



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:21 PM UTC

PDB ID : 8P8B / pdb_00008p8b
EMDB ID : EMD-17134
Title : Mycoplasma pneumoniae large ribosomal subunit in chloramphenicol-treated cells
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-05-31
Resolution : 2.90 Å (reported)
Based on initial models : 7OOC, 7OOD

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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

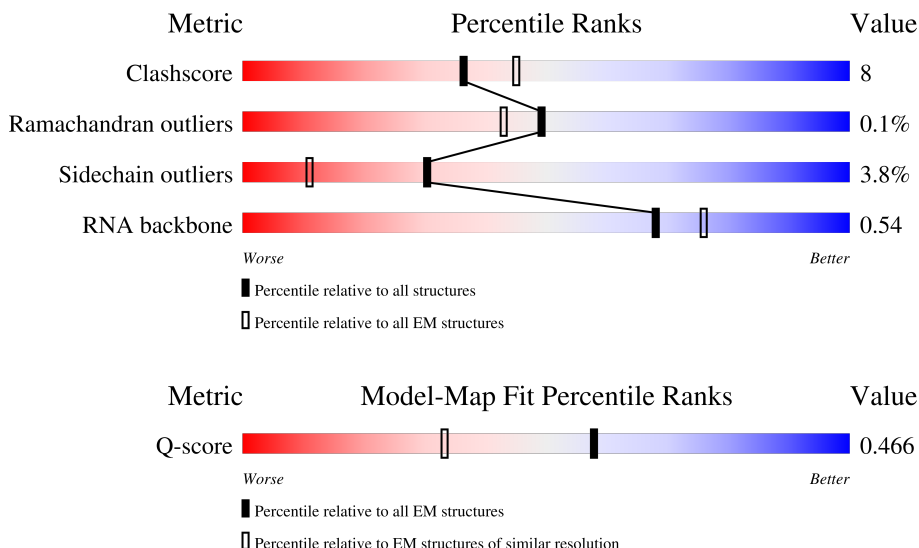
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	0	48	6% 79% 21%
2	1	59	80% 20%
3	2	37	89% 11%

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Mol	Chain	Length	Quality of chain
4	3	2907	
5	4	108	
6	5	1520	
7	6	76	
8	7	75	
9	8	76	
10	X	444	
11	Y	9	
12	Z	36	
13	a	287	
14	b	287	
15	c	212	
16	d	180	
17	e	184	
18	f	149	
19	g	161	
20	h	137	
21	i	146	
22	j	122	
23	k	151	
24	l	139	
25	m	124	
26	n	116	
27	o	119	
28	p	127	

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Mol	Chain	Length	Quality of chain
29	q	100	
30	r	159	
31	s	237	
32	t	111	
33	u	104	
34	v	65	
35	w	111	
36	x	97	
37	y	57	
38	z	53	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 97182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	48	Total	C	N	O	S	0	0
			392	242	85	63	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	2893	Total	C	N	O	P	0	0
			61995	27704	11293	20105	2893		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	108	Total	C	N	O	P	0	0
			2305	1030	415	752	108		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	32	Total	C	N	O	P	0	0
			683	307	124	220	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	75	Total	C	N	O	P	0	0
			1599	712	279	533	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	76	Total	C	N	O	P	0	0
			1615	722	284	533	76		

- Molecule 10 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	30	Total	C	N	O	S	0	0
			242	155	43	43	1		

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	9	Total	C	N	O	P	0	0
			195	87	38	61	9		

- Molecule 12 is a protein called nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	36	Total	C	N	O	0	0
			187	112	37	38		

- Molecule 13 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 14 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	231	Total	C	N	O	S	0	0
			1778	1129	320	322	7		

- Molecule 15 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 16 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 17 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 18 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	149	Total	C	N	O	S	0	0
			1210	780	212	215	3		

- Molecule 19 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 20 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 22 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 23 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 24 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 25 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 28 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 29 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 32 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 33 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	88	Total	C	N	O	S	0	0
			670	416	132	121	1		

- Molecule 34 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 35 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	w	110	Total	C	N	O	S	0	0
			906	576	168	162			

- Molecule 36 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	46	Total	C	N	O	S	0	0
			366	235	59	68	4		

- Molecule 37 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 38 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

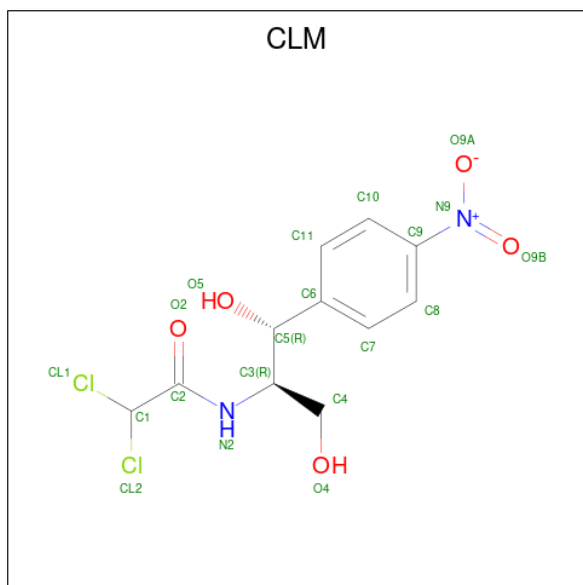
Mol	Chain	Residues	Atoms		AltConf
39	2	1	Total	Zn	0
			1	1	
39	x	1	Total	Zn	0
			1	1	
39	y	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
39	z	1	Total	Zn	0
			1	1	

- Molecule 40 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
40	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 41 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
41	3	1	Total	K	0
			1	1	

- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

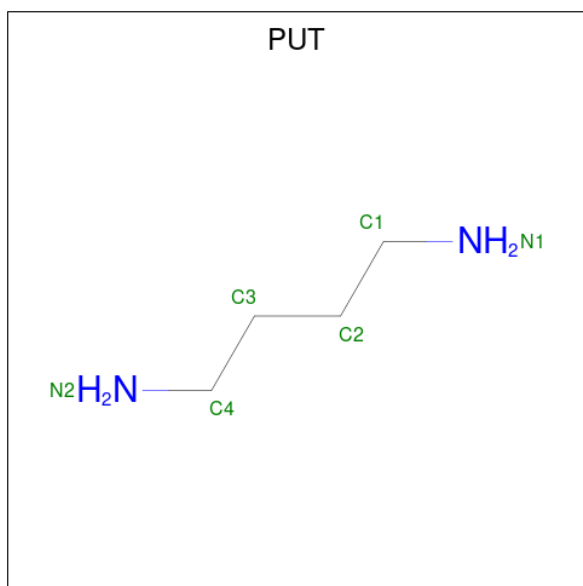
Mol	Chain	Residues	Atoms		AltConf
42	3	219	Total	Mg	0
			219	219	
42	4	1	Total	Mg	0
			1	1	
42	6	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
42	7	1	Total	Mg	0
			1	1	
42	8	2	Total	Mg	0
			2	2	
42	b	2	Total	Mg	0
			2	2	
42	i	1	Total	Mg	0
			1	1	
42	y	2	Total	Mg	0
			2	2	

- Molecule 43 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



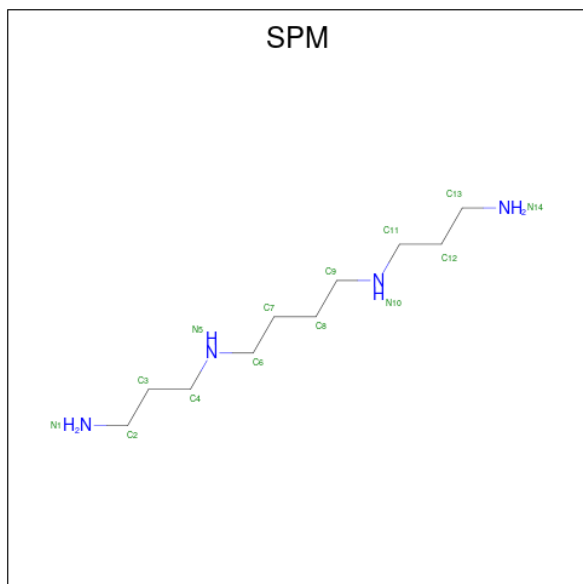
Mol	Chain	Residues	Atoms			AltConf
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	

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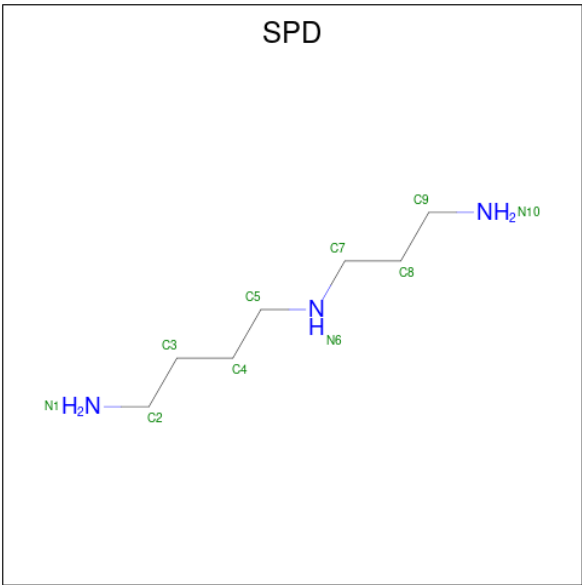
Mol	Chain	Residues	Atoms			AltConf
43	3	1	Total	C	N	0
			6	4	2	

- Molecule 44 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
44	3	1	Total	C	N	0
			14	10	4	
44	3	1	Total	C	N	0
			14	10	4	
44	3	1	Total	C	N	0
			14	10	4	
44	b	1	Total	C	N	0
			14	10	4	

- Molecule 45 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



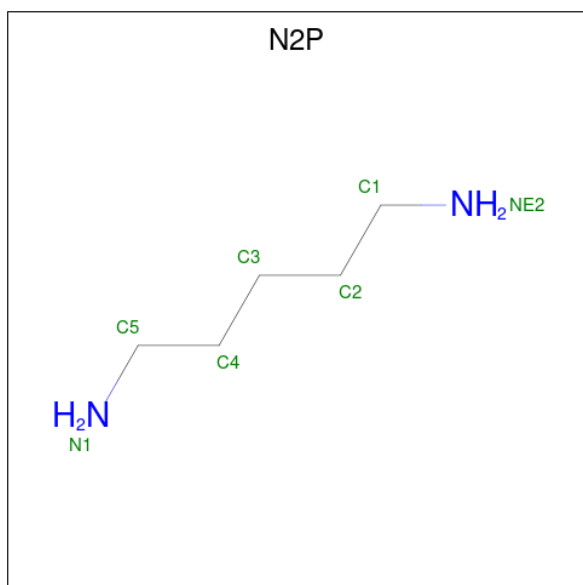
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	

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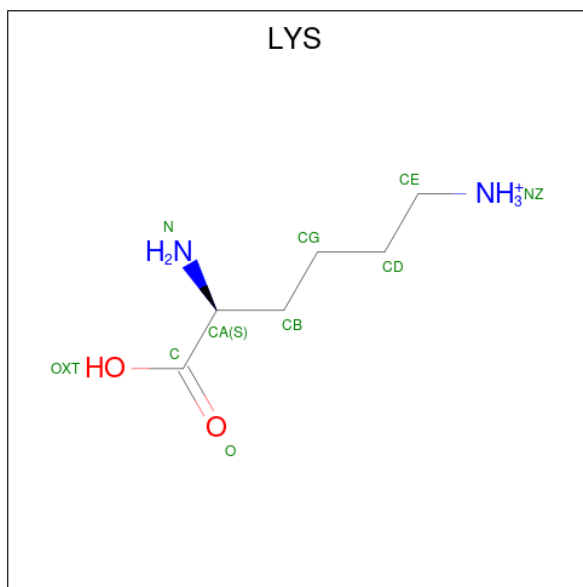
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	

- Molecule 46 is PENTANE-1,5-DIAMINE (CCD ID: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			AltConf
46	3	1	Total	C	N	0
			7	5	2	
46	3	1	Total	C	N	0
			7	5	2	
46	3	1	Total	C	N	0
			7	5	2	

- Molecule 47 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).

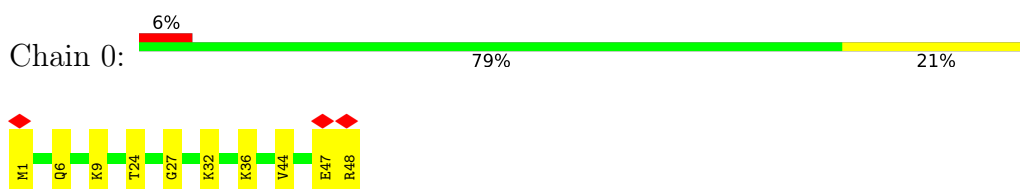


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
47	8	1	9	6	2	1	0

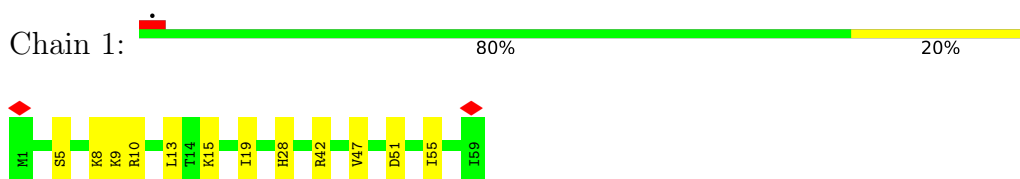
3 Residue-property plots [i](#)

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

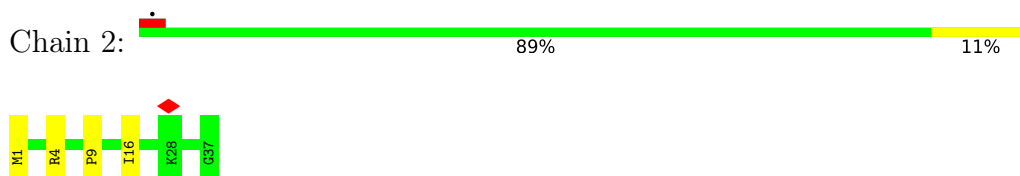
- Molecule 1: 50S ribosomal protein L34



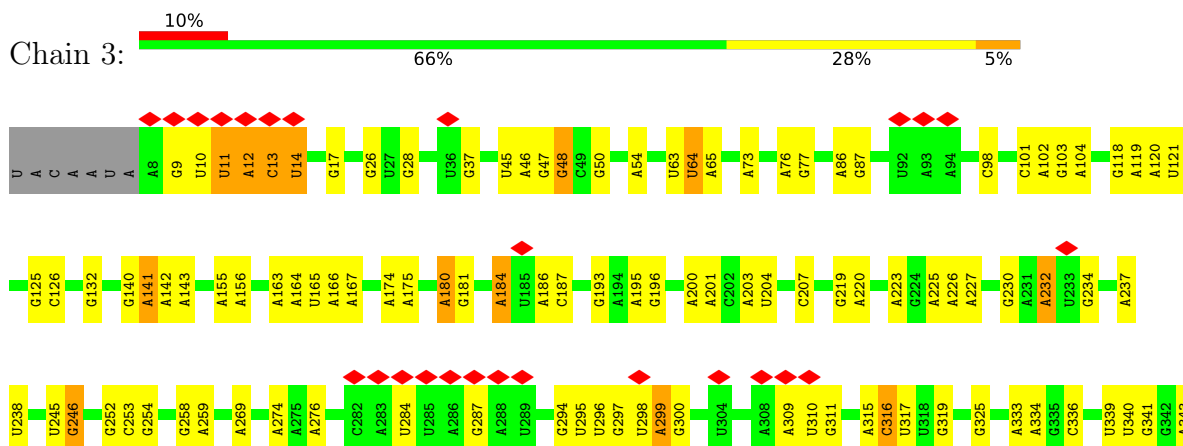
- Molecule 2: 50S ribosomal protein L35

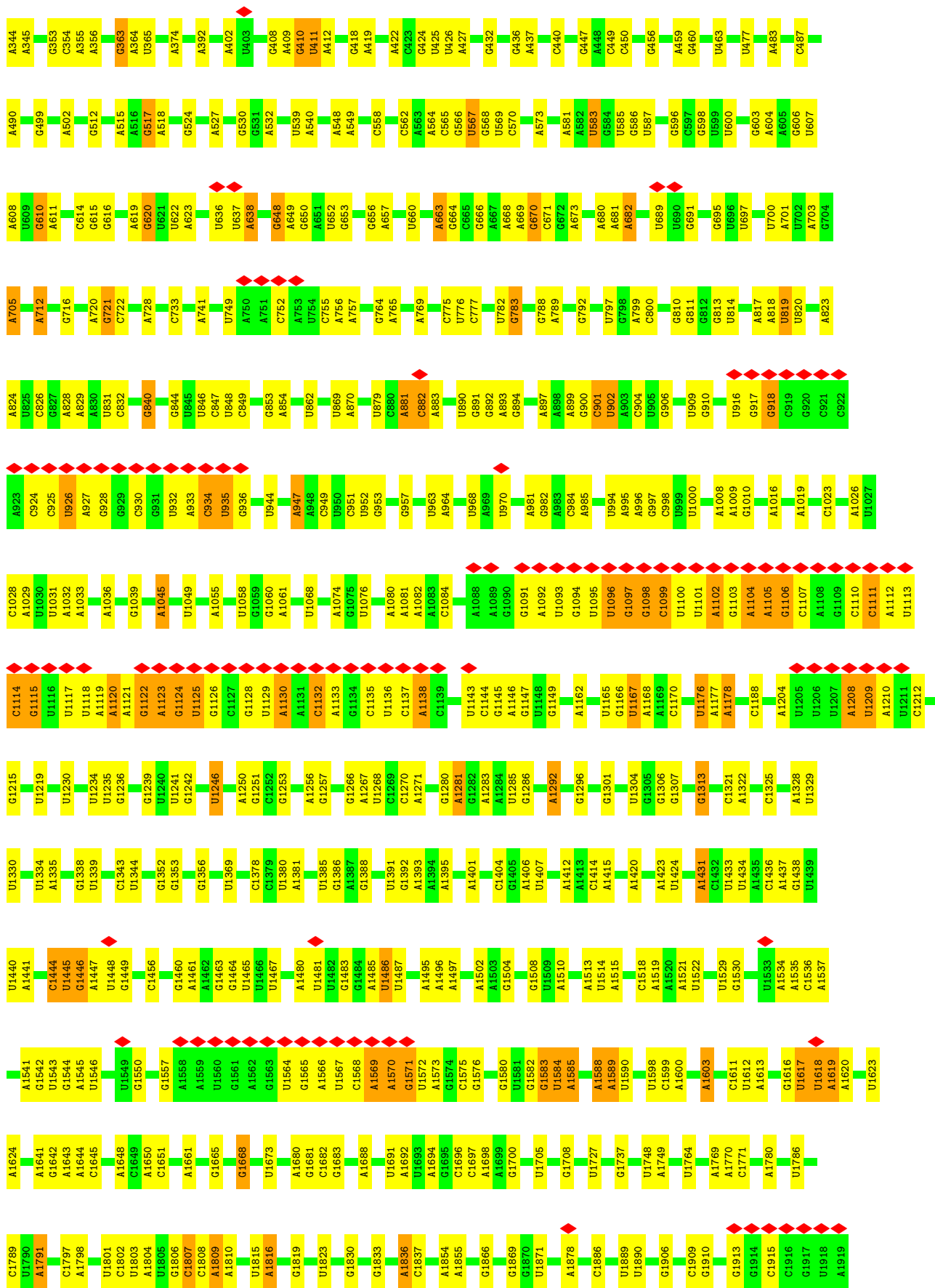


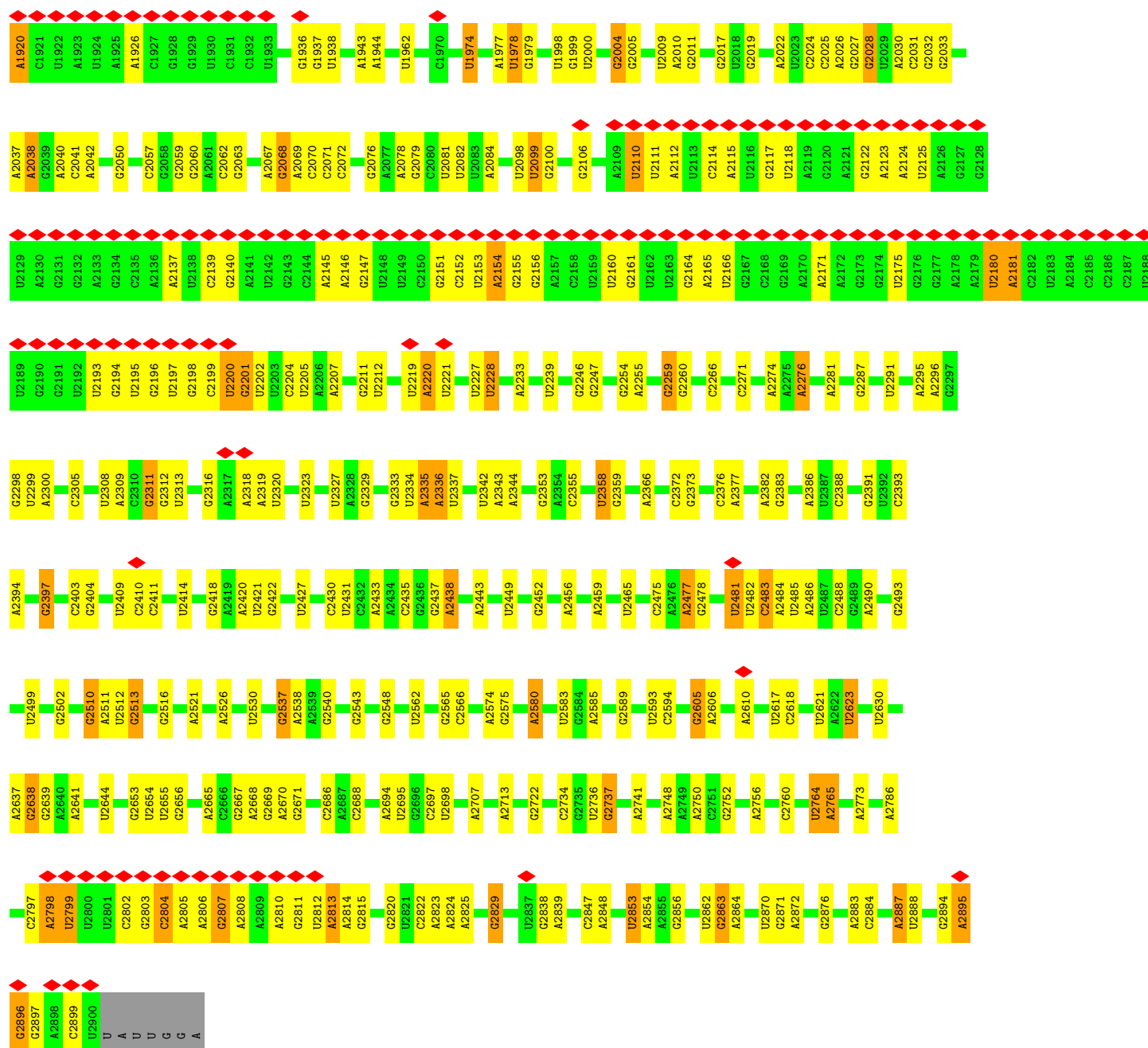
- Molecule 3: 50S ribosomal protein L36



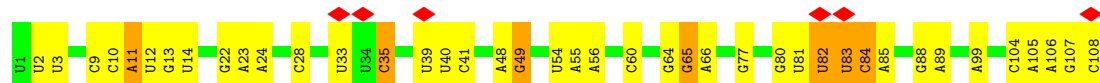
- Molecule 4: 23S ribosomal RNA



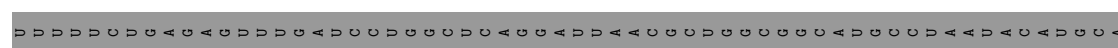




• Molecule 5: 5S ribosomal RNA

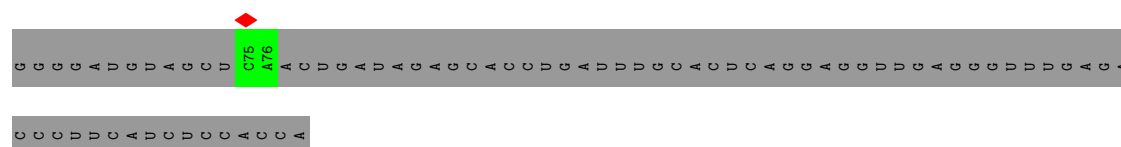


• Molecule 6: 16S ribosomal RNA

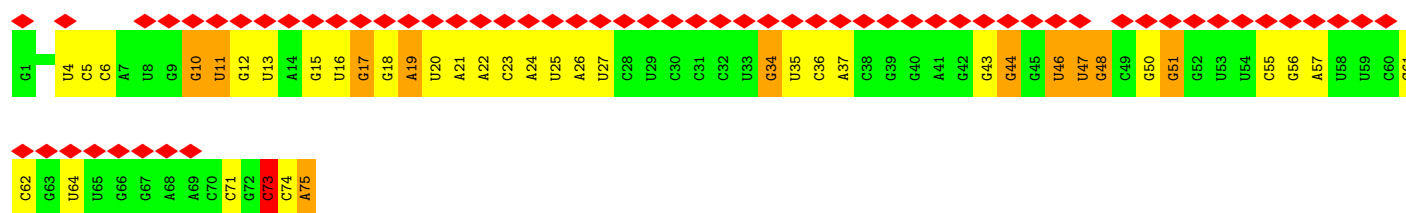
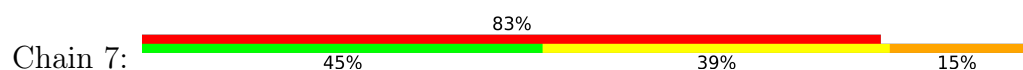




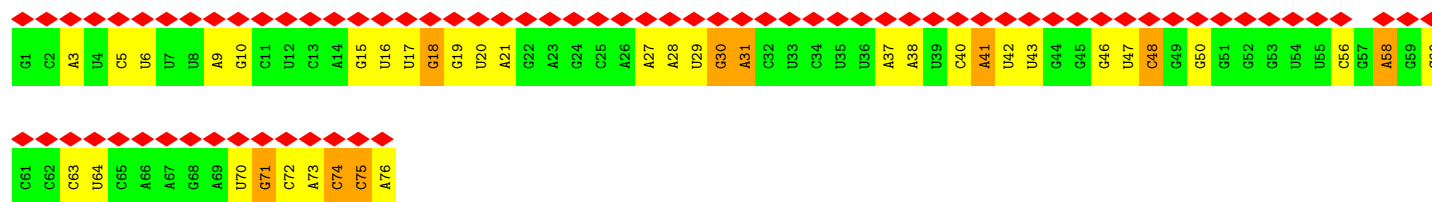
- Molecule 7: tRNA-Ala (E-site)



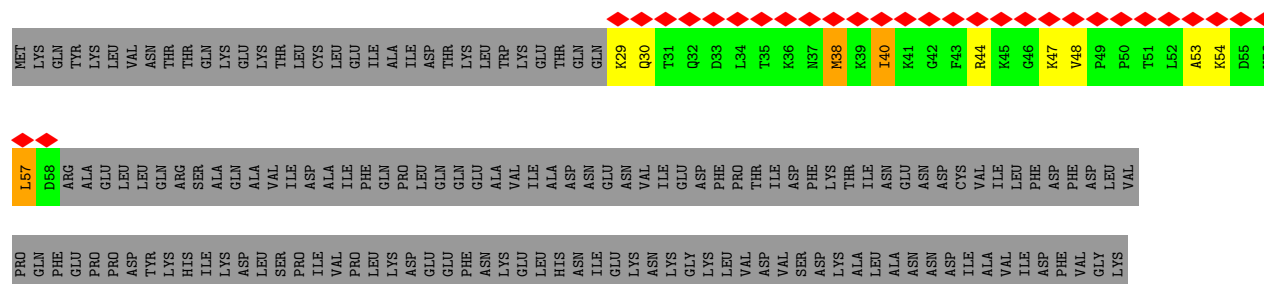
- Molecule 8: tRNA-Asp (P-site)

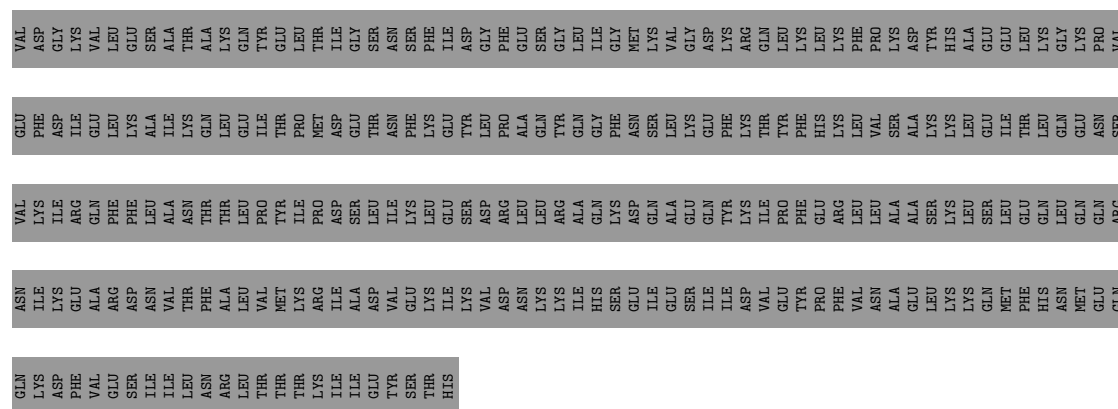


- Molecule 9: tRNA-Lys (A-site)

