



Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 08:11 PM EDT

PDB ID : 8FZD / pdb_00008fzd
EMDB ID : EMD-29620
Title : Cryo-EM structure of an E. coli non-rotated ribosome termination complex bound with apoRF3, RF1, P- and E-site tRNAPhe (Composite state I-B)
Authors : Rybak, M.Y.; Li, L.; Lin, J.; Gagnon, M.G.
Deposited on : 2023-01-28
Resolution : 3.10 Å(reported)
Based on initial model : 7K00

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

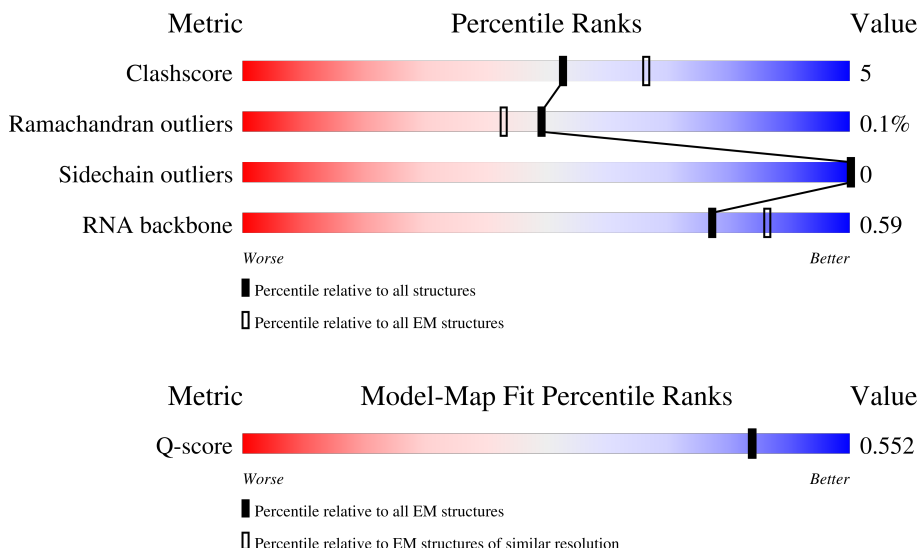
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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.



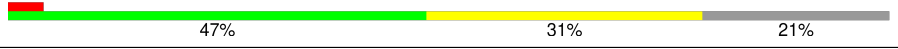
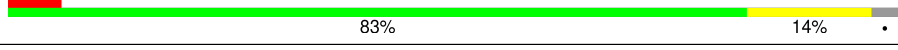
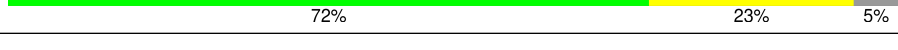
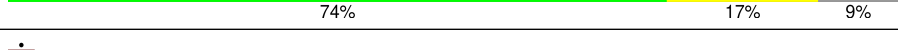
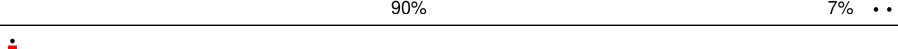
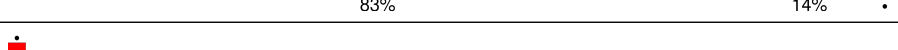
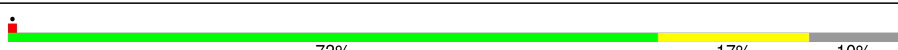
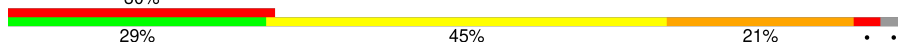
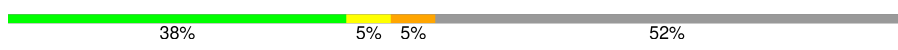
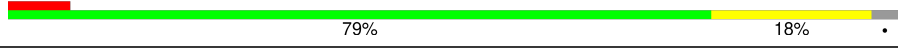
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	a	1542	
2	b	241	
3	c	233	

