55
53:3:31:ILE:O	53:3:35:LYS:NZ	2.33	0.55
5:e:110:MET:HE1	5:e:126:ALA:HB2	1.89	0.55
11:k:23:HIS:HB3	11:k:30:ILE:HG23	1.88	0.55
24:A:598:U:H2'	24:A:599:A:H8	1.71	0.55
8:h:28:SER:HB3	8:h:56:PRO:HB2	1.88	0.55
24:A:1798:U:OP1	26:C:269:ARG:NH2	2.40	0.55
1:a:269:C:H2'	1:a:270:A:C8	2.43	0.54
1:a:1345:U:OP1	9:i:121:ARG:NH1	2.40	0.54
35:L:111:ILE:HD12	35:L:111:ILE:H	1.71	0.54
1:a:672:U:H2'	1:a:673:A:H8	1.72	0.54
1:a:908:A:H2'	1:a:909:A:C8	2.43	0.54
27:D:121:THR:HG21	27:D:143:PRO:HB3	1.89	0.54
1:a:553:A:O2'	12:l:25:ALA:O	2.18	0.54
9:i:54:VAL:HG11	9:i:93:LEU:HD22	1.90	0.54
24:A:13:A:O2'	24:A:15:G:N7	2.40	0.54
34:K:24:VAL:HG13	34:K:33:ALA:HB2	1.88	0.54
48:Y:24:GLU:HB3	48:Y:46:VAL:HG21	1.90	0.54
7:g:68:VAL:HG12	7:g:134:VAL:HG13	1.90	0.54
19:s:5:LYS:HG3	19:s:6:LYS:HG2	1.89	0.54
36:M:110:GLU:OE2	36:M:114:ARG:NH1	2.40	0.54
24:A:1071:G:H21	24:A:1089:A:HO2'	1.56	0.54
1:a:1356:G:H2'	1:a:1357:A:C8	2.43	0.54
12:l:13:ARG:NH1	12:l:14:LYS:O	2.40	0.54
26:C:16:VAL:HB	26:C:203:VAL:HG22	1.90	0.54
7:g:26:VAL:HG22	7:g:42:VAL:HG21	1.90	0.54
3:c:39:ARG:NH1	3:c:54:ILE:O	2.40	0.53
1:a:340:U:OP2	34:K:98:ARG:NH2	2.41	0.53
24:A:1936:A:H2	24:A:1943:U:H3	1.54	0.53
29:F:28:PRO:HB2	29:F:168:LEU:HD22	1.89	0.53
1:a:1077:G:N2	1:a:1080:A:OP2	2.30	0.53
1:a:1151:A:H1'	10:j:41:PRO:HB2	1.90	0.53
24:A:2297:A:N1	24:A:2321:U:H5	2.06	0.53
1:a:1064:G:O2'	1:a:1190:G:N2	2.40	0.53
24:A:613:A:H4'	24:A:614:A:C8	2.44	0.53
1:a:459:A:H2'	1:a:460:A:C8	2.44	0.53
3:c:19:SER:HB3	3:c:21:TRP:HE1	1.74	0.53
24:A:2849:U:OP1	39:P:92:ARG:NH2	2.41	0.53
29:F:43:ILE:HG21	29:F:78:ILE:HG22	1.90	0.53
1:a:675:A:H1'	11:k:117:HIS:CD2	2.44	0.53
9:i:104:THR:HG22	9:i:106:ASP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2359:C:O2'	53:3:53:ASP:OD2	2.24	0.53
24:A:371:A:N6	24:A:402:A:OP2	2.41	0.53
24:A:1901:A:H4'	26:C:252:LYS:HD3	1.91	0.53
41:R:2:TYR:HA	41:R:14:VAL:O	2.08	0.53
13:m:28:ARG:HH21	13:m:62:PHE:HB2	1.74	0.53
24:A:1386:C:H2'	24:A:1387:A:H8	1.74	0.53
1:a:680:C:O2'	26:C:268:ARG:NH2	2.32	0.53
4:d:155:LYS:HA	4:d:158:LEU:HD12	1.91	0.53
5:e:35:LEU:HD21	5:e:133:ILE:HA	1.91	0.53
24:A:1434:A:H2'	24:A:1435:G:C8	2.44	0.53
13:m:15:VAL:HG23	13:m:16:ILE:HD12	1.91	0.52
24:A:2318:G:O2'	24:A:2321:U:O4	2.27	0.52
14:n:25:GLU:HA	14:n:28:ALA:HB3	1.91	0.52
27:D:25:THR:HG21	27:D:193:VAL:HG22	1.90	0.52
39:P:25:VAL:HG22	39:P:85:VAL:HG22	1.91	0.52
24:A:743:A:O2'	24:A:1659:G:OP1	2.28	0.52
24:A:1791:A:N6	24:A:1828:G:O2'	2.40	0.52
1:a:1363:A:O2'	1:a:1365:G:N7	2.38	0.52
15:o:34:GLN:HB3	15:o:58:MET:HE1	1.90	0.52
11:k:84:MET:SD	11:k:110:THR:OG1	2.64	0.52
29:F:9:ASP:OD1	29:F:9:ASP:N	2.42	0.52
1:a:539:A:H2'	1:a:540:G:C8	2.44	0.52
25:B:78:A:OP2	45:V:14:LYS:NZ	2.40	0.52
1:a:1060:U:OP1	14:n:84:ARG:NH2	2.43	0.52
13:m:10:ASP:OD1	13:m:45:SER:OG	2.26	0.52
1:a:1401:G:O6	1:a:1504:G:N2	2.43	0.52
4:d:22:SER:OG	4:d:23:GLY:N	2.43	0.52
8:h:46:GLU:O	8:h:61:THR:HB	2.10	0.52
1:a:544:G:OP2	4:d:13:ARG:NH1	2.43	0.52
11:k:111:ASP:HB3	21:u:3:ILE:HG23	1.91	0.52
12:l:72:ASN:ND2	12:l:104:SER:OG	2.43	0.52
24:A:1798:U:OP2	26:C:270:ARG:NH2	2.42	0.52
1:a:1279:G:OP1	10:j:9:ARG:NH2	2.40	0.52
1:a:1391:U:H2'	1:a:1392:G:C8	2.45	0.52
32:H:32:PRO:HA	47:X:38:TRP:CD1	2.45	0.52
35:L:76:GLU:HB2	35:L:111:ILE:HD13	1.92	0.52
55:6:37:CYS:SG	55:6:38:SER:N	2.83	0.52
9:i:62:LEU:HD23	9:i:64:ILE:HD11	1.91	0.51
17:q:50:ASN:ND2	17:q:52:CYS:O	2.42	0.51
33:J:18:VAL:HG11	33:J:28:LEU:HD11	1.92	0.51
1:a:1513:A:H2'	1:a:1514:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1405:U:H2'	24:A:1406:U:C6	2.46	0.51
24:A:2511:U:H1'	27:D:130:GLN:HE21	1.76	0.51
14:n:64:ARG:HH21	14:n:77:GLY:HA3	1.75	0.51
1:a:362:G:N2	1:a:365:U:OP2	2.43	0.51
24:A:1045:C:H5''	24:A:1046:A:H5''	1.93	0.51
1:a:501:C:H2'	1:a:502:A:H8	1.74	0.51
1:a:1241:G:H2'	1:a:1242:G:H8	1.75	0.51
24:A:1162:G:O2'	41:R:23:GLU:OE2	2.17	0.51
1:a:1219:A:H2'	1:a:1220:G:C8	2.46	0.51
1:a:1494[C]:G:OP1	24:A:1913[C]:A:N6	2.44	0.51
24:A:1912:A:H62	24:A:1917:PSU:HN3	1.59	0.51
1:a:422:C:O2'	1:a:423:G:N2	2.44	0.51
1:a:1287:A:H2'	1:a:1288:A:C8	2.45	0.51
24:A:1796:U:H2'	24:A:1797:G:C8	2.46	0.51
24:A:2120:G:H2'	24:A:2121:G:C8	2.46	0.51
26:C:131:MET:HG2	26:C:134:ILE:HD12	1.93	0.51
36:M:53:MET:HG3	36:M:116:ALA:HB1	1.93	0.51
15:o:28:VAL:HG11	15:o:66:LEU:HD21	1.92	0.50
18:r:42:ARG:NH2	23:x:91:A:OP1	2.44	0.50
24:A:2120:G:H2'	24:A:2121:G:H8	1.76	0.50
7:g:144:ALA:O	7:g:146:ALA:N	2.43	0.50
24:A:190:A:OP2	47:X:25:LYS:NZ	2.44	0.50
24:A:276:U:H1'	24:A:278:A:H62	1.76	0.50
1:a:393:A:OP2	16:p:12:LYS:NZ	2.42	0.50
2:b:113:LEU:HB2	2:b:143:LEU:HD23	1.93	0.50
24:A:9:G:O2'	24:A:2800:A:N6	2.44	0.50
24:A:771:G:OP2	52:2:11:LYS:NZ	2.44	0.50
1:a:1191:A:OP1	3:c:2:GLN:NE2	2.44	0.50
10:j:8:ILE:HD11	10:j:87:LEU:HD13	1.94	0.50
12:l:82:ARG:HD3	12:l:97:VAL:HG22	1.92	0.50
35:L:90:VAL:HG13	35:L:95:LEU:HD21	1.92	0.50
39:P:74:GLN:HB2	39:P:77:SER:HB2	1.94	0.50
1:a:1144:G:N2	1:a:1146:A:H62	2.10	0.50
29:F:114:ARG:HD2	55:6:47:LYS:HG2	1.93	0.50
46:W:33:ILE:HG22	46:W:34:VAL:HG23	1.92	0.50
5:e:18:ASN:OD1	5:e:19:ARG:N	2.45	0.50
18:r:20:ILE:O	18:r:53:GLN:NE2	2.45	0.50
24:A:594:U:H2'	24:A:595:C:C6	2.47	0.50
30:G:109:SER:OG	30:G:110:HIS:N	2.37	0.50
13:m:18:LEU:HD21	13:m:55:LEU:HD21	1.93	0.50
24:A:52:A:H2'	24:A:53:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:832:U:H2'	24:A:833:A:H8	1.77	0.50
24:A:2136:G:O6	24:A:2156:G:N2	2.45	0.50
24:A:2291:U:H2'	24:A:2292:U:C6	2.47	0.50
26:C:145:MET:HG2	26:C:152:GLN:HG3	1.93	0.50
1:a:299:G:H2'	1:a:300:A:C8	2.47	0.50
22:v:21:A:H61	22:v:46:A:H2'	1.76	0.50
24:A:2515:C:H2'	24:A:2516:A:H8	1.76	0.50
34:K:38:ILE:HD11	34:K:112:PHE:HZ	1.77	0.50
24:A:598:U:H2'	24:A:599:A:C8	2.47	0.50
38:O:40:ILE:HG12	38:O:47:VAL:HG12	1.94	0.50
1:a:147:G:H2'	1:a:148:G:C8	2.47	0.49
1:a:922:G:H2'	1:a:923:A:C8	2.47	0.49
1:a:1071:C:H2'	1:a:1072:G:H8	1.77	0.49
24:A:1558:C:H4'	24:A:1559:U:H5''	1.92	0.49
24:A:1636:U:H2'	24:A:1637:A:H8	1.77	0.49
24:A:2303:G:O2'	29:F:120:SER:O	2.30	0.49
1:a:918:A:H2'	1:a:919:A:C8	2.47	0.49
2:b:86:CYS:SG	2:b:87:ASP:N	2.77	0.49
18:r:36:GLY:O	18:r:62:ARG:NH2	2.44	0.49
24:A:1086:A:O2'	24:A:1103:A:N1	2.38	0.49
24:A:1779:U:H5	24:A:1784:A:N7	2.10	0.49
27:D:13:ARG:HH11	39:P:55:HIS:HA	1.77	0.49
47:X:36:ARG:HG2	47:X:45:PHE:HB3	1.94	0.49
24:A:51:G:N2	24:A:118:A:H62	2.11	0.49
30:G:43:LYS:HB2	30:G:50:THR:HB	1.93	0.49
38:O:30:ARG:HA	38:O:35:ILE:HD12	1.93	0.49
1:a:176:C:H4'	20:t:23:ARG:HH22	1.77	0.49
1:a:399:G:H2'	1:a:400:C:C6	2.47	0.49
1:a:1513:A:H2'	1:a:1514:G:H8	1.77	0.49
24:A:612:G:N2	24:A:614:A:O2'	2.46	0.49
24:A:1036:G:H1	24:A:1119:U:H3	1.61	0.49
1:a:321:A:H2'	1:a:322:C:C6	2.48	0.49
1:a:407:U:H2'	1:a:408:A:H8	1.76	0.49
24:A:583:G:P	40:Q:10:ARG:HH12	2.35	0.49
42:S:58:ALA:O	42:S:62:ASP:HB2	2.11	0.49
1:a:373:A:H2'	1:a:374:A:H8	1.77	0.49
7:g:68:VAL:HG23	7:g:99:ALA:HB1	1.94	0.49
24:A:910:A:N3	24:A:2264:C:O2'	2.46	0.49
28:E:3:LEU:HD13	28:E:120:VAL:HG21	1.94	0.49
1:a:619:U:N3	4:d:130:ASN:OD1	2.29	0.49
3:c:131:ARG:HG2	23:x:116:U:H2'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:69:VAL:HG21	34:K:104:THR:HG21	1.93	0.49
1:a:1004:A:H2'	1:a:1005:A:O4'	2.13	0.49
12:l:28:GLN:HA	12:l:81:ILE:O	2.13	0.49
24:A:1088:A:H61	31:I:134:SER:HB2	1.77	0.49
24:A:1173:U:C4	24:A:1174:U:H1'	2.48	0.49
24:A:2362:C:OP1	53:3:39:ARG:NH1	2.35	0.49
1:a:269:C:H2'	1:a:270:A:H8	1.78	0.49
1:a:736:C:H2'	1:a:737:C:H6	1.76	0.49
1:a:1095:U:P	1:a:1108:G:H1	2.35	0.49
11:k:126:ARG:O	21:u:34:ARG:NH2	2.42	0.49
24:A:1869:G:N2	24:A:1872:A:OP2	2.46	0.49
1:a:331:G:O3'	20:t:2:ASN:ND2	2.43	0.49
6:f:74:LEU:O	6:f:77:THR:OG1	2.26	0.49
11:k:34:THR:HG22	11:k:40:ALA:HA	1.95	0.49
24:A:181:A:H2'	24:A:182:A:C8	2.48	0.49
24:A:196:A:OP2	35:L:47:ARG:NH1	2.43	0.49
24:A:371:A:O3'	47:X:60:LYS:NZ	2.44	0.49
24:A:2537:U:H2'	24:A:2538:C:C6	2.48	0.49
1:a:208:U:HO2'	1:a:211:G:H1	1.61	0.48
24:A:2508:G:H1	24:A:2580:PSU:HN3	1.61	0.48
44:U:24:VAL:HA	44:U:35:VAL:HG22	1.95	0.48
46:W:19:VAL:HG22	46:W:34:VAL:HG22	1.94	0.48
1:a:908:A:H2'	1:a:909:A:H8	1.78	0.48
24:A:500:G:N1	24:A:503:A:OP2	2.46	0.48
24:A:1791:A:H61	24:A:1828:G:HO2'	1.60	0.48
5:e:92:ARG:HB2	5:e:127:TYR:HB2	1.94	0.48
24:A:882:G:H1	24:A:894:U:H3	1.61	0.48
48:Y:24:GLU:O	48:Y:28:LEU:HB2	2.12	0.48
1:a:160:A:H2'	1:a:161:A:O4'	2.13	0.48
1:a:210:C:O2'	1:a:211:G:N2	2.46	0.48
12:l:73:LEU:HD21	12:l:79:ILE:HG21	1.95	0.48
24:A:814:C:H1'	24:A:1225:G:H21	1.77	0.48
50:0:37:HIS:ND1	50:0:38:LEU:O	2.32	0.48
1:a:946:A:H2'	1:a:947:G:H8	1.78	0.48
14:n:34:ASN:ND2	14:n:34:ASN:O	2.46	0.48
24:A:18:U:H2'	24:A:19:A:C8	2.49	0.48
30:G:1:SER:OG	30:G:2:ARG:N	2.46	0.48
1:a:736:C:H2'	1:a:737:C:C6	2.48	0.48
7:g:74:VAL:HA	7:g:87:PRO:HA	1.96	0.48
24:A:2328:A:H2'	24:A:2329:U:C6	2.48	0.48
26:C:154:ALA:HB2	26:C:161:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:539:A:H2'	1:a:540:G:H8	1.78	0.48
9:i:94:ARG:HA	9:i:97:LEU:HB3	1.95	0.48
15:o:45:HIS:C	15:o:47:LYS:H	2.22	0.48
24:A:582:A:H2'	24:A:583:G:H8	1.78	0.48
24:A:832:U:H2'	24:A:833:A:C8	2.49	0.48
24:A:2071:A:H2'	24:A:2072:C:C6	2.49	0.48
30:G:163:TYR:HB2	30:G:166:GLU:HB2	1.96	0.48
36:M:71:LYS:HB3	36:M:93:VAL:O	2.14	0.48
1:a:403:C:OP1	4:d:133:SER:OG	2.22	0.48
8:h:52:GLY:HA3	8:h:56:PRO:HA	1.94	0.48
21:u:64:ALA:C	21:u:66:ARG:H	2.22	0.48
24:A:1013:C:H2'	24:A:1014:A:H8	1.78	0.48
27:D:37:VAL:HG22	27:D:48:ILE:HG22	1.95	0.48
22:v:3:C:H2'	22:v:4:G:H8	1.78	0.48
24:A:1434:A:H2'	24:A:1435:G:H8	1.78	0.48
28:E:49:ARG:HE	28:E:75:SER:HA	1.77	0.48
29:F:24:VAL:O	29:F:27:VAL:HG12	2.14	0.48
39:P:29:VAL:HG12	39:P:80:VAL:HG12	1.96	0.48
24:A:690:G:O2'	24:A:780:G:OP1	2.32	0.48
33:J:13:ARG:HE	33:J:121:LYS:HZ1	1.62	0.48
40:Q:48:ASP:HA	40:Q:51:GLN:HB2	1.95	0.48
1:a:1010:U:H2'	1:a:1011:C:C6	2.49	0.47
9:i:91:GLU:HA	9:i:94:ARG:HB2	1.96	0.47
24:A:581:C:H2'	24:A:582:A:C8	2.48	0.47
30:G:51:PHE:HZ	30:G:71:LEU:HD22	1.79	0.47
1:a:1518:MA6:H103	1:a:1519:MA6:N6	2.29	0.47
9:i:83:THR:HG21	9:i:102:PHE:HB3	1.95	0.47
15:o:26:VAL:O	15:o:30:LEU:HB2	2.14	0.47
26:C:15:VAL:HG22	26:C:205:GLY:HA3	1.96	0.47
27:D:116:LYS:HG3	27:D:165:MET:HE3	1.96	0.47
55:6:58:ASP:N	55:6:58:ASP:OD1	2.47	0.47
1:a:224:U:H2'	1:a:225:C:C6	2.49	0.47
11:k:87:GLY:H	11:k:113:THR:HG22	1.79	0.47
14:n:47:LEU:HD12	14:n:50:LEU:HD12	1.97	0.47
24:A:410:G:H5''	24:A:411:G:H5'	1.95	0.47
24:A:813:U:H2'	24:A:814:C:C6	2.50	0.47
5:e:152:VAL:HG21	8:h:98:LEU:HD13	1.95	0.47
11:k:92:ARG:NH2	11:k:111:ASP:OD1	2.46	0.47
29:F:169:LEU:HB3	29:F:174:PHE:CD2	2.49	0.47
31:I:14:ALA:O	31:I:42:ASN:ND2	2.47	0.47
7:g:12:LEU:HD12	7:g:13:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:49:ALA:HA	19:s:57:VAL:O	2.14	0.47
24:A:1509:A:H2'	24:A:1510:G:C8	2.49	0.47
24:A:2247:A:H2'	24:A:2248:C:H6	1.80	0.47
27:D:125:TRP:CD1	27:D:160:LYS:HB3	2.49	0.47
41:R:76:LYS:HG3	41:R:85:LYS:HE2	1.96	0.47
1:a:447:G:N1	1:a:486:U:OP2	2.45	0.47
10:j:86:ALA:HA	10:j:90:LEU:HD12	1.96	0.47
20:t:29:THR:O	20:t:33:LYS:HB2	2.15	0.47
24:A:1197:G:H2'	24:A:1198:U:H6	1.79	0.47
29:F:5:ASP:O	29:F:8:LYS:N	2.47	0.47
1:a:672:U:H2'	1:a:673:A:C8	2.50	0.47
10:j:53:ILE:HG13	14:n:84:ARG:NE	2.30	0.47
24:A:18:U:H2'	24:A:19:A:H8	1.78	0.47
24:A:281:C:H2'	24:A:282:A:C8	2.48	0.47
24:A:1062:G:H22	24:A:1088:A:H62	1.63	0.47
24:A:1181:U:H2'	24:A:1182:G:C8	2.50	0.47
24:A:1506:U:H2'	24:A:1507:C:C6	2.50	0.47
24:A:1858:A:N6	24:A:1884:G:O2'	2.48	0.47
24:A:2285:C:OP2	51:1:5:ARG:NH1	2.48	0.47
25:B:70:C:H2'	25:B:71:C:H6	1.80	0.47
27:D:22:ILE:HG21	27:D:178:VAL:HG21	1.97	0.47
29:F:5:ASP:OD1	29:F:6:TYR:N	2.48	0.47
29:F:133:GLU:HB3	29:F:135:ILE:HG13	1.97	0.47
39:P:21:PRO:HD3	39:P:49:ILE:HD12	1.96	0.47
1:a:216:U:H2'	1:a:217:C:C6	2.49	0.47
1:a:1098:C:OP1	2:b:138:ARG:NH2	2.48	0.47
24:A:2554:U:H2'	24:A:2555:U:C6	2.50	0.47
1:a:1523:G:H5''	11:k:124:LYS:HE2	1.97	0.47
6:f:12:PRO:O	6:f:44:ARG:NH2	2.48	0.47
24:A:1263:U:H5''	50:0:12:ARG:HD3	1.97	0.47
24:A:1509:A:H2'	24:A:1510:G:H8	1.79	0.47
46:W:29:ALA:N	46:W:60:ASP:OD1	2.48	0.47
1:a:981:U:OP1	14:n:8:ARG:NH1	2.48	0.47
2:b:187:ASP:OD1	2:b:188:THR:N	2.46	0.47
9:i:41:GLU:O	9:i:44:ARG:HB3	2.15	0.47
11:k:108:ASN:HB3	21:u:6:ARG:HG2	1.97	0.47
27:D:156:PHE:CG	33:J:81:ILE:HD12	2.50	0.47
1:a:158:G:N2	1:a:163:C:O2	2.38	0.46
1:a:177:G:OP1	20:t:59:ARG:NH1	2.48	0.46
1:a:337:G:H2'	1:a:338:A:H8	1.78	0.46
24:A:2339:C:H2'	24:A:2340:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:117:ARG:NH2	28:E:183:PHE:O	2.47	0.46
1:a:1403:C:O2'	1:a:1499:A:N1	2.48	0.46
9:i:122:ARG:NH1	9:i:123:ARG:O	2.48	0.46
24:A:532:A:H5'	40:Q:27:ARG:HH12	1.79	0.46
24:A:1156:A:C8	40:Q:50:ARG:HD3	2.50	0.46
24:A:2051:A:H4'	27:D:146:ILE:HG12	1.96	0.46
27:D:125:TRP:CG	27:D:160:LYS:HB3	2.50	0.46