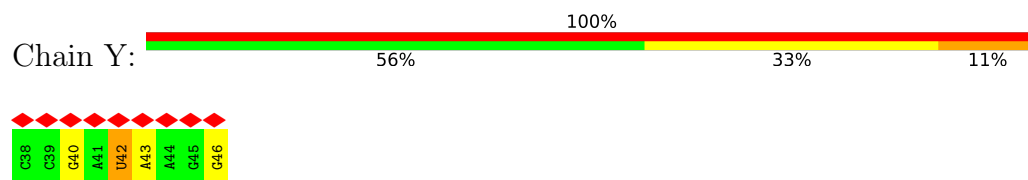


- Molecule 10: Trigger factor

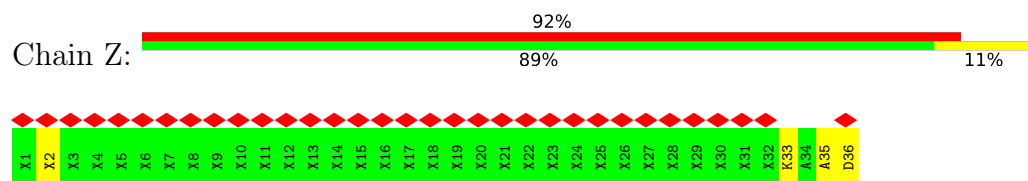




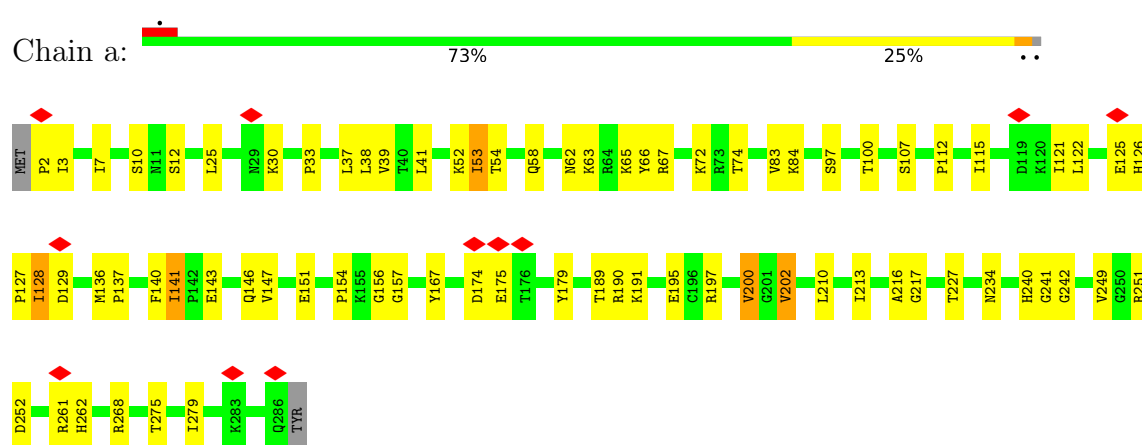
- Molecule 11: mRNA



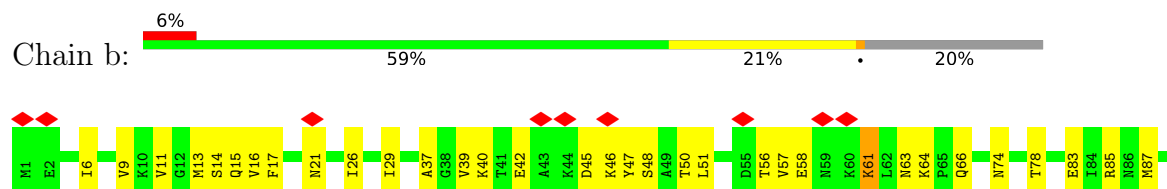
- Molecule 12: nascent peptide

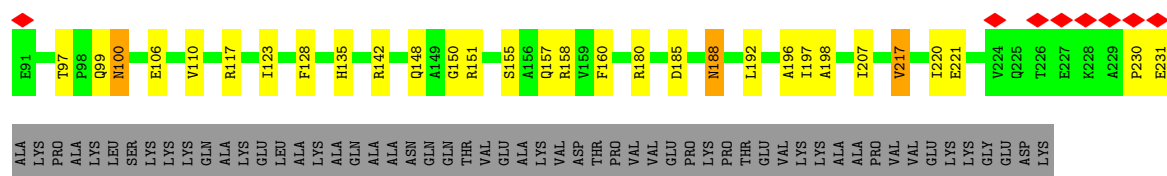


- Molecule 13: 50S ribosomal protein L2

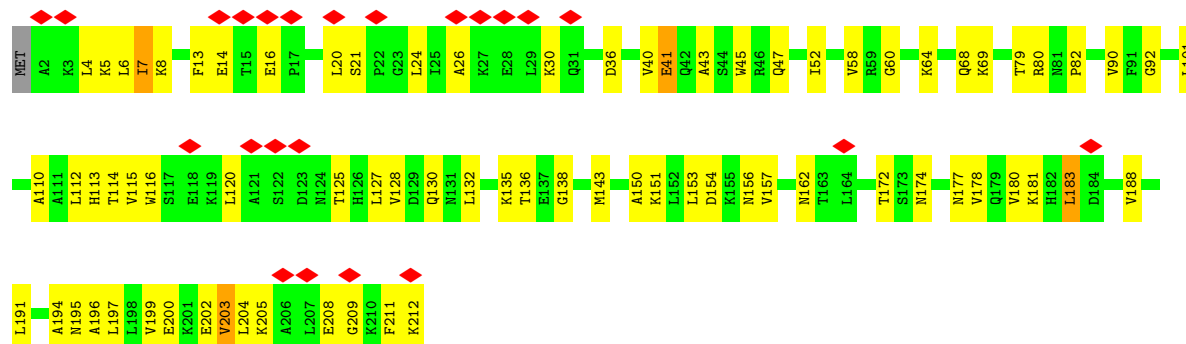


- Molecule 14: 50S ribosomal protein L3

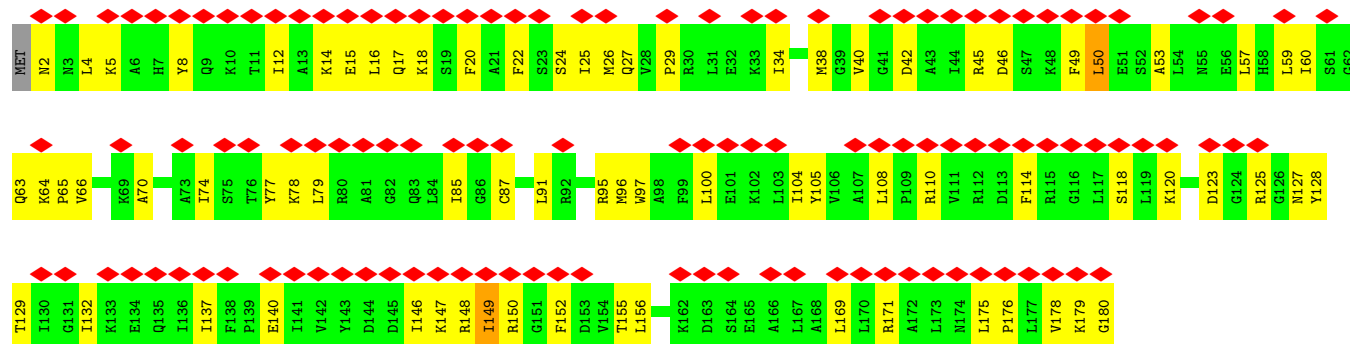




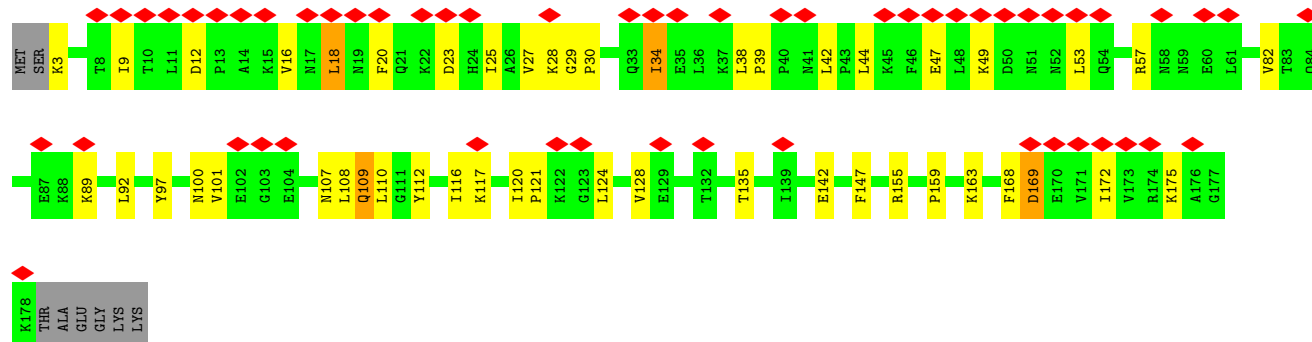
• Molecule 15: 50S ribosomal protein L4



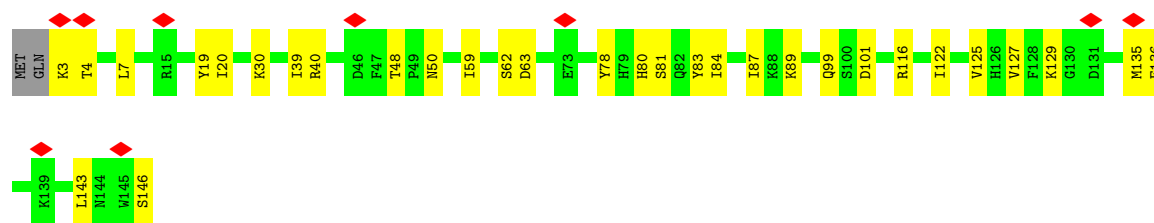
• Molecule 16: 50S ribosomal protein L5



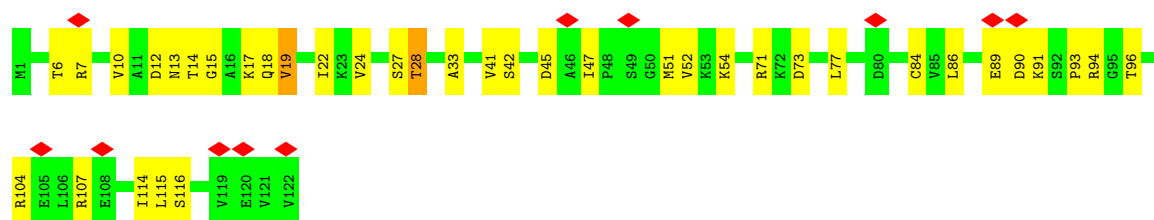
• Molecule 17: 50S ribosomal protein L6



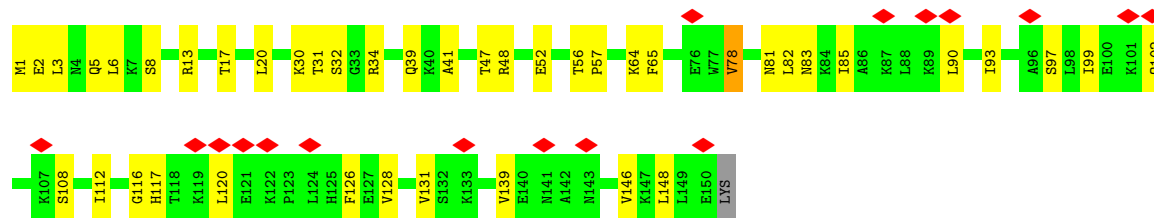




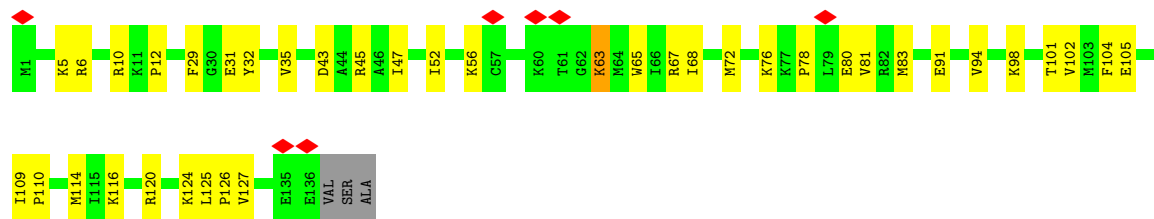
- Molecule 22: 50S ribosomal protein L14



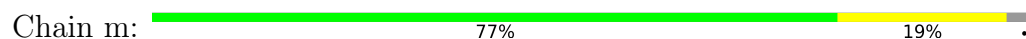
- Molecule 23: 50S ribosomal protein L15



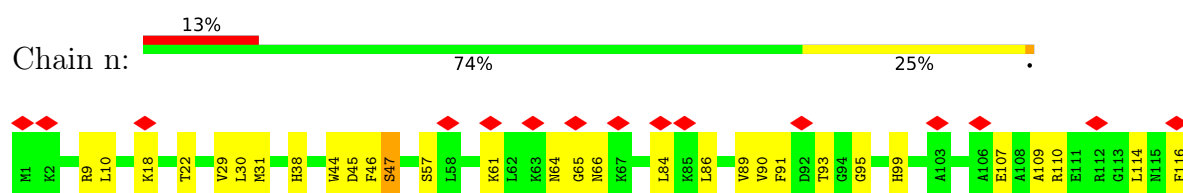
- Molecule 24: 50S ribosomal protein L16



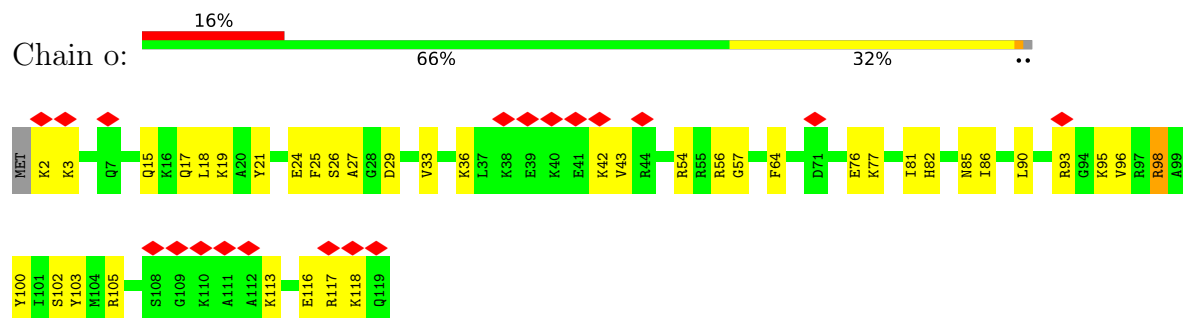
- Molecule 25: 50S ribosomal protein L17



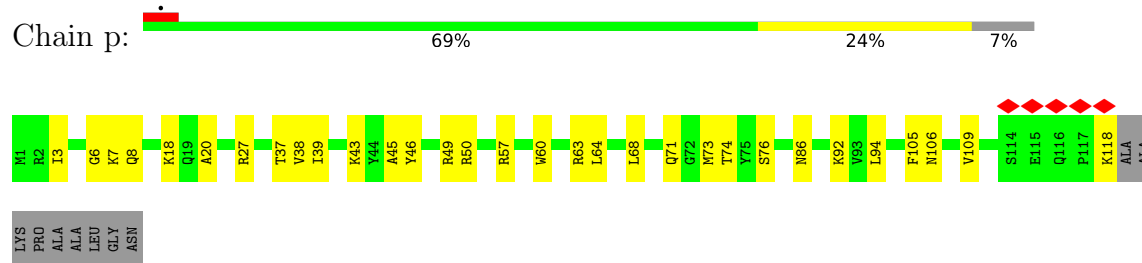
- Molecule 26: 50S ribosomal protein L18



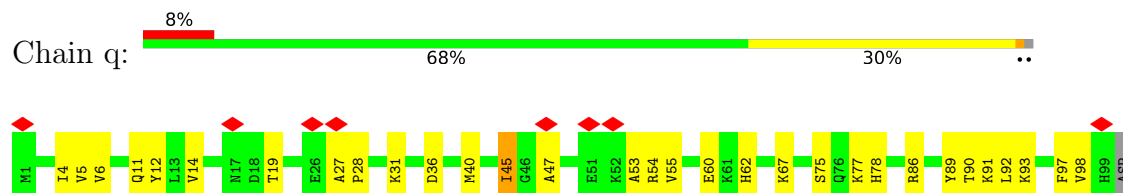
• Molecule 27: 50S ribosomal protein L19



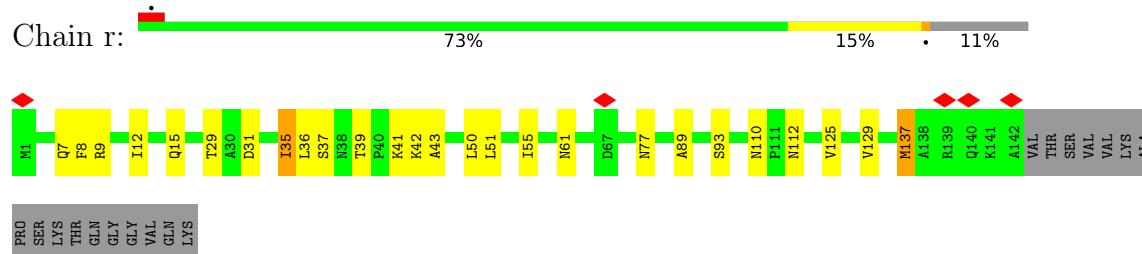
• Molecule 28: 50S ribosomal protein L20



• Molecule 29: 50S ribosomal protein L21



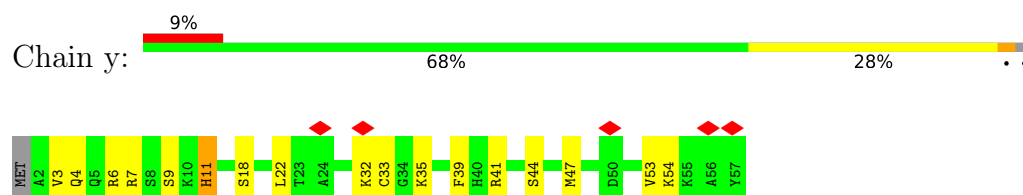
• Molecule 30: 50S ribosomal protein L22



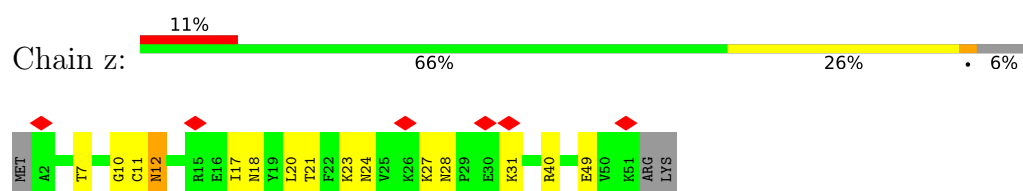
• Molecule 31: 50S ribosomal protein L23



- Molecule 37: 50S ribosomal protein L32



- Molecule 38: 50S ribosomal protein L33 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	539.574, 539.574, 539.574	wwPDB
Map dimensions	406, 406, 406	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.329, 1.329, 1.329	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, MG, 1MG, SPD, B8T, PUT, ZN, OMG, 2MA, CLM, N2P, K, SPM

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	0	0.08	0/395	0.24	0/518
2	1	0.10	0/484	0.27	0/637
3	2	0.12	0/306	0.28	0/401
4	3	0.09	0/69363	0.20	0/108161
5	4	0.08	0/2578	0.20	0/4016
6	5	0.10	0/715	0.26	0/1107
7	6	0.05	0/46	0.11	0/69
8	7	0.20	0/1785	0.40	1/2779 (0.0%)
9	8	0.23	0/1804	0.30	0/2807
10	X	0.19	0/245	0.65	1/325 (0.3%)
11	Y	0.19	0/218	0.32	0/338
12	Z	0.90	0/26	1.71	0/33
13	a	0.27	1/2267 (0.0%)	0.42	0/3044
14	b	0.20	0/1812	0.40	0/2436
15	c	0.18	0/1681	0.41	0/2257
16	d	0.22	0/1437	0.50	0/1931
17	e	0.47	4/1420 (0.3%)	0.91	4/1912 (0.2%)
18	f	0.36	1/1233 (0.1%)	0.55	1/1653 (0.1%)
19	g	0.22	0/960	0.50	0/1284
20	h	0.77	4/968 (0.4%)	1.22	8/1298 (0.6%)
21	i	0.13	0/1186	0.31	0/1592
22	j	0.15	0/953	0.37	0/1275
23	k	0.17	0/1187	0.46	0/1581
24	l	0.19	0/1104	0.41	0/1481
25	m	0.15	0/973	0.30	0/1309
26	n	0.18	0/927	0.36	0/1239
27	o	0.17	0/976	0.38	0/1296
28	p	0.15	0/996	0.35	0/1325
29	q	0.18	0/828	0.40	0/1111
30	r	0.14	0/1100	0.31	0/1471
31	s	0.14	0/752	0.39	0/1015
32	t	0.53	1/878 (0.1%)	0.89	4/1165 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	u	0.11	0/678	0.31	0/902
34	v	0.09	0/526	0.27	0/703
35	w	0.16	0/916	0.39	0/1222
36	x	0.13	0/375	0.34	0/502
37	y	0.16	0/457	0.40	0/601
38	z	0.10	0/412	0.30	0/547
All	All	0.17	11/104967 (0.0%)	0.31	19/157343 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	52	PRO	CG-CD	-14.89	1.00	1.50
32	t	95	PRO	CG-CD	-13.47	1.04	1.50
17	e	30	PRO	CB-CG	-11.76	0.90	1.49
20	h	52	PRO	N-CD	10.22	1.62	1.47
20	h	71	PRO	CG-CD	-8.97	1.20	1.50
17	e	30	PRO	N-CA	8.33	1.58	1.47
13	a	53	ILE	CG1-CD1	-7.82	1.21	1.51
18	f	104	LYS	CE-NZ	-7.47	1.26	1.49
20	h	52	PRO	CB-CG	-7.07	1.14	1.49
17	e	29	GLY	C-O	-5.36	1.16	1.24
17	e	29	GLY	C-N	-5.12	1.27	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	e	30	PRO	CB-CG-CD	23.08	179.95	106.10
20	h	52	PRO	N-CD-CG	-20.95	71.77	103.20
32	t	95	PRO	N-CD-CG	-19.84	73.44	103.20
20	h	52	PRO	CB-CG-CD	19.72	169.21	106.10
17	e	30	PRO	N-CD-CG	-19.64	73.73	103.20
17	e	30	PRO	CA-CB-CG	-16.88	72.43	104.50
32	t	95	PRO	CA-CB-CG	-15.46	75.13	104.50
20	h	52	PRO	CA-CB-CG	-13.94	78.02	104.50
20	h	71	PRO	N-CD-CG	-13.67	82.69	103.20
20	h	71	PRO	CA-N-CD	-11.13	96.41	112.00
20	h	71	PRO	CA-CB-CG	-9.89	85.71	104.50
20	h	52	PRO	CA-N-CD	-9.80	98.27	112.00
32	t	95	PRO	N-CA-CB	-9.06	94.89	103.41
17	e	30	PRO	CA-N-CD	-7.03	102.16	112.00
10	X	38	MET	CA-CB-CG	6.45	127.00	114.10
8	7	73	C	P-O3'-C3'	-6.44	110.54	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	f	104	LYS	CG-CD-CE	-6.20	97.03	111.30
32	t	95	PRO	CA-N-CD	-6.01	103.58	112.00
20	h	52	PRO	N-CA-CB	-5.32	97.80	103.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	392	0	442	8	0
2	1	477	0	530	9	0
3	2	304	0	348	4	0
4	3	61995	0	31115	475	0
5	4	2305	0	1164	14	0
6	5	683	0	339	5	0
7	6	42	0	23	0	0
8	7	1599	0	805	26	0
9	8	1615	0	816	19	0
10	X	242	0	263	10	0
11	Y	195	0	99	1	0
12	Z	187	0	68	6	0
13	a	2225	0	2301	57	0
14	b	1778	0	1821	47	0
15	c	1654	0	1744	59	0
16	d	1416	0	1500	70	0
17	e	1396	0	1481	29	0
18	f	1210	0	1259	47	0
19	g	951	0	1001	42	0
20	h	959	0	1039	49	0
21	i	1164	0	1192	36	0
22	j	944	0	1019	26	0
23	k	1170	0	1274	33	0
24	l	1079	0	1134	29	0
25	m	958	0	1011	15	0
26	n	918	0	979	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	o	966	0	1042	31	0
28	p	981	0	1062	32	0
29	q	811	0	858	27	0
30	r	1091	0	1178	20	0
31	s	740	0	819	16	0
32	t	871	0	972	25	0
33	u	670	0	704	11	0
34	v	520	0	565	12	0
35	w	906	0	981	25	0
36	x	366	0	356	12	0
37	y	452	0	471	19	0
38	z	408	0	436	8	0
39	2	1	0	0	0	0
39	x	1	0	0	0	0
39	y	1	0	0	0	0
39	z	1	0	0	0	0
40	3	20	0	11	4	0
41	3	1	0	0	0	0
42	3	219	0	0	0	0
42	4	1	0	0	0	0
42	6	1	0	0	0	0
42	7	1	0	0	0	0
42	8	2	0	0	0	0
42	b	2	0	0	0	0
42	i	1	0	0	0	0
42	y	2	0	0	0	0
43	3	42	0	84	2	0
44	3	42	0	78	7	0
44	b	14	0	26	1	0
45	3	160	0	304	3	0
46	3	21	0	42	0	0
47	8	9	0	12	0	0
All	All	97182	0	64768	1202	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 8.

All (1202) 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)
29:q:36:ASP:HB3	29:q:54:ARG:NH2	1.75	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:36:ASP:HB3	29:q:54:ARG:HH21	1.21	1.01
18:f:96:GLN:HE21	18:f:121:PHE:HB3	1.24	1.00
18:f:12:LEU:HD12	18:f:19:VAL:HB	1.42	0.97
20:h:122:LYS:HA	20:h:125:LEU:HD13	1.46	0.95
14:b:180:ARG:NH2	14:b:220:ILE:HD12	1.86	0.91
26:n:64:ASN:ND2	26:n:65:GLY:H	1.69	0.90
27:o:116:GLU:OE2	27:o:117:ARG:N	2.04	0.90
9:8:50:G:H1	9:8:64:U:H3	1.21	0.88
18:f:41:LYS:HB3	18:f:46:ASP:HB3	1.55	0.88
4:3:166:A:C6	18:f:104:LYS:NZ	2.44	0.85
29:q:36:ASP:CB	29:q:54:ARG:HH21	1.90	0.84
20:h:50:MET:SD	20:h:52:PRO:HD3	2.17	0.84
10:X:29:LYS:HE3	10:X:30:GLN:HG2	1.60	0.82
3:2:4:ARG:NH2	4:3:2485:U:O2	2.12	0.82
10:X:38:MET:SD	10:X:57:LEU:HD22	2.20	0.81
4:3:840:G:O4'	23:k:39:GLN:NE2	2.13	0.80
22:j:13:ASN:ND2	22:j:96:THR:OG1	2.13	0.80
4:3:2312:G:H22	4:3:2320:U:H3	1.28	0.80
13:a:125:GLU:OE1	13:a:125:GLU:N	2.13	0.80
28:p:6:GLY:H	28:p:8:GLN:NE2	1.80	0.79
36:x:6:HIS:HD1	36:x:7:PHE:HD1	1.28	0.79
8:7:34:G:H1	11:Y:42:U:H3	1.29	0.79
16:d:146:ILE:HG22	16:d:148:ARG:H	1.48	0.79
4:3:47:G:H5''	4:3:48:G:H5'	1.64	0.79
8:7:10:G:H1	8:7:25:U:H3	1.31	0.79
24:l:5:LYS:HD2	24:l:6:ARG:HH22	1.48	0.79
8:7:73:C:H41	33:u:18:LYS:HG3	1.48	0.78
21:i:80:HIS:ND1	21:i:81:SER:O	2.17	0.78
4:3:1344:U:O2'	10:X:44:ARG:NH2	2.15	0.78
29:q:53:ALA:C	29:q:54:ARG:HD2	2.08	0.77
15:c:162:ASN:HB3	15:c:202:GLU:OE2	1.84	0.77
30:r:31:ASP:O	30:r:35:ILE:HD12	1.84	0.77
21:i:4:THR:HA	29:q:12:TYR:HE2	1.48	0.77
16:d:104:ILE:HA	16:d:108:LEU:HD12	1.66	0.76
28:p:6:GLY:O	28:p:8:GLN:NE2	2.18	0.76
21:i:3:LYS:HG3	21:i:4:THR:H	1.51	0.76
28:p:68:LEU:HD12	28:p:73:MET:HG2	1.66	0.76
32:t:1:MET:HG2	32:t:2:GLN:H	1.52	0.75
17:e:42:LEU:HG	17:e:44:LEU:HD21	1.69	0.75
17:e:112:TYR:HB2	17:e:116:ILE:HD11	1.68	0.74
19:g:25:VAL:HG23	19:g:83:ALA:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:788:G:N2	25:m:3:TYR:OH	2.21	0.74
16:d:74:ILE:HD12	16:d:79:LEU:HD23	1.69	0.74
19:g:25:VAL:HG11	19:g:93:LEU:HD21	1.70	0.73
15:c:130:GLN:NE2	15:c:200:GLU:OE2	2.21	0.73
21:i:4:THR:HA	29:q:12:TYR:CE2	2.23	0.73
19:g:26:ILE:HG21	19:g:80:LEU:CD1	2.19	0.72
13:a:137:PRO:HA	13:a:197:ARG:HA	1.71	0.72
21:i:3:LYS:O	29:q:12:TYR:OH	2.05	0.72
16:d:40:VAL:HG22	16:d:42:ASP:H	1.55	0.72
16:d:63:GLN:HG2	16:d:95:ARG:HH21	1.55	0.72
20:h:122:LYS:HA	20:h:125:LEU:CD1	2.20	0.72
32:t:57:LYS:HE3	32:t:59:SER:HB3	1.73	0.71
18:f:5:LEU:HA	18:f:36:ALA:HA	1.71	0.71
22:j:7:ARG:HE	22:j:18:GLN:HG2	1.55	0.71
4:3:1031:U:O2'	28:p:92:LYS:NZ	2.23	0.71
13:a:179:TYR:HB3	13:a:191:LYS:HB3	1.70	0.71
8:7:48:G:H1	8:7:64:U:H3	1.37	0.71
23:k:126:PHE:HB2	23:k:146:VAL:HG22	1.72	0.70
4:3:530:G:N3	30:r:61:ASN:ND2	2.39	0.70
18:f:12:LEU:HD12	18:f:19:VAL:CB	2.21	0.70
1:0:9:LYS:NZ	4:3:1338:G:OP2	2.24	0.70
4:3:2688:C:H5'	14:b:198:ALA:HA	1.73	0.70
17:e:107:ASN:HB3	17:e:117:LYS:HG3	1.74	0.70
4:3:2799:U:OP1	4:3:2896:G:N1	2.21	0.70
4:3:2060:G:O2'	14:b:157:GLN:NE2	2.25	0.70
16:d:60:ILE:HD12	16:d:140:GLU:HB2	1.74	0.70
29:q:36:ASP:CB	29:q:54:ARG:NH2	2.51	0.69
19:g:41:ARG:NH1	19:g:51:ILE:O	2.26	0.69
24:l:72:MET:HE3	24:l:72:MET:HA	1.73	0.69
19:g:110:CYS:HA	19:g:123:LEU:HD11	1.74	0.69
4:3:1446:G:O2'	4:3:1613:A:N6	2.26	0.68
14:b:57:VAL:HG23	14:b:61:LYS:HE3	1.75	0.68
4:3:619:A:H62	4:3:1281:A:H2	1.40	0.68
19:g:29:TYR:HA	19:g:32:MET:HE1	1.75	0.68
35:w:49:ARG:HG3	35:w:49:ARG:HH11	1.59	0.68
4:3:1029:A:OP1	28:p:49:ARG:NH1	2.26	0.68
26:n:64:ASN:ND2	26:n:65:GLY:N	2.39	0.68
27:o:36:LYS:HB3	27:o:85:ASN:HB2	1.76	0.68
30:r:12:ILE:HG12	30:r:43:ALA:HB2	1.76	0.68
14:b:180:ARG:HH22	14:b:220:ILE:HD12	1.59	0.68
4:3:1806:G:OP1	13:a:268:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:83:U:H5'	5:4:84:C:H5'	1.77	0.67
4:3:656:G:H4'	4:3:657:A:H5'	1.76	0.67
24:l:47:ILE:HD11	24:l:68:ILE:HD11	1.75	0.67
26:n:64:ASN:HD22	26:n:65:GLY:N	1.92	0.67
26:n:57:SER:OG	26:n:64:ASN:OD1	2.13	0.67
13:a:143:GLU:CD	13:a:143:GLU:H	2.02	0.67
22:j:90:ASP:O	22:j:91:LYS:HB2	1.95	0.67
19:g:26:ILE:HG21	19:g:80:LEU:HD12	1.76	0.66
20:h:50:MET:SD	20:h:52:PRO:CD	2.83	0.66
1:0:24:THR:HG23	1:0:27:GLY:H	1.60	0.66
4:3:648:G:O6	15:c:181:LYS:NZ	2.27	0.66
32:t:95:PRO:HG2	32:t:96:LYS:N	2.06	0.66
32:t:90:LYS:HG3	32:t:105:LYS:HG2	1.77	0.66
4:3:2502:G:H4'	24:l:80:GLU:HG2	1.76	0.66
18:f:96:GLN:NE2	18:f:121:PHE:HB3	2.05	0.66
21:i:136:GLU:OE2	21:i:136:GLU:N	2.23	0.66
35:w:23:LYS:HD2	35:w:51:LEU:HD21	1.78	0.66
29:q:40:MET:HG3	29:q:45:ILE:HB	1.76	0.65
4:3:2465:U:H3	4:3:2502:G:H1	1.44	0.65
10:X:38:MET:SD	10:X:38:MET:O	2.54	0.65
29:q:28:PRO:HD2	29:q:31:LYS:HE3	1.78	0.65
23:k:2:GLU:OE2	23:k:5:GLN:NE2	2.29	0.65
4:3:2688:C:OP2	14:b:117:ARG:NH2	2.29	0.65
21:i:80:HIS:HE1	21:i:83:TYR:O	1.80	0.65
27:o:26:SER:N	27:o:29:ASP:OD2	2.29	0.65
4:3:1096:U:H1'	4:3:1105:A:H1'	1.78	0.65
27:o:93:ARG:HE	27:o:118:LYS:HE2	1.60	0.64
4:3:925:C:H4'	4:3:926:U:O4'	1.97	0.64
4:3:2475:C:O2	24:l:124:LYS:NZ	2.31	0.64
20:h:50:MET:CE	20:h:52:PRO:HD3	2.26	0.64
17:e:42:LEU:HG	17:e:44:LEU:CD2	2.28	0.64
24:l:32:TYR:HD2	24:l:114:MET:HE3	1.62	0.64
1:0:1:MET:HE3	4:3:788:G:H5'	1.80	0.64
4:3:2589:G:N2	4:3:2589:G:OP2	2.29	0.64
14:b:230:PRO:HG3	27:o:21:TYR:CE1	2.32	0.64
4:3:1619:A:H2'	4:3:1620:A:C8	2.33	0.64
15:c:6:LEU:HD23	15:c:127:LEU:O	1.98	0.64
31:s:52:PRO:HB3	31:s:83:ILE:HG23	1.79	0.64
4:3:2805:A:H4'	4:3:2807:G:H5''	1.80	0.64
13:a:33:PRO:HB2	13:a:38:LEU:HD11	1.79	0.64
29:q:6:VAL:HG22	29:q:11:GLN:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:881:A:HI'	4:3:882:C:H5''	1.80	0.64
4:3:1518:C:N4	4:3:2220:A:OP1	2.31	0.63
4:3:2823:A:O2'	4:3:2825:A:N7	2.30	0.63
22:j:93:PRO:HG3	22:j:114:ILE:HG12	1.81	0.63
17:e:25:ILE:HG13	17:e:38:LEU:HD21	1.81	0.63
4:3:1166:G:C4	21:i:80:HIS:CD2	2.86	0.63
8:7:19:A:H61	8:7:55:C:H42	1.46	0.63
4:3:2481:U:OP1	4:3:2483:C:N4	2.31	0.63
18:f:100:GLN:OE1	18:f:110:LYS:NZ	2.32	0.63
20:h:50:MET:HE1	20:h:52:PRO:HD3	1.80	0.63
25:m:50:THR:HA	25:m:53:LYS:HE3	1.81	0.63
4:3:1029:A:OP2	28:p:50:ARG:NH2	2.32	0.63
4:3:499:G:N2	4:3:502:A:OP2	2.29	0.62
4:3:166:A:C5	18:f:104:LYS:NZ	2.67	0.62
4:3:487:C:N4	4:3:490:A:OP2	2.27	0.62
14:b:37:ALA:HB3	14:b:51:LEU:HD23	1.80	0.62
15:c:110:ALA:O	15:c:114:THR:HG23	1.98	0.62
26:n:45:ASP:OD1	26:n:47:SER:OG	2.14	0.62
4:3:2308:U:H2'	4:3:2309:A:H8	1.64	0.62
21:i:80:HIS:CE1	21:i:81:SER:O	2.52	0.62
20:h:41:GLU:HG3	20:h:42:LYS:HG3	1.82	0.62
4:3:2026:A:OP2	37:y:6:ARG:NH2	2.33	0.61
13:a:151:GLU:OE2	13:a:156:GLY:C	2.43	0.61
4:3:2641:A:O2'	14:b:66:GLN:NE2	2.33	0.61
4:3:334:A:OP2	32:t:105:LYS:NZ	2.32	0.61
20:h:14:LEU:HD13	20:h:19:ALA:HB1	1.82	0.61
4:3:1700:G:HO2'	22:j:6:THR:HG1	1.45	0.61
4:3:1557:G:O6	4:3:1571:G:O2'	2.18	0.61
15:c:64:LYS:NZ	15:c:68:GLN:OE1	2.33	0.61
24:l:78:PRO:HG2	24:l:81:VAL:HG21	1.81	0.61
4:3:1786:U:OP2	4:3:1791:A:N6	2.25	0.61
18:f:76:GLU:HG2	18:f:142:VAL:HG13	1.82	0.61
19:g:29:TYR:HB2	19:g:79:LYS:HD3	1.82	0.61
4:3:354:C:O2	15:c:174:ASN:ND2	2.34	0.61
4:3:2667:G:N2	4:3:2670:A:OP2	2.30	0.61
4:3:619:A:N1	4:3:844:G:O2'	2.34	0.60
19:g:119:ASN:H	19:g:122:ASP:HB2	1.66	0.60
4:3:1600:A:N3	13:a:62:ASN:ND2	2.49	0.60
4:3:341:G:N1	4:3:344:A:OP2	2.32	0.60
37:y:4:GLN:OE1	37:y:7:ARG:HA	2.02	0.60
4:3:2538:A:N7	17:e:175:LYS:NZ	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:s:39:ARG:HG2	31:s:39:ARG:HH11	1.65	0.60
4:3:814:U:P	13:a:53:ILE:HD12	2.42	0.60
15:c:30:LYS:H	15:c:114:THR:HG21	1.65	0.60
15:c:150:ALA:O	15:c:151:LYS:HG2	2.02	0.60
16:d:25:ILE:HD12	16:d:25:ILE:H	1.66	0.60
19:g:100:VAL:HG12	19:g:106:MET:HG3	1.84	0.60
14:b:110:VAL:HG11	14:b:197:ILE:HD12	1.83	0.60
26:n:84:LEU:HB3	26:n:86:LEU:HD12	1.84	0.60
28:p:6:GLY:H	28:p:8:GLN:HE22	1.50	0.60
13:a:128:ILE:HG22	13:a:129:ASP:H	1.66	0.60
27:o:27:ALA:HB3	27:o:96:VAL:HG21	1.83	0.60
4:3:1095:U:H1'	4:3:1096:U:H3'	1.83	0.60
20:h:112:LEU:HD22	20:h:123:MET:SD	2.42	0.60
4:3:2490:A:O2'	9:8:63:C:O2'	2.19	0.59
4:3:13:C:H3'	4:3:14:U:H5'	1.84	0.59
4:3:2098:U:O2	34:v:34:GLN:NE2	2.35	0.59
4:3:2005:G:OP2	14:b:142:ARG:NH2	2.35	0.59
5:4:49:G:OP2	26:n:66:ASN:ND2	2.35	0.59
18:f:130:ILE:HD11	18:f:144:PRO:HG3	1.84	0.59
26:n:107:GLU:OE1	26:n:107:GLU:HA	2.02	0.59
4:3:1137:C:H2'	4:3:1138:A:H8	1.66	0.59
4:3:1031:U:HO2'	21:i:4:THR:HG21	1.68	0.59
15:c:132:LEU:HA	15:c:135:LYS:HB2	1.85	0.59
18:f:88:PRO:HG2	18:f:89:TYR:HD1	1.67	0.59
4:3:196:G:OP2	4:3:196:G:N2	2.34	0.59
4:3:2098:U:H3'	4:3:2099:U:H5''	1.84	0.59
4:3:620:G:H1	23:k:34:ARG:HH11	1.49	0.59
4:3:2068:G:OP1	15:c:69:LYS:NZ	2.28	0.59
15:c:115:VAL:HG21	15:c:188:VAL:HG13	1.85	0.59
21:i:7:LEU:HD23	21:i:7:LEU:H	1.67	0.59
27:o:25:PHE:HB3	27:o:90:LEU:HD13	1.85	0.59
4:3:477:U:O2	15:c:47:GLN:NE2	2.34	0.59
4:3:1129:U:N3	4:3:1132:C:OP2	2.25	0.59
40:3:3001:CLM:CL2	12:Z:33:LYS:HG2	2.39	0.58
14:b:185:ASP:OD2	14:b:188:ASN:ND2	2.35	0.58
20:h:70:THR:HG22	20:h:71:PRO:HD3	1.85	0.58
25:m:103:LEU:O	25:m:112:GLU:OE2	2.21	0.58
35:w:40:LYS:HD3	35:w:42:HIS:NE2	2.18	0.58
35:w:56:THR:O	35:w:60:GLU:HG2	2.03	0.58
4:3:1092:A:N6	4:3:1122:G:OP1	2.36	0.58
8:7:27:U:H3	8:7:43:G:H1	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:53:ALA:HB3	10:X:54:LYS:HE2	1.83	0.58
23:k:90:LEU:HD21	23:k:97:SER:HB3	1.85	0.58
28:p:86:ASN:OD1	28:p:118:LYS:NZ	2.32	0.58
4:3:2009:U:OP1	25:m:14:ARG:NH1	2.33	0.58
16:d:175:LEU:HD12	16:d:176:PRO:HD2	1.86	0.58
24:l:116:LYS:O	24:l:120:ARG:HG2	2.03	0.58
18:f:4:ILE:HG22	18:f:18:VAL:HG22	1.85	0.58
18:f:83:GLU:O	18:f:84:HIS:ND1	2.35	0.58
22:j:89:GLU:H	22:j:89:GLU:CD	2.11	0.58
5:4:35:C:O2	26:n:99:HIS:HE1	1.86	0.58
10:X:44:ARG:HH11	10:X:47:LYS:HE3	1.68	0.58
19:g:56:ASN:CG	19:g:60:ARG:HH21	2.11	0.58
4:3:1906:G:H21	4:3:1909:C:H41	1.50	0.57
13:a:41:LEU:HG	13:a:66:TYR:HB2	1.85	0.57
37:y:53:VAL:HG12	37:y:54:LYS:HG2	1.84	0.57
4:3:1000:U:O2'	4:3:2281:A:N3	2.34	0.57
18:f:87:ARG:HB2	18:f:88:PRO:HD3	1.86	0.57
19:g:27:PHE:O	19:g:81:ALA:N	2.37	0.57
4:3:195:A:H3'	4:3:196:G:H21	1.69	0.57
4:3:1031:U:O2'	21:i:4:THR:HG21	2.05	0.57
19:g:55:LYS:HE2	19:g:55:LYS:H	1.69	0.57
4:3:814:U:H5''	13:a:53:ILE:HD11	1.85	0.57
20:h:38:GLN:HB3	20:h:65:PHE:CZ	2.39	0.57
4:3:166:A:C6	4:3:167:A:C5	2.93	0.57
5:4:40:U:H5''	16:d:64:LYS:HD2	1.86	0.57
15:c:194:ALA:C	15:c:196:ALA:H	2.13	0.57
16:d:5:LYS:HD3	16:d:97:TRP:CD1	2.40	0.57
16:d:74:ILE:HD12	16:d:79:LEU:CD2	2.35	0.57
32:t:28:MET:HE2	32:t:31:ARG:HH12	1.69	0.57
4:3:695:G:H5''	15:c:101:LEU:HD22	1.87	0.57
4:3:1833:G:O2'	4:3:1978:U:OP2	2.23	0.57
30:r:110:ASN:OD1	30:r:112:ASN:N	2.33	0.57
19:g:37:ALA:O	19:g:40:ILE:HG22	2.03	0.56
28:p:64:LEU:HD11	28:p:94:LEU:HB3	1.87	0.56
30:r:7:GLN:HB2	30:r:50:LEU:HD11	1.87	0.56
4:3:1055:A:N1	4:3:1176:U:O2'	2.35	0.56
14:b:180:ARG:HH21	14:b:220:ILE:HD12	1.67	0.56
32:t:36:VAL:HG23	32:t:39:LEU:HB2	1.87	0.56
37:y:39:PHE:O	37:y:41:ARG:NH1	2.38	0.56
4:3:2266:C:O2'	4:3:2435:C:OP2	2.23	0.56
14:b:17:PHE:O	27:o:17:GLN:NE2	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:116:TRP:CE2	15:c:191:LEU:HD11	2.40	0.56
17:e:27:VAL:HG12	17:e:82:VAL:HG21	1.86	0.56
21:i:63:ASP:OD1	21:i:63:ASP:N	2.34	0.56
24:l:63:LYS:NZ	24:l:65:TRP:CE2	2.73	0.56
29:q:27:ALA:O	29:q:62:HIS:NE2	2.38	0.56
29:q:36:ASP:HA	29:q:54:ARG:HE	1.70	0.56
4:3:879:U:O4	4:3:968:U:O2'	2.23	0.56
4:3:697:U:H5''	23:k:17:THR:HG22	1.87	0.56
4:3:720:A:OP1	4:3:721:G:N2	2.39	0.56
4:3:2060:G:H4'	14:b:157:GLN:HG2	1.88	0.56
18:f:97:ILE:HA	18:f:100:GLN:HB2	1.88	0.56
8:7:36:C:H2'	8:7:37:A:C8	2.39	0.56
35:w:49:ARG:HG3	35:w:49:ARG:NH1	2.20	0.56
4:3:933:A:O2'	9:8:56:C:N3	2.39	0.56
8:7:50:G:H1	8:7:62:C:H42	1.53	0.56
27:o:76:GLU:OE1	27:o:105:ARG:NH1	2.39	0.56
16:d:45:ARG:HG3	16:d:46:ASP:H	1.71	0.56
4:3:512:G:N1	4:3:515:A:OP2	2.35	0.56
4:3:733:C:O2'	4:3:769:A:N6	2.39	0.56
4:3:1103:G:N2	4:3:1130:A:O2'	2.38	0.56
16:d:38:MET:HE1	16:d:53:ALA:HA	1.88	0.56
4:3:517:G:O5'	32:t:44:ARG:NH1	2.39	0.56
13:a:65:LYS:O	13:a:67:ARG:NH1	2.38	0.55
4:3:343:A:N3	4:3:363:G:O2'	2.38	0.55
4:3:585:U:H2'	4:3:586:G:H8	1.71	0.55
4:3:2383:G:N2	4:3:2386:A:OP2	2.35	0.55
14:b:180:ARG:NH2	14:b:220:ILE:CD1	2.66	0.55
16:d:49:PHE:HZ	16:d:147:LYS:HB2	1.71	0.55
4:3:1386:G:O2'	4:3:1401:A:N6	2.39	0.55
22:j:27:SER:OG	22:j:28:THR:N	2.39	0.55
36:x:32:LYS:HE3	36:x:34:ILE:HD13	1.89	0.55
27:o:116:GLU:CD	27:o:117:ARG:H	2.12	0.55
4:3:9:G:H2'	4:3:10:U:C6	2.42	0.55
4:3:436:G:O6	34:v:56:ARG:NH2	2.39	0.55
4:3:1111:C:H2'	4:3:1112:A:O4'	2.05	0.55
4:3:1909:C:O2'	13:a:251:ARG:O	2.21	0.55
8:7:36:C:H2'	8:7:37:A:H8	1.71	0.55
19:g:26:ILE:HG21	19:g:80:LEU:HD13	1.88	0.55
20:h:120:ALA:HA	20:h:123:MET:SD	2.47	0.55
29:q:55:VAL:HG22	29:q:97:PHE:CE1	2.42	0.55
4:3:193:G:OP2	34:v:26:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:39:VAL:O	13:a:66:TYR:N	2.40	0.55
13:a:137:PRO:HG2	13:a:140:PHE:CE2	2.42	0.55
4:3:1125:U:H2'	4:3:1126:G:C8	2.42	0.55
20:h:24:ALA:O	20:h:27:SER:OG	2.25	0.55
4:3:1683:G:O2'	25:m:109:ASP:OD2	2.19	0.55
4:3:2028:G:OP1	37:y:9:SER:OG	2.25	0.55
4:3:2299:U:H2'	4:3:2300:A:C8	2.42	0.55
35:w:98:LEU:HD21	35:w:102:ARG:HE	1.71	0.55
4:3:196:G:O2'	4:3:712:A:N1	2.40	0.54
4:3:814:U:OP1	13:a:53:ILE:HD12	2.07	0.54
4:3:933:A:H3'	4:3:934:C:O4'	2.08	0.54
4:3:2296:A:H1'	45:3:3248:SPD:H91	1.87	0.54
13:a:122:LEU:HD23	13:a:128:ILE:HG23	1.89	0.54
4:3:1569:A:H2'	4:3:1570:A:C2	2.42	0.54
4:3:1798:A:O2'	13:a:213:ILE:O	2.19	0.54
4:3:2513:G:C4	12:Z:33:LYS:HD2	2.43	0.54
23:k:117:HIS:O	23:k:117:HIS:ND1	2.40	0.54
31:s:3:VAL:HG23	35:w:65:TRP:HZ2	1.72	0.54
4:3:564:A:OP1	21:i:116:ARG:NH2	2.37	0.54
13:a:136:MET:HG3	13:a:141:ILE:HD11	1.89	0.54
16:d:148:ARG:HE	16:d:149:ILE:H	1.56	0.54
4:3:1076:U:H3	4:3:1149:G:H1	1.55	0.54
18:f:23:ASP:OD1	18:f:23:ASP:N	2.39	0.54
17:e:39:PRO:HG2	17:e:42:LEU:HD13	1.88	0.54
2:1:15:LYS:HD3	4:3:664:G:H5''	1.89	0.54
4:3:1097:G:H21	20:h:131:MET:HE1	1.72	0.54
18:f:84:HIS:CE1	18:f:93:ILE:HD13	2.43	0.54
20:h:112:LEU:HG	20:h:114:ALA:H	1.73	0.54
31:s:4:THR:O	31:s:4:THR:HG22	2.08	0.54
32:t:52:THR:H	32:t:55:ALA:HB3	1.72	0.54
4:3:410:G:H4'	4:3:411:U:O5'	2.07	0.54
4:3:901:C:H4'	4:3:902:U:C5'	2.38	0.54
4:3:1292:A:H61	4:3:2024:C:H42	1.55	0.54
4:3:1391:U:O2'	4:3:1816:A:N3	2.34	0.54
13:a:2:PRO:HD2	13:a:25:LEU:HD21	1.90	0.54
18:f:96:GLN:HB3	18:f:100:GLN:HE22	1.71	0.54
29:q:67:LYS:HD2	29:q:86:ARG:HD2	1.88	0.54
4:3:947:A:H62	24:l:12:PRO:HA	1.72	0.54
13:a:154:PRO:HB3	13:a:195:GLU:HG3	1.90	0.54
21:i:101:ASP:HB2	21:i:127:VAL:HG13	1.90	0.54
37:y:33:CYS:SG	37:y:35:LYS:HG2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:2:U:O2	5:4:107:G:N2	2.41	0.54
17:e:47:GLU:OE1	17:e:49:LYS:HG3	2.07	0.54
22:j:71:ARG:HH22	22:j:104:ARG:HH11	1.55	0.54
32:t:46:LYS:HE3	32:t:63:VAL:HB	1.90	0.54
9:8:29:U:H3	9:8:41:A:H61	1.54	0.54
13:a:128:ILE:HG22	13:a:129:ASP:N	2.22	0.54
23:k:131:VAL:HG12	23:k:148:LEU:HD21	1.90	0.54
31:s:50:ILE:HG12	31:s:89:ILE:CD1	2.38	0.54
38:z:24:ASN:HD22	38:z:27:LYS:HB2	1.73	0.54
4:3:600:U:OP2	23:k:30:LYS:NZ	2.40	0.53
4:3:1106:G:N2	4:3:1124:G:O2'	2.41	0.53
4:3:1166:G:N9	21:i:80:HIS:CD2	2.76	0.53
20:h:76:LEU:HD11	20:h:127:THR:HG23	1.89	0.53
4:3:583:U:O4	21:i:3:LYS:HD3	2.08	0.53
4:3:2122:G:O2'	4:3:2175:U:O2	2.25	0.53
4:3:2516:G:HO2'	4:3:2562:U:HO2'	1.56	0.53
16:d:50:LEU:O	16:d:53:ALA:HB3	2.08	0.53
21:i:78:TYR:CE1	21:i:89:LYS:HB3	2.43	0.53
8:7:73:C:N4	33:u:18:LYS:HG3	2.21	0.53
14:b:21:ASN:OD1	22:j:73:ASP:HB3	2.09	0.53
18:f:33:LYS:HD3	18:f:113:PHE:HB2	1.90	0.53
20:h:58:TYR:CE1	20:h:60:ASP:HB3	2.44	0.53
29:q:36:ASP:CA	29:q:54:ARG:HH21	2.20	0.53
4:3:201:A:N6	4:3:2438:A:O2'	2.41	0.53
4:3:897:A:N3	5:4:77:G:O2'	2.42	0.53
4:3:2797:C:O2	4:3:2895:A:O2'	2.23	0.53
4:3:2820:G:N3	4:3:2887:A:O2'	2.41	0.53
30:r:41:LYS:HE3	37:y:22:LEU:HD11	1.91	0.53
35:w:80:ASN:O	35:w:84:VAL:HG13	2.09	0.53
4:3:549:A:N3	4:3:614:C:O2'	2.41	0.53
9:8:27:A:H61	9:8:43:U:H3	1.57	0.53
14:b:150:GLY:HA3	14:b:155:SER:HB3	1.89	0.53
17:e:23:ASP:N	17:e:23:ASP:OD1	2.41	0.53
20:h:35:PHE:HB3	20:h:39:PHE:CE1	2.44	0.53
4:3:1098:G:O2'	20:h:84:LYS:NZ	2.40	0.53
4:3:1166:G:O4'	21:i:80:HIS:HD2	1.92	0.53
4:3:2137:A:O2'	4:3:2165:A:N6	2.42	0.53
4:3:2630:U:O2'	4:3:2829:G:N7	2.40	0.53
15:c:5:LYS:HE2	15:c:13:PHE:CE2	2.43	0.53
34:v:4:LYS:HD2	34:v:9:LEU:HD13	1.91	0.53
4:3:427:A:H1'	4:3:447:G:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:892:G:H2'	4:3:893:A:C8	2.43	0.53
4:3:2228:U:H5'	18:f:95:LYS:HG2	1.90	0.53
17:e:142:GLU:OE1	17:e:142:GLU:N	2.39	0.53
20:h:69:THR:HG22	20:h:70:THR:O	2.09	0.53
23:k:93:ILE:HD13	23:k:126:PHE:CE1	2.44	0.53
31:s:8:LEU:HB2	31:s:30:VAL:HG23	1.90	0.53
24:l:52:ILE:HG22	24:l:56:LYS:HE2	1.91	0.53
15:c:20:LEU:HD21	15:c:204:LEU:HD11	1.92	0.52
17:e:159:PRO:HA	17:e:172:ILE:HD13	1.90	0.52
22:j:86:LEU:HB3	22:j:94:ARG:HD2	1.91	0.52
4:3:9:G:H5'	21:i:135:MET:HE1	1.91	0.52
4:3:1521:A:N3	4:3:1611:C:O2'	2.40	0.52
14:b:45:ASP:O	14:b:46:LYS:HB2	2.10	0.52
18:f:69:LYS:O	18:f:72:ILE:HG13	2.09	0.52
4:3:184:A:O2'	4:3:186:A:N7	2.37	0.52
4:3:620:G:H5'	44:3:3227:SPM:H61	1.91	0.52
4:3:1123:A:N7	20:h:130:GLN:NE2	2.58	0.52
4:3:2477:A:H2'	4:3:2478:G:O4'	2.09	0.52
5:4:55:A:C4	16:d:26:MET:HE1	2.44	0.52
16:d:100:LEU:O	16:d:104:ILE:HG22	2.09	0.52
21:i:7:LEU:HD13	28:p:60:TRP:HE1	1.75	0.52
4:3:1588:A:H2'	4:3:1589:A:C8	2.45	0.52
4:3:2081:U:HO2'	4:3:2605:G:HO2'	1.58	0.52
16:d:108:LEU:HB3	16:d:114:PHE:CE2	2.45	0.52
23:k:102:GLN:HA	23:k:102:GLN:OE1	2.10	0.52
4:3:1648:A:N1	30:r:93:SER:OG	2.43	0.52
4:3:2004:G:OP2	45:3:3250:SPD:H41	2.10	0.52
14:b:16:VAL:HG13	14:b:26:ILE:HD13	1.91	0.52
9:8:40:C:H2'	9:8:41:A:C8	2.45	0.52
17:e:12:ASP:OD1	17:e:12:ASP:N	2.43	0.52
9:8:28:A:H2'	9:8:29:U:C6	2.44	0.51
15:c:82:PRO:HB3	15:c:90:VAL:HG23	1.91	0.51
20:h:14:LEU:HD22	20:h:19:ALA:HA	1.92	0.51
4:3:98:C:P	35:w:40:LYS:NZ	2.83	0.51
4:3:1807:C:OP2	13:a:190:ARG:NH2	2.43	0.51
4:3:2813:A:H2'	4:3:2814:A:C8	2.45	0.51
2:1:5:SER:HA	2:1:8:LYS:HE2	1.91	0.51
13:a:112:PRO:HG2	13:a:115:ILE:HG12	1.92	0.51
16:d:110:ARG:NH2	16:d:137:ILE:HA	2.25	0.51
20:h:11:LYS:HD3	20:h:54:VAL:HG22	1.92	0.51
4:3:316:C:H2'	4:3:392:A:H61	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:996:A:H61	24:l:83:MET:HE2	1.75	0.51
4:3:2736:U:O2'	4:3:2737:G:H8	1.94	0.51
17:e:120:ILE:HA	17:e:147:PHE:HE2	1.74	0.51
21:i:3:LYS:HG3	21:i:4:THR:N	2.22	0.51
22:j:90:ASP:O	22:j:90:ASP:OD1	2.27	0.51
23:k:82:LEU:HB2	23:k:116:GLY:HA3	1.93	0.51
4:3:917:G:H2'	4:3:918:G:C8	2.45	0.51
4:3:2151:G:H1'	4:3:2154:A:H61	1.76	0.51
4:3:2318:A:N1	16:d:77:TYR:HE1	2.08	0.51
15:c:153:LEU:HD12	15:c:153:LEU:H	1.76	0.51
19:g:46:LYS:HG2	19:g:48:GLY:H	1.76	0.51
22:j:17:LYS:N	22:j:45:ASP:O	2.39	0.51
4:3:788:G:H2'	4:3:789:A:H8	1.75	0.51
14:b:56:THR:HA	14:b:78:THR:HG22	1.92	0.51
17:e:168:PHE:C	17:e:169:ASP:OD1	2.54	0.51
34:v:37:LYS:HB3	34:v:45:THR:HG22	1.93	0.51
21:i:78:TYR:HE1	21:i:89:LYS:HB3	1.75	0.51
31:s:59:ILE:HD11	31:s:79:LYS:HE2	1.92	0.51
4:3:86:A:N6	4:3:101:C:O4'	2.44	0.51
4:3:620:G:H5'	44:3:3227:SPM:H82	1.92	0.51
4:3:118:G:OP2	4:3:120:A:O2'	2.27	0.51
4:3:2308:U:H2'	4:3:2309:A:C8	2.45	0.51
17:e:109:GLN:OE1	17:e:109:GLN:N	2.44	0.51
29:q:53:ALA:O	29:q:54:ARG:HD2	2.09	0.51
4:3:995:A:N6	24:l:83:MET:HE1	2.26	0.50
4:3:1028:C:OP1	28:p:46:TYR:OH	2.21	0.50
16:d:65:PRO:HB2	16:d:87:CYS:HB2	1.93	0.50
35:w:77:LYS:HG2	35:w:78:LYS:H	1.76	0.50
4:3:180:A:H5'	4:3:181:G:C8	2.46	0.50
4:3:1009:A:H5''	29:q:77:LYS:HD2	1.93	0.50
4:3:823:A:OP1	4:3:826:C:N4	2.39	0.50
16:d:8:TYR:O	16:d:12:ILE:HB	2.12	0.50
16:d:38:MET:HE1	16:d:53:ALA:CA	2.42	0.50
26:n:64:ASN:CG	26:n:65:GLY:H	2.17	0.50
4:3:853:G:N1	4:3:1219:U:OP2	2.38	0.50
4:3:1566:A:H2'	4:3:1567:U:O4'	2.12	0.50
23:k:20:LEU:O	23:k:32:SER:OG	2.18	0.50
4:3:2299:U:OP1	4:3:2388:C:O2'	2.29	0.50
23:k:52:GLU:OE1	23:k:57:PRO:HA	2.12	0.50
27:o:36:LYS:HE3	27:o:85:ASN:HA	1.93	0.50
27:o:102:SER:O	27:o:105:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:408:G:OP2	4:3:459:A:N6	2.45	0.50
4:3:1023:C:O2'	4:3:1036:A:N3	2.42	0.50
4:3:1091:G:H4'	4:3:1121:A:H8	1.76	0.50
4:3:1617:U:H5''	4:3:1619:A:C4	2.47	0.50
16:d:42:ASP:O	16:d:46:ASP:N	2.44	0.50
18:f:68:LEU:HD22	18:f:108:LEU:HD21	1.93	0.50
18:f:88:PRO:HG2	18:f:89:TYR:CD1	2.47	0.50
23:k:112:ILE:HG22	23:k:128:VAL:HG12	1.94	0.50
4:3:622:U:H2'	4:3:623:A:C8	2.47	0.50
4:3:1583:G:O2'	4:3:1584:U:OP1	2.25	0.50
23:k:81:ASN:OD1	23:k:83:ASN:ND2	2.44	0.50
31:s:50:ILE:HG12	31:s:89:ILE:HD11	1.93	0.50
4:3:663:A:N7	23:k:81:ASN:ND2	2.57	0.50
4:3:1343:C:O2'	4:3:1420:A:N3	2.36	0.50
18:f:130:ILE:HB	18:f:142:VAL:HB	1.92	0.50
24:l:43:ASP:OD2	24:l:45:ARG:NH1	2.45	0.50
4:3:1166:G:N2	4:3:1167:U:O4	2.38	0.50
4:3:1445:U:H2'	4:3:1446:G:O4'	2.11	0.50
16:d:118:SER:C	16:d:120:LYS:H	2.20	0.50
19:g:27:PHE:CZ	19:g:108:PHE:CE1	3.00	0.50
27:o:64:PHE:CD1	27:o:81:ILE:HG12	2.47	0.50
15:c:52:ILE:HG21	15:c:92:GLY:HA3	1.93	0.49
26:n:9:ARG:HG3	26:n:9:ARG:HH11	1.76	0.49
4:3:1920:A:C8	6:5:1469:G:H4'	2.46	0.49
4:3:2299:U:H2'	4:3:2300:A:H8	1.77	0.49
15:c:120:LEU:HA	15:c:125:THR:HG21	1.93	0.49
16:d:96:MET:HG3	16:d:97:TRP:N	2.27	0.49
16:d:132:ILE:HB	16:d:152:PHE:HB2	1.93	0.49
4:3:1132:C:H3'	4:3:1133:A:H8	1.77	0.49
4:3:1270:C:H2'	4:3:1271:A:H8	1.76	0.49
14:b:106:GLU:HA	14:b:217:VAL:HA	1.95	0.49
18:f:41:LYS:HE2	18:f:46:ASP:HB3	1.94	0.49
32:t:94:ASP:OD1	32:t:94:ASP:N	2.44	0.49
4:3:615:G:H2'	4:3:616:G:H8	1.77	0.49
19:g:42:LYS:HZ1	20:h:113:ASN:C	2.19	0.49
20:h:25:LEU:HB3	20:h:30:ILE:HD12	1.94	0.49
27:o:15:GLN:HA	27:o:18:LEU:HD12	1.93	0.49
32:t:3:ARG:NH2	32:t:74:LEU:O	2.45	0.49
4:3:1485:A:H4'	4:3:1486:U:C4	2.47	0.49
15:c:6:LEU:HD23	15:c:127:LEU:C	2.37	0.49
29:q:54:ARG:HB2	29:q:98:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:140:G:N2	4:3:143:A:OP2	2.28	0.49
4:3:204:U:H4'	34:v:22:LYS:HB2	1.94	0.49
4:3:917:G:H2'	4:3:918:G:H8	1.78	0.49
9:8:5:C:H2'	9:8:6:U:H6	1.78	0.49
15:c:24:LEU:HD11	15:c:208:GLU:HB3	1.93	0.49
15:c:197:LEU:HD13	15:c:199:VAL:HG23	1.94	0.49
17:e:23:ASP:HA	17:e:38:LEU:HB2	1.94	0.49
19:g:41:ARG:NH2	19:g:51:ILE:HG22	2.27	0.49
4:3:666:G:N2	4:3:669:A:OP2	2.33	0.49
4:3:1104:A:H5''	4:3:1105:A:C5	2.47	0.49
19:g:96:VAL:O	19:g:100:VAL:HG22	2.12	0.49
4:3:1830:G:OP1	13:a:58:GLN:NE2	2.46	0.49
18:f:56:GLU:OE1	18:f:56:GLU:N	2.38	0.49
28:p:86:ASN:HB2	29:q:47:ALA:HB1	1.94	0.49
4:3:164:A:OP2	4:3:165:U:O2'	2.27	0.49
4:3:1603:A:O5'	13:a:63:LYS:NZ	2.46	0.49
4:3:2797:C:H5'	4:3:2798:A:O5'	2.13	0.49
4:3:2493:G:O3'	24:l:126:PRO:HB3	2.12	0.49
14:b:97:THR:HG23	14:b:99:GLN:H	1.77	0.49
18:f:104:LYS:HB2	18:f:109:GLN:O	2.12	0.49
4:3:799:A:H5''	13:a:217:GLY:HA3	1.94	0.48
16:d:17:GLN:OE1	16:d:22:PHE:HB2	2.13	0.48
16:d:59:LEU:HG	36:x:7:PHE:HE2	1.78	0.48
18:f:106:MET:SD	18:f:107:ALA:HB2	2.53	0.48
36:x:37:ASP:OD1	36:x:38:ILE:HG13	2.12	0.48
4:3:1119:A:C8	19:g:53:VAL:HG21	2.48	0.48
4:3:1568:C:H3'	4:3:1569:A:C8	2.48	0.48
4:3:1618:U:H4'	4:3:1619:A:OP2	2.12	0.48
13:a:72:LYS:HB3	13:a:74:THR:HG22	1.94	0.48
20:h:51:ILE:HG23	20:h:68:LYS:O	2.13	0.48
21:i:40:ARG:HG2	21:i:40:ARG:HH11	1.78	0.48
4:3:246:G:O2'	4:3:258:G:O6	2.29	0.48
4:3:1143:U:H5''	19:g:77:LYS:HA	1.94	0.48
4:3:2027:G:H5'	37:y:9:SER:HB3	1.95	0.48
4:3:2854:A:N7	4:3:2872:A:O2'	2.35	0.48
15:c:112:LEU:HD23	15:c:211:PHE:HE1	1.78	0.48
4:3:1095:U:OP1	20:h:72:VAL:HG13	2.13	0.48
4:3:2032:G:OP1	14:b:158:ARG:NH1	2.46	0.48
5:4:11:A:H2'	5:4:12:U:H5''	1.95	0.48
15:c:143:MET:HE3	15:c:172:THR:CG2	2.43	0.48
16:d:49:PHE:CZ	16:d:147:LYS:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:171:ARG:HA	16:d:171:ARG:CZ	2.43	0.48
17:e:89:LYS:HB3	17:e:168:PHE:HB2	1.95	0.48
24:l:43:ASP:HA	24:l:94:VAL:HA	1.94	0.48
32:t:37:GLU:OE2	32:t:37:GLU:C	2.56	0.48
38:z:23:LYS:HE2	38:z:28:ASN:HB2	1.95	0.48
4:3:518:A:O2'	4:3:532:A:N1	2.44	0.48
4:3:638:A:H62	4:3:660:U:H3	1.60	0.48
4:3:728:A:O2'	4:3:1381:A:N3	2.40	0.48
4:3:1033:A:OP2	28:p:57:ARG:NH1	2.47	0.48
8:7:10:G:O2'	8:7:11:U:OP1	2.25	0.48
10:X:40:ILE:HD11	10:X:48:VAL:HG13	1.94	0.48
22:j:15:GLY:HA3	22:j:47:ILE:HG12	1.95	0.48
4:3:700:U:H2'	4:3:701:A:H8	1.79	0.48
4:3:840:G:C4'	23:k:39:GLN:HE21	2.27	0.48
5:4:2:U:H2'	5:4:3:U:C6	2.49	0.48
16:d:104:ILE:HG23	16:d:105:TYR:CD1	2.48	0.48
4:3:892:G:H2'	4:3:893:A:H8	1.79	0.48
4:3:1117:U:H2'	4:3:1118:U:O4'	2.14	0.48
4:3:1230:U:H1'	28:p:3:ILE:HG13	1.96	0.48
43:3:3225:PUT:H21	23:k:20:LEU:HD11	1.96	0.48
18:f:12:LEU:HB3	18:f:19:VAL:HG11	1.95	0.48
4:3:87:G:O2'	4:3:104:A:N1	2.39	0.48
4:3:1296:G:O2'	4:3:2019:G:O6	2.27	0.48
4:3:1696:C:O2'	4:3:2695:U:OP1	2.31	0.48
4:3:2644:U:H4'	14:b:83:GLU:OE2	2.12	0.48
22:j:51:MET:HG3	22:j:52:VAL:HG13	1.96	0.48
4:3:50:G:H22	4:3:180:A:H5''	1.79	0.48
4:3:916:U:H3	4:3:935:U:H3	1.61	0.48
4:3:1296:G:C8	30:r:15:GLN:HG2	2.49	0.48
4:3:2311:G:H21	16:d:129:THR:HG21	1.78	0.48
4:3:2452:G:OP2	15:c:69:LYS:HD2	2.14	0.48
19:g:63:LEU:HD21	19:g:71:ILE:HG21	1.95	0.48
33:u:61:PRO:HB3	33:u:65:VAL:HG12	1.96	0.48
4:3:12:A:H2'	4:3:13:C:O4'	2.13	0.48
4:3:2022:A:N1	37:y:3:VAL:HG23	2.29	0.48
4:3:2847:C:H2'	4:3:2848:A:H8	1.79	0.48
16:d:70:ALA:HB2	16:d:85:ILE:HD11	1.95	0.48
26:n:29:VAL:HG21	26:n:46:PHE:CD2	2.49	0.48
34:v:14:TYR:CZ	34:v:28:LYS:HD3	2.48	0.48
2:1:19:ILE:HD12	2:1:47:VAL:HG21	1.95	0.47
4:3:615:G:H2'	4:3:616:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2180:U:H4'	4:3:2181:A:OP2	2.13	0.47
40:3:3001:CLM:CL1	12:Z:35:ALA:HB2	2.50	0.47
13:a:84:LYS:HE2	13:a:100:THR:HG21	1.96	0.47
14:b:50:THR:HB	14:b:87:MET:HB3	1.96	0.47
16:d:2:ASN:HB3	16:d:5:LYS:HB2	1.95	0.47
17:e:121:PRO:HG2	17:e:124:LEU:HD22	1.96	0.47
18:f:115:ASP:HA	18:f:132:GLU:HA	1.96	0.47
4:3:619:A:OP1	44:3:3227:SPM:N14	2.47	0.47
4:3:652:U:H2'	4:3:653:G:C8	2.49	0.47
4:3:1544:G:H2'	4:3:1545:A:H8	1.79	0.47
4:3:1665:G:N1	4:3:1668:G:OP2	2.37	0.47
4:3:2254:G:H2'	4:3:2255:A:H8	1.80	0.47
15:c:8:LYS:NZ	15:c:14:GLU:OE1	2.45	0.47
19:g:27:PHE:CE2	19:g:108:PHE:CE1	3.02	0.47
28:p:39:ILE:HG22	28:p:43:LYS:HE3	1.96	0.47
28:p:71:GLN:NE2	28:p:106:ASN:OD1	2.47	0.47
32:t:40:ASN:HB2	32:t:69:ILE:HD11	1.96	0.47
4:3:818:A:H2'	4:3:819:U:H4'	1.97	0.47
24:l:5:LYS:HD2	24:l:6:ARG:NH2	2.25	0.47
25:m:46:ASP:O	25:m:50:THR:HG22	2.14	0.47
4:3:703:A:H2'	4:3:705:A:H62	1.79	0.47
4:3:2394:A:O2'	33:u:70:ASP:OD1	2.31	0.47
35:w:10:LYS:HB2	35:w:15:LEU:CD1	2.44	0.47
8:7:50:G:H2'	8:7:51:G:C8	2.49	0.47
18:f:6:LYS:HE3	18:f:37:ALA:HB2	1.95	0.47
19:g:103:LYS:HD2	19:g:106:MET:CG	2.44	0.47
25:m:115:ILE:HD13	37:y:53:VAL:HG13	1.95	0.47
4:3:1306:G:H2'	4:3:1307:G:H8	1.80	0.47
4:3:2323:U:O2	16:d:125:ARG:NH1	2.44	0.47
4:3:2580:A:OP2	14:b:151:ARG:N	2.48	0.47
13:a:151:GLU:OE2	13:a:157:GLY:CA	2.62	0.47
20:h:96:ILE:HG23	20:h:100:LYS:HG3	1.96	0.47
22:j:13:ASN:HD21	22:j:96:THR:H	1.63	0.47
23:k:47:THR:OG1	23:k:48:ARG:N	2.48	0.47
37:y:35:LYS:NZ	37:y:44:SER:H	2.13	0.47
4:3:652:U:H2'	4:3:653:G:H8	1.80	0.47
4:3:1392:G:N2	4:3:1395:A:OP2	2.42	0.47
4:3:2376:C:H2'	4:3:2377:A:H8	1.79	0.47
4:3:2427:U:H5''	38:z:20:LEU:HD22	1.95	0.47
4:3:2548:G:O2'	4:3:2748:A:N3	2.44	0.47
18:f:33:LYS:HB3	18:f:35:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:20:LEU:HB3	23:k:32:SER:HB3	1.96	0.47
24:l:29:PHE:HB3	24:l:65:TRP:CE2	2.50	0.47
28:p:64:LEU:O	28:p:68:LEU:HD23	2.14	0.47
28:p:105:PHE:O	28:p:109:VAL:HG13	2.13	0.47
4:3:355:A:O2'	4:3:374:A:N3	2.47	0.47
4:3:1103:G:O2'	4:3:1104:A:H5'	2.15	0.47
4:3:2160:U:H2'	4:3:2161:G:H8	1.80	0.47
13:a:3:ILE:HD13	13:a:210:LEU:HB2	1.97	0.47
13:a:151:GLU:OE2	13:a:156:GLY:O	2.33	0.47
20:h:58:TYR:OH	20:h:62:SER:O	2.27	0.47
20:h:123:MET:O	20:h:127:THR:HG22	2.15	0.47
38:z:11:CYS:SG	38:z:12:ASN:N	2.87	0.47
4:3:1045:A:N3	4:3:1188:C:O2'	2.45	0.47
4:3:1093:U:H3	4:3:1115:G:H1	1.62	0.47
4:3:1137:C:H2'	4:3:1138:A:C8	2.48	0.47
4:3:1246:U:OP2	28:p:7:LYS:NZ	2.48	0.47
4:3:2254:G:H2'	4:3:2255:A:C8	2.50	0.47
4:3:2653:G:OP2	4:3:2653:G:N2	2.29	0.47