29:F:30:VAL:HG23	29:F:155:ILE:HG23	1.97	0.46
30:G:37:ASN:OD1	30:G:38:ASP:N	2.49	0.46
32:H:11:ASN:CG	32:H:12:LEU:H	2.23	0.46
1:a:533:A:O2'	1:a:535:A:OP2	2.28	0.46
1:a:1317:C:H4'	14:n:47:LEU:HD21	1.97	0.46
17:q:29:LYS:HA	17:q:36:PHE:HA	1.97	0.46
26:C:132:ARG:O	26:C:166:ARG:NH1	2.48	0.46
28:E:47:LYS:HB2	28:E:51:GLU:HG2	1.96	0.46
1:a:960:U:H4'	1:a:961:U:O5'	2.14	0.46
6:f:32:ALA:HB2	6:f:70:VAL:HG11	1.97	0.46
12:l:74:GLN:O	12:l:76:HIS:N	2.49	0.46
24:A:927:A:H2'	24:A:928:A:C8	2.50	0.46
24:A:947:A:H2'	24:A:948:C:C6	2.49	0.46
24:A:1071:G:N2	24:A:1089:A:O2'	2.39	0.46
24:A:1697:G:H4'	24:A:1978:A:H5''	1.97	0.46
38:O:33:ARG:HG2	38:O:34:HIS:CD2	2.51	0.46
1:a:714:G:H2'	1:a:715:A:C8	2.50	0.46
24:A:783:A:H2'	24:A:784:G:H5'	1.98	0.46
24:A:856:G:H2'	24:A:857:G:C8	2.50	0.46
24:A:1223:G:OP1	41:R:68:ARG:NH2	2.49	0.46
29:F:127:TYR:HE2	29:F:129:MET:HE2	1.81	0.46
1:a:707:U:H4'	11:k:21:HIS:ND1	2.31	0.46
24:A:968:C:H2'	24:A:969:G:H8	1.80	0.46
24:A:1287:A:H5'	37:N:103:ARG:NH1	2.31	0.46
27:D:46:ARG:HB3	27:D:84:LEU:HD12	1.97	0.46
1:a:718:A:OP1	1:a:720:C:N4	2.48	0.46
24:A:624:C:O2'	24:A:657:U:H5''	2.16	0.46
24:A:2591:C:H2'	24:A:2592:G:C8	2.51	0.46
36:M:21:ALA:HB2	36:M:97:GLN:HB2	1.98	0.46
1:a:518:C:N4	1:a:530:G:N7	2.64	0.46
6:f:9:MET:HB3	6:f:57:ALA:HB1	1.97	0.46
24:A:1266:G:O2'	24:A:2012:G:O6	2.34	0.46
24:A:1806:C:H1'	26:C:43:ASN:HD21	1.81	0.46
24:A:2098:U:H2'	24:A:2099:U:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2271:G:H5'	46:W:16:ARG:HG2	1.98	0.46
29:F:102:LEU:O	29:F:106:ALA:HB3	2.15	0.46
24:A:250:G:H2'	24:A:251:A:C8	2.51	0.46
24:A:1790:C:H2'	24:A:1791:A:C5	2.51	0.46
25:B:28:C:H2'	25:B:29:A:C8	2.51	0.46
34:K:76:VAL:H	39:P:72:VAL:HG22	1.80	0.46
48:Y:17:GLU:HB2	48:Y:53:VAL:HG11	1.98	0.46
1:a:1039:G:H2'	1:a:1040:U:C6	2.51	0.46
4:d:124:VAL:HG22	4:d:142:VAL:HG22	1.98	0.46
22:v:3:C:H2'	22:v:4:G:C8	2.51	0.46
24:A:2187:U:H2'	24:A:2188:U:C6	2.51	0.46
35:L:29:LYS:O	35:L:31:GLY:N	2.49	0.46
38:O:29:HIS:HB3	38:O:36:TYR:HB2	1.98	0.46
1:a:384:G:H2'	1:a:385:C:C6	2.52	0.45
1:a:552:U:H2'	1:a:553:A:H8	1.81	0.45
24:A:1022:G:H22	24:A:1142:A:H2	1.65	0.45
24:A:1847:A:O2'	24:A:1848:A:H8	1.98	0.45
28:E:18:THR:HA	28:E:106:LYS:HE3	1.98	0.45
33:J:36:LEU:HD22	33:J:121:LYS:HB2	1.98	0.45
1:a:602:A:H2'	1:a:603:U:C6	2.51	0.45
1:a:841:C:O2'	1:a:843:U:O4'	2.33	0.45
2:b:163:ILE:HD11	2:b:209:VAL:HG11	1.98	0.45
12:l:65:TYR:HB2	12:l:92:VAL:HG11	1.98	0.45
19:s:67:GLY:H	55:6:56:ARG:NH1	2.14	0.45
24:A:279:A:N6	24:A:361:G:H1'	2.31	0.45
24:A:608:A:H2'	24:A:609:A:C8	2.52	0.45
1:a:519:C:H2'	1:a:520:A:O4'	2.16	0.45
1:a:677:U:H3	1:a:713:G:H22	1.63	0.45
24:A:1569:A:H2'	24:A:1570:A:C8	2.51	0.45
24:A:2230:G:H2'	24:A:2231:U:C6	2.51	0.45
24:A:2768:U:O2'	33:J:95:ARG:NH2	2.49	0.45
3:c:152:VAL:HG12	3:c:197:VAL:HG22	1.99	0.45
24:A:581:C:H2'	24:A:582:A:H8	1.81	0.45
24:A:969:G:H2'	24:A:970:U:C6	2.52	0.45
33:J:109:LEU:HD13	33:J:118:MET:HG3	1.98	0.45
1:a:263:A:H2'	1:a:264:C:C6	2.51	0.45
1:a:449:G:H2'	1:a:450:G:C8	2.51	0.45
1:a:878:A:H5'	8:h:80:PRO:HG2	1.98	0.45
6:f:29:ILE:HG21	6:f:64:VAL:HG21	1.98	0.45
24:A:2059:A:C8	24:A:2503:2MA:HM22	2.52	0.45
24:A:2788:C:H2'	24:A:2789:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:114:GLU:HG2	32:H:134:VAL:HG12	1.98	0.45
43:T:80:TRP:CZ3	43:T:82:LYS:HB3	2.52	0.45
1:a:208:U:O2'	1:a:211:G:N1	2.44	0.45
19:s:30:LEU:HD13	19:s:48:ILE:HG22	1.98	0.45
20:t:26:MET:O	20:t:29:THR:OG1	2.26	0.45
21:u:3:ILE:HD11	21:u:23:GLU:HG3	1.98	0.45
24:A:848:C:H2'	24:A:849:A:C8	2.51	0.45
26:C:52:HIS:O	26:C:216:ARG:N	2.45	0.45
36:M:102:LEU:HD11	36:M:126:ILE:HD11	1.99	0.45
1:a:900:A:H2'	1:a:901:A:C8	2.51	0.45
1:a:1347:G:H22	1:a:1373:G:H2'	1.81	0.45
1:a:1477:U:H2'	1:a:1478:U:C6	2.52	0.45
9:i:93:LEU:O	9:i:97:LEU:HB2	2.16	0.45
14:n:80:ARG:HA	14:n:83:VAL:HG12	1.98	0.45
24:A:28:A:N6	24:A:512:G:H1'	2.31	0.45
24:A:910:A:H2'	24:A:911:A:C8	2.51	0.45
24:A:1736:U:H2'	24:A:1737:G:O4'	2.17	0.45
24:A:1759:A:HO2'	24:A:2714:G:HO2'	1.65	0.45
25:B:66:A:O2'	25:B:67:G:O5'	2.34	0.45
29:F:140:ILE:HG22	29:F:142:TYR:H	1.80	0.45
15:o:17:ASP:N	15:o:17:ASP:OD1	2.49	0.45
24:A:126:A:H5'	52:2:19:ARG:HG3	1.97	0.45
24:A:151:C:H2'	24:A:152:A:H8	1.80	0.45
31:I:85:ILE:HD11	31:I:99:LYS:H	1.82	0.45
34:K:109:SER:O	34:K:111:LYS:N	2.50	0.45
1:a:1414:U:H2'	1:a:1415:G:H8	1.82	0.45
1:a:1486:G:H2'	1:a:1487:G:O4'	2.16	0.45
24:A:247:G:O2'	24:A:386:G:N1	2.49	0.45
24:A:1060:U:N3	24:A:1088:A:N7	2.56	0.45
37:N:37:THR:HG22	37:N:110:MET:HE1	1.98	0.45
4:d:169:TRP:CD1	4:d:185:PRO:HG3	2.52	0.45
7:g:111:GLY:HA2	7:g:118:ARG:HD3	1.99	0.45
20:t:4:LYS:HG3	20:t:6:ALA:H	1.82	0.45
24:A:635:C:H2'	24:A:636:G:O4'	2.16	0.45
24:A:782:A:C6	26:C:224:MET:HE2	2.52	0.45
24:A:859:G:O2'	24:A:916:G:O6	2.28	0.45
24:A:1047:G:H2'	24:A:1110:G:C2	2.52	0.45
51:1:8:ILE:HD13	51:1:24:LYS:HE3	1.98	0.45
24:A:575:A:OP2	24:A:2055:C:N4	2.49	0.44
24:A:1932:A:H2'	24:A:1933:G:O4'	2.17	0.44
24:A:2291:U:OP1	24:A:2380:C:O2'	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:15:SER:HB2	28:E:18:THR:HB	1.99	0.44
47:X:38:TRP:NE1	47:X:40:GLU:OE1	2.50	0.44
1:a:715:A:H2'	1:a:716:A:C8	2.53	0.44
1:a:779:C:O2'	11:k:121:ARG:NH1	2.49	0.44
1:a:1347:G:N2	1:a:1373:G:H2'	2.32	0.44
3:c:163:ARG:NE	23:x:111:G:H1	2.15	0.44
9:i:31:GLN:NE2	9:i:63:TYR:OH	2.51	0.44
24:A:1433:A:H2'	24:A:1434:A:C8	2.53	0.44
24:A:2024:G:O3'	27:D:154:LYS:NZ	2.44	0.44
28:E:143:LEU:HB3	28:E:146:VAL:HG11	1.99	0.44
31:I:89:SER:HB2	31:I:135:MET:O	2.18	0.44
36:M:69:PRO:HA	36:M:94:ALA:HB2	1.98	0.44
52:2:12:ARG:NE	52:2:44:VAL:HG21	2.29	0.44
55:6:30:HIS:ND1	55:6:31:ASP:OD1	2.41	0.44
1:a:54:C:H2'	1:a:352:C:H41	1.81	0.44
1:a:413:G:H22	1:a:428:G:H1'	1.83	0.44
12:l:33:CYS:HA	12:l:54:VAL:HG22	1.99	0.44
24:A:482:A:N6	24:A:506:G:O2'	2.50	0.44
24:A:2415:G:H2'	24:A:2416:C:C6	2.53	0.44
24:A:2655:G:O2'	24:A:2664:G:O6	2.27	0.44
1:a:1014:A:H4'	19:s:13:HIS:CE1	2.52	0.44
3:c:19:SER:HB3	3:c:21:TRP:NE1	2.33	0.44
11:k:87:GLY:N	11:k:113:THR:HG22	2.32	0.44
12:l:72:ASN:HD21	12:l:104:SER:H	1.66	0.44
13:m:2:ARG:HH12	55:6:36:VAL:HG22	1.82	0.44
24:A:1802:A:H2'	24:A:1803:A:C8	2.53	0.44
1:a:553:A:H2'	1:a:554:A:H8	1.83	0.44
1:a:728:A:H2'	1:a:729:A:C8	2.52	0.44
3:c:109:GLU:HB2	3:c:143:LEU:HD11	1.99	0.44
24:A:2140:G:H2'	24:A:2141:G:H8	1.83	0.44
24:A:2859:G:H2'	24:A:2860:A:C8	2.53	0.44
48:Y:39:GLN:N	48:Y:39:GLN:OE1	2.50	0.44
24:A:582:A:H2'	24:A:583:G:C8	2.53	0.44
26:C:161:VAL:HG11	26:C:173:LEU:HD13	1.98	0.44
28:E:149:ILE:HD11	28:E:172:ALA:HA	1.99	0.44
37:N:24:MET:HE3	37:N:44:LEU:HD22	2.00	0.44
44:U:52:ASN:OD1	44:U:53:GLN:N	2.51	0.44
51:1:35:LEU:HD13	51:1:37:LYS:HE2	2.00	0.44
1:a:1172:C:H2'	1:a:1173:U:C6	2.53	0.44
24:A:968:C:H2'	24:A:969:G:C8	2.53	0.44
24:A:1723:G:H2'	24:A:1724:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2395:C:H2'	24:A:2396:G:O4'	2.18	0.44
29:F:141:ASP:C	29:F:143:ASP:H	2.26	0.44
41:R:63:VAL:HG22	41:R:96:VAL:HG12	2.00	0.44
1:a:740:U:OP1	15:o:37:HIS:NE2	2.45	0.44
2:b:56:LEU:HD13	2:b:216:VAL:HG13	1.99	0.44
6:f:2:ARG:HD3	6:f:92:THR:HG21	2.00	0.44
20:t:59:ARG:O	20:t:63:LYS:HG2	2.18	0.44
24:A:1443:U:H2'	24:A:1444:G:H8	1.82	0.44
24:A:2015:A:C6	50:0:2:VAL:HG23	2.53	0.44
24:A:443:A:C4	28:E:40:ARG:HD3	2.53	0.44
24:A:1654:A:OP2	37:N:1:MET:N	2.51	0.44
24:A:2033:A:O2'	24:A:2035:G:OP2	2.31	0.44
25:B:114:C:H2'	25:B:115:A:H8	1.83	0.44
29:F:3:LEU:O	29:F:6:TYR:HB3	2.18	0.44
1:a:20:U:H2'	1:a:21:G:O4'	2.19	0.43
1:a:102:G:H2'	1:a:103:U:C6	2.53	0.43
1:a:414:A:OP2	1:a:428:G:N2	2.49	0.43
1:a:1152:A:OP1	10:j:70:HIS:NE2	2.50	0.43
1:a:1223:C:H5''	1:a:1224:U:H5''	1.99	0.43
1:a:1244:G:H2'	1:a:1245:C:C6	2.52	0.43
24:A:742:A:H2'	24:A:743:A:C8	2.53	0.43
24:A:871:U:H2'	24:A:872:U:C6	2.52	0.43
29:F:72:SER:OG	29:F:80:GLN:N	2.50	0.43
33:J:43:GLU:OE1	33:J:43:GLU:N	2.49	0.43
35:L:29:LYS:C	35:L:31:GLY:H	2.25	0.43
55:6:3:LYS:HB3	55:6:4:ASP:H	1.62	0.43
55:6:22:MET:HE2	55:6:22:MET:HB3	1.79	0.43
1:a:337:G:H2'	1:a:338:A:C8	2.53	0.43
1:a:621:A:H2'	1:a:622:A:C8	2.52	0.43
14:n:12:ARG:O	14:n:16:ALA:CB	2.66	0.43
24:A:370:G:O2'	24:A:424:G:OP1	2.36	0.43
24:A:1316:U:H2'	24:A:1317:G:H8	1.83	0.43
28:E:94:GLN:N	28:E:94:GLN:OE1	2.51	0.43
37:N:10:LEU:O	37:N:12:ARG:HG3	2.19	0.43
1:a:1007:U:H2'	1:a:1008:U:H6	1.83	0.43
1:a:1425:U:H2'	1:a:1426:G:H8	1.83	0.43
24:A:588:U:H2'	24:A:589:U:C6	2.53	0.43
24:A:1289:C:H2'	24:A:1290:C:C6	2.53	0.43
24:A:2584:U:H2'	24:A:2585:U:H5''	2.00	0.43
24:A:2623:G:H2'	24:A:2624:G:H8	1.84	0.43
24:A:2699:C:H2'	24:A:2700:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:15:GLY:O	34:K:47:ILE:HG12	2.17	0.43
46:W:20:LYS:O	46:W:21:ARG:NH1	2.50	0.43
1:a:255:G:H2'	1:a:256:U:C6	2.53	0.43
1:a:825:A:O2'	8:h:8:ASP:OD1	2.35	0.43
1:a:1492[C]:A:H3'	1:a:1493[C]:A:H8	1.84	0.43
24:A:7:G:H2'	24:A:8:C:C6	2.54	0.43
24:A:1412:U:H2'	24:A:1413:A:H8	1.84	0.43
24:A:1474:U:O4	24:A:1475:G:N2	2.52	0.43
24:A:2543:G:H21	24:A:2646:C:H5''	1.83	0.43
5:e:110:MET:HE3	5:e:110:MET:HB2	1.91	0.43
22:v:18:G:H1	22:v:55:PSU:H6	1.66	0.43
24:A:304:U:H2'	24:A:305:C:C6	2.53	0.43
24:A:2324:U:H5''	24:A:2325:G:H5''	2.01	0.43
24:A:2347:C:H2'	24:A:2348:U:C6	2.53	0.43
33:J:49:ASP:HB2	33:J:114:LEU:HD11	2.00	0.43
42:S:4:ILE:HG22	42:S:106:VAL:HG22	2.01	0.43
54:4:16:ILE:HD13	54:4:25:VAL:HG22	2.01	0.43
1:a:1437:A:H2'	1:a:1438:G:H8	1.82	0.43
4:d:123:MET:HA	4:d:128:VAL:HA	2.01	0.43
6:f:77:THR:O	6:f:81:ASN:HB2	2.18	0.43
17:q:56:ASP:HB3	17:q:81:ALA:H	1.82	0.43
24:A:287:G:H2'	24:A:288:U:C6	2.53	0.43
24:A:2411:A:H2'	24:A:2412:A:C8	2.54	0.43
24:A:2557:G:H2'	24:A:2558:C:C6	2.53	0.43
24:A:2830:C:H5''	27:D:56:LYS:NZ	2.34	0.43
25:B:105:G:H2'	25:B:106:G:H8	1.84	0.43
31:I:34:ILE:HA	31:I:37:PHE:HD2	1.84	0.43
1:a:1038:C:H2'	1:a:1039:G:C8	2.53	0.43
3:c:68:HIS:HD2	3:c:103:ALA:HB3	1.84	0.43
8:h:76:ARG:NH1	8:h:125:ILE:HG23	2.33	0.43
24:A:483:A:C8	44:U:44:HIS:HD2	2.37	0.43
24:A:566:U:H5''	35:L:29:LYS:HE3	2.01	0.43
24:A:1138:G:N2	33:J:108:MET:SD	2.77	0.43
53:3:22:LYS:HA	53:3:47:ALA:O	2.18	0.43
2:b:56:LEU:HD23	2:b:59:ILE:HD11	2.01	0.43
24:A:319:G:H22	24:A:323:C:H5	1.65	0.43
24:A:364:C:H2'	24:A:365:U:C6	2.53	0.43
24:A:1353:A:H2'	24:A:1354:A:C8	2.53	0.43
24:A:1412:U:H2'	24:A:1413:A:C8	2.54	0.43
24:A:1478:G:H1	24:A:1513:U:H3	1.66	0.43
24:A:2074:U:H2'	24:A:2075:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2485:G:H5''	36:M:45:GLN:HE21	1.84	0.43
24:A:2784:U:H2'	24:A:2785:C:H6	1.84	0.43
34:K:21:CYS:SG	34:K:22:ILE:N	2.91	0.43
1:a:1391:U:H2'	1:a:1392:G:H8	1.84	0.43
20:t:34:VAL:HG11	20:t:78:LEU:HD21	2.01	0.43
24:A:308:G:H2'	24:A:309:A:C8	2.54	0.43
24:A:771:G:OP1	52:2:14:ARG:NH2	2.52	0.43
24:A:1082:U:O2	24:A:1086:A:N6	2.52	0.43
24:A:1184:U:OP2	49:Z:30:ARG:NH1	2.52	0.43
24:A:1248:G:P	28:E:44:ARG:HH12	2.42	0.43
24:A:1258:U:H2'	24:A:1259:G:C8	2.54	0.43
24:A:1264:A:H5'	50:0:7:PRO:HG2	2.00	0.43
33:J:95:ARG:HG2	33:J:96:ARG:HG2	2.00	0.43
44:U:3:LYS:O	44:U:93:ARG:NH2	2.48	0.43
45:V:9:ARG:HG2	45:V:41:GLU:HB2	2.00	0.43
48:Y:21:LEU:HA	48:Y:25:GLN:HB3	2.00	0.43
1:a:499:A:H61	1:a:547:A:H5''	1.82	0.43
1:a:509:A:N3	1:a:543:U:O2'	2.50	0.43
1:a:1329:A:H5''	13:m:25:GLY:N	2.34	0.43
24:A:1326:U:O2'	24:A:2010:G:O2'	2.34	0.43
37:N:78:LYS:O	37:N:82:GLU:HB2	2.19	0.43
1:a:230:G:H4'	16:p:25:ARG:HH22	1.84	0.42
1:a:447:G:O2'	1:a:487:A:N6	2.52	0.42
1:a:553:A:H2'	1:a:554:A:C8	2.54	0.42
4:d:96:ARG:NH2	4:d:114:ARG:HH21	2.17	0.42
9:i:79:ARG:HD2	9:i:102:PHE:CD1	2.53	0.42
9:i:115:VAL:HG23	10:j:62:ARG:HH11	1.84	0.42
13:m:26:LYS:O	13:m:29:SER:OG	2.37	0.42
24:A:848:C:H2'	24:A:849:A:H8	1.84	0.42
24:A:1437:C:HO2'	24:A:1516:G:HO2'	1.62	0.42
24:A:1683:U:H2'	24:A:1684:G:C8	2.53	0.42
24:A:1704:C:H2'	24:A:1705:A:C8	2.54	0.42
24:A:2513:A:H2'	24:A:2514:U:C6	2.54	0.42
26:C:242:HIS:HA	26:C:243:PRO:HD3	1.90	0.42
42:S:44:ALA:HA	42:S:47:VAL:HG12	2.01	0.42
55:6:44:PHE:CD1	55:6:45:THR:HG23	2.53	0.42
2:b:185:ILE:HA	2:b:199:ILE:HB	2.00	0.42
4:d:105:GLY:HA3	4:d:161:ALA:HB2	2.01	0.42
24:A:172:A:H2'	24:A:173:A:H8	1.84	0.42
24:A:560:C:O2'	40:Q:47:ARG:NH2	2.49	0.42
24:A:1679:A:H2'	24:A:1680:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1693:U:OP2	24:A:1694:C:N4	2.48	0.42
24:A:2800:A:C2	24:A:2895:G:H1'	2.54	0.42
34:K:35:VAL:HG13	34:K:69:VAL:HG11	2.00	0.42
37:N:45:ARG:HG2	37:N:95:THR:HG21	1.99	0.42
45:V:32:GLY:H	45:V:93:ARG:HH21	1.67	0.42
1:a:429:U:H3'	4:d:21:LYS:HE2	2.01	0.42
2:b:144:GLU:O	2:b:148:GLY:HA3	2.18	0.42
5:e:32:PHE:CD2	5:e:55:VAL:HG23	2.54	0.42
24:A:1443:U:H2'	24:A:1444:G:C8	2.55	0.42
24:A:1915:3TD:H10A	24:A:1916:A:C6	2.55	0.42
24:A:2861:U:H2'	24:A:2862:G:H8	1.84	0.42
27:D:131:ASP:O	27:D:136:ASN:ND2	2.52	0.42
36:M:74:THR:HA	36:M:89:VAL:HA	2.01	0.42
41:R:77:PHE:HD1	41:R:84:ARG:HB3	1.85	0.42
47:X:34:SER:HA	47:X:48:LEU:O	2.18	0.42
3:c:19:SER:HA	3:c:56:ILE:O	2.18	0.42
6:f:15:SER:OG	6:f:44:ARG:NH2	2.53	0.42
9:i:3:ASN:CG	9:i:4:GLN:H	2.28	0.42
24:A:1636:U:H2'	24:A:1637:A:C8	2.54	0.42
27:D:48:ILE:O	27:D:81:GLU:HA	2.19	0.42
28:E:3:LEU:HD21	28:E:19:PHE:HE2	1.85	0.42
37:N:20:MET:HE3	37:N:20:MET:HB2	1.77	0.42
41:R:49:ILE:HD12	41:R:52:PRO:HA	2.01	0.42
42:S:41:LYS:H	42:S:41:LYS:HG2	1.63	0.42
47:X:36:ARG:HG3	47:X:47:THR:OG1	2.19	0.42
1:a:285:C:H2'	1:a:286:C:C6	2.54	0.42
1:a:523:A:N6	12:l:49:ARG:HH12	2.17	0.42
1:a:721:G:H4'	1:a:722:G:O4'	2.20	0.42
1:a:1007:U:H2'	1:a:1008:U:C6	2.54	0.42
1:a:1326:U:H2'	1:a:1327:C:C6	2.53	0.42
2:b:22:TRP:CZ3	2:b:24:PRO:HA	2.54	0.42
6:f:29:ILE:HD13	6:f:64:VAL:HG21	2.02	0.42
10:j:52:LEU:HD23	10:j:52:LEU:HA	1.89	0.42
19:s:64:GLU:O	55:6:56:ARG:NH2	2.52	0.42
20:t:17:ARG:HA	20:t:20:ASN:HB3	2.01	0.42
24:A:739:A:H1'	24:A:740:C:H5	1.84	0.42
24:A:2627:G:O2'	24:A:2781:A:N1	2.43	0.42
3:c:184:ASN:OD1	3:c:185:THR:N	2.53	0.42
24:A:172:A:H2'	24:A:173:A:C8	2.55	0.42
24:A:306:U:H2'	24:A:307:G:O4'	2.19	0.42
24:A:639:U:H2'	24:A:640:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2233:U:H2'	24:A:2234:G:C8	2.54	0.42
24:A:2446:G:H2'	24:A:2447:G:H5''	2.01	0.42
24:A:2684:U:O4'	34:K:70:ARG:NH1	2.53	0.42
25:B:30:C:H2'	25:B:31:C:H5'	2.02	0.42
27:D:84:LEU:HA	27:D:84:LEU:HD23	1.85	0.42
51:1:4:ILE:H	51:1:4:ILE:HG13	1.61	0.42
1:a:985:C:H2'	1:a:986:U:C6	2.55	0.42
1:a:1247:U:O2	1:a:1290:G:O6	2.37	0.42
13:m:47:LEU:HD22	13:m:52:ILE:HG13	2.01	0.42
22:v:53:G:H3'	22:v:54:5MU:H73	2.02	0.42
24:A:549:G:H2'	24:A:550:C:C6	2.54	0.42
24:A:1410:G:H2'	24:A:1411:U:H6	1.83	0.42
24:A:1837:C:H2'	24:A:1899:A:H61	1.84	0.42
28:E:143:LEU:HD13	28:E:146:VAL:HG11	2.01	0.42
37:N:30:ARG:HG2	37:N:31:HIS:CD2	2.55	0.42
1:a:88:U:H2'	1:a:89:U:C5	2.55	0.42
1:a:147:G:H2'	1:a:148:G:H8	1.85	0.42
1:a:151:A:H2'	1:a:152:A:O4'	2.20	0.42
1:a:1371:G:H2'	1:a:1372:U:C6	2.55	0.42
3:c:91:ALA:HB1	3:c:96:VAL:HG22	2.01	0.42
6:f:90:MET:HB3	6:f:91:ARG:H	1.72	0.42
8:h:54:THR:HG23	8:h:55:LYS:HG3	2.01	0.42
24:A:619:G:OP2	24:A:620:G:N2	2.50	0.42
25:B:35:C:H2'	25:B:36:C:O4'	2.19	0.42
27:D:13:ARG:HA	27:D:22:ILE:O	2.19	0.42
1:a:503:C:O2'	1:a:510:A:N1	2.50	0.42
8:h:42:GLU:HG2	8:h:100:ILE:HG12	2.02	0.42
16:p:20:VAL:HG23	16:p:35:ARG:HA	2.01	0.42
16:p:70:ARG:HA	16:p:70:ARG:HD2	1.79	0.42
24:A:144:A:H2'	24:A:145:C:C6	2.55	0.42
24:A:527:C:C4	24:A:2779:U:H2'	2.54	0.42
24:A:1199:U:H2'	24:A:1200:C:C6	2.54	0.42
24:A:1683:U:H2'	24:A:1684:G:H8	1.84	0.42
24:A:2164:C:H41	24:A:2171:A:H61	1.68	0.42
24:A:2696:U:H2'	24:A:2697:G:C8	2.55	0.42
28:E:189:THR:HG22	28:E:191:ASP:H	1.85	0.42
1:a:399:G:H2'	1:a:400:C:H6	1.85	0.42
1:a:577:G:H2'	1:a:578:C:C6	2.54	0.42
6:f:23:GLU:O	6:f:26:THR:HG22	2.19	0.42
24:A:372:G:P	47:X:60:LYS:HZ1	2.42	0.42
24:A:1028:A:N3	24:A:2486:C:O2'	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1669:A:O3'	24:A:2549:G:H5'	2.19	0.42
35:L:82:LEU:HD21	35:L:120:VAL:HG11	2.02	0.42
37:N:103:ARG:NH2	37:N:110:MET:SD	2.93	0.42
45:V:31:TYR:HB3	45:V:37:PRO:HB3	2.02	0.42
1:a:34:C:H2'	1:a:35:G:H8	1.84	0.41
1:a:680:C:H2'	1:a:681:A:H8	1.85	0.41
10:j:8:ILE:HB	10:j:74:VAL:HB	2.01	0.41
10:j:52:LEU:HB2	14:n:80:ARG:HD2	2.02	0.41
24:A:692:C:H2'	24:A:693:A:C8	2.55	0.41
24:A:1424:G:H2'	24:A:1425:G:O4'	2.20	0.41
24:A:1794:A:H2'	24:A:1795:C:C6	2.55	0.41
25:B:5:U:H2'	25:B:6:G:H8	1.86	0.41
25:B:93:C:H2'	25:B:94:A:C8	2.55	0.41
27:D:51:THR:HG21	27:D:68:PHE:HE1	1.85	0.41
41:R:76:LYS:HB2	41:R:85:LYS:HB3	2.02	0.41
55:6:20:ASN:HD22	55:6:39:LYS:HE2	1.84	0.41
1:a:381:C:H2'	1:a:382:A:O4'	2.19	0.41
7:g:14:ASP:HB2	7:g:23:ALA:HB2	2.02	0.41
14:n:11:LYS:HE2	14:n:11:LYS:HB2	1.85	0.41
24:A:415:A:H2'	24:A:416:U:C6	2.55	0.41
24:A:438:G:H2'	24:A:439:A:C8	2.54	0.41
24:A:660:C:OP1	28:E:94:GLN:HB2	2.21	0.41
24:A:1197:G:H2'	24:A:1198:U:C6	2.55	0.41
24:A:2394:C:OP1	35:L:63:LYS:HG2	2.20	0.41
26:C:86:ARG:NH1	26:C:155:ARG:HH21	2.14	0.41
1:a:10:A:H2'	1:a:11:G:C8	2.55	0.41
13:m:84:CYS:HB3	19:s:73:PHE:HE1	1.84	0.41
13:m:94:LEU:HB3	13:m:95:PRO:HD2	2.01	0.41
24:A:280:U:H2'	24:A:281:C:C6	2.55	0.41
24:A:574:A:H2	27:D:150:GLN:HE22	1.68	0.41
42:S:72:THR:OG1	42:S:73:LYS:N	2.53	0.41
1:a:657:U:H2'	1:a:658:C:C6	2.55	0.41
24:A:458:G:O2'	24:A:469:G:O6	2.37	0.41
24:A:1857:G:N2	24:A:1884:G:H2'	2.36	0.41
24:A:2039:U:H2'	24:A:2040:G:C8	2.55	0.41
24:A:2233:U:H2'	24:A:2234:G:H8	1.86	0.41
24:A:2246:G:H2'	24:A:2247:A:C8	2.55	0.41
31:I:12:VAL:HG11	31:I:22:PRO:HB2	2.01	0.41
32:H:108:VAL:HG12	32:H:110:VAL:H	1.85	0.41
37:N:55:ALA:HA	37:N:80:PHE:CE1	2.55	0.41
41:R:11:GLN:N	41:R:11:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:33:A:H2'	1:a:34:C:C6	2.55	0.41
1:a:109:A:H2'	1:a:326:G:N2	2.36	0.41
1:a:335:C:H2'	1:a:336:A:H8	1.85	0.41
1:a:673:A:H2'	1:a:674:G:C8	2.56	0.41
1:a:1323:G:H2'	1:a:1324:A:C8	2.54	0.41
4:d:151:GLN:C	4:d:153:ARG:H	2.28	0.41
24:A:184:C:H2'	24:A:185:G:C8	2.56	0.41
24:A:794:A:H2'	24:A:795:C:C6	2.56	0.41
29:F:28:PRO:HB3	29:F:159:ALA:HB2	2.02	0.41
45:V:72:VAL:HG12	45:V:93:ARG:HA	2.02	0.41
4:d:31:CYS:SG	4:d:33:ILE:HG23	2.60	0.41
24:A:499:U:H5''	44:U:42:LYS:HE2	2.03	0.41
24:A:310:A:O2'	24:A:311:A:H2'	2.20	0.41
25:B:30:C:H1'	25:B:57:A:H61	1.85	0.41
43:T:44:LYS:HG3	43:T:55:VAL:HG11	2.01	0.41
3:c:135:ARG:NH2	23:x:117:C:O4'	2.53	0.41
24:A:545:U:O2	24:A:548:G:N2	2.46	0.41
24:A:814:C:H1'	24:A:1225:G:N2	2.36	0.41
24:A:1824:G:H5''	26:C:51:ARG:HH21	1.86	0.41
34:K:25:LEU:HD12	34:K:38:ILE:HG22	2.03	0.41
34:K:68:GLY:HA2	34:K:77:ILE:O	2.21	0.41
1:a:88:U:H2'	1:a:89:U:C6	2.56	0.41
1:a:102:G:H2'	1:a:103:U:H6	1.85	0.41
1:a:453:G:H2'	1:a:454:G:O4'	2.21	0.41
1:a:667:G:H4'	15:o:50:HIS:CE1	2.55	0.41
1:a:708:C:H2'	1:a:709:U:H6	1.86	0.41
1:a:933:G:O6	7:g:2:ARG:NH2	2.53	0.41
1:a:1070:U:H2'	1:a:1071:C:C6	2.55	0.41
1:a:1129:C:H2'	1:a:1139:G:N7	2.36	0.41
10:j:57:VAL:HG22	10:j:58:ASN:H	1.84	0.41
11:k:46:ALA:HA	11:k:65:ALA:HB2	2.03	0.41
24:A:1993:U:H4'	27:D:133:THR:CG2	2.51	0.41
24:A:2064:C:H2'	24:A:2065:C:C6	2.56	0.41
24:A:2843:G:H2'	24:A:2844:G:O4'	2.21	0.41
26:C:180:MET:HB2	26:C:268:ARG:H	1.86	0.41
27:D:16:THR:OG1	27:D:20:VAL:O	2.35	0.41
36:M:48:ALA:O	36:M:52:ALA:HB2	2.20	0.41
40:Q:88:GLU:CD	41:R:52:PRO:HB3	2.46	0.41
42:S:17:VAL:HA	42:S:43:ALA:HB1	2.03	0.41
1:a:311:C:OP1	16:p:31:ARG:NH1	2.54	0.41
1:a:607:A:H2'	1:a:608:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:10:LEU:HD13	4:d:62:ARG:HD2	2.03	0.41
4:d:85:THR:HB	5:e:102:THR:HG21	2.03	0.41
6:f:13:ASP:OD1	6:f:14:GLN:HG3	2.20	0.41
7:g:2:ARG:HA	7:g:2:ARG:HD3	1.85	0.41
7:g:62:GLU:O	7:g:66:GLU:HG2	2.21	0.41
24:A:39:G:H2'	24:A:40:U:C6	2.56	0.41
24:A:120:U:H4'	24:A:121:G:H5''	2.03	0.41
24:A:655:A:H4'	24:A:656:G:H5'	2.02	0.41
24:A:1057:A:N6	24:A:1080:A:H61	2.19	0.41
24:A:1062:G:H22	24:A:1088:A:N6	2.19	0.41
24:A:2285:C:P	51:l:25:ASN:HD22	2.44	0.41
24:A:2476:A:H2	24:A:2481:G:H1	1.67	0.41
26:C:35:LYS:HE3	26:C:35:LYS:HB2	1.82	0.41
31:I:108:ILE:O	31:I:111:THR:OG1	2.33	0.41
33:J:17:VAL:HG23	33:J:137:PRO:HB2	2.02	0.41
45:V:72:VAL:HG21	45:V:91:PHE:HB3	2.02	0.41
46:W:15:LYS:HB2	46:W:37:ARG:HH22	1.86	0.41
52:2:13:ASN:O	52:2:17:GLY:HA3	2.21	0.41
1:a:203:G:O2'	1:a:465:A:N1	2.45	0.40
1:a:254:G:H21	17:q:17:GLU:CD	2.29	0.40
1:a:321:A:H2	1:a:332:G:H22	1.69	0.40
1:a:778:G:O2'	11:k:120:CYS:HB2	2.22	0.40
13:m:70:ARG:NH1	29:F:114:ARG:HH11	2.19	0.40
24:A:558:U:H2'	24:A:559:G:C8	2.56	0.40
24:A:720:U:H2'	24:A:721:A:C8	2.56	0.40
24:A:1278:C:H2'	24:A:1279:G:H8	1.87	0.40
24:A:1972:G:H2'	24:A:1973:G:H8	1.86	0.40
24:A:2183:A:H2'	24:A:2184:A:C8	2.56	0.40
1:a:110:C:H2'	1:a:111:G:O4'	2.21	0.40
1:a:204:G:H2'	1:a:205:A:H8	1.86	0.40
1:a:401:C:O2'	1:a:621:A:N3	2.47	0.40
1:a:1120:C:H2'	1:a:1121:U:C6	2.56	0.40
4:d:191:SER:C	4:d:193:ASP:H	2.30	0.40
7:g:91:ARG:HD3	7:g:92:PRO:HD2	2.03	0.40
11:k:93:GLU:O	11:k:96:ILE:HG12	2.21	0.40
24:A:1361:G:H2'	24:A:1362:C:C6	2.57	0.40
24:A:1538:G:H2'	24:A:1539:U:C6	2.56	0.40
24:A:2141:G:H2'	24:A:2142:A:H8	1.86	0.40
1:a:61:G:OP2	20:t:4:LYS:NZ	2.52	0.40
1:a:692:U:O2'	1:a:694:A:N7	2.43	0.40
1:a:953:G:H2'	1:a:954:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:994:A:C8	1:a:1216:A:H4'	2.57	0.40
1:a:1436:U:H2'	1:a:1437:A:H8	1.86	0.40
24:A:973:A:H5'	24:A:1188:U:H1'	2.03	0.40
24:A:1295:C:H2'	24:A:1296:G:H8	1.87	0.40
24:A:2163:A:H2'	24:A:2164:C:H5'	2.02	0.40
24:A:2267:A:H5''	24:A:2268:A:H5''	2.02	0.40
30:G:154:GLU:O	30:G:158:GLY:N	2.54	0.40
42:S:77:ASP:OD1	42:S:77:ASP:N	2.38	0.40
46:W:42:HIS:NE2	46:W:73:ARG:HD3	2.37	0.40
51:1:5:ARG:NH1	51:1:25:ASN:HB2	2.36	0.40
4:d:197:HIS:CE1	5:e:104:ILE:H	2.39	0.40
8:h:12:ARG:HB3	8:h:24:VAL:HG11	2.03	0.40
12:l:45:ASN:ND2	12:l:88:ASP:OD1	2.53	0.40
18:r:72:ARG:HA	18:r:72:ARG:HD3	1.77	0.40
24:A:138:U:C4	43:T:3:ARG:HG2	2.56	0.40
24:A:643:A:H1'	51:1:43:ARG:NH2	2.37	0.40
24:A:1289:C:H2'	24:A:1290:C:H6	1.86	0.40
24:A:1316:U:H2'	24:A:1317:G:C8	2.57	0.40
24:A:1341:G:OP2	24:A:1394:U:O2'	2.36	0.40
24:A:1656:C:H2'	24:A:1657:U:H6	1.86	0.40
24:A:2215:C:H2'	24:A:2216:G:H8	1.87	0.40
24:A:2819:G:H2'	24:A:2821:A:N7	2.36	0.40
29:F:95:MET:HE3	29:F:95:MET:HB2	1.88	0.40
45:V:64:VAL:HA	45:V:68:LYS:O	2.21	0.40
48:Y:56:LEU:HD23	48:Y:56:LEU:HA	1.89	0.40
51:1:10:LEU:HD23	51:1:50:GLU:HA	2.02	0.40
1:a:1426:G:H2'	1:a:1427:C:O4'	2.21	0.40
2:b:19:THR:OG1	2:b:20:ARG:N	2.54	0.40
2:b:156:LEU:HA	2:b:157:PRO:HD3	1.98	0.40
3:c:69:THR:HG21	3:c:75:VAL:HG21	2.02	0.40
12:l:98:ARG:HB2	12:l:116:TYR:HA	2.02	0.40
15:o:65:LEU:HD23	15:o:65:LEU:HA	1.91	0.40
23:x:111:G:H21	23:x:112:C:H41	1.68	0.40
24:A:729:G:C5	26:C:206:LYS:HB2	2.56	0.40
39:P:91:VAL:HG21	39:P:96:LEU:HD21	2.02	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	
2	b	216/218 (99%)	189 (88%)	23 (11%)	4 (2%)	6	33
3	c	204/206 (99%)	190 (93%)	13 (6%)	1 (0%)	24	57
4	d	203/205 (99%)	187 (92%)	14 (7%)	2 (1%)	12	45
5	e	155/157 (99%)	134 (86%)	16 (10%)	5 (3%)	3	24
6	f	98/100 (98%)	82 (84%)	10 (10%)	6 (6%)	1	13
7	g	149/151 (99%)	135 (91%)	11 (7%)	3 (2%)	6	32
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	49
9	i	125/127 (98%)	104 (83%)	15 (12%)	6 (5%)	2	16
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	2	19
11	k	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	4	27
12	l	121/123 (98%)	98 (81%)	14 (12%)	9 (7%)	1	9
13	m	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	4	27
14	n	98/100 (98%)	83 (85%)	13 (13%)	2 (2%)	6	32
15	o	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	5	30
16	p	80/82 (98%)	71 (89%)	6 (8%)	3 (4%)	2	21
17	q	78/80 (98%)	66 (85%)	10 (13%)	2 (3%)	4	27
18	r	63/65 (97%)	57 (90%)	2 (3%)	4 (6%)	1	12
19	s	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	39
20	t	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
21	u	63/65 (97%)	50 (79%)	9 (14%)	4 (6%)	1	12
26	C	269/271 (99%)	246 (91%)	20 (7%)	3 (1%)	11	43
27	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	24	57
28	E	199/201 (99%)	184 (92%)	12 (6%)	3 (2%)	8	37
29	F	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	5	30
30	G	174/176 (99%)	157 (90%)	11 (6%)	6 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5	30
32	H	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	4	27
33	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	K	120/122 (98%)	105 (88%)	10 (8%)	5 (4%)	2	19
35	L	141/143 (99%)	129 (92%)	9 (6%)	3 (2%)	5	31
36	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	5	30
37	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
38	O	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	6	34
39	P	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	14	46
40	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
41	R	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	6	32
42	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
43	T	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	3	24
44	U	100/102 (98%)	89 (89%)	6 (6%)	5 (5%)	1	16
45	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	9	38
47	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
48	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
49	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
50	0	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	6	33
51	1	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	5	31
52	2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	30
53	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	36
54	4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	26
55	6	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	7	36
All	All	5717/5817 (98%)	5150 (90%)	447 (8%)	120 (2%)	8	31