9:8:28:A:H2'	9:8:29:U:H6	1.79	0.47
20:h:38:GLN:HB3	20:h:65:PHE:HZ	1.78	0.47
26:n:18:LYS:O	26:n:22:THR:HG23	2.15	0.47
4:3:1306:G:H4'	25:m:31:ILE:HD12	1.95	0.47
14:b:47:TYR:HB2	14:b:85:ARG:HH21	1.80	0.47
18:f:30:LEU:HB3	18:f:36:ALA:HB3	1.97	0.47
24:l:104:PHE:HE2	24:l:125:LEU:HD11	1.80	0.47
27:o:24:GLU:C	27:o:24:GLU:OE1	2.58	0.47
4:3:1124:G:N2	4:3:1125:U:O4	2.48	0.46
4:3:1436:C:H2'	4:3:1437:A:C8	2.50	0.46
20:h:70:THR:HG22	20:h:71:PRO:CD	2.44	0.46
31:s:66:ARG:HD2	31:s:66:ARG:HA	1.58	0.46
38:z:10:GLY:HA2	38:z:17:ILE:HA	1.97	0.46
4:3:125:G:OP1	4:3:1404:C:O2'	2.28	0.46
4:3:933:A:H2'	4:3:933:A:N3	2.29	0.46
4:3:1431:A:O2'	4:3:1497:A:O2'	2.30	0.46
4:3:1871:U:OP1	4:3:2418:G:O2'	2.33	0.46
4:3:2838:G:H2'	4:3:2883:A:H61	1.79	0.46
9:8:37:A:H3'	9:8:38:A:H8	1.79	0.46
15:c:194:ALA:O	15:c:195:ASN:HB3	2.15	0.46
4:3:1797:C:O2'	13:a:216:ALA:HB2	2.15	0.46
12:Z:2:UNK:HA	32:t:50:GLN:HB2	1.97	0.46
2:1:42:ARG:NH1	4:3:2358:U:OP2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1121:A:H5''	4:3:1122:G:H5'	1.96	0.46
14:b:63:ASN:OD1	14:b:64:LYS:N	2.47	0.46
15:c:5:LYS:HE2	15:c:13:PHE:HE2	1.80	0.46
18:f:104:LYS:HB3	18:f:104:LYS:HE3	1.54	0.46
19:g:63:LEU:HD12	19:g:68:PHE:HD2	1.80	0.46
27:o:98:ARG:HD2	27:o:103:TYR:HE1	1.81	0.46
32:t:1:MET:HG2	32:t:2:GLN:N	2.26	0.46
32:t:28:MET:HE1	32:t:68:PRO:HB3	1.98	0.46
4:3:755:C:H2'	4:3:756:A:H8	1.79	0.46
4:3:1166:G:N9	21:i:80:HIS:HD2	2.14	0.46
4:3:1437:A:H2'	4:3:1438:G:C8	2.51	0.46
6:5:1463:A:H2'	6:5:1464:G:C8	2.51	0.46
16:d:57:LEU:O	16:d:60:ILE:HG22	2.16	0.46
18:f:104:LYS:HE3	18:f:104:LYS:O	2.16	0.46
4:3:1091:G:H4'	4:3:1121:A:C8	2.50	0.46
4:3:1583:G:H2'	4:3:1584:U:C6	2.51	0.46
4:3:2540:G:N2	4:3:2671:G:O2'	2.48	0.46
16:d:34:ILE:CD1	16:d:96:MET:HB2	2.46	0.46
17:e:9:ILE:HG21	17:e:53:LEU:HB3	1.98	0.46
23:k:1:MET:HE3	23:k:6:LEU:HA	1.96	0.46
26:n:29:VAL:HG21	26:n:46:PHE:CE2	2.51	0.46
26:n:38:HIS:HB3	26:n:57:SER:HB2	1.98	0.46
29:q:54:ARG:HD2	29:q:54:ARG:N	2.25	0.46
36:x:30:LYS:HB2	36:x:34:ILE:HD11	1.97	0.46
1:0:48:ARG:HH12	4:3:1339:U:H2'	1.81	0.46
4:3:230:G:O2'	4:3:232:A:N6	2.48	0.46
4:3:253:C:O2'	23:k:64:LYS:NZ	2.35	0.46
4:3:1465:U:HO2'	4:3:1542:G:HO2'	1.60	0.46
4:3:2118:U:OP2	4:3:2152:C:N4	2.49	0.46
4:3:2583:U:H4'	14:b:148:GLN:HE21	1.81	0.46
9:8:18:G:N2	9:8:58:A:OP2	2.45	0.46
10:X:44:ARG:NH1	10:X:47:LYS:HE3	2.31	0.46
25:m:33:THR:OG1	25:m:34:THR:N	2.49	0.46
30:r:29:THR:HG23	30:r:55:ILE:CD1	2.46	0.46
4:3:1081:A:H2	19:g:11:VAL:HG11	1.81	0.46
4:3:1440:U:H2'	4:3:1441:A:C8	2.51	0.46
4:3:2530:U:O2'	4:3:2655:U:OP1	2.30	0.46
44:3:3249:SPM:H62	44:3:3249:SPM:H92	1.78	0.46
8:7:35:U:H2'	8:7:36:C:C6	2.50	0.46
14:b:26:ILE:HD12	14:b:192:LEU:HG	1.97	0.46
16:d:104:ILE:HG23	16:d:105:TYR:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:10:GLN:O	19:g:14:VAL:HG22	2.16	0.46
36:x:2:LYS:HG3	36:x:3:LYS:H	1.81	0.46
4:3:1797:C:H2'	4:3:1798:A:C8	2.51	0.46
4:3:2863:G:OP2	4:3:2863:G:H8	1.99	0.46
15:c:209:GLY:O	15:c:212:LYS:HG3	2.16	0.46
23:k:13:ARG:HD2	23:k:13:ARG:HA	1.57	0.46
4:3:813:G:H5''	13:a:52:LYS:HE3	1.98	0.45
4:3:1436:C:H2'	4:3:1437:A:H8	1.80	0.45
4:3:1529:U:H2'	4:3:1530:G:H8	1.81	0.45
4:3:2665:A:O2'	17:e:163:LYS:NZ	2.48	0.45
15:c:191:LEU:HD23	15:c:191:LEU:HA	1.80	0.45
17:e:100:ASN:HA	17:e:128:VAL:HG11	1.98	0.45
27:o:54:ARG:HB2	27:o:100:TYR:CD1	2.51	0.45
4:3:196:G:O6	4:3:207:C:O2'	2.23	0.45
4:3:356:A:H5'	4:3:374:A:H1'	1.98	0.45
4:3:569:U:H2'	4:3:570:C:C6	2.50	0.45
4:3:604:A:O2'	4:3:606:G:OP2	2.28	0.45
14:b:14:SER:OG	14:b:15:GLN:N	2.49	0.45
16:d:110:ARG:HH21	16:d:137:ILE:C	2.23	0.45
16:d:148:ARG:NE	16:d:149:ILE:H	2.13	0.45
22:j:12:ASP:OD1	22:j:14:THR:N	2.47	0.45
28:p:46:TYR:HA	28:p:49:ARG:NH1	2.31	0.45
1:0:6:GLN:O	4:3:721:G:H8	1.99	0.45
4:3:606:G:N2	4:3:2038:A:OP1	2.49	0.45
4:3:756:A:H2'	4:3:757:A:C8	2.51	0.45
4:3:901:C:H4'	4:3:902:U:O5'	2.17	0.45
4:3:916:U:H2'	4:3:917:G:C8	2.52	0.45
4:3:963:U:H2'	4:3:964:A:H8	1.81	0.45
4:3:1437:A:H2'	4:3:1438:G:H8	1.82	0.45
4:3:2372:C:H2'	4:3:2373:G:O4'	2.16	0.45
44:3:3227:SPM:H121	44:3:3227:SPM:H92	1.76	0.45
9:8:41:A:H2'	9:8:42:U:O4'	2.16	0.45
13:a:167:TYR:HB3	13:a:202:VAL:HG13	1.97	0.45
15:c:128:VAL:HG23	15:c:132:LEU:HD21	1.97	0.45
16:d:50:LEU:HD13	16:d:50:LEU:C	2.42	0.45
26:n:10:LEU:HD12	26:n:10:LEU:HA	1.84	0.45
27:o:95:LYS:HA	27:o:95:LYS:HD2	1.73	0.45
31:s:63:THR:H	31:s:75:SER:HB3	1.81	0.45
4:3:223:A:N3	4:3:238:U:O2'	2.39	0.45
4:3:527:A:N1	30:r:7:GLN:NE2	2.63	0.45
4:3:894:G:N3	4:3:2276:A:H2'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:1384:A:H2'	6:5:1385:A:C8	2.51	0.45
9:8:74:C:OP1	9:8:75:C:H5'	2.17	0.45
4:3:340:U:H2'	4:3:341:G:O4'	2.17	0.45
15:c:7:ILE:HG22	15:c:127:LEU:O	2.16	0.45
19:g:42:LYS:HZ3	19:g:42:LYS:HG3	1.70	0.45
30:r:125:VAL:O	30:r:129:VAL:HG23	2.17	0.45
4:3:668:A:H2'	4:3:669:A:C8	2.52	0.45
4:3:799:A:H5''	13:a:217:GLY:CA	2.46	0.45
4:3:2299:U:O2'	4:3:2382:A:N3	2.48	0.45
4:3:2813:A:H61	4:3:2894:G:H2'	1.81	0.45
15:c:14:GLU:HG3	15:c:16:GLU:H	1.82	0.45
23:k:120:LEU:H	23:k:120:LEU:HD23	1.81	0.45
27:o:56:ARG:HG2	27:o:57:GLY:N	2.31	0.45
28:p:6:GLY:C	28:p:8:GLN:NE2	2.74	0.45
30:r:137:MET:HE2	30:r:137:MET:HB3	1.91	0.45
31:s:29:PHE:CE1	31:s:83:ILE:HD12	2.52	0.45
4:3:1926:A:N1	6:5:1470:U:O2'	2.47	0.45
18:f:104:LYS:HE3	18:f:104:LYS:C	2.41	0.45
25:m:106:ARG:HG3	25:m:113:MET:SD	2.56	0.45
31:s:50:ILE:HG21	31:s:89:ILE:HD13	1.97	0.45
4:3:299:A:H2'	4:3:300:G:C8	2.51	0.45
4:3:356:A:OP2	15:c:174:ASN:HB2	2.16	0.45
4:3:411:U:H2'	4:3:412:A:H8	1.82	0.45
4:3:1135:C:H2'	4:3:1136:U:O4'	2.17	0.45
5:4:3:U:O2'	5:4:24:A:N1	2.47	0.45
16:d:38:MET:HE1	16:d:53:ALA:CB	2.46	0.45
20:h:57:ALA:HA	20:h:63:PHE:CE2	2.52	0.45
28:p:6:GLY:O	28:p:7:LYS:HB3	2.16	0.45
32:t:10:VAL:HG21	32:t:74:LEU:HB3	1.99	0.45
36:x:10:GLN:NE2	36:x:11:SER:O	2.50	0.45
4:3:1974:U:OP1	43:3:3231:PUT:N1	2.49	0.45
13:a:83:VAL:HG22	13:a:121:ILE:HD11	1.98	0.45
15:c:41:GLU:OE1	15:c:41:GLU:HA	2.17	0.45
16:d:34:ILE:HG23	16:d:155:THR:O	2.16	0.45
16:d:38:MET:HE1	16:d:53:ALA:HB1	1.98	0.45
19:g:18:LEU:HD13	19:g:68:PHE:HE2	1.81	0.45
21:i:99:GLN:O	21:i:99:GLN:HG2	2.17	0.45
26:n:31:MET:CE	26:n:44:TRP:HB2	2.47	0.45
31:s:59:ILE:O	31:s:61:LYS:NZ	2.49	0.45
4:3:1096:U:C5	20:h:11:LYS:HG3	2.51	0.45
4:3:1575:C:H2'	4:3:1576:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2260:G:O6	33:u:18:LYS:NZ	2.35	0.45
9:8:70:U:H2'	9:8:71:G:C8	2.51	0.45
15:c:125:THR:O	15:c:125:THR:HG22	2.16	0.45
19:g:43:LYS:HE3	19:g:43:LYS:HB3	1.88	0.45
25:m:112:GLU:OE1	37:y:41:ARG:NE	2.39	0.45
36:x:16:CYS:SG	36:x:17:ALA:N	2.90	0.45
4:3:166:A:N6	4:3:167:A:C6	2.85	0.44
4:3:680:A:H2'	4:3:682:A:N7	2.32	0.44
4:3:1092:A:H2'	4:3:1093:U:C6	2.52	0.44
5:4:104:C:H2'	5:4:105:A:C8	2.52	0.44
16:d:24:SER:OG	16:d:26:MET:SD	2.62	0.44
20:h:72:VAL:O	20:h:73:SER:OG	2.27	0.44
33:u:78:ASP:HB3	33:u:100:HIS:NE2	2.32	0.44
15:c:154:ASP:OD1	15:c:154:ASP:N	2.34	0.44
16:d:123:ASP:OD2	16:d:127:ASN:ND2	2.50	0.44
18:f:5:LEU:HD23	18:f:5:LEU:H	1.81	0.44
24:l:56:LYS:HB2	24:l:56:LYS:HE3	1.83	0.44
30:r:8:PHE:CD2	30:r:9:ARG:HB2	2.52	0.44
31:s:48:TYR:HD1	31:s:91:ILE:HD13	1.82	0.44
2:l:9:LYS:O	23:k:65:PHE:N	2.43	0.44
14:b:57:VAL:HG22	14:b:58:GLU:N	2.32	0.44
24:l:32:TYR:HD2	24:l:114:MET:CE	2.27	0.44
1:0:1:MET:CE	4:3:788:G:H5'	2.44	0.44
4:3:1102:A:N3	4:3:1102:A:H2'	2.31	0.44
4:3:1598:U:H2'	4:3:1599:C:C6	2.52	0.44
4:3:2017:G:H5''	30:r:42:LYS:HB2	2.00	0.44
4:3:2110:U:H3	4:3:2194:G:H1	1.65	0.44
13:a:72:LYS:HG2	13:a:156:GLY:O	2.17	0.44
15:c:162:ASN:O	15:c:162:ASN:ND2	2.37	0.44
16:d:178:VAL:C	16:d:179:LYS:HG2	2.42	0.44
21:i:19:TYR:HD2	21:i:143:LEU:HD22	1.82	0.44
26:n:109:ALA:HB1	26:n:114:LEU:HD12	1.99	0.44
27:o:54:ARG:HB2	27:o:100:TYR:HD1	1.83	0.44
28:p:27:ARG:HD3	28:p:37:THR:HG21	1.98	0.44
4:3:1094:G:H5''	20:h:68:LYS:HZ1	1.82	0.44
4:3:1099:C:H3'	4:3:1100:U:H6	1.83	0.44
4:3:1128:G:H2'	4:3:1129:U:C6	2.53	0.44
4:3:2863:G:H2'	4:3:2864:A:C8	2.53	0.44
8:7:46:U:O2'	8:7:47:U:OP1	2.24	0.44
13:a:252:ASP:OD2	13:a:261:ARG:NH1	2.50	0.44
15:c:60:GLY:HA3	15:c:80:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:140:GLU:OE2	36:x:27:SER:HB2	2.17	0.44
3:2:9:PRO:HD3	3:2:16:ILE:HD11	2.00	0.44
4:3:2802:C:N4	4:3:2803:G:H21	2.15	0.44
26:n:61:LYS:HE3	26:n:61:LYS:HB3	1.52	0.44
28:p:106:ASN:O	28:p:109:VAL:HG22	2.18	0.44
35:w:65:TRP:CE2	35:w:66:GLN:HG3	2.52	0.44
37:y:35:LYS:HZ2	37:y:44:SER:H	1.66	0.44
4:3:524:G:N2	4:3:527:A:OP2	2.34	0.44
4:3:603:G:H2'	4:3:2037:A:N7	2.32	0.44
4:3:1344:U:HO2'	10:X:44:ARG:HH21	1.58	0.44
44:3:3241:SPM:H121	44:3:3241:SPM:H92	1.77	0.44
5:4:82:U:H2'	5:4:83:U:H4'	1.98	0.44
20:h:100:LYS:HA	20:h:103:GLU:OE2	2.17	0.44
25:m:74:ASP:O	25:m:78:LEU:HB2	2.16	0.44
15:c:205:LYS:HA	15:c:208:GLU:OE2	2.18	0.44
17:e:16:VAL:HA	17:e:28:LYS:O	2.18	0.44
18:f:82:LYS:HZ1	18:f:146:ASN:HB3	1.83	0.44
27:o:85:ASN:O	27:o:86:ILE:HD13	2.18	0.44
4:3:1801:U:H2'	4:3:1802:C:C6	2.53	0.44
10:X:40:ILE:HD12	10:X:40:ILE:H	1.83	0.44
16:d:5:LYS:HD3	16:d:97:TRP:CG	2.53	0.44
23:k:3:LEU:HD23	23:k:3:LEU:HA	1.87	0.44
33:u:39:LYS:NZ	33:u:45:ILE:HG13	2.33	0.44
35:w:12:SER:O	35:w:16:VAL:HG23	2.18	0.44
4:3:174:A:H2'	4:3:175:A:H8	1.83	0.43
4:3:333:A:N3	4:3:353:G:O2'	2.45	0.43
4:3:1691:U:H2'	4:3:1692:A:C8	2.53	0.43
4:3:1705:U:H1'	14:b:135:HIS:CE1	2.53	0.43
4:3:2811:G:H2'	4:3:2812:U:C6	2.53	0.43
20:h:15:LEU:HD23	20:h:50:MET:HG2	2.00	0.43
26:n:9:ARG:HG3	26:n:9:ARG:NH1	2.33	0.43
35:w:98:LEU:C	35:w:98:LEU:HD23	2.43	0.43
4:3:299:A:H2'	4:3:300:G:H8	1.84	0.43
4:3:340:U:H1'	4:3:1241:U:H5	1.82	0.43
4:3:1447:A:O2'	4:3:1449:G:N7	2.44	0.43
4:3:2059:G:H4'	14:b:148:GLN:OE1	2.18	0.43
4:3:2155:G:H2'	4:3:2156:G:H8	1.81	0.43
4:3:2386:A:H1'	26:n:90:VAL:HG23	2.00	0.43
4:3:2459:A:C2	40:3:3001:CLM:H8	2.53	0.43
4:3:2896:G:H3'	4:3:2897:G:H5'	2.00	0.43
15:c:40:VAL:HG12	15:c:101:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:12:ILE:O	16:d:16:LEU:HB2	2.18	0.43
16:d:29:PRO:HG2	16:d:169:LEU:HB2	1.99	0.43
16:d:128:TYR:HB3	16:d:156:LEU:HD23	2.00	0.43
24:l:5:LYS:HB3	24:l:6:ARG:NH2	2.32	0.43
38:z:7:THR:OG1	38:z:49:GLU:OE2	2.23	0.43
1:0:44:VAL:O	1:0:47:GLU:HG3	2.18	0.43
4:3:756:A:H2'	4:3:757:A:H8	1.83	0.43
4:3:1414:C:H2'	4:3:1415:A:C8	2.52	0.43
4:3:1529:U:H2'	4:3:1530:G:C8	2.53	0.43
4:3:2409:U:OP1	38:z:40:ARG:NH2	2.52	0.43
8:7:61:C:H2'	8:7:62:C:H6	1.83	0.43
13:a:147:VAL:HA	13:a:200:VAL:HA	2.00	0.43
18:f:77:LEU:O	18:f:78:HIS:C	2.61	0.43
22:j:77:LEU:HD13	27:o:77:LYS:HE2	2.01	0.43
33:u:45:ILE:HD13	33:u:75:ALA:HB2	1.99	0.43
4:3:610:G:H5''	4:3:2510:G:C2	2.53	0.43
4:3:1415:A:H5'	4:3:1495:A:H1'	2.00	0.43
4:3:2565:G:H2'	4:3:2566:C:C6	2.53	0.43
14:b:123:ILE:HG23	14:b:128:PHE:O	2.19	0.43
15:c:26:ALA:HB2	15:c:113:HIS:NE2	2.33	0.43
16:d:14:LYS:HG3	16:d:18:LYS:HE2	1.99	0.43
21:i:129:LYS:HB2	21:i:129:LYS:HE3	1.91	0.43
24:l:31:GLU:OE2	24:l:114:MET:HE1	2.18	0.43
1:0:32:LYS:O	1:0:36:LYS:HG3	2.19	0.43
4:3:1623:U:H2'	4:3:1624:A:C8	2.53	0.43
13:a:126:HIS:HB3	13:a:127:PRO:HD2	2.00	0.43
13:a:252:ASP:OD1	13:a:252:ASP:N	2.41	0.43
16:d:171:ARG:HD3	16:d:180:GLY:HA2	2.00	0.43
18:f:84:HIS:HE1	18:f:93:ILE:HD13	1.84	0.43
22:j:7:ARG:HG3	22:j:7:ARG:HH11	1.82	0.43
29:q:60:GLU:HB2	29:q:91:LYS:HD3	2.00	0.43
4:3:2623:U:H1'	37:y:4:GLN:HB3	1.99	0.43
4:3:2853:U:O2'	4:3:2870:U:O2	2.31	0.43
13:a:234:ASN:O	13:a:241:GLY:HA3	2.18	0.43
15:c:157:VAL:HA	15:c:196:ALA:O	2.19	0.43
28:p:8:GLN:N	28:p:8:GLN:CD	2.77	0.43
28:p:45:ALA:O	28:p:49:ARG:HG3	2.19	0.43
4:3:339:U:H2'	4:3:340:U:C6	2.53	0.43
4:3:610:G:H2'	4:3:611:A:C8	2.54	0.43
4:3:764:G:OP1	13:a:10:SER:OG	2.36	0.43
4:3:2146:A:H2'	4:3:2147:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:37:ALA:HB3	14:b:51:LEU:CD2	2.46	0.43
15:c:156:ASN:HA	15:c:177:ASN:OD1	2.18	0.43
30:r:110:ASN:OD1	30:r:110:ASN:C	2.61	0.43
35:w:63:LEU:HD11	35:w:68:GLU:HB2	1.99	0.43
37:y:9:SER:HB2	37:y:11:HIS:CD2	2.53	0.43
37:y:32:LYS:HD3	37:y:47:MET:HE2	2.01	0.43
4:3:26:G:H1'	30:r:77:ASN:HB3	2.00	0.43
4:3:1306:G:H2'	4:3:1307:G:C8	2.54	0.43
4:3:2031:C:OP1	45:3:3237:SPD:H81	2.18	0.43
4:3:2081:U:H2'	4:3:2082:U:C6	2.53	0.43
4:3:2813:A:H2'	4:3:2814:A:H8	1.84	0.43
13:a:189:THR:HB	13:a:279:ILE:HB	2.00	0.43
16:d:96:MET:HE3	16:d:97:TRP:NE1	2.34	0.43
22:j:12:ASP:OD1	22:j:12:ASP:C	2.62	0.43
22:j:107:ARG:HA	22:j:115:LEU:HD11	2.01	0.43
28:p:6:GLY:H	28:p:8:GLN:HE21	1.63	0.43
4:3:1119:A:C4	19:g:53:VAL:HG21	2.54	0.43
4:3:1495:A:H2'	4:3:1496:A:C8	2.54	0.43
8:7:23:C:H2'	8:7:24:A:C8	2.54	0.43
14:b:6:ILE:HG22	14:b:207:ILE:HB	2.00	0.43
16:d:95:ARG:H	16:d:95:ARG:HG3	1.54	0.43
23:k:2:GLU:CD	23:k:2:GLU:N	2.77	0.43
4:3:848:U:H2'	4:3:849:C:C6	2.53	0.43
4:3:1585:A:N3	4:3:1585:A:H2'	2.34	0.43
4:3:1619:A:H8	4:3:1619:A:H5''	1.82	0.43
4:3:1915:C:O2'	8:7:12:G:H5''	2.19	0.43
4:3:2032:G:H2'	4:3:2033:G:C8	2.54	0.43
4:3:2798:A:O3'	4:3:2896:G:N2	2.52	0.43
9:8:63:C:H6	9:8:63:C:H5''	1.84	0.43
16:d:91:LEU:C	16:d:96:MET:HB3	2.44	0.43
21:i:122:ILE:HD12	21:i:122:ILE:HA	1.83	0.43
23:k:82:LEU:HA	23:k:85:ILE:HG22	2.01	0.43
27:o:54:ARG:HD3	27:o:56:ARG:HB2	2.01	0.43
34:v:15:GLY:HA3	34:v:29:TRP:HZ3	1.84	0.43
35:w:13:GLU:HG2	35:w:14:GLU:N	2.34	0.43
4:3:1414:C:H2'	4:3:1415:A:H8	1.84	0.42
8:7:26:A:H61	8:7:44:G:H1	1.67	0.42
16:d:45:ARG:HG3	16:d:46:ASP:N	2.33	0.42
16:d:114:PHE:CD1	16:d:114:PHE:C	2.96	0.42
17:e:3:LYS:NZ	17:e:57:ARG:HH12	2.16	0.42
18:f:82:LYS:NZ	18:f:146:ASN:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:w:16:VAL:O	35:w:20:ILE:HG22	2.18	0.42
36:x:14:PHE:O	36:x:22:SER:HA	2.19	0.42
3:2:1:MET:CE	4:3:2750:A:H5''	2.49	0.42
4:3:1119:A:N9	19:g:53:VAL:HG21	2.35	0.42
4:3:1697:C:HO2'	4:3:1698:A:H8	1.66	0.42
4:3:1815:U:O2'	4:3:1816:A:O4'	2.37	0.42
4:3:2336:A:H2'	4:3:2337:U:C6	2.54	0.42
4:3:2358:U:H2'	4:3:2359:G:O4'	2.18	0.42
4:3:2655:U:H2'	4:3:2656:G:H8	1.84	0.42
4:3:2815:G:H5''	14:b:63:ASN:HD21	1.83	0.42
14:b:40:LYS:O	14:b:48:SER:HA	2.19	0.42
29:q:4:ILE:HG13	29:q:40:MET:HB3	2.00	0.42
3:2:1:MET:HE3	4:3:2750:A:H5''	2.02	0.42
4:3:17:G:H4'	37:y:18:SER:HB2	2.00	0.42
4:3:831:U:H2'	4:3:832:C:C6	2.53	0.42
4:3:1836:A:H3'	4:3:1837:C:H6	1.84	0.42
4:3:2239:U:H5''	34:v:29:TRP:HD1	1.83	0.42
4:3:2537:G:H5''	4:3:2538:A:H5''	2.01	0.42
4:3:2764:U:H1'	4:3:2765:A:H5''	2.01	0.42
13:a:12:SER:O	13:a:12:SER:OG	2.28	0.42
15:c:162:ASN:HD22	15:c:162:ASN:C	2.20	0.42
16:d:20:PHE:CD2	16:d:22:PHE:CE2	3.08	0.42
17:e:18:LEU:HD12	17:e:20:PHE:CZ	2.54	0.42
20:h:61:LYS:HA	20:h:63:PHE:CE1	2.55	0.42
4:3:63:U:O2'	4:3:64:U:O2	2.37	0.42
4:3:1096:U:H3	20:h:13:ASN:HD21	1.67	0.42
4:3:1101:U:H2'	4:3:1103:G:N7	2.34	0.42
4:3:1798:A:H8	4:3:1798:A:P	2.43	0.42
4:3:2271:C:H4'	4:3:2337:U:H4'	2.00	0.42
4:3:2713:A:O2'	4:3:2856:G:OP1	2.33	0.42
20:h:84:LYS:HA	20:h:84:LYS:HD2	1.92	0.42
22:j:10:VAL:HA	22:j:84:CYS:O	2.20	0.42
22:j:19:VAL:HG13	22:j:41:VAL:HB	2.00	0.42
22:j:54:LYS:HE3	22:j:54:LYS:HB3	1.83	0.42
26:n:110:ARG:HD3	26:n:116:PHE:O	2.18	0.42
36:x:46:TYR:CD1	36:x:46:TYR:N	2.85	0.42
4:3:54:A:OP2	4:3:118:G:N1	2.43	0.42
4:3:1120:A:H2'	4:3:1121:A:N9	2.34	0.42
4:3:1321:C:H2'	4:3:1322:A:O4'	2.19	0.42
4:3:1385:U:H2'	4:3:1386:G:O4'	2.19	0.42
6:5:1385:A:H2'	6:5:1386:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:61:C:H2'	8:7:62:C:C6	2.54	0.42
20:h:105:ALA:HA	20:h:123:MET:CE	2.50	0.42
23:k:78:VAL:HG13	23:k:112:ILE:HA	2.01	0.42
27:o:3:LYS:HE3	27:o:3:LYS:HB2	1.79	0.42
27:o:18:LEU:HD23	27:o:82:HIS:CG	2.55	0.42
29:q:14:VAL:HG23	29:q:97:PHE:HZ	1.85	0.42
4:3:899:A:H2'	4:3:900:G:C8	2.54	0.42
4:3:2438:A:H2'	4:3:2438:A:N3	2.33	0.42
4:3:2638:G:H2'	4:3:2639:G:H8	1.85	0.42
9:8:48:C:OP2	9:8:48:C:H6	2.02	0.42
14:b:50:THR:OG1	14:b:87:MET:O	2.22	0.42
19:g:99:VAL:O	19:g:103:LYS:HG3	2.19	0.42
29:q:19:THR:HG22	29:q:93:LYS:HB2	2.01	0.42
29:q:36:ASP:HA	29:q:54:ARG:HH21	1.85	0.42
32:t:3:ARG:NH2	32:t:4:ILE:HD11	2.34	0.42
38:z:31:LYS:HE2	38:z:31:LYS:HB3	1.93	0.42
4:3:558:C:H1'	4:3:587:U:H1'	2.01	0.42
4:3:1096:U:H5	20:h:11:LYS:HG3	1.82	0.42
4:3:1536:C:H2'	4:3:1537:A:C8	2.54	0.42
4:3:1572:U:H2'	4:3:1573:A:H8	1.85	0.42
4:3:1809:A:H2'	4:3:1810:A:C8	2.55	0.42
4:3:2334:U:H3	4:3:2397:G:H1	1.67	0.42
40:3:3001:CLM:CL1	12:Z:35:ALA:CB	3.04	0.42
15:c:43:ALA:C	15:c:45:TRP:H	2.28	0.42
15:c:143:MET:HE3	15:c:172:THR:HG21	2.02	0.42
18:f:58:TYR:HA	18:f:61:ASN:HD21	1.84	0.42
24:l:10:ARG:HH11	24:l:10:ARG:HG2	1.84	0.42
26:n:114:LEU:HD23	26:n:114:LEU:HA	1.89	0.42
32:t:13:ILE:H	32:t:13:ILE:HG13	1.75	0.42
4:3:141:A:H2	4:3:1437:A:H1'	1.83	0.42
4:3:449:C:H2'	4:3:450:C:C6	2.55	0.42
4:3:1673:U:O2'	4:3:2707:A:H4'	2.20	0.42
4:3:1691:U:H2'	4:3:1692:A:H8	1.85	0.42
4:3:2070:C:H1'	12:Z:36:ASP:HA	2.02	0.42
13:a:38:LEU:HD23	13:a:38:LEU:HA	1.80	0.42
22:j:71:ARG:HH22	22:j:104:ARG:NH1	2.16	0.42
24:l:109:ILE:HG12	24:l:110:PRO:HD2	2.01	0.42
28:p:71:GLN:OE1	28:p:109:VAL:HG21	2.20	0.42
4:3:776:U:H2'	4:3:777:C:H6	1.85	0.42
4:3:1166:G:O4'	21:i:80:HIS:CD2	2.72	0.42
4:3:1460:G:H2'	4:3:1461:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2204:C:H2'	4:3:2205:U:C6	2.54	0.42
4:3:2606:A:H5''	13:a:242:GLY:HA3	2.01	0.42
19:g:99:VAL:HG12	19:g:103:LYS:HE2	2.02	0.42
19:g:103:LYS:HD2	19:g:106:MET:HG3	2.02	0.42
20:h:39:PHE:N	20:h:39:PHE:CD1	2.87	0.42
20:h:77:LYS:HD3	20:h:83:GLU:O	2.19	0.42
28:p:20:ALA:HB2	28:p:38:VAL:HG23	2.02	0.42
4:3:606:G:N1	4:3:2038:A:OP1	2.53	0.42
4:3:783:1MG:C8	30:r:89:ALA:HB1	2.55	0.42
4:3:1114:C:H3'	4:3:1115:G:H8	1.84	0.42
4:3:1239:G:O2'	4:3:1267:A:N1	2.37	0.42
16:d:46:ASP:OD1	16:d:46:ASP:C	2.63	0.42
19:g:37:ALA:O	19:g:41:ARG:HG2	2.20	0.42
19:g:51:ILE:HD13	19:g:51:ILE:HA	1.95	0.42
20:h:118:GLU:O	20:h:122:LYS:HG2	2.20	0.42
28:p:73:MET:HG3	28:p:74:THR:N	2.35	0.42
32:t:95:PRO:HG2	32:t:96:LYS:H	1.79	0.42
33:u:99:LYS:HE3	33:u:101:LYS:HE2	2.00	0.42
34:v:4:LYS:HG3	34:v:5:ASP:O	2.19	0.42
4:3:622:U:H2'	4:3:623:A:H8	1.81	0.41
4:3:1444:C:N4	4:3:1616:G:O6	2.53	0.41
4:3:1819:G:N2	13:a:54:THR:HG21	2.34	0.41
15:c:183:LEU:HD12	15:c:203:VAL:HG13	2.00	0.41
17:e:110:LEU:HG	17:e:155:ARG:HG3	2.02	0.41
18:f:97:ILE:O	18:f:101:ALA:N	2.53	0.41
21:i:39:ILE:HG12	21:i:125:VAL:HG22	2.01	0.41
36:x:6:HIS:O	36:x:8:PRO:HD3	2.19	0.41
2:1:10:ARG:HG2	23:k:64:LYS:HA	2.02	0.41
4:3:155:A:H2'	4:3:156:A:H8	1.84	0.41
4:3:2376:C:H2'	4:3:2377:A:C8	2.55	0.41
4:3:2420:A:H2'	4:3:2421:U:O4'	2.20	0.41
16:d:4:LEU:O	16:d:4:LEU:HD23	2.20	0.41
16:d:24:SER:HB3	16:d:27:GLN:HG3	2.02	0.41
20:h:102:LYS:HB2	20:h:102:LYS:HE2	1.79	0.41
28:p:18:LYS:HB2	28:p:18:LYS:HE3	1.75	0.41
30:r:51:LEU:O	30:r:55:ILE:HG13	2.20	0.41
32:t:84:GLN:H	32:t:84:GLN:HG3	1.55	0.41
37:y:35:LYS:NZ	37:y:44:SER:HB3	2.34	0.41
2:1:10:ARG:NH1	4:3:254:G:OP2	2.46	0.41
4:3:259:A:O2'	4:3:422:A:OP1	2.36	0.41
4:3:274:A:OP2	4:3:294:G:N1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1313:G:N2	4:3:1356:G:H5''	2.35	0.41
17:e:57:ARG:H	17:e:57:ARG:HG2	1.73	0.41
32:t:47:LYS:H	32:t:47:LYS:HD3	1.85	0.41
33:u:78:ASP:HB3	33:u:100:HIS:CD2	2.55	0.41
35:w:16:VAL:O	35:w:19:VAL:HG12	2.19	0.41
35:w:39:ASP:O	35:w:41:PRO:HD3	2.21	0.41
4:3:1464:G:H1	4:3:1590:U:H3	1.67	0.41
13:a:240:HIS:CE1	13:a:249:VAL:HG13	2.55	0.41
15:c:113:HIS:HA	15:c:211:PHE:CZ	2.55	0.41
15:c:205:LYS:HA	15:c:208:GLU:CD	2.46	0.41
24:l:98:LYS:O	24:l:101:THR:HG23	2.20	0.41
27:o:42:LYS:HG2	27:o:43:VAL:H	1.84	0.41
32:t:24:VAL:HG22	32:t:36:VAL:HG12	2.01	0.41
33:u:39:LYS:HZ2	33:u:45:ILE:HG13	1.85	0.41
35:w:8:ARG:HD2	35:w:57:ILE:HG12	2.02	0.41
4:3:166:A:C6	4:3:167:A:C6	3.09	0.41
4:3:749:U:H1'	4:3:752:C:H5	1.85	0.41
4:3:890:U:H2'	4:3:891:G:C8	2.55	0.41
4:3:2403:C:H2'	4:3:2404:G:C8	2.55	0.41
5:4:65:G:H2'	5:4:66:A:H8	1.86	0.41
13:a:30:LYS:HE3	13:a:30:LYS:HB3	1.95	0.41
13:a:174:ASP:OD1	13:a:175:GLU:OE2	2.38	0.41
15:c:20:LEU:HD23	15:c:20:LEU:HA	1.90	0.41
18:f:104:LYS:HA	18:f:109:GLN:HA	2.02	0.41
22:j:22:ILE:HD11	22:j:42:SER:HB3	2.01	0.41
23:k:90:LEU:HD12	23:k:90:LEU:HA	1.86	0.41
31:s:21:MET:HA	31:s:25:LYS:NZ	2.36	0.41
4:3:155:A:H2'	4:3:156:A:C8	2.55	0.41
8:7:10:G:HO2'	8:7:11:U:P	2.43	0.41
9:8:5:C:H2'	9:8:6:U:C6	2.55	0.41
15:c:205:LYS:HA	15:c:208:GLU:OE1	2.20	0.41
19:g:26:ILE:HA	19:g:81:ALA:O	2.20	0.41
26:n:93:THR:C	26:n:95:GLY:H	2.28	0.41
27:o:19:LYS:HE2	27:o:82:HIS:HA	2.03	0.41
35:w:88:LYS:HE3	35:w:88:LYS:HB2	1.87	0.41
37:y:53:VAL:HG12	37:y:54:LYS:CG	2.50	0.41
4:3:10:U:H2'	4:3:11:U:H4'	2.02	0.41
4:3:1697:C:O2'	4:3:2694:A:H4'	2.21	0.41
4:3:1803:U:H2'	4:3:1804:A:C8	2.55	0.41
4:3:2071:C:H2'	4:3:2072:C:C6	2.55	0.41
4:3:2638:G:H2'	4:3:2639:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:2803:G:O2'	4:3:2804:C:O5'	2.35	0.41
14:b:97:THR:HG22	14:b:100:ASN:OD1	2.20	0.41
16:d:17:GLN:OE1	16:d:17:GLN:HA	2.20	0.41
20:h:106:GLN:OE1	20:h:106:GLN:N	2.53	0.41
21:i:59:ILE:HB	21:i:127:VAL:HG23	2.03	0.41
31:s:44:PHE:CE2	31:s:85:LEU:HD11	2.55	0.41
2:1:28:HIS:HE1	4:3:2430:C:C5	2.39	0.41
4:3:1208:A:H2'	4:3:1209:U:H4'	2.01	0.41
4:3:2025:C:H2'	4:3:2026:A:H8	1.86	0.41
4:3:2814:A:H4'	14:b:64:LYS:HD2	2.02	0.41
15:c:4:LEU:HD12	15:c:4:LEU:HA	1.81	0.41
15:c:136:THR:HG22	15:c:138:GLY:H	1.85	0.41
16:d:29:PRO:CG	16:d:169:LEU:HB2	2.51	0.41
23:k:34:ARG:HB3	23:k:41:ALA:HA	2.03	0.41
26:n:30:LEU:HD23	26:n:91:PHE:HD1	1.85	0.41
4:3:45:U:H2'	4:3:46:A:O4'	2.21	0.41
4:3:893:A:H61	4:3:957:G:H1	1.69	0.41
4:3:1081:A:C2	19:g:61:ARG:HD2	2.56	0.41
4:3:1334:U:H2'	4:3:1335:A:H8	1.86	0.41
4:3:1485:A:H4'	4:3:1486:U:C5	2.56	0.41
4:3:1564:U:H2'	4:3:1565:G:C8	2.56	0.41
4:3:1619:A:H2'	4:3:1620:A:H8	1.81	0.41
4:3:2335:A:H2'	4:3:2336:A:C8	2.56	0.41
5:4:81:U:H2'	5:4:82:U:O4'	2.20	0.41
8:7:18:G:O2'	8:7:56:G:N2	2.32	0.41
13:a:146:GLN:H	13:a:146:GLN:HG2	1.69	0.41
16:d:45:ARG:HB3	16:d:78:LYS:NZ	2.36	0.41
17:e:34:ILE:HD13	17:e:34:ILE:HA	1.83	0.41
22:j:24:VAL:HG13	22:j:33:ALA:HB2	2.01	0.41
24:l:67:ARG:HD3	24:l:105:GLU:OE2	2.20	0.41
24:l:76:LYS:HB3	24:l:91:GLU:HG3	2.03	0.41
25:m:57:PHE:O	25:m:61:ARG:HG3	2.21	0.41
25:m:89:LYS:HD2	25:m:90:TYR:CZ	2.56	0.41
27:o:113:LYS:HD3	27:o:113:LYS:HA	1.92	0.41
30:r:36:LEU:HD12	30:r:36:LEU:HA	1.90	0.41
35:w:11:SER:OG	35:w:13:GLU:OE2	2.35	0.41
4:3:227:A:O2'	4:3:456:G:N3	2.45	0.41
4:3:410:G:C8	34:v:60:LYS:HD2	2.56	0.41
4:3:788:G:N2	25:m:3:TYR:HH	2.18	0.41
4:3:814:U:P	13:a:53:ILE:CD1	3.08	0.41
4:3:869:U:H2'	4:3:870:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:909:U:H2'	4:3:910:G:C8	2.56	0.41
4:3:1144:C:P	19:g:77:LYS:HG2	2.61	0.41
4:3:1178:A:N7	21:i:30:LYS:NZ	2.58	0.41
13:a:83:VAL:HG13	13:a:97:SER:HB3	2.03	0.41
16:d:40:VAL:HG21	16:d:150:ARG:NH1	2.36	0.41
17:e:92:LEU:HD21	17:e:97:TYR:HB3	2.02	0.41
30:r:29:THR:HG23	30:r:55:ILE:HD13	2.02	0.41
35:w:38:LEU:HD23	35:w:38:LEU:HA	1.81	0.41
2:1:51:ASP:O	2:1:55:ILE:HG12	2.21	0.40
4:3:98:C:O5'	35:w:40:LYS:NZ	2.54	0.40
4:3:984:C:H2'	4:3:985:A:H8	1.85	0.40
4:3:1162:A:N3	44:3:3249:SPM:H21	2.36	0.40
4:3:1583:G:HO2'	4:3:1584:U:P	2.43	0.40
4:3:2010:A:H2'	4:3:2011:G:O4'	2.21	0.40
8:7:17:G:H4'	8:7:18:G:H5''	2.03	0.40
14:b:160:PHE:CZ	21:i:84:ILE:HD11	2.56	0.40
15:c:128:VAL:O	15:c:200:GLU:HA	2.20	0.40
21:i:7:LEU:HD12	28:p:63:ARG:NH1	2.36	0.40
4:3:567:U:H4'	4:3:568:G:C8	2.56	0.40
4:3:2078:A:H2'	4:3:2079:G:C8	2.56	0.40
8:7:5:C:H2'	8:7:6:C:H6	1.86	0.40
9:8:71:G:H2'	9:8:72:C:C6	2.57	0.40
14:b:29:ILE:HD13	14:b:207:ILE:HD11	2.04	0.40
21:i:48:THR:HG22	21:i:50:ASN:OD1	2.21	0.40
27:o:93:ARG:NH2	27:o:118:LYS:O	2.54	0.40
32:t:9:LYS:HD2	32:t:21:SER:OG	2.21	0.40
4:3:166:A:N6	18:f:104:LYS:NZ	2.68	0.40
4:3:881:A:H2	4:3:968:U:H3	1.63	0.40
8:7:10:G:H2'	8:7:11:U:C6	2.56	0.40
19:g:93:LEU:HA	19:g:96:VAL:HG22	2.04	0.40
24:l:35:VAL:HG22	24:l:102:VAL:HG22	2.02	0.40
27:o:2:LYS:HA	27:o:2:LYS:HD3	1.87	0.40
27:o:64:PHE:HD1	27:o:81:ILE:HG12	1.85	0.40
29:q:89:TYR:CD1	29:q:89:TYR:C	2.99	0.40
4:3:741:A:H4'	13:a:7:ILE:HD13	2.03	0.40
4:3:1543:U:H2'	4:3:1544:G:C8	2.57	0.40
4:3:1889:U:H2'	4:3:1890:U:C6	2.57	0.40
4:3:2145:A:H2'	4:3:2146:A:H8	1.85	0.40
4:3:2200:U:H2'	4:3:2201:G:H5'	2.04	0.40
4:3:2686:C:H4'	44:b:303:SPM:HN41	1.87	0.40
8:7:74:C:H5''	8:7:75:A:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:13:MET:HE1	14:b:196:ALA:HA	2.02	0.40
15:c:194:ALA:C	15:c:196:ALA:N	2.78	0.40
16:d:155:THR:O	16:d:156:LEU:HD13	2.21	0.40
18:f:3:VAL:HG23	18:f:37:ALA:O	2.22	0.40
4:3:670:G:H2'	4:3:671:C:C6	2.56	0.40
4:3:1433:U:H2'	4:3:1434:U:C6	2.57	0.40
8:7:5:C:H2'	8:7:6:C:C6	2.56	0.40
9:8:30:G:H3'	9:8:31:A:H8	1.87	0.40
14:b:13:MET:HB2	14:b:13:MET:HE3	1.73	0.40
20:h:35:PHE:O	20:h:39:PHE:CD1	2.75	0.40
34:v:48:ILE:H	34:v:48:ILE:HG12	1.68	0.40
35:w:107:ASP:OD1	35:w:107:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
12	Z	3/36 (8%)	3 (100%)	0	0	100	100
13	a	283/287 (99%)	268 (95%)	14 (5%)	1 (0%)	30	59
14	b	229/287 (80%)	221 (96%)	8 (4%)	0	100	100
15	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
16	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100
17	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	f	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	30
19	g	123/161 (76%)	116 (94%)	7 (6%)	0	100	100
20	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
21	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
22	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
23	k	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
24	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
25	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
26	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
27	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
28	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
29	q	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
30	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
31	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
32	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
33	u	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
34	v	62/65 (95%)	62 (100%)	0	0	100	100
35	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
36	x	44/97 (45%)	35 (80%)	8 (18%)	1 (2%)	5	19
37	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
38	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	3485/4359 (80%)	3310 (95%)	171 (5%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	a	128	ILE
18	f	12	LEU
18	f	74	GLN
36	x	18	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	41/41 (100%)	41 (100%)	0	100	100
2	1	51/51 (100%)	50 (98%)	1 (2%)	48	78
3	2	35/35 (100%)	35 (100%)	0	100	100
10	X	27/406 (7%)	25 (93%)	2 (7%)	13	38
12	Z	2/2 (100%)	2 (100%)	0	100	100
13	a	241/243 (99%)	233 (97%)	8 (3%)	33	67
14	b	188/233 (81%)	177 (94%)	11 (6%)	18	48
15	c	183/184 (100%)	173 (94%)	10 (6%)	19	50
16	d	153/154 (99%)	149 (97%)	4 (3%)	40	73
17	e	153/159 (96%)	146 (95%)	7 (5%)	24	57
18	f	134/134 (100%)	130 (97%)	4 (3%)	36	70
19	g	100/129 (78%)	96 (96%)	4 (4%)	28	62
20	h	102/110 (93%)	97 (95%)	5 (5%)	22	54
21	i	126/128 (98%)	122 (97%)	4 (3%)	34	68
22	j	103/103 (100%)	100 (97%)	3 (3%)	37	71
23	k	125/126 (99%)	118 (94%)	7 (6%)	19	50
24	l	113/115 (98%)	111 (98%)	2 (2%)	51	80
25	m	105/109 (96%)	101 (96%)	4 (4%)	29	64
26	n	99/99 (100%)	97 (98%)	2 (2%)	48	78
27	o	104/105 (99%)	102 (98%)	2 (2%)	50	79
28	p	104/108 (96%)	103 (99%)	1 (1%)	68	89
29	q	90/91 (99%)	84 (93%)	6 (7%)	15	43
30	r	118/132 (89%)	114 (97%)	4 (3%)	32	66
31	s	84/208 (40%)	77 (92%)	7 (8%)	10	32
32	t	96/96 (100%)	94 (98%)	2 (2%)	47	77
33	u	70/85 (82%)	67 (96%)	3 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	v	59/60 (98%)	57 (97%)	2 (3%)	32	66
35	w	97/98 (99%)	93 (96%)	4 (4%)	27	61
36	x	44/86 (51%)	42 (96%)	2 (4%)	24	58
37	y	48/49 (98%)	47 (98%)	1 (2%)	47	77
38	z	47/50 (94%)	44 (94%)	3 (6%)	16	44
All	All	3042/3729 (82%)	2927 (96%)	115 (4%)	30	64