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	73	ARG

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Mol	Chain	Res	Type
4	d	192	ALA
5	e	77	ASN
5	e	89	THR
5	e	122	VAL
5	e	158	LYS
6	f	53	LYS
6	f	54	LEU
6	f	86	ARG
7	g	110	ARG
8	h	47	ASP
9	i	90	ASP
10	j	34	ALA
10	j	57	VAL
10	j	92	LEU
11	k	92	ARG
12	l	101	LEU
13	m	65	GLU
15	o	46	LYS
16	p	44	SER
16	p	79	ASN
17	q	49	ASN
17	q	69	THR
18	r	11	ARG
18	r	17	VAL
19	s	4	LEU
21	u	8	ASN
21	u	34	ARG
21	u	37	TYR
26	C	121	ALA
26	C	204	LEU
28	E	83	VAL
29	F	174	PHE
30	G	46	ASP
30	G	108	PHE
30	G	118	ALA
30	G	174	LYS
32	H	9	VAL
34	K	92	GLU
35	L	29	LYS
35	L	36	LYS
35	L	111	ILE
38	O	63	LYS

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Mol	Chain	Res	Type
44	U	6	ARG
44	U	51	LEU
44	U	88	ASP
50	0	2	VAL
51	1	4	ILE
53	3	31	ILE
5	e	93	VAL
7	g	29	LEU
7	g	95	ARG
9	i	57	VAL
9	i	125	GLN
10	j	42	LEU
11	k	88	PRO
12	l	75	GLU
13	m	4	ALA
13	m	6	ILE
14	n	2	LYS
29	F	20	ASN
30	G	45	ALA
32	H	3	VAL
32	H	11	ASN
32	H	41	LYS
34	K	35	VAL
34	K	110	GLU
36	M	58	LYS
36	M	70	ASP
41	R	54	VAL
41	R	55	ASP
43	T	38	ALA
43	T	52	GLU
55	6	3	LYS
9	i	12	LYS
9	i	122	ARG
14	n	34	ASN
16	p	43	ALA
18	r	18	GLN
26	C	52	HIS
27	D	149	ASN
28	E	184	ASP
31	I	22	PRO
36	M	14	LYS
43	T	88	LYS

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Mol	Chain	Res	Type
44	U	39	ASN
46	W	17	LEU
54	4	37	GLN
3	c	96	VAL
4	d	191	SER
6	f	92	THR
6	f	99	ALA
12	l	2	THR
12	l	23	LEU
12	l	45	ASN
12	l	46	SER
12	l	77	SER
12	l	88	ASP
15	o	27	GLN
18	r	46	THR
21	u	65	ARG
29	F	149	ARG
29	F	176	PHE
34	K	109	SER
6	f	93	LYS
28	E	122	GLU
30	G	109	SER
31	I	20	SER
38	O	34	HIS
39	P	86	LYS
52	2	23	ALA
34	K	93	GLN
9	i	71	ILE
44	U	54	PRO
11	k	90	PRO
12	l	41	PRO
2	b	28	PRO
31	I	92	PRO

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	
2	b	180/180 (100%)	179 (99%)	1 (1%)	78	79
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	171 (99%)	1 (1%)	78	79
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	86 (99%)	1 (1%)	65	74
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	103 (99%)	1 (1%)	68	75
9	i	105/105 (100%)	104 (99%)	1 (1%)	68	75
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	68	75
13	m	92/92 (100%)	91 (99%)	1 (1%)	65	74
14	n	79/83 (95%)	77 (98%)	2 (2%)	42	63
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	63 (97%)	2 (3%)	35	59
17	q	74/74 (100%)	73 (99%)	1 (1%)	59	71
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	68 (97%)	2 (3%)	37	60
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
26	C	216/216 (100%)	214 (99%)	2 (1%)	70	76
27	D	164/164 (100%)	163 (99%)	1 (1%)	78	79
28	E	165/165 (100%)	165 (100%)	0	100	100
29	F	148/148 (100%)	148 (100%)	0	100	100
30	G	137/137 (100%)	137 (100%)	0	100	100
31	I	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	J	116/116 (100%)	116 (100%)	0	100	100
34	K	103/103 (100%)	103 (100%)	0	100	100
35	L	102/102 (100%)	101 (99%)	1 (1%)	68	75
36	M	109/109 (100%)	108 (99%)	1 (1%)	70	76
37	N	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	O	86/86 (100%)	86 (100%)	0	100	100
39	P	99/99 (100%)	99 (100%)	0	100	100
40	Q	89/89 (100%)	89 (100%)	0	100	100
41	R	84/84 (100%)	84 (100%)	0	100	100
42	S	93/93 (100%)	93 (100%)	0	100	100
43	T	80/80 (100%)	80 (100%)	0	100	100
44	U	83/83 (100%)	83 (100%)	0	100	100
45	V	78/78 (100%)	77 (99%)	1 (1%)	61	72
46	W	57/57 (100%)	57 (100%)	0	100	100
47	X	67/67 (100%)	66 (98%)	1 (2%)	57	70
48	Y	55/55 (100%)	55 (100%)	0	100	100
49	Z	48/48 (100%)	48 (100%)	0	100	100
50	0	47/47 (100%)	46 (98%)	1 (2%)	47	65
51	1	45/45 (100%)	45 (100%)	0	100	100
52	2	38/38 (100%)	38 (100%)	0	100	100
53	3	51/51 (100%)	51 (100%)	0	100	100
54	4	34/34 (100%)	34 (100%)	0	100	100
55	6	59/59 (100%)	59 (100%)	0	100	100
All	All	4728/4751 (100%)	4706 (100%)	22 (0%)	78	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	178	LEU
4	d	173	ASP
6	f	64	VAL
8	h	103	VAL
9	i	60	LEU
12	l	33	CYS
13	m	6	ILE
14	n	33	VAL
14	n	34	ASN
16	p	2	VAL
16	p	36	VAL
17	q	4	ILE
19	s	4	LEU

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Mol	Chain	Res	Type
19	s	48	ILE
26	C	52	HIS
26	C	103	ILE
27	D	48	ILE
35	L	27	LEU
36	M	20	LEU
45	V	65	VAL
47	X	4	CYS
50	0	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	177	ASN
3	c	122	GLN
4	d	70	GLN
8	h	20	ASN
8	h	117	GLN
9	i	30	ASN
9	i	31	GLN
11	k	14	GLN
11	k	23	HIS
12	l	5	GLN
12	l	72	ASN
13	m	90	HIS
14	n	34	ASN
15	o	36	ASN
15	o	41	HIS
16	p	26	ASN
16	p	63	GLN
16	p	79	ASN
20	t	12	GLN
20	t	19	HIS
20	t	81	GLN
26	C	44	ASN
26	C	114	GLN
26	C	199	HIS
27	D	49	GLN
27	D	150	GLN
27	D	164	GLN
28	E	90	GLN
28	E	195	GLN

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Mol	Chain	Res	Type
29	F	51	ASN
30	G	21	GLN
30	G	47	ASN
32	H	2	GLN
32	H	66	ASN
34	K	5	GLN
34	K	93	GLN
35	L	38	GLN
35	L	99	ASN
37	N	62	ASN
40	Q	51	GLN
41	R	12	HIS
43	T	48	GLN
44	U	39	ASN
44	U	65	GLN
45	V	51	GLN
46	W	8	ASN
46	W	46	ASN
48	Y	20	ASN
48	Y	25	GLN
49	Z	8	GLN
53	3	27	ASN
54	4	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1534/1539 (99%)	260 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	21 (44%)	0
24	A	2897/2903 (99%)	544 (18%)	34 (1%)
25	B	119/120 (99%)	17 (14%)	3 (2%)
All	All	4673/4687 (99%)	857 (18%)	37 (0%)

All (857) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A

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Mol	Chain	Res	Type
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	59	A
1	a	61	G
1	a	69	G
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	83	C
1	a	85	U
1	a	86	G
1	a	88	U
1	a	92	U
1	a	94	G
1	a	95	C
1	a	116	A
1	a	121	U
1	a	122	G
1	a	126	G
1	a	127	G
1	a	128	G
1	a	131	A
1	a	134	G
1	a	141	G
1	a	144	G
1	a	149	A
1	a	173	U
1	a	183	C
1	a	184	G
1	a	189	A
1	a	195	A
1	a	197	A
1	a	207	C
1	a	209	U
1	a	210	C
1	a	211	G

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Mol	Chain	Res	Type
1	a	212	G
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	280	C
1	a	281	G
1	a	289	G
1	a	300	A
1	a	306	A
1	a	316	C
1	a	328	C
1	a	329	A
1	a	330	C
1	a	345	C
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	376	G
1	a	388	G
1	a	398	U
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	429	U
1	a	439	U
1	a	441	A
1	a	446	G
1	a	448	A
1	a	467	U
1	a	468	A
1	a	474	G

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Mol	Chain	Res	Type
1	a	479	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	496	A
1	a	497	G
1	a	499	A
1	a	505	G
1	a	509	A
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	528	C
1	a	529	G
1	a	531	U
1	a	532	A
1	a	547	A
1	a	548	G
1	a	559	A
1	a	562	U
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	615	G
1	a	633	G
1	a	639	G
1	a	653	U
1	a	654	G
1	a	665	A
1	a	687	A
1	a	695	A
1	a	701	U
1	a	702	A
1	a	713	G
1	a	718	A
1	a	723	U
1	a	724	G
1	a	731	G
1	a	733	G
1	a	777	A

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Mol	Chain	Res	Type
1	a	787	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	802	A
1	a	810	C
1	a	815	A
1	a	817	C
1	a	818	G
1	a	820	U
1	a	821	G
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	849	G
1	a	872	A
1	a	890	G
1	a	891	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	933	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	967	5MC
1	a	968	A
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	983	A
1	a	989	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	1004	A

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Mol	Chain	Res	Type
1	a	1020	G
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1036	A
1	a	1042	A
1	a	1050	G
1	a	1053	G
1	a	1054	C
1	a	1066	C
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1100	C
1	a	1101	A
1	a	1130	A
1	a	1133	G
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1145	A
1	a	1146	A
1	a	1151	A
1	a	1152	A
1	a	1158	C
1	a	1159	U
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1191	A
1	a	1196	A
1	a	1212	U
1	a	1213	A
1	a	1225	A
1	a	1226	C
1	a	1227	A

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Mol	Chain	Res	Type
1	a	1236	A
1	a	1238	A
1	a	1239	A
1	a	1240	U
1	a	1241	G
1	a	1253	G
1	a	1258	G
1	a	1260	G
1	a	1280	A
1	a	1281	C
1	a	1287	A
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1303	C
1	a	1305	G
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1332	A
1	a	1353	G
1	a	1360	A
1	a	1363	A
1	a	1364	U
1	a	1394	A
1	a	1398	A
1	a	1419	G
1	a	1422	G
1	a	1429	A
1	a	1433	A
1	a	1440	U
1	a	1441	A
1	a	1446	A
1	a	1452	C
1	a	1499	A
1	a	1503	A
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G

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Mol	Chain	Res	Type
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1537	U
22	v	9	G
22	v	14	A
22	v	16	C
22	v	17	C
22	v	17(A)	U
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	21	A
22	v	22	G
22	v	47	U
22	v	48	C
22	v	58	A
22	v	75	C
22	v	76	A
23	x	88	A
23	x	90	G
23	x	91	A
23	x	93	G
23	x	96	C
23	x	98	U
23	x	99	U
23	x	104	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	115	A
23	x	117	C
23	x	118	G
23	x	120	U
23	x	121	U
23	x	126	G
23	x	127	U
23	x	129	U
23	x	130	G
23	x	134	C
24	A	10	A
24	A	14	A

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Mol	Chain	Res	Type
24	A	34	U
24	A	35	G
24	A	43	G
24	A	45	G
24	A	46	G
24	A	50	U
24	A	51	G
24	A	52	A
24	A	63	A
24	A	71	A
24	A	73	A
24	A	74	A
24	A	75	G
24	A	84	A
24	A	92	U
24	A	96	C
24	A	98	G
24	A	102	U
24	A	103	A
24	A	114	U
24	A	118	A
24	A	119	A
24	A	120	U
24	A	131	A
24	A	138	U
24	A	139	U
24	A	141	G
24	A	142	A
24	A	161	A
24	A	162	U
24	A	163	C
24	A	165	A
24	A	178	G
24	A	196	A
24	A	204	A
24	A	205	G
24	A	206	U
24	A	215	G
24	A	216	A
24	A	221	A
24	A	222	A
24	A	228	C

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Mol	Chain	Res	Type
24	A	229	C
24	A	241	A
24	A	245	G
24	A	247	G
24	A	248	G
24	A	250	G
24	A	255	A
24	A	266	G
24	A	276	U
24	A	277	G
24	A	278	A
24	A	281	C
24	A	282	A
24	A	285	G
24	A	294	A
24	A	295	G
24	A	310	A
24	A	317	G
24	A	322	A
24	A	323	C
24	A	329	G
24	A	330	A
24	A	346	A
24	A	349	U
24	A	359	G
24	A	361	G
24	A	362	A
24	A	371	A
24	A	372	G
24	A	373	U
24	A	386	G
24	A	387	U
24	A	404	A
24	A	406	G
24	A	411	G
24	A	412	A
24	A	424	G
24	A	456	C
24	A	457	A
24	A	481	G
24	A	490	C
24	A	491	G

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Mol	Chain	Res	Type
24	A	496	G
24	A	504	A
24	A	505	A
24	A	509	C
24	A	510	C
24	A	513	A
24	A	522	A
24	A	527	C
24	A	529	A
24	A	531	C
24	A	532	A
24	A	533	G
24	A	544	C
24	A	545	U
24	A	549	G
24	A	556	A
24	A	563	A
24	A	573	U
24	A	575	A
24	A	588	U
24	A	592	A
24	A	603	A
24	A	613	A
24	A	614	A
24	A	627	A
24	A	632	A
24	A	637	A
24	A	645	C
24	A	646	U
24	A	647	G
24	A	654	A
24	A	655	A
24	A	656	G
24	A	669	G
24	A	677	A
24	A	686	U
24	A	690	G
24	A	694	U
24	A	695	G
24	A	699	A
24	A	714	U
24	A	729	G

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Mol	Chain	Res	Type
24	A	730	A
24	A	746	PSU
24	A	747	5MU
24	A	752	A
24	A	764	A
24	A	774	G
24	A	775	G
24	A	776	G
24	A	782	A
24	A	784	G
24	A	785	G
24	A	805	G
24	A	812	C
24	A	819	A
24	A	827	U
24	A	828	U
24	A	844	A
24	A	845	A
24	A	846	U
24	A	858	G
24	A	859	G
24	A	869	G
24	A	878	A
24	A	884	U
24	A	886	A
24	A	892	A
24	A	896	A
24	A	897	C
24	A	910	A
24	A	941	A
24	A	944	C
24	A	945	A
24	A	946	C
24	A	961	C
24	A	962	G
24	A	974	G
24	A	983	A
24	A	985	C
24	A	990	A
24	A	995	C
24	A	996	A
24	A	1003	G

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Mol	Chain	Res	Type
24	A	1012	U
24	A	1013	C
24	A	1021	A
24	A	1022	G
24	A	1023	U
24	A	1026	G
24	A	1033	U
24	A	1040	A
24	A	1046	A
24	A	1053	C
24	A	1054	A
24	A	1060	U
24	A	1061	U
24	A	1062	G
24	A	1064	C
24	A	1065	U
24	A	1066	U
24	A	1067	A
24	A	1068	G
24	A	1069	A
24	A	1070	A
24	A	1071	G
24	A	1072	C
24	A	1073	A
24	A	1075	C
24	A	1076	C
24	A	1077	A
24	A	1079	C
24	A	1084	A
24	A	1087	G
24	A	1088	A
24	A	1097	U
24	A	1104	C
24	A	1111	A
24	A	1112	G
24	A	1116	G
24	A	1119	U
24	A	1130	U
24	A	1131	G
24	A	1132	U
24	A	1135	C
24	A	1136	G

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Mol	Chain	Res	Type
24	A	1142	A
24	A	1143	A
24	A	1151	A
24	A	1165	A
24	A	1172	C
24	A	1174	U
24	A	1175	A
24	A	1178	C
24	A	1179	G
24	A	1180	U
24	A	1183	U
24	A	1205	A
24	A	1206	G
24	A	1210	G
24	A	1212	G
24	A	1213	A
24	A	1221	C
24	A	1237	A
24	A	1247	A
24	A	1248	G
24	A	1250	G
24	A	1251	C
24	A	1253	A
24	A	1256	G
24	A	1270	C
24	A	1271	G
24	A	1272	A
24	A	1273	U
24	A	1300	G
24	A	1301	A
24	A	1306	C
24	A	1311	G
24	A	1313	U
24	A	1314	C
24	A	1325	U
24	A	1332	G
24	A	1341	G
24	A	1345	C
24	A	1359	A
24	A	1365	A
24	A	1368	G
24	A	1378	A

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Mol	Chain	Res	Type
24	A	1379	U
24	A	1383	A
24	A	1386	C
24	A	1395	A
24	A	1396	U
24	A	1403	A
24	A	1407	G
24	A	1414	C
24	A	1416	G
24	A	1421	G
24	A	1428	C
24	A	1437	C
24	A	1454	C
24	A	1458	U
24	A	1459	G
24	A	1461	C
24	A	1475	G
24	A	1482	G
24	A	1490	A
24	A	1493	C
24	A	1498	C
24	A	1504	A
24	A	1509	A
24	A	1515	A
24	A	1523	U
24	A	1524	G
24	A	1529	G
24	A	1533	C
24	A	1534	U
24	A	1535	A
24	A	1536	C
24	A	1537	G
24	A	1559	U
24	A	1560	G
24	A	1565	C
24	A	1568	G
24	A	1569	A
24	A	1578	U
24	A	1584	U
24	A	1614	A
24	A	1616	A
24	A	1618	6MZ

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Mol	Chain	Res	Type
24	A	1633	G
24	A	1634	A
24	A	1643	G
24	A	1647	U
24	A	1648	U
24	A	1649	G
24	A	1674	G
24	A	1695	G
24	A	1698	A
24	A	1703	G
24	A	1713	A
24	A	1715	G
24	A	1718	G
24	A	1729	U
24	A	1730	C
24	A	1738	G
24	A	1757	A
24	A	1758	U
24	A	1764	C
24	A	1773	A
24	A	1780	A
24	A	1782	U
24	A	1784	A
24	A	1785	A
24	A	1791	A
24	A	1800	C
24	A	1801	A
24	A	1808	A
24	A	1809	A
24	A	1816	C
24	A	1829	A
24	A	1833	C
24	A	1847	A
24	A	1857	G
24	A	1870	C
24	A	1884	G
24	A	1891	G
24	A	1901	A
24	A	1906	G
24	A	1907	G
24	A	1914	C
24	A	1915	3TD

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Mol	Chain	Res	Type
24	A	1929	G
24	A	1930	G
24	A	1931	U
24	A	1936	A
24	A	1937	A
24	A	1939	5MU
24	A	1940	U
24	A	1941	C
24	A	1943	U
24	A	1955	U
24	A	1964	G
24	A	1967	C
24	A	1970	A
24	A	1971	U
24	A	1972	G
24	A	1991	U
24	A	1993	U
24	A	1997	C
24	A	2022	U
24	A	2023	C
24	A	2030	6MZ
24	A	2031	A
24	A	2033	A
24	A	2036	C
24	A	2043	C
24	A	2049	G
24	A	2055	C
24	A	2056	G
24	A	2059	A
24	A	2060	A
24	A	2061	G
24	A	2062	A
24	A	2069	G7M
24	A	2070	A
24	A	2072	C
24	A	2077	A
24	A	2080	A
24	A	2093	G
24	A	2096	C
24	A	2100	G
24	A	2108	A
24	A	2110	G

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Mol	Chain	Res	Type
24	A	2111	U
24	A	2112	G
24	A	2113	U
24	A	2117	A
24	A	2118	U
24	A	2119	A
24	A	2120	G
24	A	2125	G
24	A	2127	G
24	A	2130	U
24	A	2132	U
24	A	2133	G
24	A	2134	A
24	A	2137	U
24	A	2145	C
24	A	2146	C
24	A	2147	A
24	A	2154	A
24	A	2158	A
24	A	2162	G
24	A	2163	A
24	A	2164	C
24	A	2166	U
24	A	2167	U
24	A	2168	G
24	A	2169	A
24	A	2170	A
24	A	2171	A
24	A	2172	U
24	A	2173	A
24	A	2178	C
24	A	2189	U
24	A	2198	A
24	A	2199	A
24	A	2204	G
24	A	2211	A
24	A	2214	C
24	A	2220	U
24	A	2223	G
24	A	2225	A
24	A	2238	G
24	A	2239	G

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Mol	Chain	Res	Type
24	A	2250	G
24	A	2268	A
24	A	2279	G
24	A	2283	C
24	A	2286	G
24	A	2287	A
24	A	2288	A
24	A	2294	G
24	A	2298	A
24	A	2305	U
24	A	2309	A
24	A	2310	C
24	A	2319	G
24	A	2322	A
24	A	2331	G
24	A	2333	A
24	A	2335	A
24	A	2347	C
24	A	2350	C
24	A	2354	C
24	A	2357	G
24	A	2383	G
24	A	2385	C
24	A	2389	G
24	A	2392	A
24	A	2402	U
24	A	2403	C
24	A	2406	A
24	A	2407	A
24	A	2429	G
24	A	2430	A
24	A	2431	U
24	A	2441	U
24	A	2448	A
24	A	2464	G
24	A	2468	A
24	A	2475	C
24	A	2476	A
24	A	2480	C
24	A	2484	G
24	A	2491	U
24	A	2494	G

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Mol	Chain	Res	Type
24	A	2498	OMC
24	A	2501	C
24	A	2502	G
24	A	2503	2MA
24	A	2504	PSU
24	A	2505	G
24	A	2506	U
24	A	2513	A
24	A	2518	A
24	A	2520	C
24	A	2525	G
24	A	2535	G
24	A	2547	A
24	A	2548	U
24	A	2554	U
24	A	2567	G
24	A	2569	G
24	A	2572	A
24	A	2573	C
24	A	2578	G
24	A	2582	G
24	A	2585	U
24	A	2586	U
24	A	2602	A
24	A	2603	G
24	A	2609	U
24	A	2610	C
24	A	2611	C
24	A	2613	U
24	A	2615	U
24	A	2621	G
24	A	2629	U
24	A	2636	C
24	A	2646	C
24	A	2656	U
24	A	2685	G
24	A	2689	U
24	A	2690	U
24	A	2714	G
24	A	2718	G
24	A	2720	U
24	A	2726	A

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Mol	Chain	Res	Type
24	A	2729	G
24	A	2733	A
24	A	2739	U
24	A	2744	G
24	A	2748	A
24	A	2751	G
24	A	2757	A
24	A	2764	A
24	A	2765	A
24	A	2766	A
24	A	2769	U
24	A	2778	A
24	A	2779	U
24	A	2790	U
24	A	2791	G
24	A	2793	C
24	A	2794	C
24	A	2797	U
24	A	2798	U
24	A	2799	A
24	A	2800	A
24	A	2801	G
24	A	2803	G
24	A	2808	G
24	A	2818	U
24	A	2820	A
24	A	2821	A
24	A	2833	U
24	A	2834	G
24	A	2849	U
24	A	2867	G
24	A	2868	A
24	A	2872	A
24	A	2873	A
24	A	2880	C
24	A	2883	A
24	A	2885	G
24	A	2891	U
25	B	4	C
25	B	13	G
25	B	16	G
25	B	25	U

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Mol	Chain	Res	Type
25	B	30	C
25	B	35	C
25	B	41	G
25	B	44	G
25	B	57	A
25	B	67	G
25	B	68	C
25	B	73	A
25	B	89	U
25	B	90	C
25	B	96	G
25	B	108	A
25	B	109	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	51	G
24	A	91	A
24	A	205	G
24	A	228	C
24	A	385	C
24	A	512	G
24	A	555	G
24	A	572	A
24	A	774	G
24	A	830	G
24	A	989	G
24	A	1020	A
24	A	1070	A
24	A	1111	A
24	A	1182	G
24	A	1190	G
24	A	1211	C
24	A	1212	G
24	A	1251	C
24	A	1432	G
24	A	1458	U
24	A	1567	G
24	A	1930	G
24	A	1940	U
24	A	2061	G

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Mol	Chain	Res	Type
24	A	2308	G
24	A	2391	G
24	A	2447	G
24	A	2566	A
24	A	2610	C
24	A	2756	U
24	A	2820	A
24	A	2832	U
24	A	2867	G
25	B	3	C
25	B	66	A
25	B	88	C

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

39 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
22	H2U	v	20	22	18,21,22	0.94	2 (11%)	21,30,33	1.26	3 (14%)
24	3TD	A	1915	24	18,22,23	4.06	7 (38%)	22,32,35	1.79	3 (13%)
1	2MG	a	1516	1	23,26,27	1.26	4 (17%)	32,38,41	2.21	6 (18%)
24	1MG	A	745	24	22,26,27	1.16	2 (9%)	33,39,42	1.78	6 (18%)
24	6MZ	A	1618	24	22,25,26	1.55	4 (18%)	30,36,39	2.26	10 (33%)
24	PSU	A	1917	24	18,21,22	1.42	3 (16%)	22,30,33	1.93	3 (13%)
24	2MG	A	1835	24	23,26,27	1.22	3 (13%)	32,38,41	2.43	9 (28%)
24	OMC	A	2498	24	19,22,23	0.88	1 (5%)	26,31,34	1.13	2 (7%)
24	2MA	A	2503	24	22,25,26	1.42	4 (18%)	33,37,40	2.27	7 (21%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	0.98	2 (7%)
24	PSU	A	2604	24	18,21,22	1.48	3 (16%)	22,30,33	1.84	4 (18%)
24	PSU	A	2605	24	18,21,22	1.40	3 (16%)	22,30,33	1.90	4 (18%)
24	PSU	A	2504	24	18,21,22	1.44	3 (16%)	22,30,33	1.84	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	a	1518	1	23,26,27	1.57	4 (17%)	34,38,41	2.31	11 (32%)
1	5MC	a	967	1	18,22,23	0.92	2 (11%)	26,32,35	1.10	3 (11%)
24	OMG	A	2251	22,24	23,26,27	1.26	3 (13%)	33,38,41	2.05	6 (18%)
24	PSU	A	1911	24	18,21,22	1.38	3 (16%)	22,30,33	1.94	3 (13%)
22	PSU	v	55	22	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
24	5MC	A	1962	24	18,22,23	1.00	1 (5%)	26,32,35	1.49	3 (11%)
1	MA6	a	1519	1	23,26,27	1.52	4 (17%)	34,38,41	2.42	12 (35%)
1	G7M	a	527	1	23,26,27	1.83	6 (26%)	35,39,42	2.03	8 (22%)
24	PSU	A	2457	24	18,21,22	1.55	4 (22%)	22,30,33	2.11	5 (22%)
24	G7M	A	2069	24	23,26,27	1.63	4 (17%)	35,39,42	2.14	8 (22%)
24	5MU	A	1939	24	19,22,23	1.45	4 (21%)	28,32,35	2.18	5 (17%)
24	6MZ	A	2030	24	22,25,26	1.55	3 (13%)	30,36,39	2.61	10 (33%)
24	OMU	A	2552	24	19,22,23	1.23	2 (10%)	26,31,34	1.94	7 (26%)
24	PSU	A	746	24	18,21,22	1.34	2 (11%)	22,30,33	1.74	4 (18%)
22	5MU	v	54	22	19,22,23	1.40	6 (31%)	28,32,35	2.05	6 (21%)
1	2MG	a	1207	1	23,26,27	1.33	4 (17%)	32,38,41	2.15	6 (18%)
1	UR3	a	1498	1	19,22,23	1.13	2 (10%)	26,32,35	2.06	5 (19%)
24	PSU	A	955	24	18,21,22	1.42	4 (22%)	22,30,33	1.94	3 (13%)
24	2MG	A	2445	24	23,26,27	1.26	3 (13%)	32,38,41	2.28	8 (25%)
1	2MG	a	966	1	23,26,27	1.26	3 (13%)	32,38,41	2.40	8 (25%)
24	5MU	A	747	24	19,22,23	1.42	5 (26%)	28,32,35	2.06	8 (28%)
24	H2U	A	2449	24	18,21,22	1.05	2 (11%)	21,30,33	1.76	3 (14%)
1	5MC	a	1407	1	18,22,23	0.89	2 (11%)	26,32,35	1.19	3 (11%)
22	4SU	v	8	22	18,21,22	1.80	4 (22%)	26,30,33	2.35	5 (19%)
1	PSU	a	516	1	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
24	PSU	A	2580	24	18,21,22	1.51	3 (16%)	22,30,33	1.94	3 (13%)

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
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
24	3TD	A	1915	24	-	5/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	A	745	24	-	0/7/25/26	0/3/3/3
24	6MZ	A	1618	24	-	0/9/27/28	0/3/3/3
24	PSU	A	1917	24	-	0/7/25/26	0/2/2/2
24	2MG	A	1835	24	-	2/9/27/28	0/3/3/3
24	OMC	A	2498	24	-	2/9/27/28	0/2/2/2
24	2MA	A	2503	24	-	4/7/25/26	0/3/3/3
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
24	PSU	A	2604	24	-	1/7/25/26	0/2/2/2
24	PSU	A	2605	24	-	0/7/25/26	0/2/2/2
24	PSU	A	2504	24	-	2/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	5/11/29/30	0/3/3/3
1	5MC	a	967	1	-	2/7/25/26	0/2/2/2
24	OMG	A	2251	22,24	-	3/9/27/28	0/3/3/3
24	PSU	A	1911	24	-	0/7/25/26	0/2/2/2
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
24	5MC	A	1962	24	-	4/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/11/29/30	0/3/3/3
1	G7M	a	527	1	2/2/5/5	1/7/25/26	0/3/3/3
24	PSU	A	2457	24	-	2/7/25/26	0/2/2/2
24	G7M	A	2069	24	2/2/5/5	2/7/25/26	0/3/3/3
24	5MU	A	1939	24	-	2/7/25/26	0/2/2/2
24	6MZ	A	2030	24	-	3/9/27/28	0/3/3/3
24	OMU	A	2552	24	-	2/9/27/28	0/2/2/2
24	PSU	A	746	24	-	2/7/25/26	0/2/2/2
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
24	PSU	A	955	24	-	0/7/25/26	0/2/2/2
24	2MG	A	2445	24	-	3/9/27/28	0/3/3/3
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
24	5MU	A	747	24	-	1/7/25/26	0/2/2/2
24	H2U	A	2449	24	-	0/7/38/39	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
24	PSU	A	2580	24	-	2/7/25/26	0/2/2/2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1915	3TD	C6-C5	11.98	1.49	1.35
24	A	1915	3TD	C2-N1	8.97	1.48	1.37
24	A	1915	3TD	C6-N1	5.66	1.45	1.36
24	A	2030	6MZ	C5-C4	5.26	1.48	1.39
24	A	1618	6MZ	C5-C4	5.14	1.48	1.39
1	a	1518	MA6	C5-C4	4.81	1.48	1.39
24	A	2069	G7M	C5-N7	-4.69	1.33	1.39
22	v	8	4SU	C4-S4	-4.62	1.59	1.68
1	a	527	G7M	C5-N7	-4.49	1.34	1.39
1	a	1519	MA6	C5-C4	4.43	1.47	1.39
24	A	2503	2MA	C5-C4	4.24	1.46	1.39
1	a	527	G7M	C5-C4	4.13	1.48	1.38
24	A	745	1MG	C5-C4	3.55	1.48	1.38
24	A	1915	3TD	C2-N3	3.50	1.46	1.38
24	A	2504	PSU	C6-C5	3.37	1.39	1.35
24	A	2457	PSU	C4-N3	-3.29	1.32	1.38
24	A	1917	PSU	C6-C5	3.28	1.39	1.35
24	A	2069	G7M	C5-C4	3.23	1.46	1.38
22	v	8	4SU	C4-N3	-3.19	1.34	1.37
24	A	746	PSU	C6-C5	3.19	1.39	1.35
24	A	2580	PSU	C4-N3	-3.17	1.33	1.38
22	v	55	PSU	C6-C5	3.16	1.39	1.35
1	a	1518	MA6	C5-C6	3.15	1.49	1.41
24	A	2604	PSU	C4-N3	-3.10	1.33	1.38
24	A	2605	PSU	C6-C5	3.09	1.38	1.35
1	a	1519	MA6	C5-C6	3.08	1.49	1.41
1	a	527	G7M	C5-C6	3.07	1.51	1.43
1	a	1207	2MG	C5-C4	3.06	1.47	1.38
24	A	955	PSU	C4-N3	-3.04	1.33	1.38
24	A	1962	5MC	C6-C5	3.04	1.39	1.34
24	A	747	5MU	C4-N3	-3.03	1.33	1.38
24	A	1939	5MU	C4-N3	-3.02	1.33	1.38
24	A	2457	PSU	C6-C5	3.00	1.38	1.35
24	A	2580	PSU	C6-C5	2.99	1.38	1.35
1	a	527	G7M	O6-C6	2.99	1.29	1.23
22	v	8	4SU	C5-C4	-2.98	1.38	1.42
24	A	2251	OMG	C5-C4	2.98	1.47	1.38
1	a	966	2MG	C5-C4	2.96	1.47	1.38
24	A	1911	PSU	C4-N3	-2.95	1.33	1.38
1	a	1498	UR3	C2-N1	2.94	1.42	1.38
22	v	55	PSU	C4-N3	-2.91	1.33	1.38
1	a	516	PSU	C6-C5	2.91	1.38	1.35
24	A	2605	PSU	C4-N3	-2.90	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	2251	OMG	C6-N1	-2.88	1.33	1.38
24	A	2504	PSU	C4-N3	-2.87	1.33	1.38
24	A	1915	3TD	C4-N3	2.83	1.46	1.40
1	a	516	PSU	C4-N3	-2.83	1.33	1.38
24	A	1835	2MG	C5-C4	2.83	1.46	1.38
1	a	1207	2MG	C6-N1	-2.81	1.33	1.38
1	a	1516	2MG	C5-C4	2.81	1.46	1.38
24	A	2445	2MG	C6-N1	-2.80	1.33	1.38
24	A	747	5MU	C6-C5	2.78	1.39	1.34
24	A	1618	6MZ	C5-C6	2.78	1.49	1.41
22	v	54	5MU	C4-N3	-2.77	1.33	1.38
24	A	2604	PSU	C6-C5	2.76	1.38	1.35
24	A	2445	2MG	C5-C4	2.74	1.46	1.38
24	A	2030	6MZ	C5-C6	2.73	1.49	1.41
24	A	1917	PSU	C4-N3	-2.68	1.33	1.38
24	A	2449	H2U	C2-N3	-2.67	1.33	1.38
1	a	527	G7M	C6-N1	-2.67	1.33	1.38
1	a	967	5MC	C6-C5	2.63	1.38	1.34
24	A	2552	OMU	C4-N3	-2.63	1.33	1.38
24	A	2069	G7M	C6-N1	-2.63	1.34	1.38
1	a	966	2MG	C6-N1	-2.62	1.34	1.38
24	A	2449	H2U	C4-N3	-2.62	1.33	1.37
22	v	54	5MU	C6-C5	2.60	1.38	1.34
24	A	2604	PSU	C2-N3	-2.58	1.33	1.37
24	A	746	PSU	C4-N3	-2.58	1.34	1.38
24	A	1835	2MG	C6-N1	-2.57	1.34	1.38
1	a	1516	2MG	C6-N1	-2.55	1.34	1.38
24	A	1911	PSU	C6-C5	2.55	1.38	1.35
24	A	1939	5MU	C6-N1	-2.55	1.33	1.38
24	A	2251	OMG	C5-N7	-2.53	1.34	1.39
24	A	1939	5MU	C2-N3	-2.48	1.33	1.38
24	A	1915	3TD	O2-C2	-2.47	1.18	1.23
24	A	2503	2MA	C5-C6	2.47	1.47	1.41
22	v	20	H2U	C2-N3	-2.44	1.33	1.38
22	v	54	5MU	C6-N1	-2.38	1.34	1.38
24	A	2503	2MA	C5-N7	-2.38	1.34	1.39
24	A	1915	3TD	O4-C4	-2.37	1.18	1.23
24	A	1939	5MU	C6-C5	2.36	1.38	1.34
22	v	8	4SU	C2-N1	2.35	1.42	1.38
1	a	1519	MA6	C4-N9	-2.34	1.32	1.37
1	a	1516	2MG	C5-N7	-2.34	1.34	1.39
24	A	747	5MU	C2-N1	2.31	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	967	5MC	C6-N1	-2.31	1.34	1.38
24	A	2445	2MG	C5-N7	-2.29	1.34	1.39
24	A	2605	PSU	C2-N3	-2.28	1.33	1.37
1	a	1207	2MG	C5-N7	-2.28	1.34	1.39
24	A	955	PSU	C6-C5	2.27	1.38	1.35
24	A	2457	PSU	C2-N3	-2.26	1.33	1.37
24	A	1835	2MG	C5-N7	-2.26	1.34	1.39
24	A	2552	OMU	C2-N3	-2.26	1.33	1.38
1	a	1407	5MC	C6-N1	-2.25	1.34	1.38
24	A	1911	PSU	C2-N3	-2.25	1.33	1.37
24	A	2069	G7M	O2'-C2'	-2.24	1.37	1.43
1	a	1518	MA6	C8-N9	-2.23	1.33	1.37
1	a	966	2MG	C5-N7	-2.22	1.34	1.39
22	v	54	5MU	C2-N1	2.21	1.42	1.38
22	v	55	PSU	C2-N3	-2.21	1.33	1.37
24	A	747	5MU	C6-N1	-2.18	1.34	1.38
24	A	747	5MU	C2-N3	-2.17	1.34	1.38
1	a	1407	5MC	C6-C5	2.16	1.38	1.34
24	A	1618	6MZ	C8-N7	2.14	1.35	1.31
22	v	54	5MU	C4-C5	2.14	1.48	1.44
1	a	1207	2MG	C2-N3	2.14	1.36	1.31
1	a	516	PSU	C2-N3	-2.13	1.33	1.37
24	A	2580	PSU	C2-N3	-2.12	1.33	1.37
24	A	2503	2MA	C8-N7	2.12	1.35	1.31
24	A	955	PSU	C2-N1	-2.11	1.33	1.36
1	a	1518	MA6	C4-N9	-2.11	1.33	1.37
24	A	2030	6MZ	C8-N7	2.09	1.35	1.31
1	a	527	G7M	O2'-C2'	-2.08	1.38	1.43
22	v	54	5MU	C2-N3	-2.07	1.34	1.38
22	v	20	H2U	C4-N3	-2.07	1.34	1.37
24	A	2457	PSU	C2-N1	-2.05	1.34	1.36
1	a	1519	MA6	C8-N9	-2.03	1.33	1.37
24	A	2504	PSU	C2-N3	-2.03	1.34	1.37
1	a	1516	2MG	C2-N3	2.03	1.35	1.31
24	A	955	PSU	C2-N3	-2.02	1.34	1.37
24	A	2498	OMC	C6-C5	2.01	1.39	1.35
24	A	1618	6MZ	C5-N7	-2.01	1.35	1.39
24	A	745	1MG	C5-N7	-2.01	1.35	1.39
24	A	1917	PSU	C2-N1	-2.01	1.34	1.36
1	a	1498	UR3	C5-C4	-2.00	1.38	1.43