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	13	LEU
10	X	40	ILE
10	X	57	LEU
13	a	37	LEU
13	a	107	SER
13	a	141	ILE
13	a	200	VAL
13	a	202	VAL
13	a	227	THR
13	a	262	HIS
13	a	275	THR
14	b	9	VAL
14	b	11	VAL
14	b	39	VAL
14	b	42	GLU
14	b	61	LYS
14	b	74	ASN
14	b	100	ASN
14	b	188	ASN
14	b	217	VAL
14	b	221	GLU
14	b	231	GLU
15	c	7	ILE
15	c	21	SER
15	c	36	ASP
15	c	41	GLU
15	c	58	VAL
15	c	79	THR
15	c	178	VAL
15	c	180	VAL

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Mol	Chain	Res	Type
15	c	183	LEU
15	c	203	VAL
16	d	15	GLU
16	d	50	LEU
16	d	66	VAL
16	d	149	ILE
17	e	18	LEU
17	e	34	ILE
17	e	101	VAL
17	e	108	LEU
17	e	109	GLN
17	e	135	THR
17	e	169	ASP
18	f	3	VAL
18	f	8	ASP
18	f	23	ASP
18	f	84	HIS
19	g	25	VAL
19	g	60	ARG
19	g	63	LEU
19	g	76	ILE
20	h	12	ILE
20	h	58	TYR
20	h	74	ILE
20	h	100	LYS
20	h	123	MET
21	i	20	ILE
21	i	62	SER
21	i	87	ILE
21	i	146	SER
22	j	19	VAL
22	j	28	THR
22	j	116	SER
23	k	8	SER
23	k	31	THR
23	k	56	THR
23	k	78	VAL
23	k	99	ILE
23	k	108	SER
23	k	139	VAL
24	l	63	LYS
24	l	127	VAL