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1835	2MG	C2-N3-C4	8.53	122.62	112.04
24	A	2503	2MA	C5-C4-N3	-8.23	117.93	127.19
1	a	966	2MG	C2-N3-C4	8.18	122.17	112.04
24	A	2445	2MG	C2-N3-C4	7.52	121.36	112.04
1	a	1516	2MG	C2-N3-C4	7.42	121.23	112.04
24	A	2030	6MZ	C9-N6-C6	-7.16	116.71	122.87
1	a	1207	2MG	C2-N3-C4	7.10	120.84	112.04
24	A	2457	PSU	N1-C2-N3	6.97	123.03	115.13
22	v	8	4SU	C4-N3-C2	-6.82	120.71	127.34
24	A	2251	OMG	C5-C4-N3	-6.75	117.51	128.46
1	a	966	2MG	C5-C4-N3	-6.74	117.53	128.46
24	A	2503	2MA	N3-C4-N9	6.66	136.22	126.99
24	A	2449	H2U	C4-N3-C2	-6.55	120.36	125.79
24	A	2580	PSU	N1-C2-N3	6.55	122.55	115.13
24	A	1835	2MG	C5-C4-N3	-6.51	117.90	128.46
24	A	2445	2MG	C5-C4-N3	-6.39	118.09	128.46
24	A	2030	6MZ	C5-C4-N3	-6.31	118.52	126.75
24	A	955	PSU	N1-C2-N3	6.14	122.09	115.13
22	v	8	4SU	C5-C4-N3	6.14	120.39	114.69
1	a	1207	2MG	C5-C4-N3	-6.12	118.53	128.46
24	A	2069	G7M	N9-C4-N3	6.11	138.21	125.94
24	A	1911	PSU	N1-C2-N3	6.05	121.99	115.13
24	A	1917	PSU	N1-C2-N3	6.02	121.95	115.13
1	a	1516	2MG	C5-C4-N3	-6.00	118.72	128.46
1	a	516	PSU	N1-C2-N3	5.97	121.89	115.13
24	A	2504	PSU	N1-C2-N3	5.96	121.89	115.13
24	A	1618	6MZ	C5-C4-N3	-5.83	119.14	126.75
1	a	527	G7M	C5-C4-N3	-5.83	116.97	128.15
24	A	1915	3TD	N1-C2-N3	5.81	120.72	116.14
24	A	2604	PSU	N1-C2-N3	5.74	121.64	115.13
1	a	1498	UR3	C1'-N1-C2	5.70	126.61	116.99
22	v	55	PSU	N1-C2-N3	5.65	121.53	115.13
1	a	1518	MA6	C5-C4-N3	-5.55	119.51	126.75
24	A	747	5MU	N3-C2-N1	5.53	122.23	114.89
24	A	2069	G7M	C5-C4-N3	-5.52	117.57	128.15
24	A	2605	PSU	N1-C2-N3	5.45	121.31	115.13
24	A	1939	5MU	C4-N3-C2	-5.42	120.33	127.35
1	a	966	2MG	N9-C4-N3	5.24	136.47	125.94
24	A	745	1MG	C5-C4-N3	-5.16	120.09	128.46
1	a	1519	MA6	C4-C5-N7	-5.15	104.34	110.62
24	A	1939	5MU	C5-C4-N3	5.15	119.70	115.31
24	A	2030	6MZ	N3-C4-N9	5.12	135.52	127.08
24	A	2251	OMG	N9-C4-N3	5.12	136.22	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	54	5MU	C4-N3-C2	-5.05	120.82	127.35
1	a	1498	UR3	C4-N3-C2	-5.03	119.83	124.56
24	A	2251	OMG	C2-N3-C4	5.00	121.20	112.30
1	a	1519	MA6	C2-N1-C6	4.98	123.52	111.75
1	a	1519	MA6	C5-C4-N3	-4.94	120.30	126.75
22	v	54	5MU	N3-C2-N1	4.91	121.41	114.89
24	A	747	5MU	C4-N3-C2	-4.89	121.03	127.35
1	a	1518	MA6	C2-N1-C6	4.86	123.23	111.75
24	A	2069	G7M	C2-N3-C4	4.85	120.95	112.30
24	A	746	PSU	N1-C2-N3	4.84	120.61	115.13
1	a	1207	2MG	N9-C4-N3	4.84	135.66	125.94
22	v	8	4SU	C5-C4-S4	-4.79	118.29	124.47
1	a	527	G7M	N9-C4-N3	4.76	135.51	125.94
1	a	1518	MA6	C4-C5-N7	-4.75	104.83	110.62
24	A	1939	5MU	N3-C2-N1	4.75	121.19	114.89
24	A	1835	2MG	N9-C4-N3	4.66	135.30	125.94
24	A	2445	2MG	N9-C4-N3	4.65	135.27	125.94
1	a	1519	MA6	C10-N6-C6	-4.56	108.58	120.40
1	a	1498	UR3	O2-C2-N3	-4.55	114.92	121.34
24	A	1618	6MZ	C6-C5-N7	4.52	137.28	132.39
24	A	2552	OMU	N3-C2-N1	4.49	120.86	114.89
1	a	527	G7M	C2-N3-C4	4.48	120.29	112.30
24	A	1618	6MZ	C9-N6-C6	-4.44	119.05	122.87
24	A	2030	6MZ	C6-C5-N7	4.42	137.17	132.39
22	v	54	5MU	C5-C4-N3	4.40	119.07	115.31
24	A	1618	6MZ	N3-C4-N9	4.37	134.29	127.08
24	A	745	1MG	C2-N3-C4	4.36	121.77	111.98
1	a	1516	2MG	N9-C4-N3	4.35	134.68	125.94
24	A	1962	5MC	C5-C6-N1	-4.28	118.94	123.34
24	A	2457	PSU	C4-N3-C2	-4.24	120.23	126.34
24	A	745	1MG	N9-C4-N3	4.22	134.42	125.94
24	A	1917	PSU	O2-C2-N1	-4.22	118.14	122.79
24	A	1939	5MU	O4-C4-C5	-4.22	120.01	124.90
24	A	1939	5MU	C5-C6-N1	-4.21	119.00	123.34
24	A	2552	OMU	C4-N3-C2	-4.21	121.03	126.58
24	A	2552	OMU	C1'-N1-C2	4.16	125.10	117.57
24	A	2605	PSU	C4-N3-C2	-4.15	120.35	126.34
1	a	1519	MA6	C5-N7-C8	4.03	109.24	103.51
22	v	54	5MU	O4-C4-C5	-4.03	120.23	124.90
24	A	2069	G7M	O3'-C3'-C4'	4.00	122.61	111.05
24	A	955	PSU	O2-C2-N1	-3.97	118.42	122.79
24	A	747	5MU	O4-C4-C5	-3.92	120.35	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	8	4SU	N3-C2-N1	3.91	120.08	114.89
24	A	2030	6MZ	C2-N3-C4	3.91	120.99	111.75
24	A	1915	3TD	C4-N3-C2	-3.91	120.37	124.61
24	A	2498	OMC	O2-C2-N3	-3.89	116.01	122.33
24	A	955	PSU	C4-N3-C2	-3.88	120.74	126.34
24	A	1962	5MC	O2-C2-N3	-3.88	116.02	122.33
1	a	1518	MA6	C9-N6-C6	-3.86	110.38	120.40
24	A	1911	PSU	C4-N3-C2	-3.83	120.82	126.34
1	a	1518	MA6	N3-C4-N9	3.83	133.40	127.08
1	a	516	PSU	C4-N3-C2	-3.82	120.83	126.34
22	v	55	PSU	C4-N3-C2	-3.80	120.87	126.34
24	A	747	5MU	C5-C4-N3	3.79	118.55	115.31
24	A	1618	6MZ	C4-C5-N7	-3.76	106.03	110.62
24	A	1911	PSU	O2-C2-N1	-3.75	118.67	122.79
24	A	1917	PSU	C4-N3-C2	-3.74	120.95	126.34
1	a	1518	MA6	C2-N3-C4	3.72	120.54	111.75
24	A	2504	PSU	C4-N3-C2	-3.71	120.99	126.34
24	A	2030	6MZ	C4-C5-N7	-3.70	106.11	110.62
24	A	1618	6MZ	C2-N3-C4	3.65	120.36	111.75
22	v	20	H2U	C4-N3-C2	-3.61	122.79	125.79
1	a	1519	MA6	C2-N3-C4	3.61	120.29	111.75
1	a	1519	MA6	C6-C5-N7	3.61	139.34	133.28
24	A	2604	PSU	C4-N3-C2	-3.57	121.19	126.34
24	A	746	PSU	C4-N3-C2	-3.56	121.21	126.34
24	A	2580	PSU	C4-N3-C2	-3.56	121.21	126.34
24	A	1835	2MG	C6-C5-N7	3.53	136.81	130.25
1	a	527	G7M	O3'-C3'-C4'	3.53	121.25	111.05
1	a	967	5MC	C5-C6-N1	-3.51	119.73	123.34
24	A	2552	OMU	C5-C4-N3	3.49	120.07	114.84
1	a	1519	MA6	N1-C2-N3	-3.46	123.19	128.60
1	a	1518	MA6	C5-N7-C8	3.36	108.29	103.51
1	a	527	G7M	O3'-C3'-C2'	3.30	122.51	111.82
24	A	2457	PSU	O2-C2-N1	-3.30	119.15	122.79
1	a	1498	UR3	C6-N1-C2	-3.30	118.83	121.79
22	v	54	5MU	C5-C6-N1	-3.29	119.96	123.34
1	a	1518	MA6	N1-C2-N3	-3.28	123.47	128.60
1	a	1516	2MG	C6-C5-N7	3.25	136.28	130.25
1	a	1519	MA6	N3-C4-N9	3.21	132.37	127.08
1	a	1519	MA6	C4-N9-C8	3.14	109.14	105.73
24	A	2580	PSU	O2-C2-N1	-3.11	119.36	122.79
1	a	516	PSU	O2-C2-N1	-3.11	119.37	122.79
24	A	2552	OMU	O2-C2-N3	-3.08	115.76	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C6-C5-N7	3.07	135.95	130.25
1	a	1518	MA6	C6-C5-N7	3.01	138.34	133.28
1	a	1407	5MC	C5-C6-N1	-3.01	120.25	123.34
24	A	2445	2MG	C6-C5-N7	3.00	135.84	130.25
24	A	745	1MG	C6-C5-N7	3.00	136.14	129.35
24	A	747	5MU	C5-C6-N1	-2.99	120.27	123.34
24	A	2030	6MZ	N1-C2-N3	-2.97	123.95	128.60
22	v	8	4SU	C1'-N1-C2	2.97	122.95	117.57
1	a	1407	5MC	O2-C2-N3	-2.95	117.53	122.33
1	a	1519	MA6	C10-N6-C9	-2.95	106.61	116.12
24	A	2605	PSU	C6-C5-C4	-2.94	116.14	118.20
1	a	1519	MA6	N9-C8-N7	-2.90	109.95	113.91
1	a	1498	UR3	C1'-N1-C6	-2.88	114.55	120.84
24	A	2030	6MZ	C5-N7-C8	2.87	107.58	103.51
24	A	2503	2MA	C4-C5-N7	-2.82	107.18	110.62
1	a	1207	2MG	C6-C5-N7	2.82	135.49	130.25
24	A	1618	6MZ	N1-C2-N3	-2.82	124.20	128.60
24	A	2069	G7M	CN7-N7-C5	2.81	130.25	126.77
24	A	746	PSU	C6-C5-C4	-2.80	116.24	118.20
24	A	745	1MG	C4-C5-N7	-2.78	106.32	110.72
24	A	2030	6MZ	C4-N9-C8	2.77	108.73	105.73
24	A	2503	2MA	N6-C6-N1	2.76	120.93	117.03
24	A	746	PSU	O2-C2-N1	-2.75	119.76	122.79
1	a	1402	4OC	O2-C2-N3	-2.66	118.00	122.33
24	A	2251	OMG	C6-C5-N7	2.65	135.18	130.25
24	A	1835	2MG	C4-C5-N7	-2.64	106.54	110.72
24	A	1962	5MC	C5-C4-N3	-2.64	118.82	121.67
1	a	1518	MA6	C10-N6-C9	-2.64	107.62	116.12
24	A	2504	PSU	O2-C2-N1	-2.63	119.89	122.79
22	v	55	PSU	C6-C5-C4	-2.62	116.36	118.20
24	A	2445	2MG	C4-C5-N7	-2.62	106.58	110.72
1	a	1516	2MG	C4-C5-N7	-2.58	106.64	110.72
24	A	2503	2MA	C4-N9-C8	2.56	108.50	105.73
24	A	2605	PSU	O2-C2-N1	-2.55	119.98	122.79
22	v	55	PSU	O2-C2-N1	-2.55	119.98	122.79
24	A	2449	H2U	C5-C6-N1	-2.55	103.21	111.61
24	A	1618	6MZ	C5-N7-C8	2.55	107.13	103.51
24	A	2552	OMU	O4-C4-C5	-2.52	120.73	125.16
24	A	2503	2MA	C2-N1-C6	2.51	122.00	118.08
24	A	2604	PSU	O2-C2-N1	-2.49	120.05	122.79
1	a	966	2MG	C4-C5-N7	-2.49	106.78	110.72
24	A	2251	OMG	C4-C5-N7	-2.49	106.78	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	2503	2MA	C5-N7-C8	2.48	107.03	103.51
24	A	2445	2MG	C2-N1-C6	-2.46	121.65	124.48
24	A	2445	2MG	CM2-N2-C2	-2.45	118.45	123.86
1	a	527	G7M	C5'-C4'-C3'	2.43	124.30	115.18
1	a	967	5MC	C5-C4-N3	-2.40	119.08	121.67
1	a	527	G7M	O2'-C2'-C1'	2.40	118.05	110.02
1	a	1518	MA6	C4-N9-C8	2.39	108.32	105.73
24	A	747	5MU	O2-C2-N3	-2.39	117.05	121.50
24	A	1835	2MG	C2-N1-C6	-2.38	121.74	124.48
24	A	2604	PSU	C6-C5-C4	-2.37	116.54	118.20
24	A	2069	G7M	O2'-C2'-C1'	2.35	117.87	110.02
24	A	747	5MU	C6-N1-C2	-2.29	118.97	121.30
24	A	1835	2MG	CM2-N2-C2	-2.29	118.81	123.86
24	A	2069	G7M	C5-C6-N1	2.28	116.54	111.79
24	A	747	5MU	C1'-N1-C2	2.26	121.67	117.57
24	A	2449	H2U	O4-C4-N3	2.25	123.84	120.28
24	A	2251	OMG	O6-C6-C5	-2.24	120.64	126.60
1	a	1516	2MG	O6-C6-C5	-2.23	120.68	126.60
24	A	1835	2MG	C5-C6-N1	2.22	118.83	113.19
1	a	1207	2MG	O6-C6-C5	-2.21	120.72	126.60
24	A	745	1MG	C6-C5-C4	-2.20	117.54	119.97
24	A	2457	PSU	C5-C6-N1	-2.19	118.83	122.11
24	A	2552	OMU	C6-N1-C2	-2.17	118.21	120.99
22	v	20	H2U	C5-C6-N1	-2.16	104.50	111.61
1	a	966	2MG	O6-C6-C5	-2.15	120.90	126.60
24	A	2445	2MG	O6-C6-C5	-2.15	120.90	126.60
22	v	20	H2U	C5-C4-N3	2.15	119.06	116.65
1	a	1407	5MC	C5-C4-N3	-2.14	119.36	121.67
1	a	966	2MG	C2-N1-C6	-2.14	122.02	124.48
24	A	1915	3TD	O4-C4-N3	-2.14	116.38	120.30
1	a	1207	2MG	C4-C5-N7	-2.13	107.34	110.72
24	A	2457	PSU	O2-C2-N3	-2.13	117.80	121.82
22	v	54	5MU	O2-C2-N1	-2.13	119.96	122.79
1	a	966	2MG	C5-C6-N1	2.12	118.58	113.19
24	A	2069	G7M	C1'-N9-C8	-2.11	119.62	126.74
24	A	1618	6MZ	C2-N1-C6	2.10	122.29	115.25
24	A	2498	OMC	O2-C2-N1	2.07	123.18	118.89
1	a	516	PSU	O4'-C1'-C2'	2.06	108.05	105.14
24	A	1835	2MG	O6-C6-C5	-2.06	121.15	126.60
1	a	1402	4OC	CM4-N4-C4	-2.05	118.44	122.45
24	A	2030	6MZ	C2-N1-C6	2.04	122.09	115.25
24	A	1618	6MZ	C4-N9-C8	2.03	107.92	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	527	G7M	O2'-C2'-C3'	2.02	118.37	111.82
1	a	967	5MC	O2-C2-N3	-2.00	119.08	122.33

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3'
1	a	527	G7M	C4'
24	A	2069	G7M	C3'
24	A	2069	G7M	C4'

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	967	5MC	O4'-C4'-C5'-O5'
1	a	967	5MC	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C10
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	A	1915	3TD	O4'-C1'-C5-C4
24	A	1915	3TD	O4'-C1'-C5-C6
24	A	1915	3TD	C3'-C4'-C5'-O5'
24	A	1915	3TD	O4'-C4'-C5'-O5'
24	A	1962	5MC	C2'-C1'-N1-C2
24	A	1962	5MC	C2'-C1'-N1-C6
24	A	2445	2MG	O4'-C4'-C5'-O5'
24	A	2445	2MG	C3'-C4'-C5'-O5'
24	A	2503	2MA	O4'-C1'-N9-C8
24	A	2503	2MA	O4'-C1'-N9-C4
24	A	2504	PSU	C3'-C4'-C5'-O5'
24	A	2504	PSU	O4'-C4'-C5'-O5'
24	A	2552	OMU	O4'-C1'-N1-C2
24	A	746	PSU	C3'-C4'-C5'-O5'
24	A	746	PSU	O4'-C4'-C5'-O5'
24	A	2030	6MZ	C3'-C4'-C5'-O5'
24	A	2498	OMC	C3'-C4'-C5'-O5'
24	A	2498	OMC	O4'-C4'-C5'-O5'
24	A	2457	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	N1-C6-N6-C10
24	A	2552	OMU	O4'-C1'-N1-C6
24	A	2069	G7M	O4'-C4'-C5'-O5'
24	A	2069	G7M	C3'-C4'-C5'-O5'
24	A	2580	PSU	O4'-C4'-C5'-O5'
24	A	2030	6MZ	O4'-C4'-C5'-O5'
24	A	2251	OMG	O4'-C4'-C5'-O5'
24	A	1915	3TD	C4'-C5'-O5'-P
24	A	1962	5MC	O4'-C1'-N1-C6
24	A	1835	2MG	O4'-C4'-C5'-O5'
24	A	2030	6MZ	C4'-C5'-O5'-P
24	A	2251	OMG	C4'-C5'-O5'-P
24	A	1939	5MU	C3'-C4'-C5'-O5'
1	a	527	G7M	C4'-C5'-O5'-P
24	A	1962	5MC	O4'-C1'-N1-C2
1	a	1518	MA6	O4'-C1'-N9-C8
24	A	2503	2MA	C4'-C5'-O5'-P
24	A	1835	2MG	C3'-C4'-C5'-O5'
24	A	747	5MU	C3'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C4
24	A	2457	PSU	C3'-C4'-C5'-O5'
24	A	2580	PSU	C3'-C4'-C5'-O5'
1	a	1519	MA6	C3'-C4'-C5'-O5'
24	A	2604	PSU	O4'-C4'-C5'-O5'
24	A	2445	2MG	C4'-C5'-O5'-P
24	A	1939	5MU	O4'-C4'-C5'-O5'
24	A	2251	OMG	C3'-C4'-C5'-O5'
24	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1915	3TD	1	0
24	A	1917	PSU	1	0
24	A	2503	2MA	1	0
1	a	1518	MA6	2	0
22	v	55	PSU	1	0
1	a	1519	MA6	1	0
22	v	54	5MU	1	0
24	A	2580	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

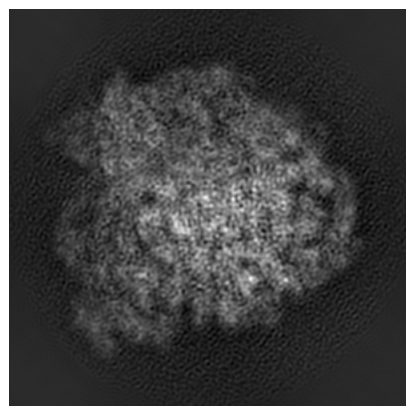
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4121. These allow visual inspection of the internal detail of the map and identification of artifacts.

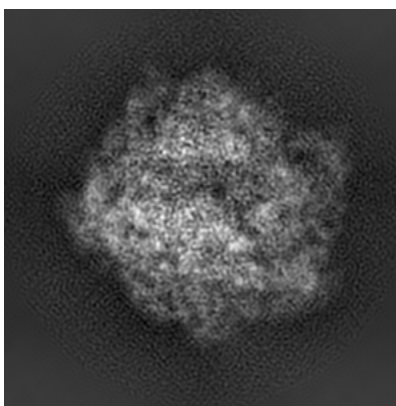
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

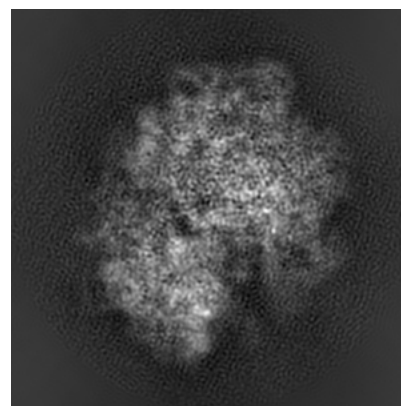
6.1.1 Primary map



X

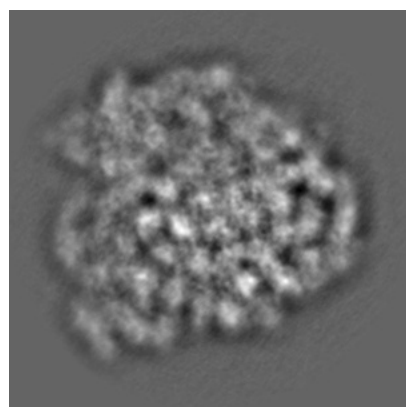


Y

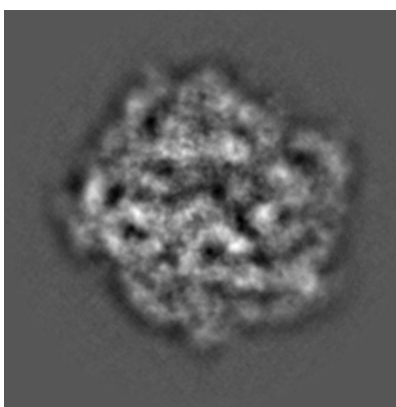


Z

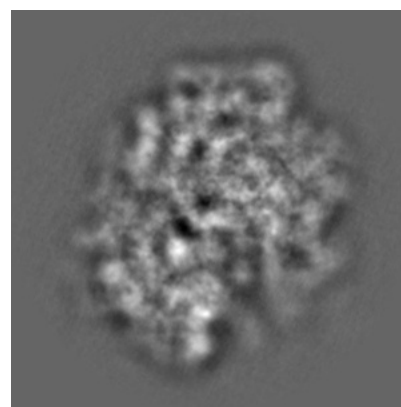
6.1.2 Raw map



X



Y

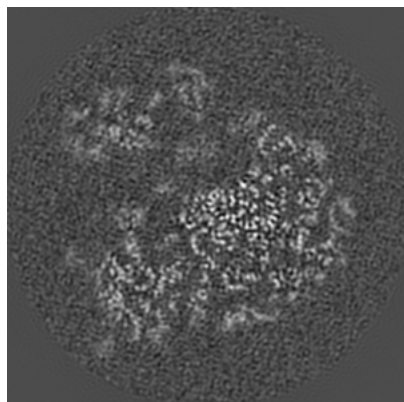


Z

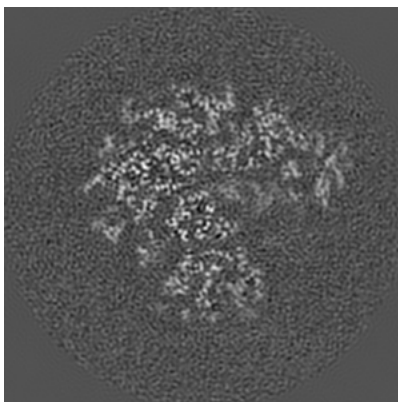
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

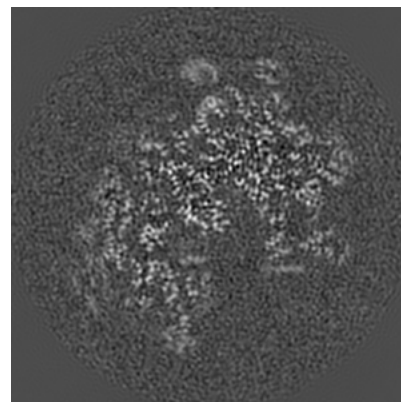
6.2.1 Primary map



X Index: 136

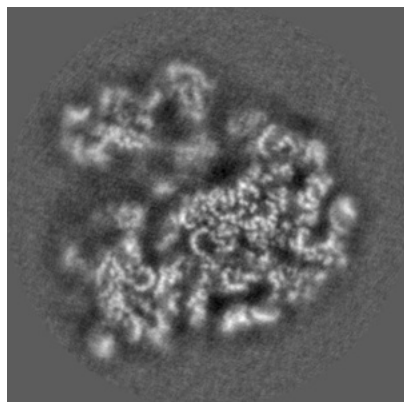


Y Index: 136

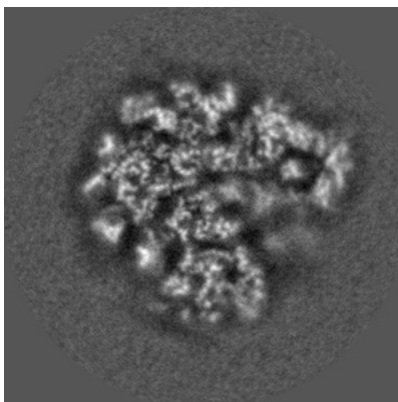


Z Index: 136

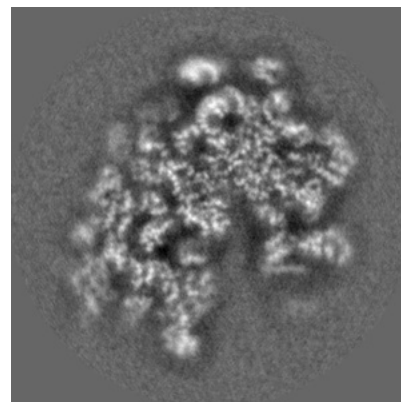
6.2.2 Raw map



X Index: 136



Y Index: 136

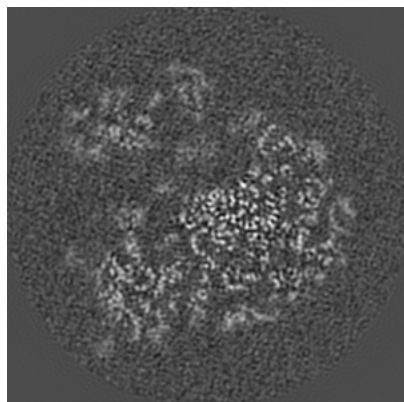


Z Index: 136

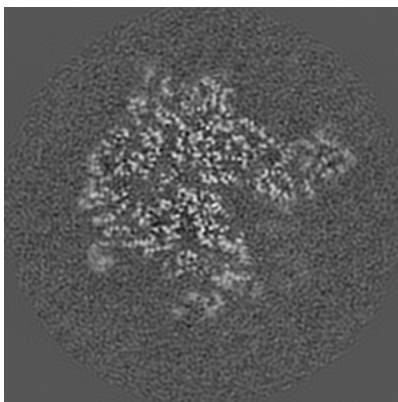
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

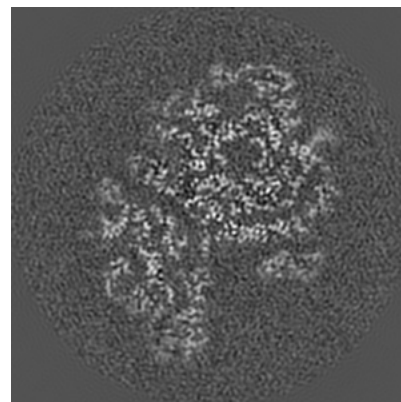
6.3.1 Primary map



X Index: 136

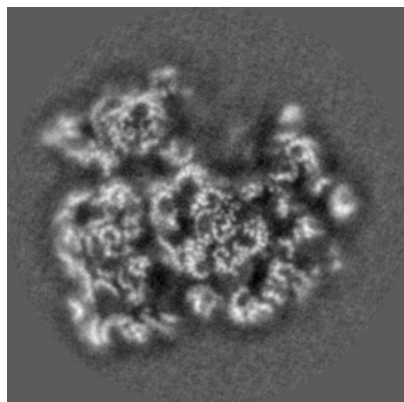


Y Index: 152

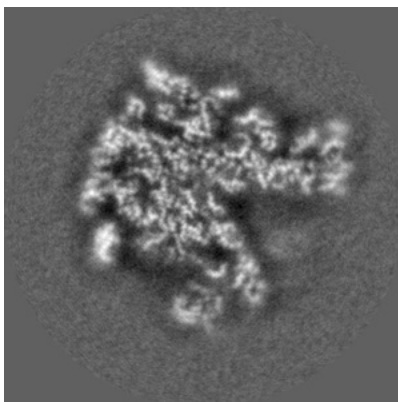


Z Index: 119

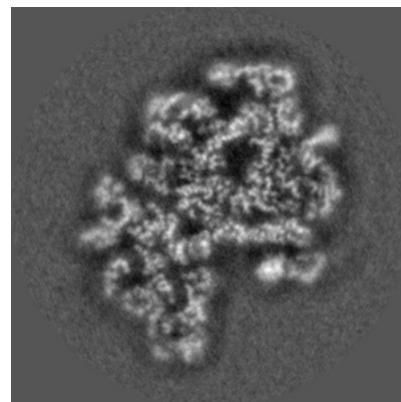
6.3.2 Raw map



X Index: 125



Y Index: 146

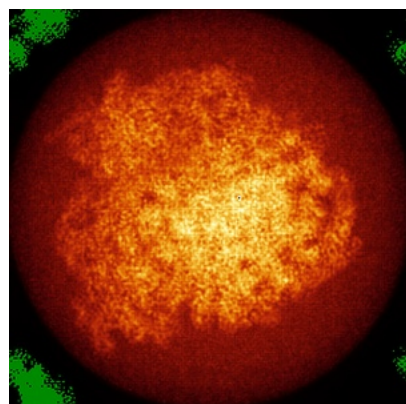


Z Index: 121

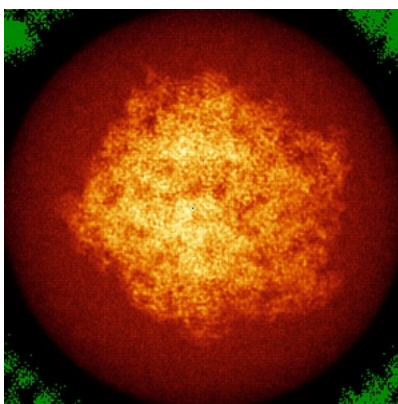
The images above show the largest variance slices of the map in three orthogonal directions.

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

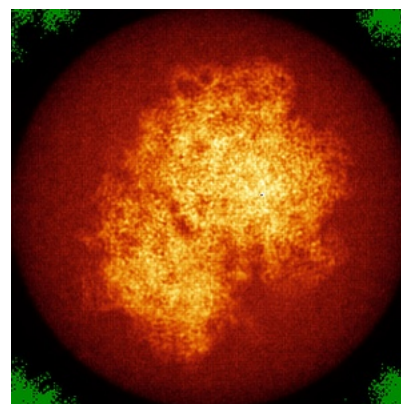
6.4.1 Primary map



X

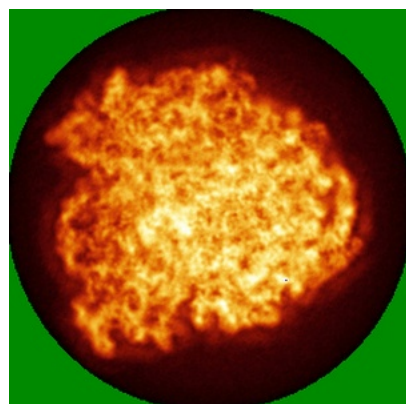


Y

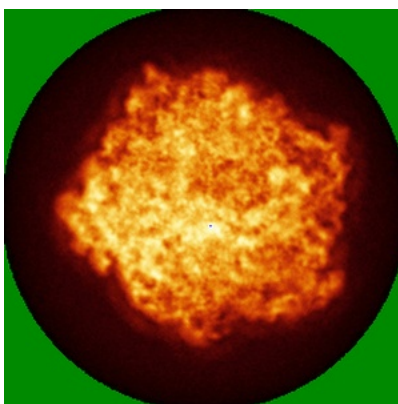


Z

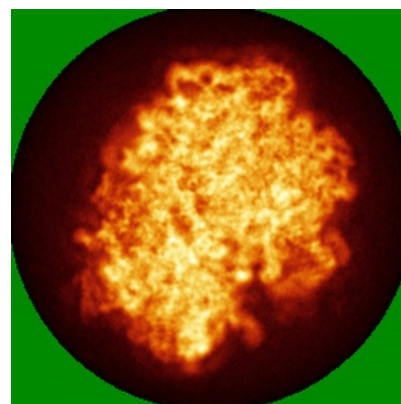
6.4.2 Raw map



X



Y

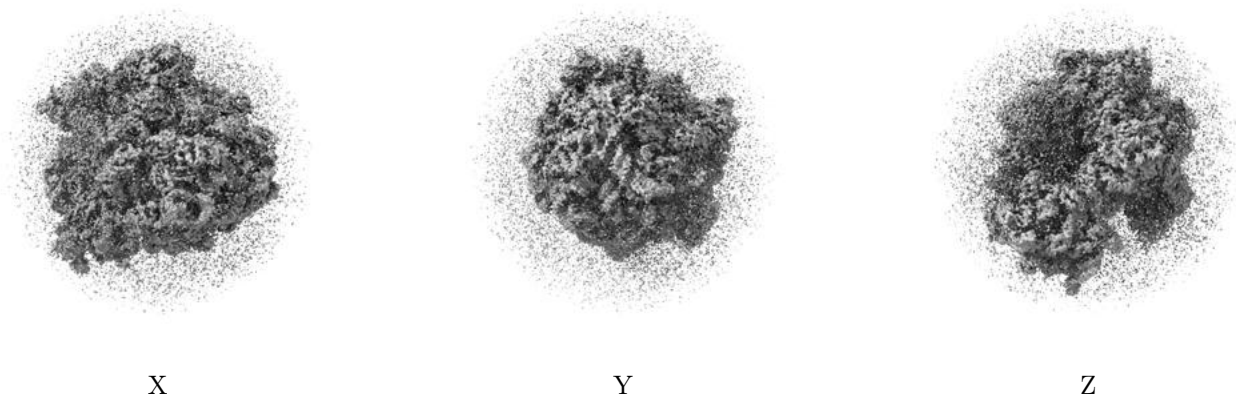


Z

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.

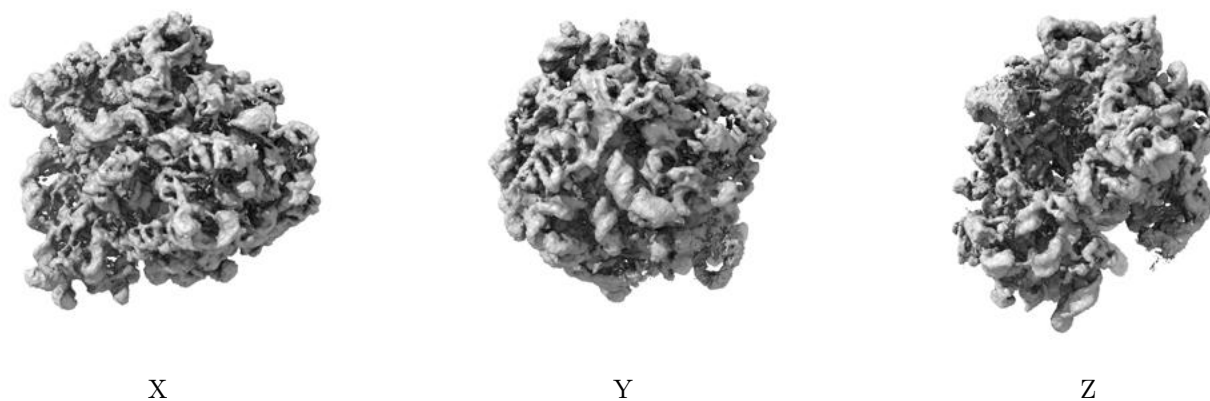
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.52. 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.

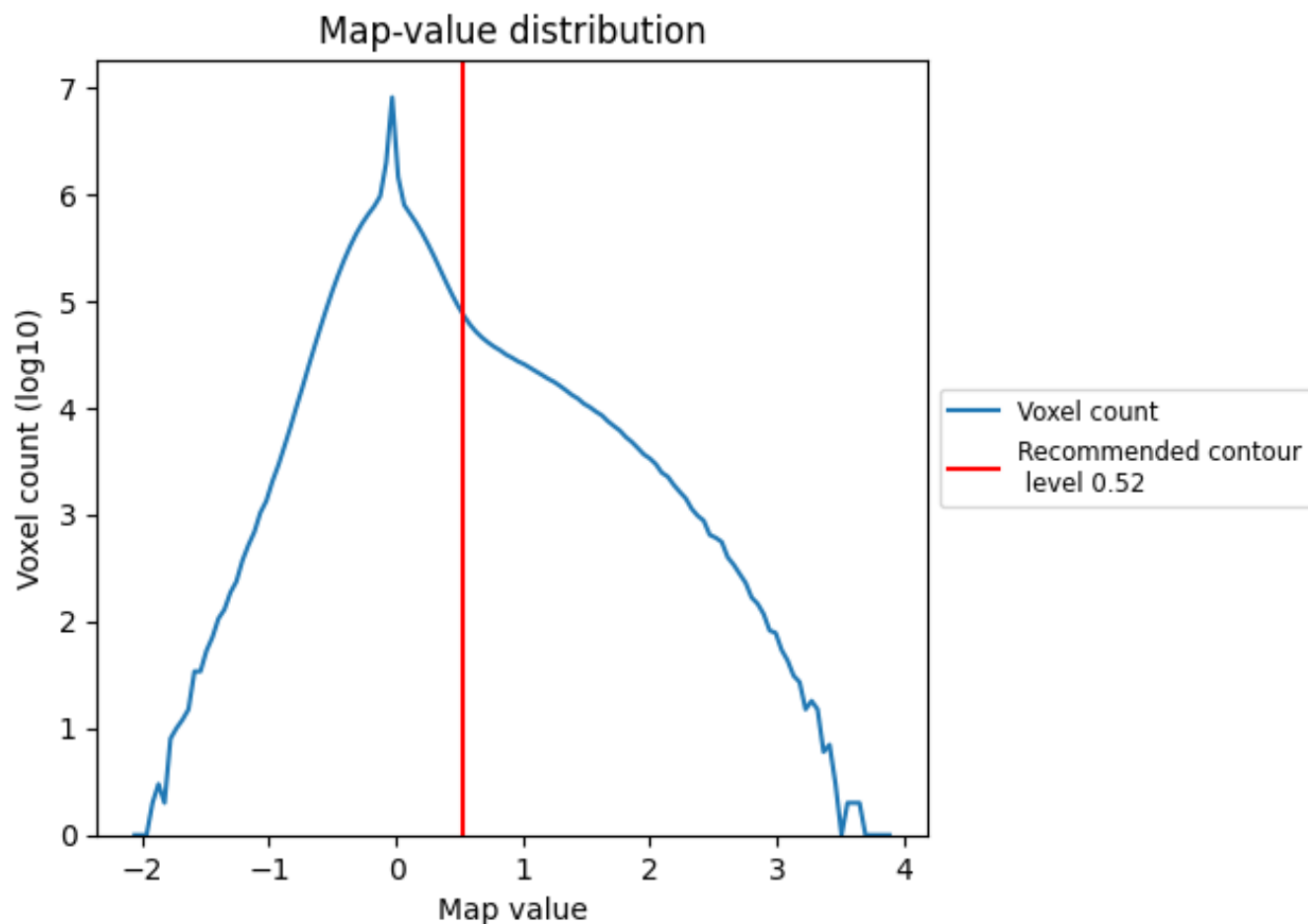
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

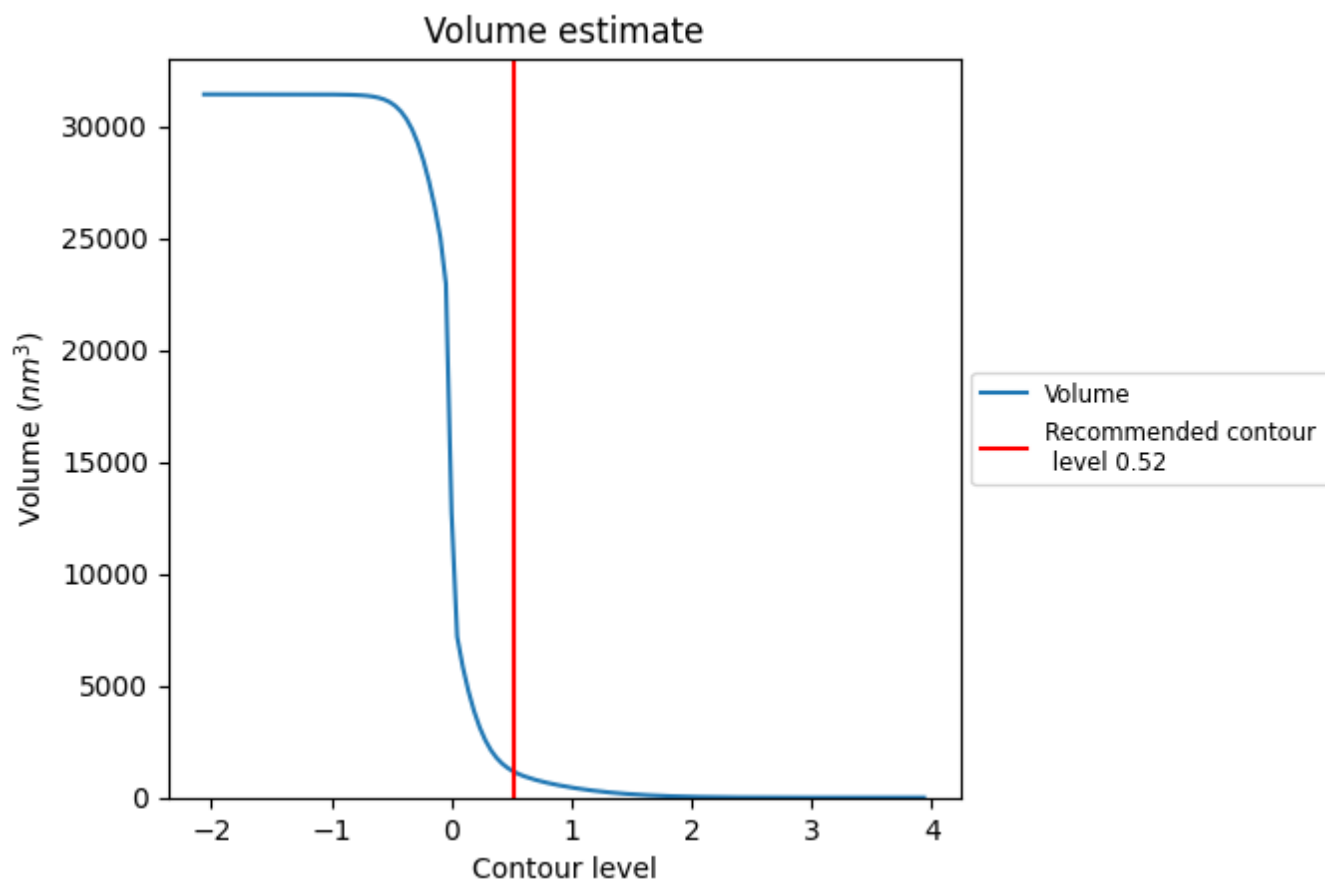
This section contains the results of statistical analysis of the map.