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Mol	Chain	Res	Type
25	m	5	ASN
25	m	10	THR
25	m	21	GLN
25	m	23	SER
26	n	47	SER
26	n	89	VAL
27	o	33	VAL
27	o	98	ARG
28	p	76	SER
29	q	5	VAL
29	q	45	ILE
29	q	75	SER
29	q	78	HIS
29	q	90	THR
29	q	92	LEU
30	r	35	ILE
30	r	37	SER
30	r	39	THR
30	r	137	MET
31	s	12	LEU
31	s	14	GLU
31	s	24	THR
31	s	47	VAL
31	s	59	ILE
31	s	64	THR
31	s	84	THR
32	t	47	LYS
32	t	92	VAL
33	u	81	VAL
33	u	84	GLN
33	u	96	SER
34	v	9	LEU
34	v	48	ILE
35	w	15	LEU
35	w	38	LEU
35	w	76	THR
35	w	107	ASP
36	x	18	SER
36	x	27	SER
37	y	11	HIS
38	z	12	ASN
38	z	18	ASN

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Mol	Chain	Res	Type
38	z	21	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	20	HIS
3	2	36	GLN
14	b	66	GLN
14	b	73	ASN
14	b	148	GLN
14	b	157	GLN
14	b	171	HIS
14	b	188	ASN
15	c	96	ASN
16	d	83	GLN
17	e	63	GLN
18	f	96	GLN
20	h	13	ASN
21	i	80	HIS
21	i	134	ASN
23	k	67	ASN
23	k	125	HIS
23	k	129	HIS
25	m	77	GLN
26	n	64	ASN
28	p	8	GLN
28	p	40	GLN
28	p	71	GLN
28	p	106	ASN
29	q	78	HIS
30	r	7	GLN
30	r	33	GLN
30	r	38	ASN
32	t	98	ASN
33	u	43	GLN
33	u	84	GLN
33	u	100	HIS
38	z	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Y	8/9 (88%)	4 (50%)	1 (12%)
4	3	2892/2907 (99%)	505 (17%)	12 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	30/1520 (1%)	6 (20%)	0
7	6	1/76 (1%)	0	0
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	3187/4771 (66%)	587 (18%)	15 (0%)

All (587) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G
4	3	37	G
4	3	48	G
4	3	64	U
4	3	65	A
4	3	73	A
4	3	76	A
4	3	77	G
4	3	102	A
4	3	103	G
4	3	119	A
4	3	121	U
4	3	126	C
4	3	132	G
4	3	141	A
4	3	142	A
4	3	163	A
4	3	180	A
4	3	184	A
4	3	187	C
4	3	200	A
4	3	203	A
4	3	219	G
4	3	220	A
4	3	225	A
4	3	226	A
4	3	232	A

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Mol	Chain	Res	Type
4	3	234	G
4	3	237	A
4	3	245	U
4	3	246	G
4	3	252	G
4	3	269	A
4	3	276	A
4	3	284	U
4	3	287	G
4	3	295	U
4	3	296	U
4	3	297	G
4	3	298	U
4	3	299	A
4	3	309	A
4	3	310	U
4	3	311	G
4	3	315	A
4	3	316	C
4	3	317	U
4	3	319	G
4	3	325	G
4	3	336	C
4	3	345	A
4	3	363	G
4	3	364	A
4	3	365	U
4	3	402	A
4	3	409	A
4	3	410	G
4	3	411	U
4	3	418	G
4	3	419	A
4	3	424	G
4	3	425	U
4	3	426	U
4	3	432	G
4	3	437	A
4	3	440	C
4	3	460	G
4	3	463	U
4	3	483	A

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Mol	Chain	Res	Type
4	3	517	G
4	3	539	U
4	3	540	A
4	3	548	A
4	3	562	C
4	3	565	C
4	3	566	G
4	3	567	U
4	3	573	A
4	3	581	A
4	3	583	U
4	3	596	G
4	3	598	G
4	3	607	U
4	3	608	A
4	3	610	G
4	3	620	G
4	3	636	U
4	3	637	U
4	3	638	A
4	3	648	G
4	3	649	A
4	3	650	G
4	3	663	A
4	3	670	G
4	3	673	A
4	3	681	A
4	3	682	A
4	3	689	U
4	3	691	G
4	3	705	A
4	3	712	A
4	3	716	G
4	3	721	G
4	3	722	C
4	3	765	A
4	3	775	C
4	3	782	U
4	3	792	G
4	3	797	U
4	3	800	C
4	3	810	G

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Mol	Chain	Res	Type
4	3	811	G
4	3	817	A
4	3	819	U
4	3	820	U
4	3	824	A
4	3	828	A
4	3	829	A
4	3	840	G
4	3	846	U
4	3	847	C
4	3	854	A
4	3	862	U
4	3	881	A
4	3	882	C
4	3	883	A
4	3	901	C
4	3	902	U
4	3	904	C
4	3	906	G
4	3	918	G
4	3	924	C
4	3	926	U
4	3	927	A
4	3	928	G
4	3	930	C
4	3	932	U
4	3	934	C
4	3	935	U
4	3	936	G
4	3	944	U
4	3	947	A
4	3	949	C
4	3	951	C
4	3	952	U
4	3	953	G
4	3	970	U
4	3	981	A
4	3	982	G
4	3	994	U
4	3	997	G
4	3	998	C
4	3	1008	A

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Mol	Chain	Res	Type
4	3	1010	G
4	3	1016	A
4	3	1019	A
4	3	1026	A
4	3	1032	A
4	3	1039	G
4	3	1045	A
4	3	1049	U
4	3	1058	U
4	3	1060	G
4	3	1061	A
4	3	1068	U
4	3	1074	A
4	3	1080	A
4	3	1082	A
4	3	1084	C
4	3	1096	U
4	3	1097	G
4	3	1098	G
4	3	1099	C
4	3	1102	A
4	3	1104	A
4	3	1105	A
4	3	1106	G
4	3	1107	C
4	3	1110	C
4	3	1111	C
4	3	1113	U
4	3	1114	C
4	3	1115	G
4	3	1120	A
4	3	1122	G
4	3	1123	A
4	3	1125	U
4	3	1130	A
4	3	1132	C
4	3	1138	A
4	3	1145	G
4	3	1146	A
4	3	1147	G
4	3	1165	U
4	3	1167	U

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Mol	Chain	Res	Type
4	3	1168	A
4	3	1170	C
4	3	1176	U
4	3	1177	A
4	3	1178	A
4	3	1204	A
4	3	1208	A
4	3	1209	U
4	3	1210	A
4	3	1212	C
4	3	1215	G
4	3	1234	U
4	3	1235	U
4	3	1236	G
4	3	1242	G
4	3	1246	U
4	3	1250	A
4	3	1251	G
4	3	1253	G
4	3	1256	A
4	3	1257	G
4	3	1266	G
4	3	1268	U
4	3	1280	G
4	3	1281	A
4	3	1283	A
4	3	1285	U
4	3	1286	G
4	3	1292	A
4	3	1301	G
4	3	1304	U
4	3	1313	G
4	3	1325	C
4	3	1328	A
4	3	1329	U
4	3	1330	U
4	3	1352	G
4	3	1353	G
4	3	1369	U
4	3	1378	C
4	3	1380	U
4	3	1388	G

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Mol	Chain	Res	Type
4	3	1393	A
4	3	1406	A
4	3	1407	U
4	3	1412	A
4	3	1423	A
4	3	1424	U
4	3	1431	A
4	3	1444	C
4	3	1445	U
4	3	1446	G
4	3	1448	U
4	3	1456	C
4	3	1463	G
4	3	1467	U
4	3	1480	A
4	3	1481	U
4	3	1483	G
4	3	1486	U
4	3	1487	U
4	3	1502	A
4	3	1504	G
4	3	1508	G
4	3	1510	A
4	3	1513	A
4	3	1514	U
4	3	1515	A
4	3	1519	A
4	3	1522	U
4	3	1534	A
4	3	1535	A
4	3	1541	A
4	3	1546	U
4	3	1550	G
4	3	1569	A
4	3	1570	A
4	3	1571	G
4	3	1580	G
4	3	1582	G
4	3	1584	U
4	3	1585	A
4	3	1588	A
4	3	1589	A

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Mol	Chain	Res	Type
4	3	1603	A
4	3	1612	U
4	3	1617	U
4	3	1618	U
4	3	1619	A
4	3	1641	A
4	3	1642	G
4	3	1643	A
4	3	1644	A
4	3	1645	C
4	3	1650	A
4	3	1651	C
4	3	1661	A
4	3	1668	G
4	3	1680	A
4	3	1681	G
4	3	1682	C
4	3	1688	A
4	3	1694	A
4	3	1708	G
4	3	1727	U
4	3	1737	G
4	3	1748	U
4	3	1749	A
4	3	1764	U
4	3	1769	A
4	3	1770	A
4	3	1771	C
4	3	1780	A
4	3	1789	C
4	3	1791	A
4	3	1807	C
4	3	1808	C
4	3	1809	A
4	3	1816	A
4	3	1823	U
4	3	1836	A
4	3	1854	A
4	3	1855	A
4	3	1866	G
4	3	1869	G
4	3	1878	A

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Mol	Chain	Res	Type
4	3	1886	C
4	3	1910	G
4	3	1913	G
4	3	1920	A
4	3	1936	G
4	3	1937	G
4	3	1938	U
4	3	1943	A
4	3	1944	A
4	3	1962	U
4	3	1974	U
4	3	1977	A
4	3	1978	U
4	3	1979	G
4	3	1998	U
4	3	1999	G
4	3	2000	U
4	3	2004	G
4	3	2028	G
4	3	2030	A
4	3	2038	A
4	3	2040	A
4	3	2041	C
4	3	2042	A
4	3	2050	G
4	3	2057	C
4	3	2062	C
4	3	2063	G
4	3	2067	A
4	3	2068	G
4	3	2069	A
4	3	2076	G
4	3	2084	A
4	3	2099	U
4	3	2100	G
4	3	2106	G
4	3	2110	U
4	3	2111	U
4	3	2112	A
4	3	2114	C
4	3	2115	A
4	3	2117	G

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Mol	Chain	Res	Type
4	3	2123	A
4	3	2124	A
4	3	2125	U
4	3	2139	C
4	3	2140	G
4	3	2153	U
4	3	2154	A
4	3	2164	G
4	3	2166	U
4	3	2171	A
4	3	2180	U
4	3	2181	A
4	3	2193	U
4	3	2195	U
4	3	2196	G
4	3	2197	U
4	3	2198	G
4	3	2199	C
4	3	2200	U
4	3	2201	G
4	3	2202	U
4	3	2207	A
4	3	2211	G
4	3	2212	U
4	3	2219	U
4	3	2220	A
4	3	2221	U
4	3	2227	U
4	3	2228	U
4	3	2233	A
4	3	2246	G
4	3	2247	G
4	3	2259	OMG
4	3	2274	A
4	3	2276	A
4	3	2287	G
4	3	2291	U
4	3	2295	A
4	3	2298	G
4	3	2305	C
4	3	2311	G
4	3	2313	U

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Mol	Chain	Res	Type
4	3	2316	G
4	3	2319	A
4	3	2327	U
4	3	2329	G
4	3	2333	G
4	3	2335	A
4	3	2336	A
4	3	2342	U
4	3	2343	A
4	3	2344	A
4	3	2353	G
4	3	2355	C
4	3	2358	U
4	3	2366	A
4	3	2391	G
4	3	2393	C
4	3	2397	G
4	3	2410	C
4	3	2411	C
4	3	2414	U
4	3	2422	G
4	3	2431	U
4	3	2433	A
4	3	2437	G
4	3	2438	A
4	3	2443	A
4	3	2449	U
4	3	2456	A
4	3	2477	A
4	3	2481	U
4	3	2482	U
4	3	2483	C
4	3	2484	A
4	3	2486	A
4	3	2488	C
4	3	2499	U
4	3	2510	G
4	3	2512	U
4	3	2513	G
4	3	2521	A
4	3	2526	A
4	3	2537	G

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Mol	Chain	Res	Type
4	3	2543	G
4	3	2574	A
4	3	2575	G
4	3	2580	A
4	3	2585	A
4	3	2593	U
4	3	2594	C
4	3	2605	G
4	3	2610	A
4	3	2617	U
4	3	2618	C
4	3	2621	U
4	3	2623	U
4	3	2637	A
4	3	2638	G
4	3	2654	U
4	3	2668	A
4	3	2669	G
4	3	2697	C
4	3	2698	U
4	3	2722	G
4	3	2734	C
4	3	2737	G
4	3	2741	A
4	3	2752	G
4	3	2756	A
4	3	2760	C
4	3	2764	U
4	3	2765	A
4	3	2773	A
4	3	2786	A
4	3	2798	A
4	3	2799	U
4	3	2804	C
4	3	2806	A
4	3	2807	G
4	3	2808	A
4	3	2810	A
4	3	2813	A
4	3	2822	C
4	3	2824	A
4	3	2829	G

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Mol	Chain	Res	Type
4	3	2839	A
4	3	2853	U
4	3	2862	U
4	3	2863	G
4	3	2871	G
4	3	2876	G
4	3	2884	C
4	3	2887	A
4	3	2888	U
4	3	2895	A
4	3	2896	G
4	3	2899	C
5	4	9	C
5	4	10	C
5	4	11	A
5	4	13	G
5	4	14	U
5	4	22	G
5	4	23	A
5	4	28	C
5	4	33	U
5	4	35	C
5	4	39	U
5	4	41	C
5	4	48	A
5	4	49	G
5	4	54	U
5	4	56	A
5	4	60	C
5	4	64	G
5	4	65	G
5	4	80	G
5	4	82	U
5	4	83	U
5	4	84	C
5	4	85	A
5	4	88	G
5	4	89	A
5	4	99	A
5	4	106	A
5	4	108	C
6	5	1466	U

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Mol	Chain	Res	Type
6	5	1467	A
6	5	1469	G
6	5	1472	G
6	5	1478	A
6	5	1480	G
8	7	4	U
8	7	11	U
8	7	13	U
8	7	15	G
8	7	16	U
8	7	17	G
8	7	19	A
8	7	20	U
8	7	21	A
8	7	22	A
8	7	34	G
8	7	44	G
8	7	46	U
8	7	47	U
8	7	48	G
8	7	51	G
8	7	57	A
8	7	71	C
8	7	73	C
8	7	75	A
9	8	3	A
9	8	9	A
9	8	10	G
9	8	15	G
9	8	16	U
9	8	17	U
9	8	18	G
9	8	19	G
9	8	20	U
9	8	21	A
9	8	30	G
9	8	31	A
9	8	41	A
9	8	46	G
9	8	47	U
9	8	48	C
9	8	58	A

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Mol	Chain	Res	Type
9	8	60	C
9	8	71	G
9	8	73	A
9	8	74	C
9	8	75	C
9	8	76	A
11	Y	40	G
11	Y	42	U
11	Y	43	A
11	Y	46	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	315	A
4	3	410	G
4	3	881	A
4	3	901	C
4	3	1124	G
4	3	1209	U
4	3	1352	G
4	3	1583	G
4	3	1618	U
4	3	2180	U
4	3	2410	C
4	3	2764	U
8	7	10	G
8	7	46	U
11	Y	42	U

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

5 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
4	2MA	3	2511	4,42	22,25,26	4.12	10 (45%)	32,37,40	3.50	12 (37%)
6	B8T	5	1377	6	19,22,23	3.31	8 (42%)	25,31,34	0.85	1 (4%)
6	5MC	5	1375	6	19,22,23	4.56	8 (42%)	26,32,35	1.02	2 (7%)
4	1MG	3	783	4	23,26,27	3.02	6 (26%)	33,39,42	2.33	8 (24%)
4	OMG	3	2259	4,8,42	23,26,27	2.61	7 (30%)	32,38,41	2.43	10 (31%)

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
4	2MA	3	2511	4,42	-	1/7/25/26	0/3/3/3
6	B8T	5	1377	6	-	1/7/27/28	0/2/2/2
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2
4	1MG	3	783	4	-	0/7/25/26	0/3/3/3
4	OMG	3	2259	4,8,42	-	3/9/27/28	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	2511	2MA	C4-N3	11.93	1.49	1.34
6	5	1375	5MC	C6-C5	10.07	1.51	1.34
6	5	1375	5MC	C5-C4	9.17	1.51	1.44
4	3	783	1MG	C2-N3	8.59	1.47	1.33
4	3	2511	2MA	C2-N3	8.00	1.47	1.34
6	5	1375	5MC	C4-N3	7.93	1.46	1.34
6	5	1377	B8T	C4-N3	7.51	1.45	1.32
4	3	2511	2MA	C6-N1	7.39	1.44	1.35
4	3	2259	OMG	C2-N2	7.27	1.51	1.34
6	5	1375	5MC	C2-N3	7.19	1.50	1.36
4	3	783	1MG	C4-N3	6.72	1.49	1.34
4	3	783	1MG	C2-N2	6.59	1.45	1.34
6	5	1377	B8T	C2-N3	6.55	1.49	1.36
4	3	2511	2MA	C2-N1	6.45	1.45	1.34
4	3	2259	OMG	C4-N3	6.18	1.48	1.34
6	5	1377	B8T	C6-C5	6.08	1.49	1.35
6	5	1375	5MC	C4-N4	5.78	1.48	1.34
6	5	1375	5MC	C6-N1	5.63	1.47	1.38
4	3	2511	2MA	C5-C6	5.33	1.55	1.41
4	3	2259	OMG	C2-N3	5.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1375	5MC	C2-N1	4.78	1.50	1.40
6	5	1377	B8T	C4-N4	4.63	1.45	1.36
6	5	1377	B8T	C2-N1	4.45	1.49	1.40
4	3	783	1MG	C2-N1	4.10	1.44	1.37
6	5	1377	B8T	C5-C4	3.69	1.49	1.41
4	3	2511	2MA	C5-N7	-3.68	1.32	1.39
4	3	783	1MG	C5-C6	3.47	1.54	1.45
4	3	2511	2MA	C8-N7	3.37	1.38	1.31
4	3	2259	OMG	C2-N1	3.35	1.45	1.37
6	5	1377	B8T	C6-N1	3.14	1.45	1.38
4	3	783	1MG	C5-N7	-2.62	1.33	1.39
6	5	1377	B8T	O2-C2	-2.61	1.18	1.23
4	3	2259	OMG	C5-C6	2.38	1.53	1.44
6	5	1375	5MC	O2-C2	-2.21	1.19	1.23
4	3	2511	2MA	C4-N9	-2.18	1.33	1.37
4	3	2511	2MA	C6-N6	-2.14	1.28	1.34
4	3	2259	OMG	C8-N7	2.04	1.38	1.32
4	3	2511	2MA	C8-N9	-2.03	1.34	1.37
4	3	2259	OMG	O2'-CM2	-2.02	1.35	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2511	2MA	C1'-N9-C8	-12.31	99.78	127.09
4	3	2511	2MA	C4-N9-C1'	10.67	151.59	126.63
4	3	2259	OMG	C1'-N9-C8	-6.76	107.54	126.73
4	3	783	1MG	C1'-N9-C4	-6.72	106.64	126.49
4	3	783	1MG	C1'-N9-C8	6.30	144.62	126.73
4	3	2511	2MA	C5-C4-N3	-5.76	121.11	127.18
4	3	2259	OMG	C1'-N9-C4	5.53	142.82	126.49
4	3	783	1MG	C5-C4-N3	-5.19	120.13	128.39
4	3	2511	2MA	N9-C8-N7	-4.72	107.23	113.94
4	3	2259	OMG	C5-C4-N3	-4.54	121.16	128.39
4	3	2259	OMG	C2-N3-C4	4.34	119.77	112.30
4	3	783	1MG	C2-N3-C4	3.62	120.12	111.98
4	3	2259	OMG	N9-C8-N7	-3.60	106.72	113.40
4	3	2511	2MA	N3-C2-N1	-3.29	119.97	125.77
4	3	783	1MG	N9-C4-N3	3.23	132.42	125.95
4	3	783	1MG	N9-C8-N7	-3.12	107.61	113.40
4	3	2511	2MA	C5-N7-C8	3.02	108.19	103.45
6	5	1375	5MC	C5-C6-N1	-2.97	120.09	123.31
4	3	2259	OMG	C2-N1-C6	-2.94	119.77	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2511	2MA	N3-C4-N9	2.81	130.56	126.99
4	3	783	1MG	C5-C6-N1	2.75	120.09	115.02
4	3	2511	2MA	C4-N9-C8	2.74	108.62	105.74
4	3	2259	OMG	N9-C4-N3	2.74	131.43	125.95
4	3	2511	2MA	CM2-C2-N1	2.71	121.19	117.13
4	3	2259	OMG	C5-C6-N1	2.66	120.03	113.25
4	3	2511	2MA	C4-C5-N7	-2.59	107.62	110.58
6	5	1377	B8T	C6-C5-C4	2.52	120.04	117.00
4	3	2259	OMG	O6-C6-C5	-2.45	120.08	126.53
4	3	2259	OMG	C8-N7-C5	2.33	108.40	104.26
4	3	2511	2MA	C5-C4-N9	2.31	108.33	105.81
4	3	783	1MG	C8-N7-C5	2.21	108.19	104.26
4	3	2511	2MA	N6-C6-N1	2.20	120.00	117.03
6	5	1375	5MC	CM5-C5-C6	-2.19	119.88	122.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-C4'-C5'-O5'
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	1377	B8T	O4'-C4'-C5'-O5'
4	3	2511	2MA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	783	1MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 234 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
40	CLM	3	3001	-	20,20,20	0.68	1 (5%)	23,27,27	0.61	0
44	SPM	b	303	-	13,13,13	0.17	0	12,12,12	0.31	0
47	LYS	8	103	9	7,8,9	1.63	1 (14%)	3,8,10	0.37	0
44	SPM	3	3241	-	13,13,13	0.34	0	12,12,12	0.92	0
43	PUT	3	3224	-	5,5,5	0.24	0	4,4,4	0.52	0
43	PUT	3	3222	-	5,5,5	0.23	0	4,4,4	0.53	0
45	SPD	3	3233	-	9,9,9	0.32	0	8,8,8	0.88	0
45	SPD	3	3235	-	9,9,9	0.33	0	8,8,8	0.86	0
45	SPD	3	3240	-	9,9,9	0.31	0	8,8,8	0.85	0
45	SPD	3	3238	-	9,9,9	0.32	0	8,8,8	0.84	0
44	SPM	3	3227	-	13,13,13	0.35	0	12,12,12	0.89	0
45	SPD	3	3250	-	9,9,9	0.18	0	8,8,8	0.18	0
45	SPD	3	3230	-	9,9,9	0.33	0	8,8,8	0.79	0
46	N2P	3	3244	-	6,6,6	0.24	0	5,5,5	0.61	0
45	SPD	3	3232	-	9,9,9	0.35	0	8,8,8	0.74	0
45	SPD	3	3246	-	9,9,9	0.33	0	8,8,8	0.81	0
45	SPD	3	3229	-	9,9,9	0.32	0	8,8,8	0.86	0
43	PUT	3	3242	-	5,5,5	0.24	0	4,4,4	0.52	0
44	SPM	3	3249	-	13,13,13	0.35	0	12,12,12	0.87	0
46	N2P	3	3247	-	6,6,6	0.23	0	5,5,5	0.65	0
43	PUT	3	3223	-	5,5,5	0.22	0	4,4,4	0.54	0
45	SPD	3	3245	-	9,9,9	0.32	0	8,8,8	0.88	0
43	PUT	3	3226	-	5,5,5	0.25	0	4,4,4	0.50	0
45	SPD	3	3234	-	9,9,9	0.32	0	8,8,8	0.77	0
45	SPD	3	3228	-	9,9,9	0.32	0	8,8,8	0.86	0
45	SPD	3	3239	-	9,9,9	0.32	0	8,8,8	0.87	0
43	PUT	3	3225	-	5,5,5	0.24	0	4,4,4	0.50	0
45	SPD	3	3236	-	9,9,9	0.33	0	8,8,8	0.81	0
45	SPD	3	3237	-	9,9,9	0.31	0	8,8,8	0.95	0
45	SPD	3	3248	-	9,9,9	0.31	0	8,8,8	0.87	0
46	N2P	3	3243	-	6,6,6	0.24	0	5,5,5	0.63	0
43	PUT	3	3231	-	5,5,5	0.24	0	4,4,4	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLM	3	3001	-	-	2/20/22/22	0/1/1/1
44	SPM	b	303	-	-	2/11/11/11	-
47	LYS	8	103	9	-	3/6/7/9	-
44	SPM	3	3241	-	-	2/11/11/11	-
43	PUT	3	3224	-	-	0/3/3/3	-
43	PUT	3	3222	-	-	0/3/3/3	-
45	SPD	3	3233	-	-	0/7/7/7	-
45	SPD	3	3235	-	-	0/7/7/7	-
45	SPD	3	3240	-	-	0/7/7/7	-
45	SPD	3	3238	-	-	0/7/7/7	-
44	SPM	3	3227	-	-	4/11/11/11	-
45	SPD	3	3250	-	-	0/7/7/7	-
45	SPD	3	3230	-	-	0/7/7/7	-
46	N2P	3	3244	-	-	2/4/4/4	-
45	SPD	3	3232	-	-	1/7/7/7	-
45	SPD	3	3246	-	-	1/7/7/7	-
45	SPD	3	3229	-	-	1/7/7/7	-
43	PUT	3	3242	-	-	0/3/3/3	-
44	SPM	3	3249	-	-	1/11/11/11	-
46	N2P	3	3247	-	-	1/4/4/4	-
43	PUT	3	3223	-	-	0/3/3/3	-
45	SPD	3	3245	-	-	0/7/7/7	-
43	PUT	3	3226	-	-	0/3/3/3	-
45	SPD	3	3234	-	-	2/7/7/7	-
45	SPD	3	3228	-	-	0/7/7/7	-
45	SPD	3	3239	-	-	2/7/7/7	-
43	PUT	3	3225	-	-	1/3/3/3	-
45	SPD	3	3236	-	-	0/7/7/7	-
45	SPD	3	3237	-	-	1/7/7/7	-
45	SPD	3	3248	-	-	0/7/7/7	-
46	N2P	3	3243	-	-	1/4/4/4	-
43	PUT	3	3231	-	-	0/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	103	LYS	CB-CA	3.68	1.59	1.53
40	3	3001	CLM	C1-C2	-2.09	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	8	103	LYS	O-C-CA-CB
47	8	103	LYS	C-CA-CB-CG
46	3	3243	N2P	C2-C3-C4-C5
45	3	3229	SPD	N6-C7-C8-C9
40	3	3001	CLM	C5-C3-N2-C2
44	3	3227	SPM	C7-C8-C9-N10
44	3	3241	SPM	C7-C6-N5-C4
46	3	3247	N2P	C2-C3-C4-C5
46	3	3244	N2P	C2-C3-C4-C5
44	3	3249	SPM	C6-C7-C8-C9
45	3	3234	SPD	C8-C7-N6-C5
44	3	3227	SPM	C7-C6-N5-C4
45	3	3232	SPD	N1-C2-C3-C4
45	3	3239	SPD	C8-C7-N6-C5
45	3	3237	SPD	C8-C7-N6-C5
43	3	3225	PUT	C1-C2-C3-C4
40	3	3001	CLM	C4-C3-N2-C2
46	3	3244	N2P	C3-C4-C5-N1
44	b	303	SPM	C3-C4-N5-C6
44	3	3227	SPM	N10-C11-C12-C13
44	3	3241	SPM	N10-C11-C12-C13
44	b	303	SPM	C7-C6-N5-C4
45	3	3239	SPD	C2-C3-C4-C5
45	3	3234	SPD	C4-C5-N6-C7
44	3	3227	SPM	C6-C7-C8-C9
47	8	103	LYS	N-CA-CB-CG
45	3	3246	SPD	C3-C4-C5-N6

There are no ring outliers.

10 monomers are involved in 17 short contacts:

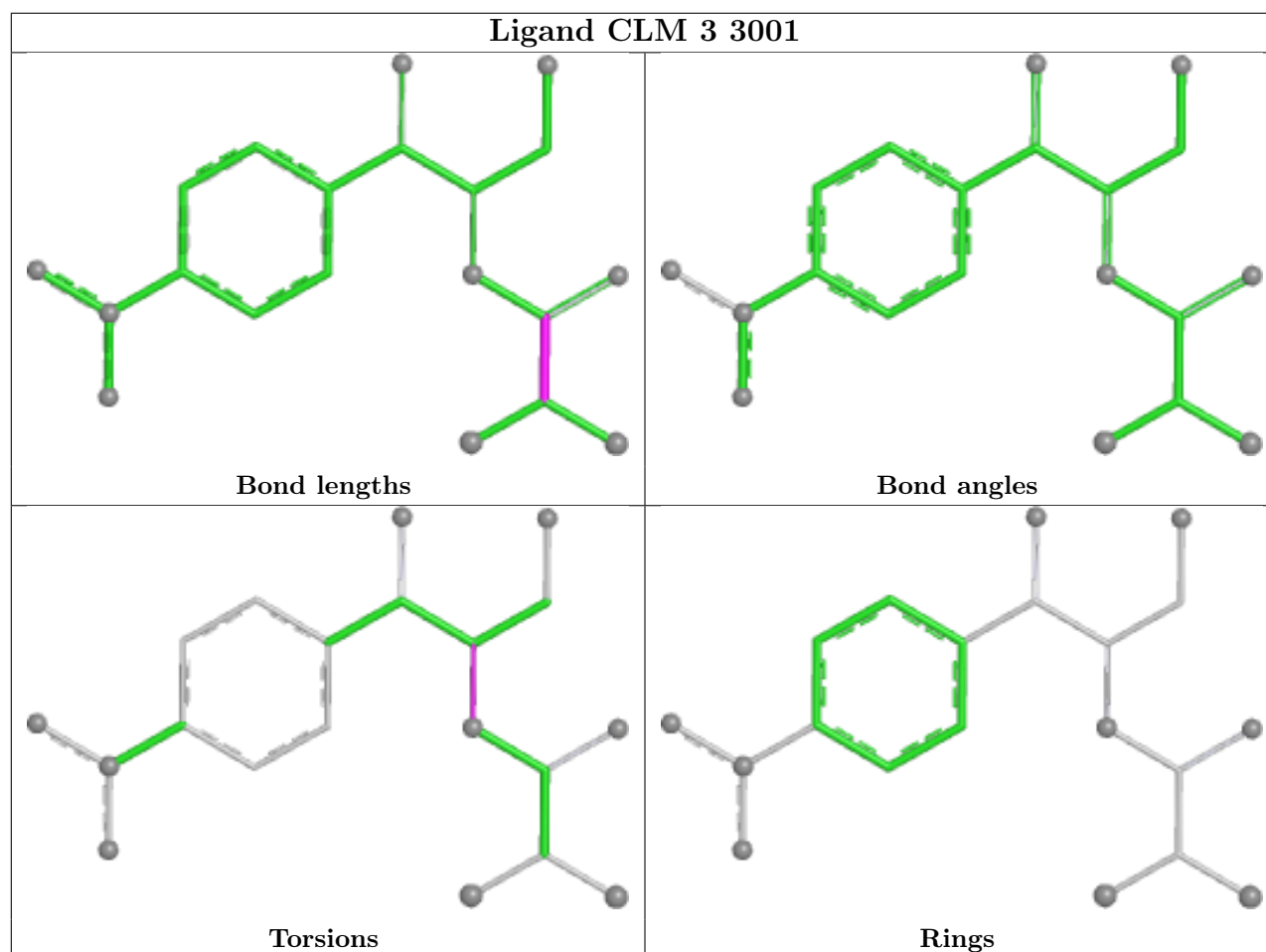
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	3	3001	CLM	4	0
44	b	303	SPM	1	0
44	3	3241	SPM	1	0
44	3	3227	SPM	4	0
45	3	3250	SPD	1	0
44	3	3249	SPM	2	0
43	3	3225	PUT	1	0
45	3	3237	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	3	3248	SPD	1	0
43	3	3231	PUT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

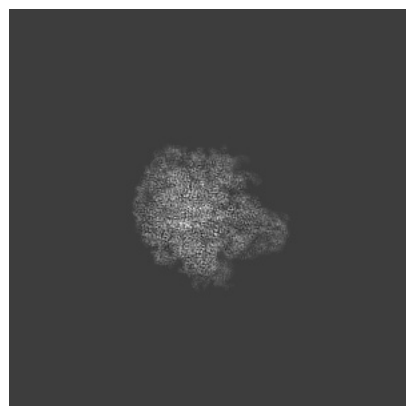
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17134. These allow visual inspection of the internal detail of the map and identification of artifacts.

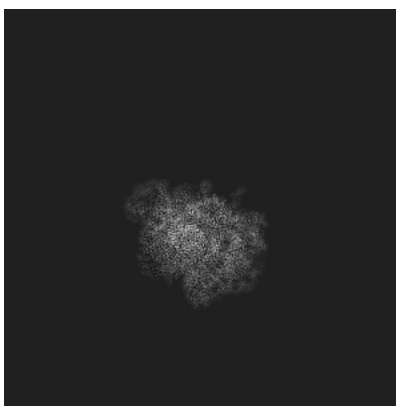
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

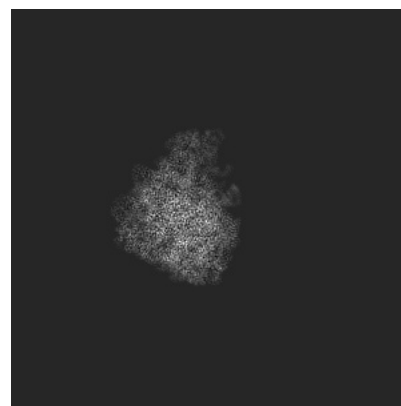
6.1.1 Primary map



X

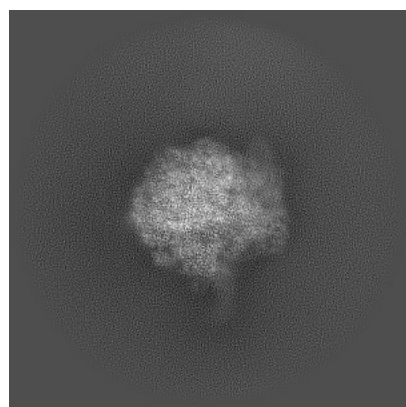


Y

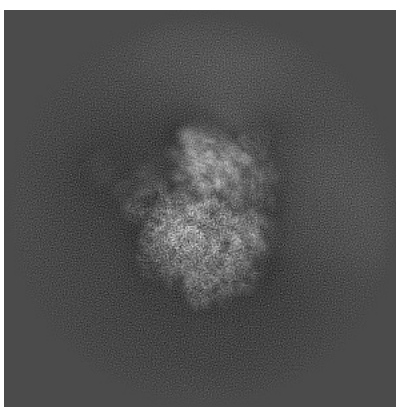


Z

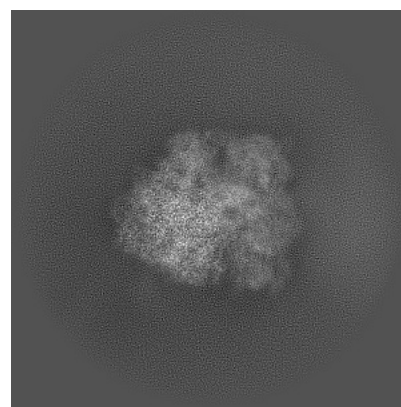
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

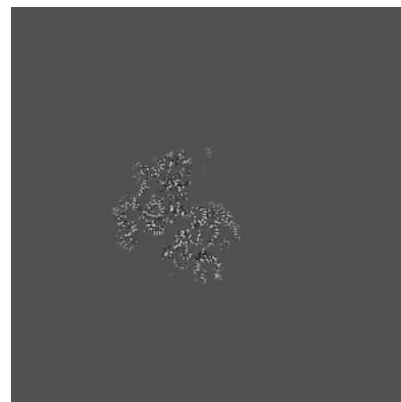
6.2.1 Primary map



X Index: 203

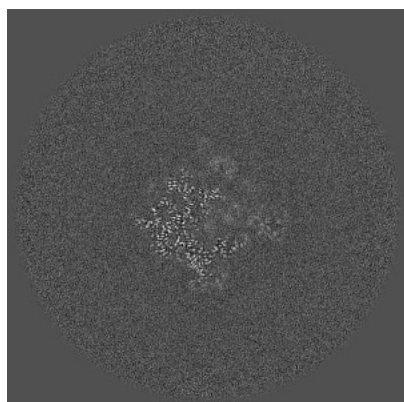


Y Index: 203

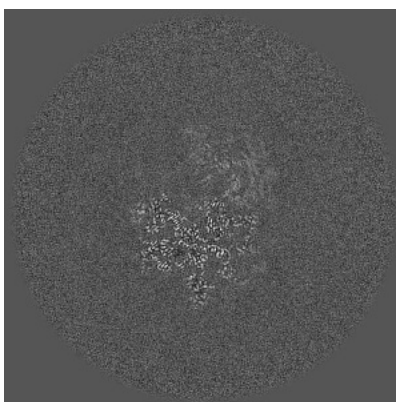


Z Index: 203

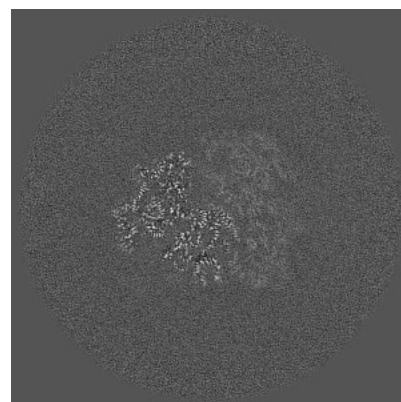
6.2.2 Raw map



X Index: 203



Y Index: 203



Z Index: 203

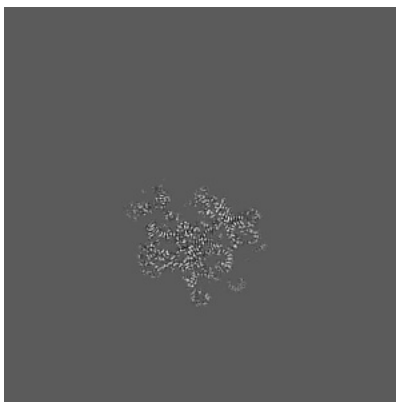
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

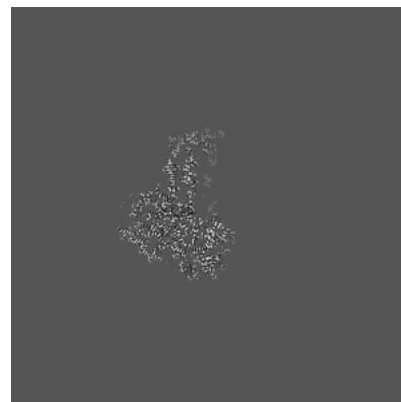
6.3.1 Primary map



X Index: 174

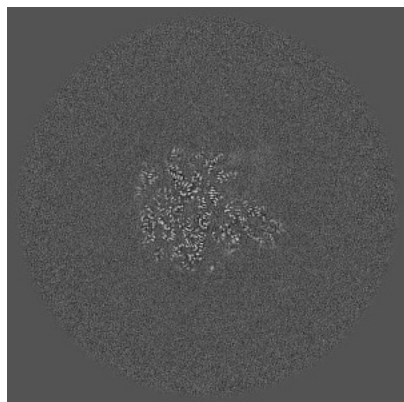


Y Index: 196

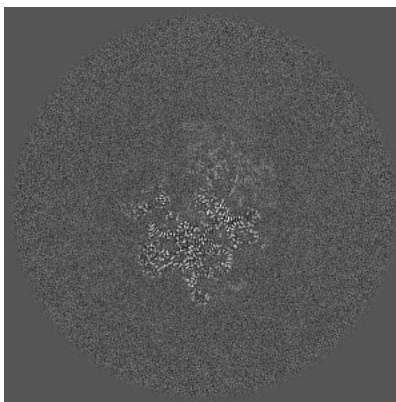


Z Index: 188

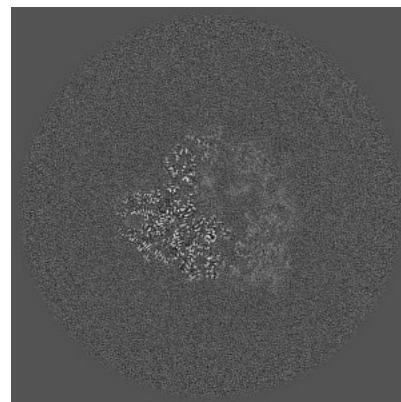
6.3.2 Raw map



X Index: 174



Y Index: 196

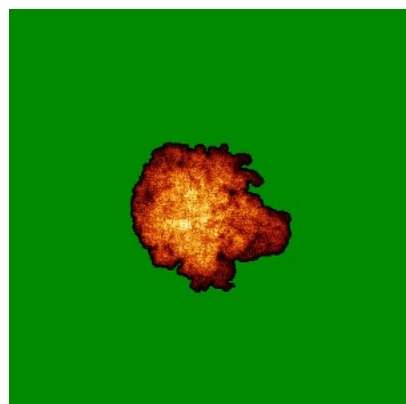


Z Index: 191

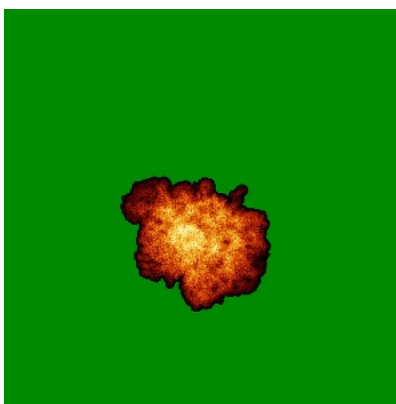
The images above show the largest variance slices of the map in three orthogonal directions.

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

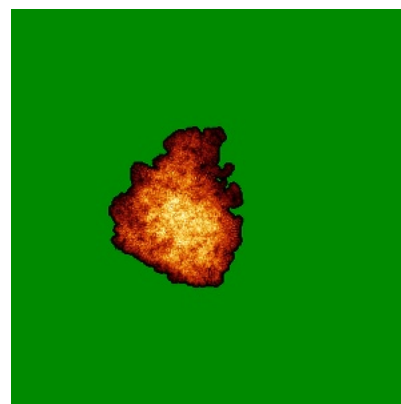
6.4.1 Primary map



X

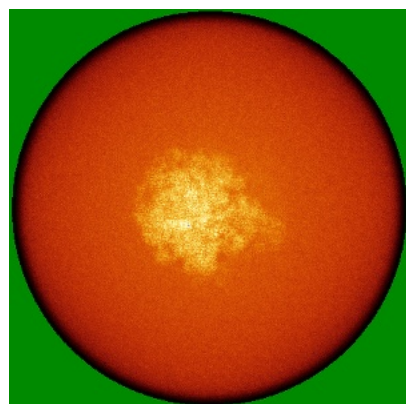


Y

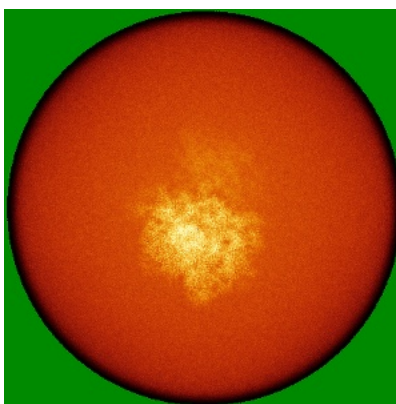


Z

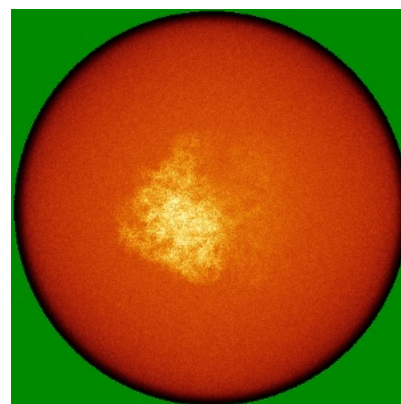
6.4.2 Raw map



X



Y

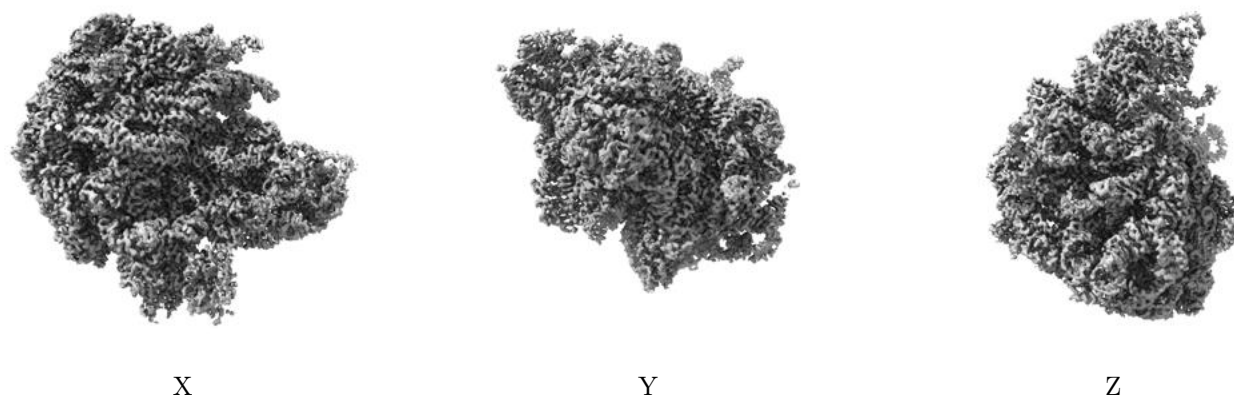


Z

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.