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.

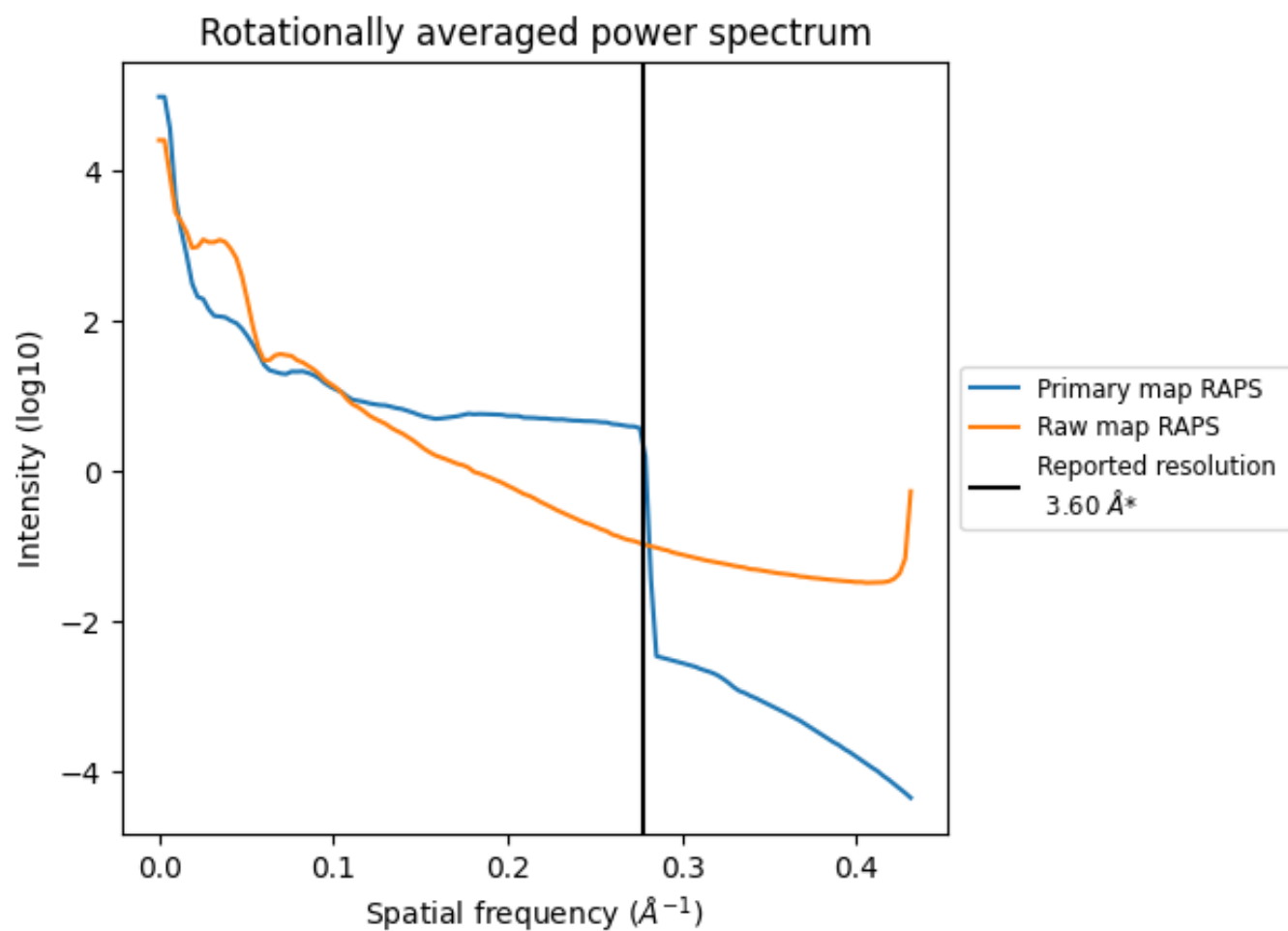
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1155 nm³; this corresponds to an approximate mass of 1043 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

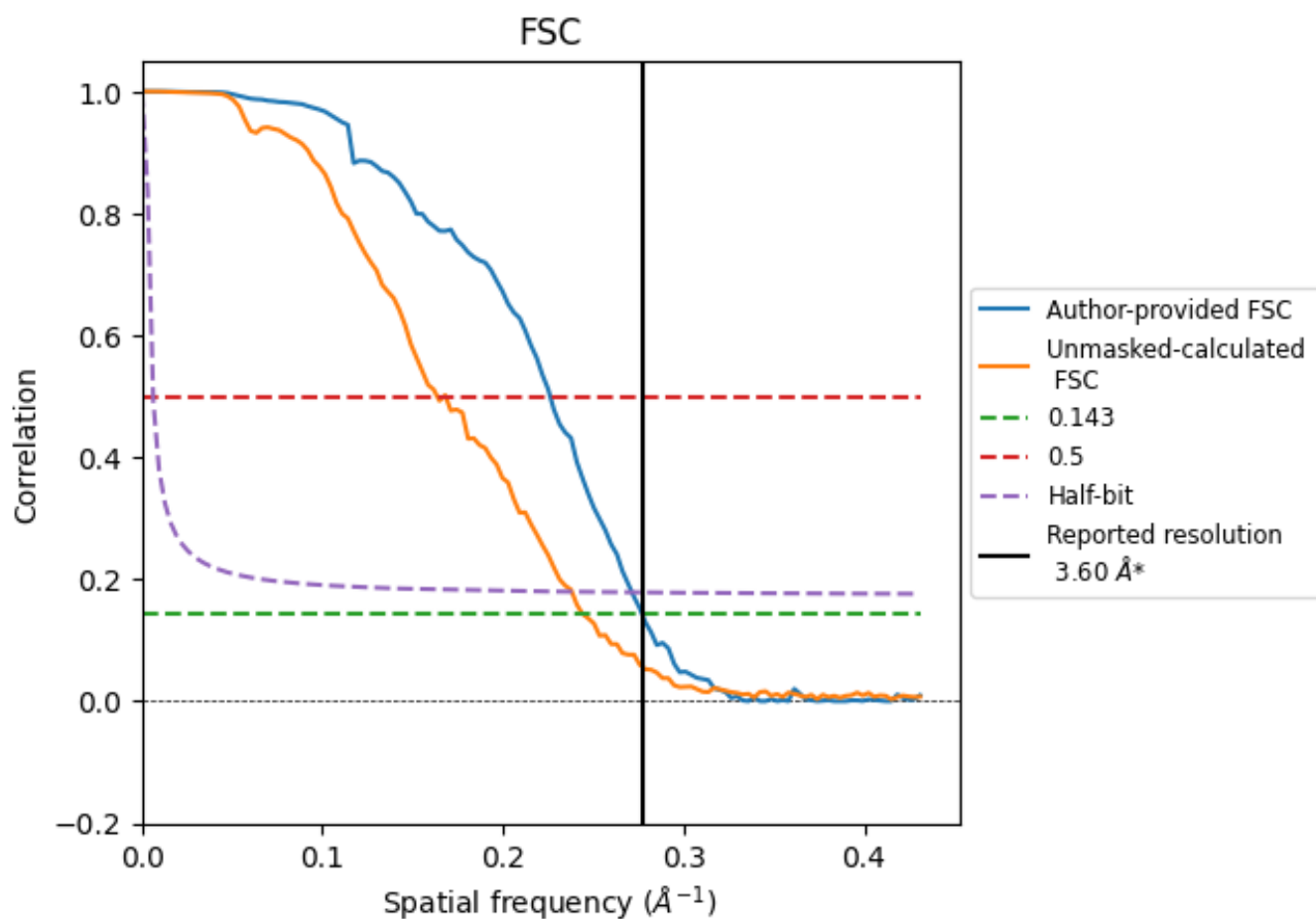


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

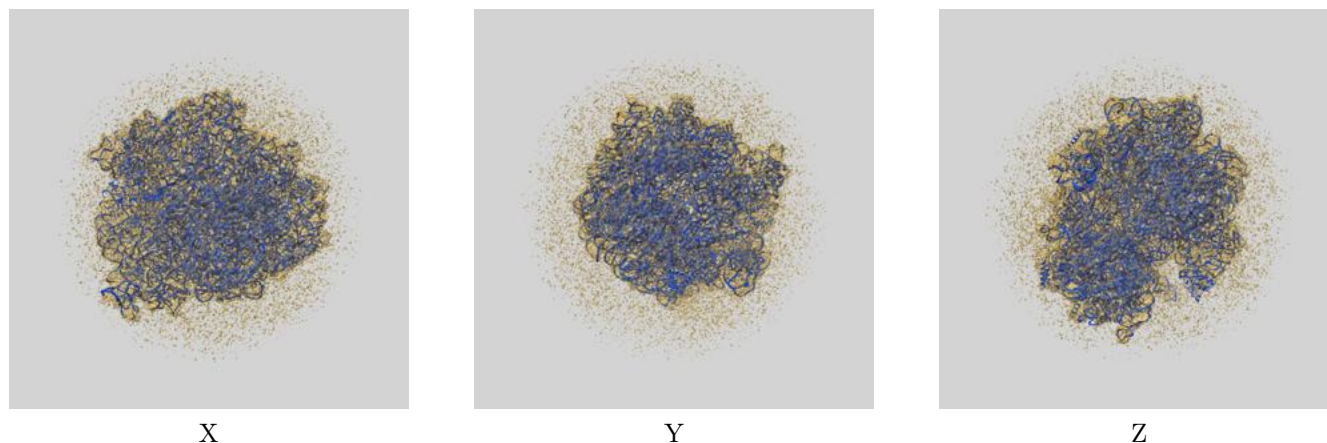
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.42	3.68
Unmasked-calculated*	4.10	6.12	4.20

*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 4.10 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

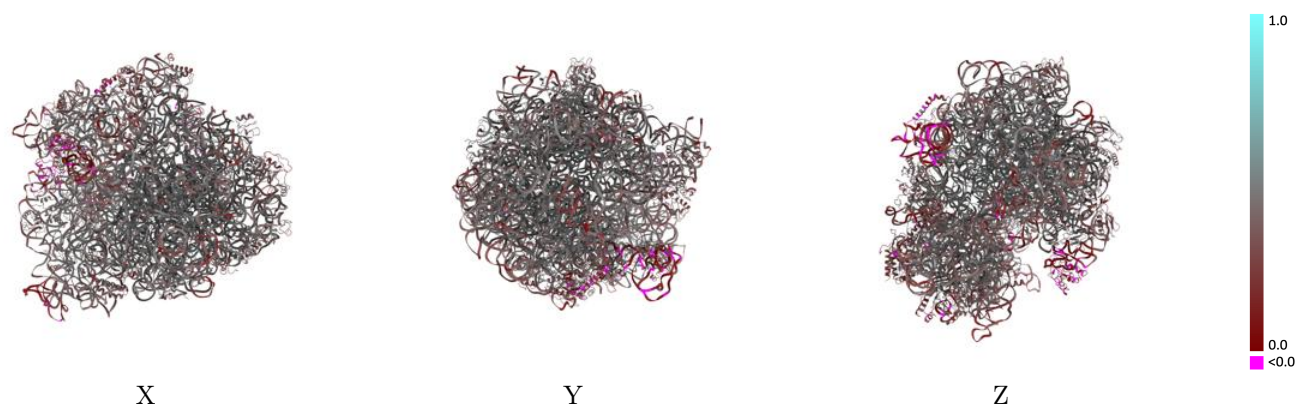
This section contains information regarding the fit between EMDB map EMD-4121 and PDB model 5LZA. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



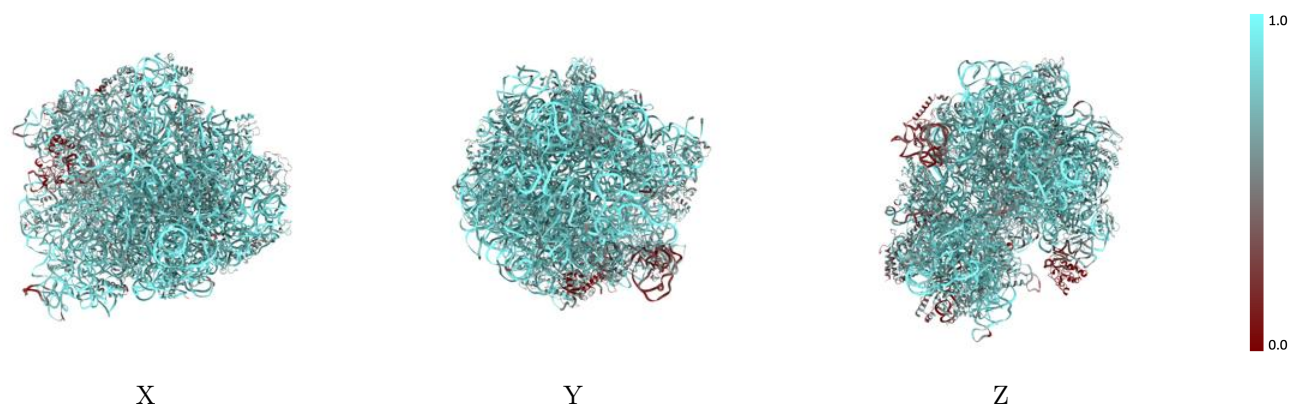
The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



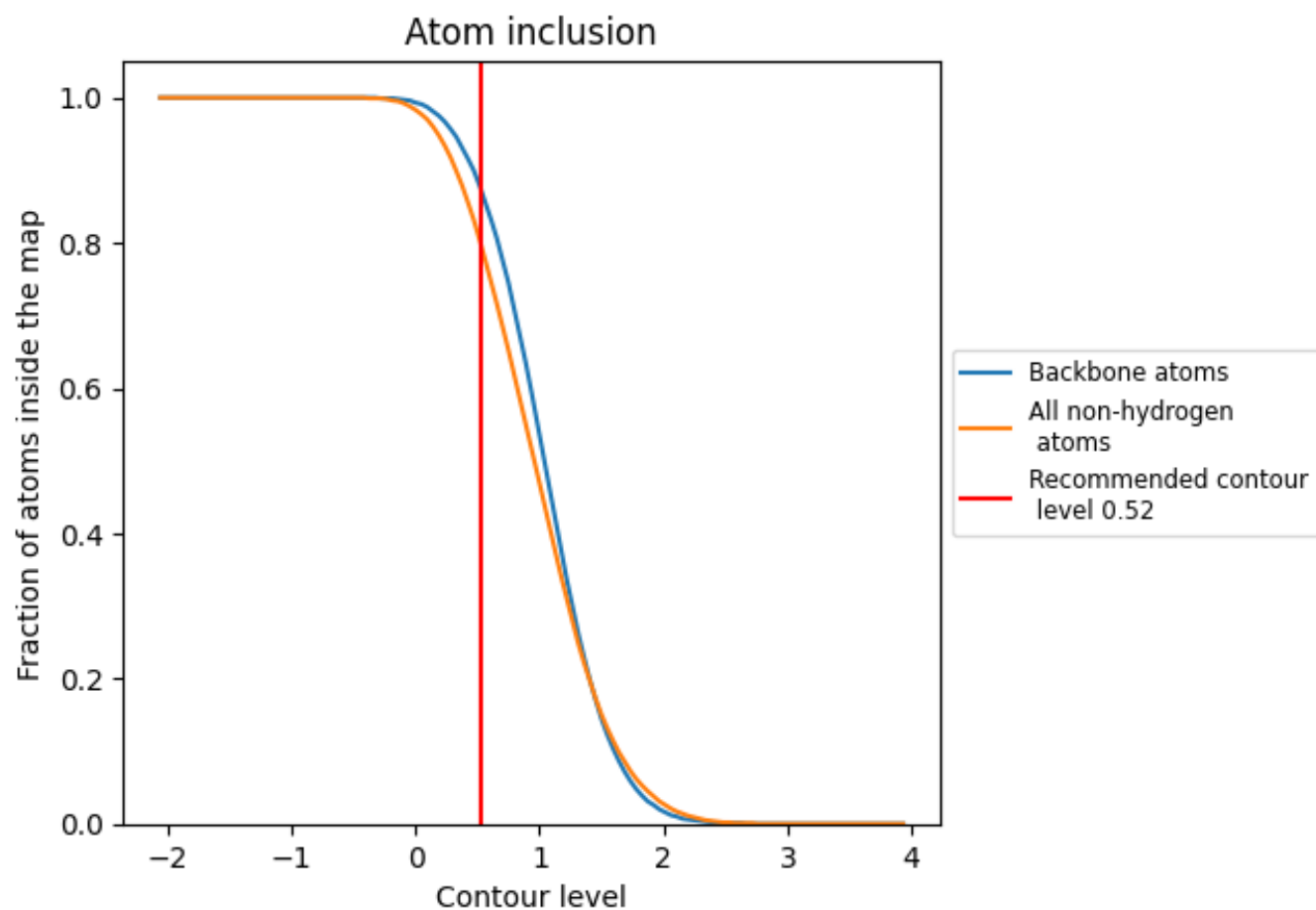
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.52).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.4070
0	 0.7310	 0.4610
1	 0.6120	 0.3830
2	 0.7940	 0.4860
3	 0.7640	 0.4790
4	 0.7270	 0.4640
6	 0.5110	 0.2440
A	 0.8750	 0.4260
B	 0.8940	 0.4000
C	 0.7710	 0.4680
D	 0.7260	 0.4450
E	 0.6780	 0.3990
F	 0.6640	 0.3560
G	 0.6680	 0.3660
H	 0.2190	 0.2180
I	 0.0500	 0.0810
J	 0.7220	 0.4380
K	 0.7180	 0.4370
L	 0.7320	 0.4350
M	 0.7420	 0.4440
N	 0.7410	 0.4440
O	 0.6670	 0.3800
P	 0.7140	 0.4120
Q	 0.7340	 0.4480
R	 0.7190	 0.4200
S	 0.7050	 0.4270
T	 0.6720	 0.3980
U	 0.6630	 0.3880
V	 0.6910	 0.3840
W	 0.7340	 0.4540
X	 0.7170	 0.4400
Y	 0.6660	 0.3720
Z	 0.7050	 0.4150
a	 0.8810	 0.4160
b	 0.4780	 0.3010



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Chain	Atom inclusion	Q-score
c	 0.6520	 0.3940
d	 0.6130	 0.3520
e	 0.6960	 0.4120
f	 0.6860	 0.3480
g	 0.6340	 0.3380
h	 0.6900	 0.4030
i	 0.6120	 0.3400
j	 0.5490	 0.3390
k	 0.7100	 0.3950
l	 0.7240	 0.4100
m	 0.6640	 0.3530
n	 0.6920	 0.3970
o	 0.7250	 0.4000
p	 0.6750	 0.4080
q	 0.6540	 0.3540
r	 0.6980	 0.4040
s	 0.6580	 0.3670
t	 0.6830	 0.3690
u	 0.5200	 0.2610
v	 0.7140	 0.3550
x	 0.1990	 0.1580