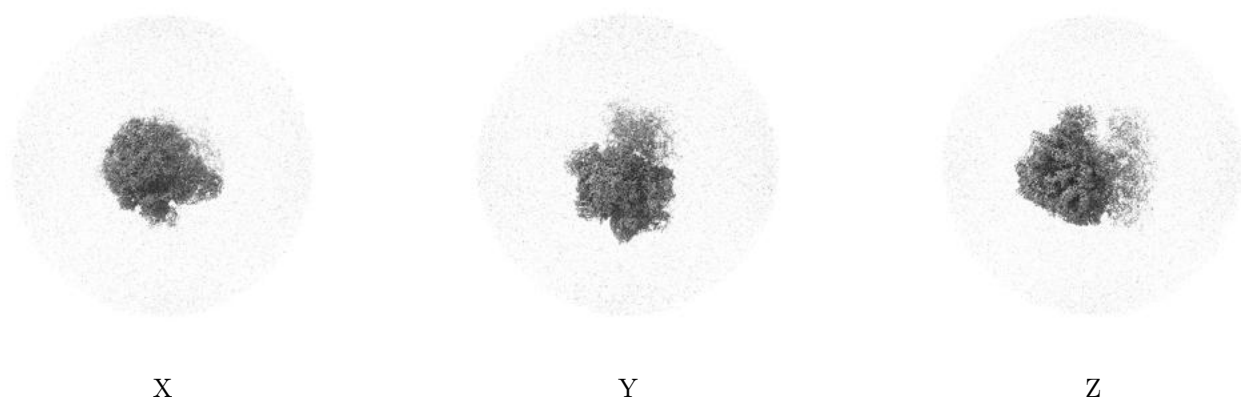
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.002. 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.

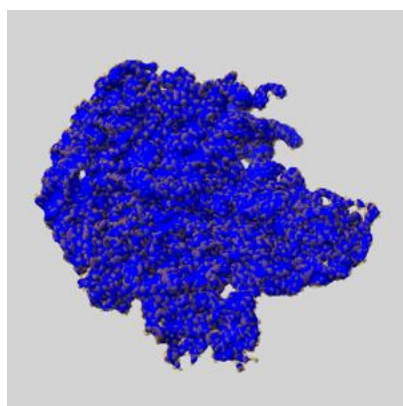
6.6 Mask visualisation [i](#)

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

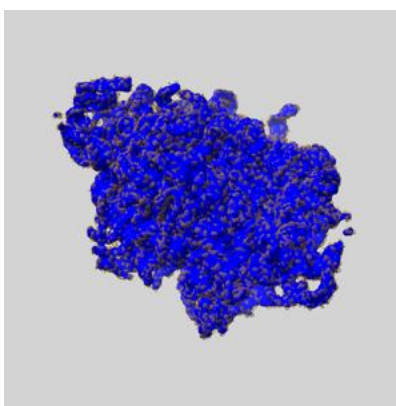
A mask typically either:

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

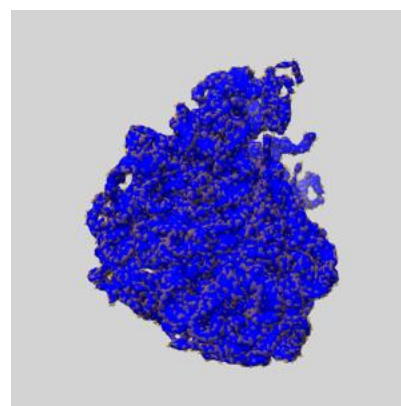
6.6.1 emd_17134_msk_1.map [i](#)



X



Y

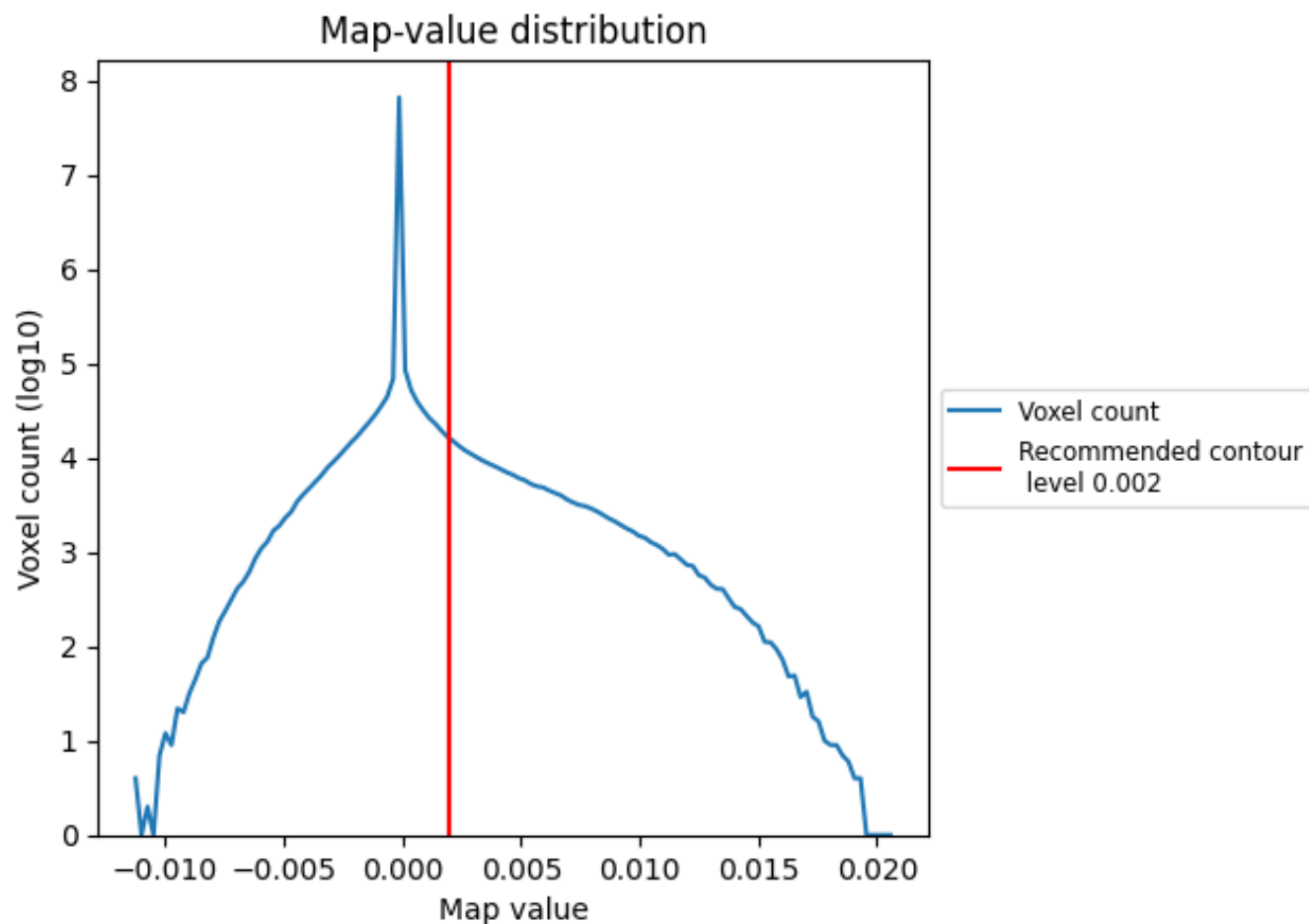


Z

7 Map analysis [i](#)

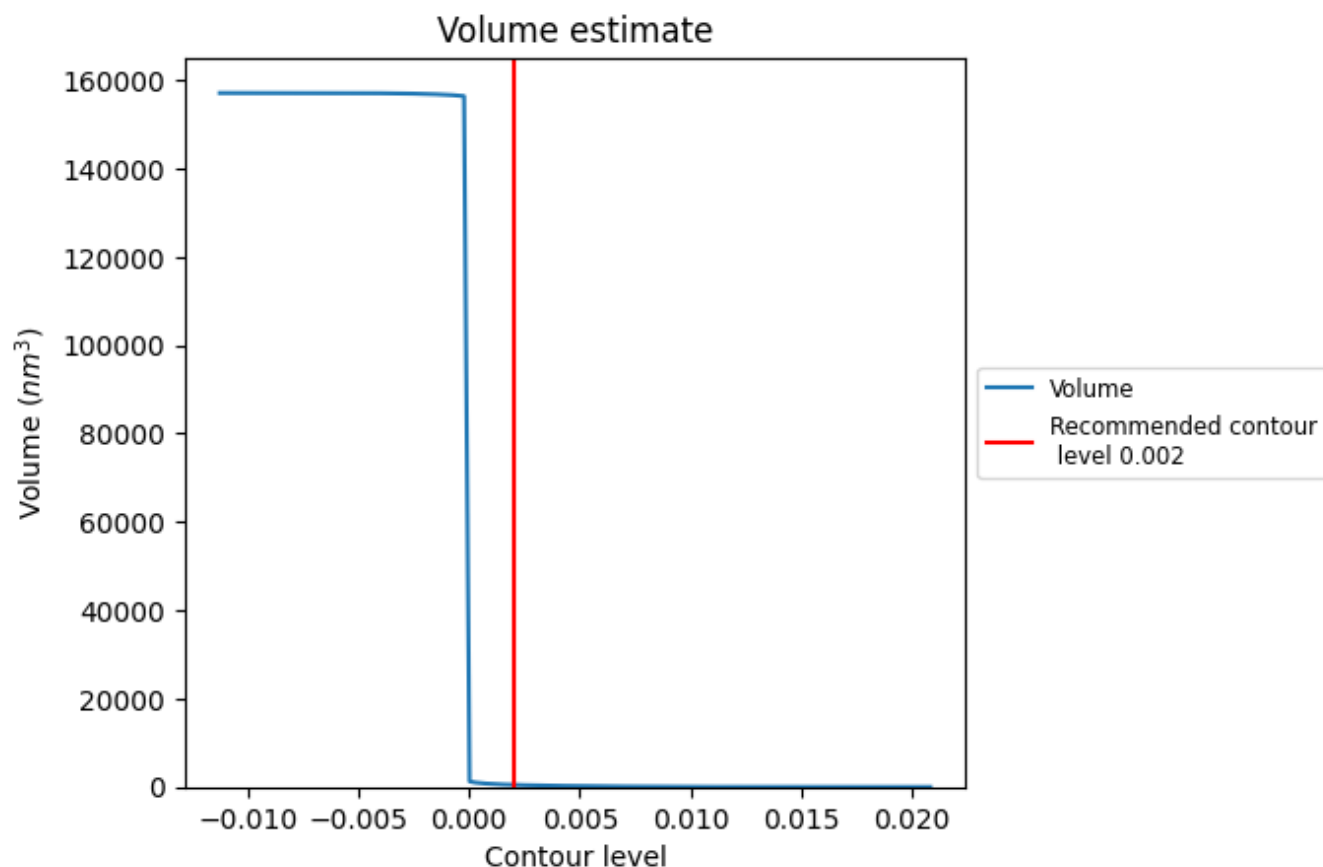
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

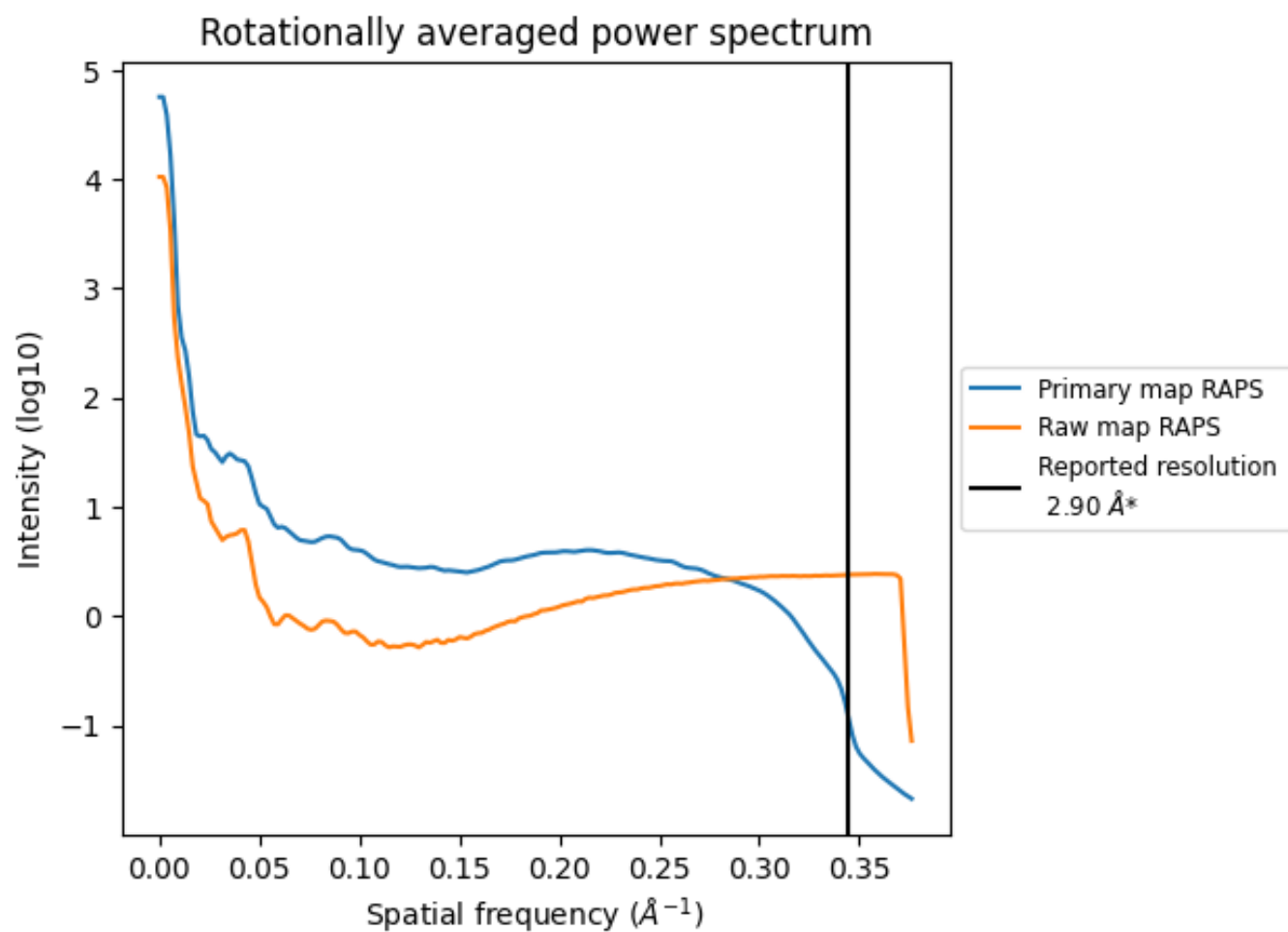
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 475 nm^3 ; this corresponds to an approximate mass of 429 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 ⓘ

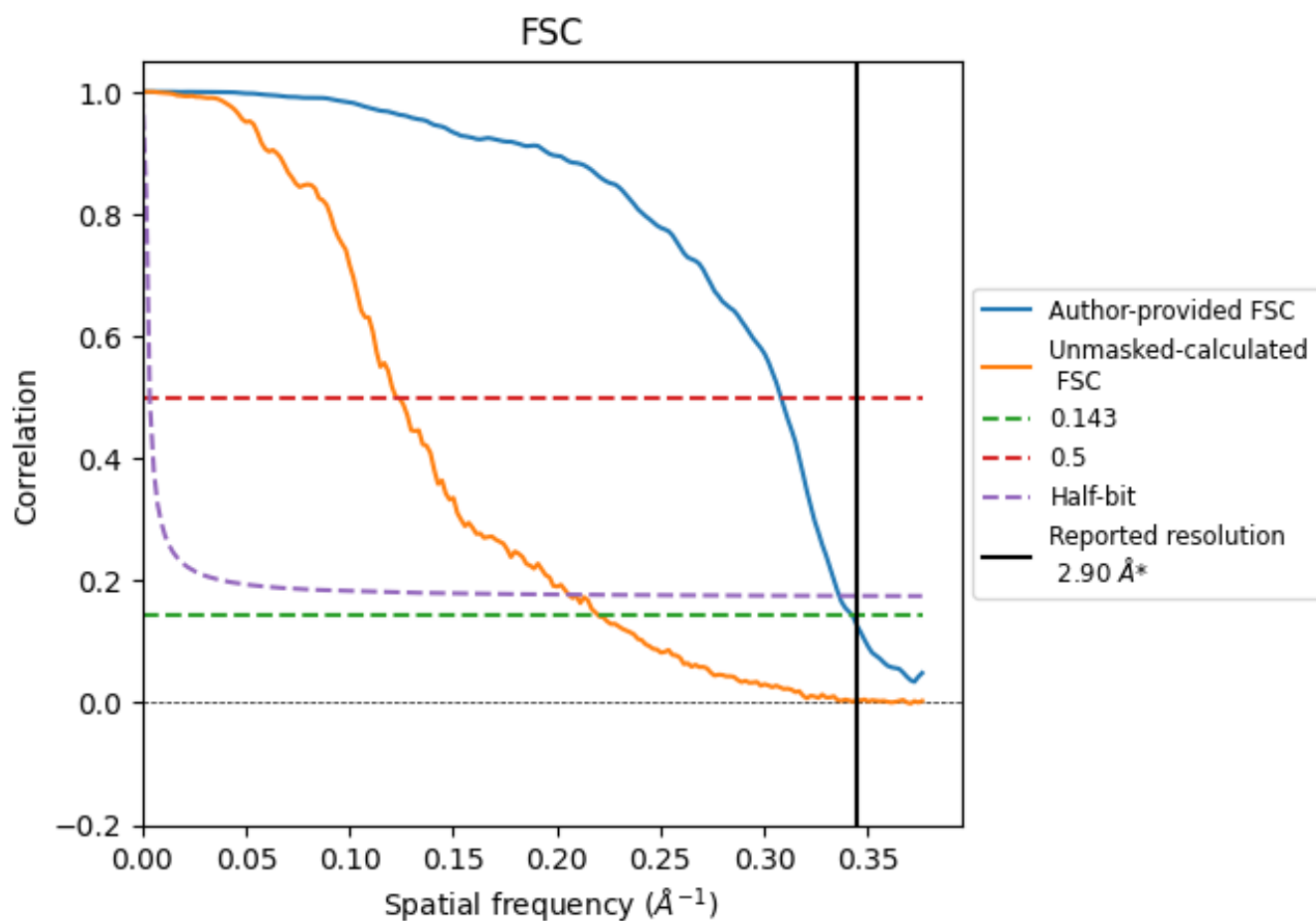


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

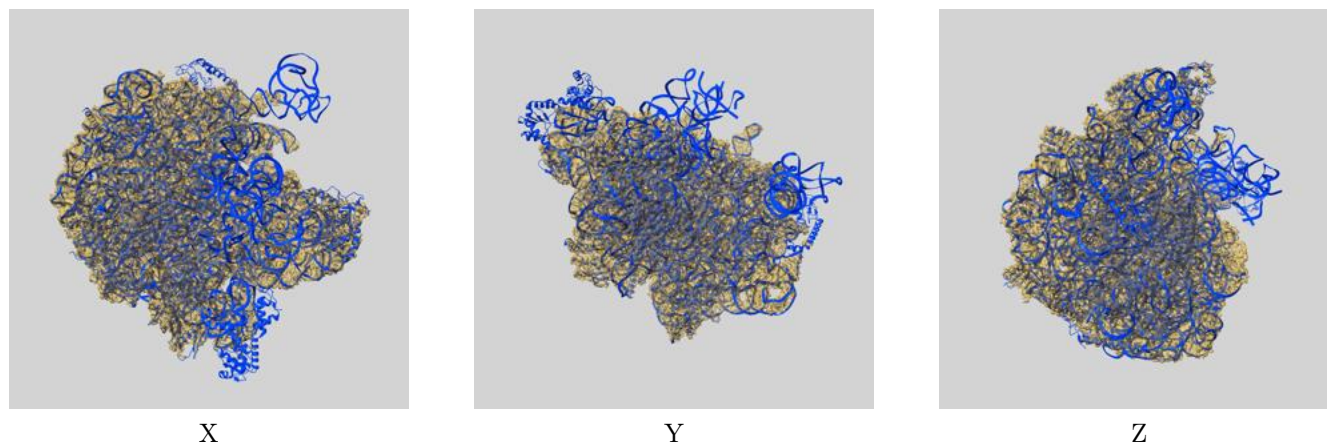
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.25	2.97
Unmasked-calculated*	4.55	8.15	4.86

*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 4.55 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

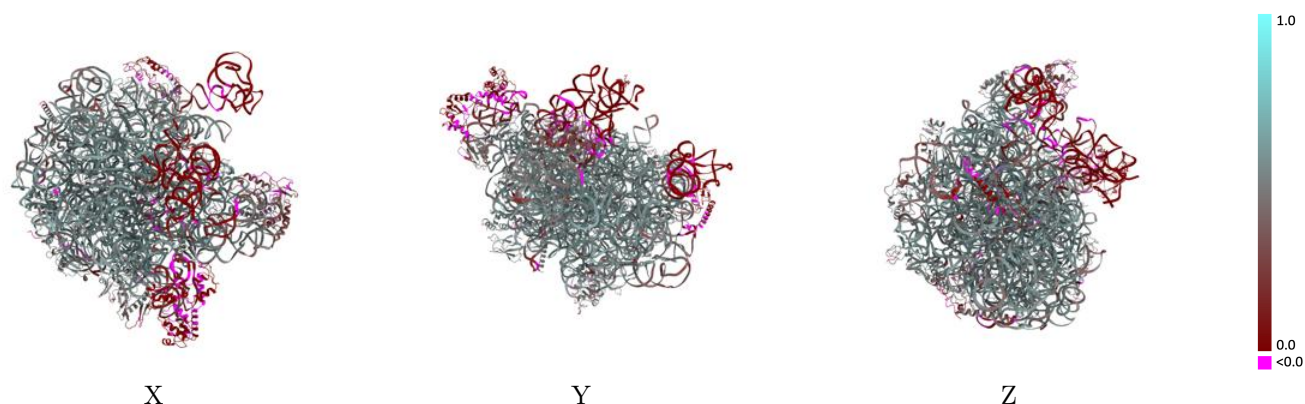
This section contains information regarding the fit between EMDB map EMD-17134 and PDB model 8P8B. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



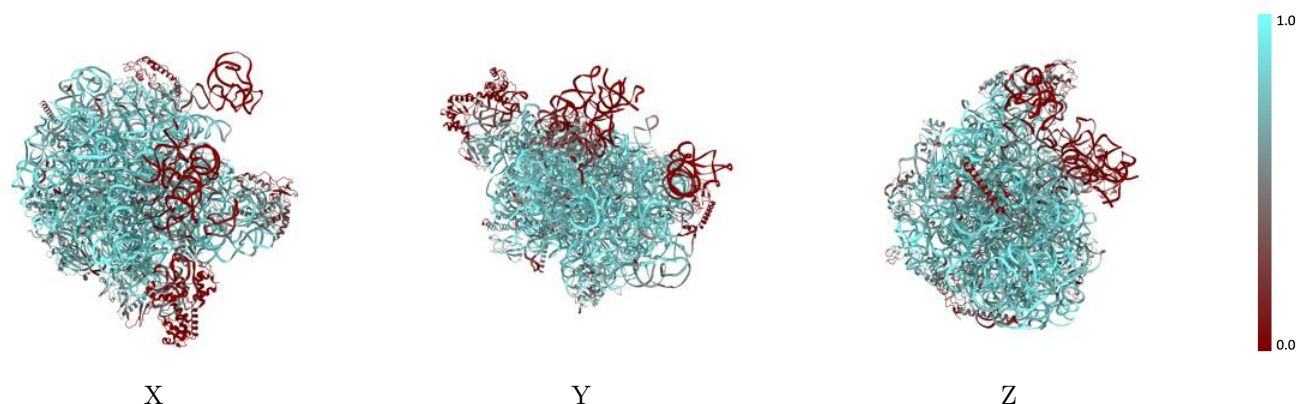
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



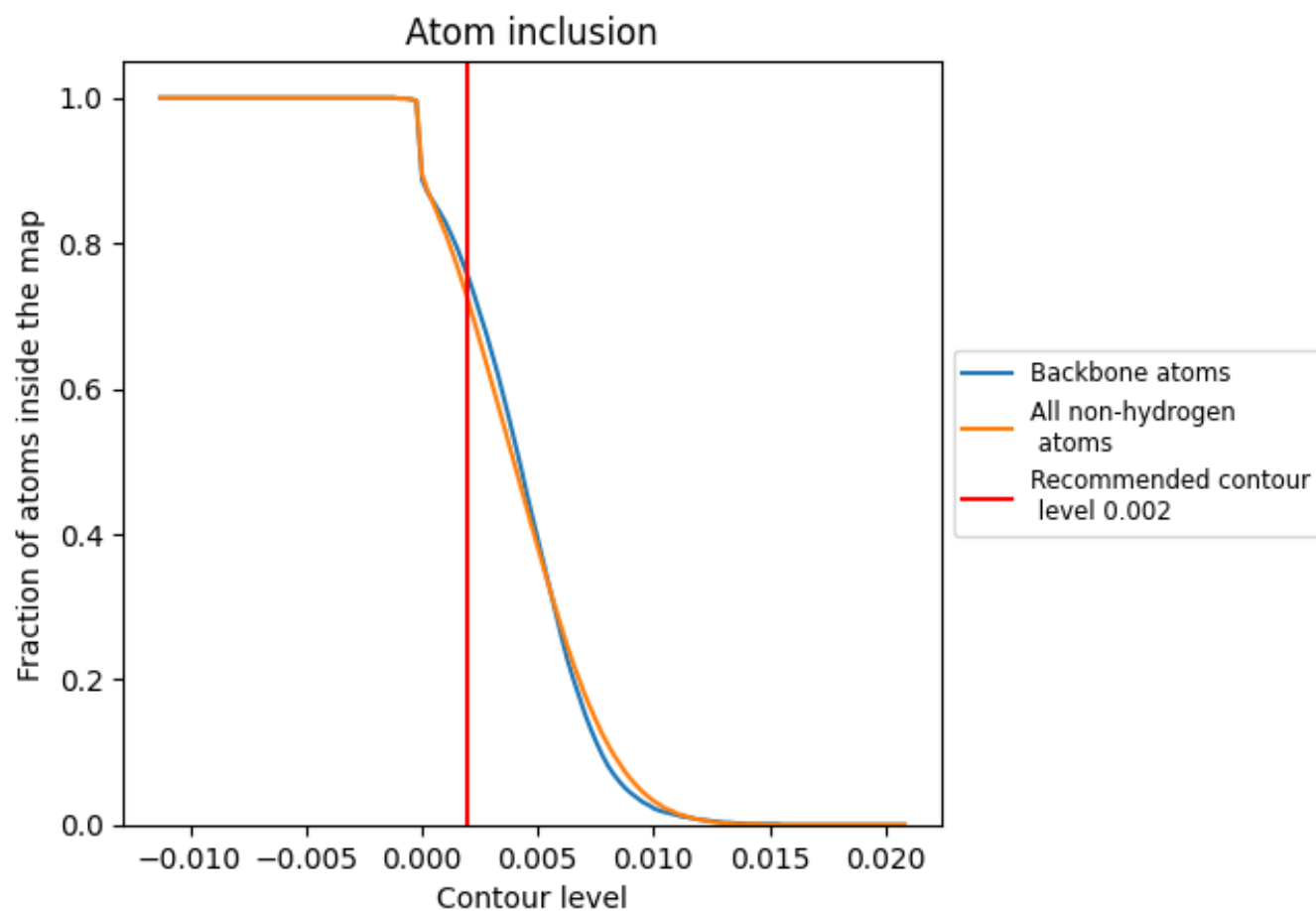
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.002).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.4660
0	 0.7790	 0.5500
1	 0.7510	 0.5530
2	 0.7510	 0.5370
3	 0.8260	 0.5100
4	 0.7480	 0.4430
5	 0.0000	 0.0000
6	 0.5120	 0.4240
7	 0.1950	 0.1240
8	 0.0660	 0.0720
X	 0.0040	 0.0520
Y	 0.0000	 0.0000
Z	 0.1020	 0.0650
a	 0.7450	 0.5320
b	 0.7300	 0.5210
c	 0.6810	 0.4950
d	 0.3320	 0.2890
e	 0.4910	 0.3980
f	 0.1180	 0.0770
g	 0.0070	 0.0040
h	 0.0010	 -0.0110
i	 0.7380	 0.5230
j	 0.7000	 0.5230
k	 0.6820	 0.4910
l	 0.7290	 0.5280
m	 0.7500	 0.5420
n	 0.6230	 0.4820
o	 0.6290	 0.4690
p	 0.7400	 0.5450
q	 0.7250	 0.5220
r	 0.7250	 0.5260
s	 0.6610	 0.4850
t	 0.5090	 0.3920
u	 0.6980	 0.4960
v	 0.6710	 0.4860



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Chain	Atom inclusion	Q-score
w	 0.4970	 0.4120
x	 0.1310	 0.1920
y	 0.7480	 0.5360
z	 0.6760	 0.5110