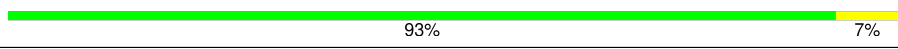
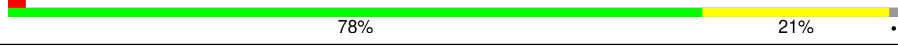
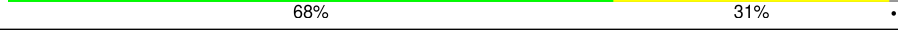
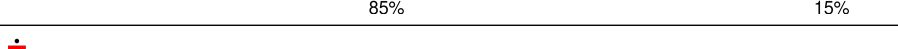
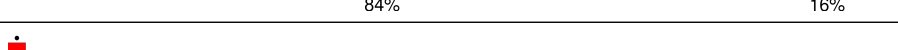
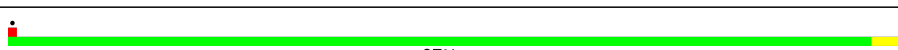
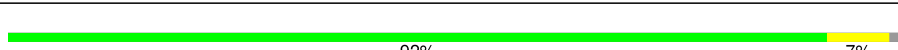
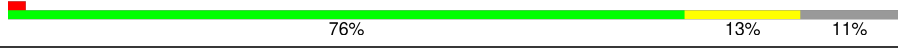
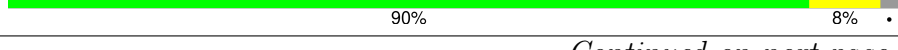
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Mol	Chain	Length	Quality of chain
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	101	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	x	76	
23	y	76	
24	z	21	
25	w	360	
26	v	529	
27	A	2904	
28	B	120	

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Mol	Chain	Length	Quality of chain
29	C	273	
30	D	209	
31	E	201	
32	F	179	
33	G	177	
34	H	149	
35	I	165	
36	J	142	
37	L	142	
38	M	123	
39	N	144	
40	O	136	
41	P	127	
42	Q	117	
43	R	115	
44	S	118	
45	T	103	
46	U	110	
47	V	100	
48	W	104	
49	X	94	
50	Y	85	
51	Z	78	
52	1	63	
53	2	59	

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Mol	Chain	Length	Quality of chain
54	3	70	9% 70% 16% 14%
55	4	57	88% 9%
56	5	55	87% 5% 7%
57	6	46	93% 7%
58	7	65	83% 15%
59	8	38	79% 21%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1528	Total	C	N	O	P	0	0
			32803	14637	6019	10619	1528		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1754	1110	315	321	8		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP A0A0H3PWX2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 22 is a RNA chain called P-site phenylalanyl-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	x	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

- Molecule 23 is a RNA chain called P-site phenylalanyl-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	y	74	Total	C	N	O	P	S	0	0
			1584	707	285	517	74	1		

- Molecule 24 is a RNA chain called F-UAA mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	z	10	Total	C	N	O	P	0	0
			210	95	36	69	10		

- Molecule 25 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	349	Total	C	N	O	S	0	0
			2750	1679	513	545	13		

- Molecule 26 is a protein called Peptide chain release factor RF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	493	Total	C	N	O	S	0	0
			3898	2469	671	738	20		

- Molecule 27 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 28 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	H	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 35 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	I	131	Total	C	N	O	S	0	0
			984	622	174	183	5		

- Molecule 36 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	J	141	Total	C	N	O	S	0	0
			1028	649	178	195	6		

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	conflict	UNP E6BI61

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 54 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	60	Total	C	N	O	S	0	0
			468	290	87	85	6		

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 56 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 57 is a protein called 50S ribosomal protein L34.

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

- Molecule 58 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 59 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	a	130	Total	Mg	0
			130	130	
60	n	1	Total	Mg	0
			1	1	
60	x	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
60	A	428	Total 428	Mg 428	0
60	B	11	Total 11	Mg 11	0
60	C	2	Total 2	Mg 2	0
60	N	1	Total 1	Mg 1	0
60	S	2	Total 2	Mg 2	0
60	V	1	Total 1	Mg 1	0
60	4	1	Total 1	Mg 1	0
60	6	1	Total 1	Mg 1	0
60	7	1	Total 1	Mg 1	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total 1	Zn 1	0
61	8	1	Total 1	Zn 1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	a	23	Total 23	O 23	0
62	y	1	Total 1	O 1	0
62	z	1	Total 1	O 1	0
62	A	122	Total 122	O 122	0
62	B	5	Total 5	O 5	0
62	C	1	Total 1	O 1	0

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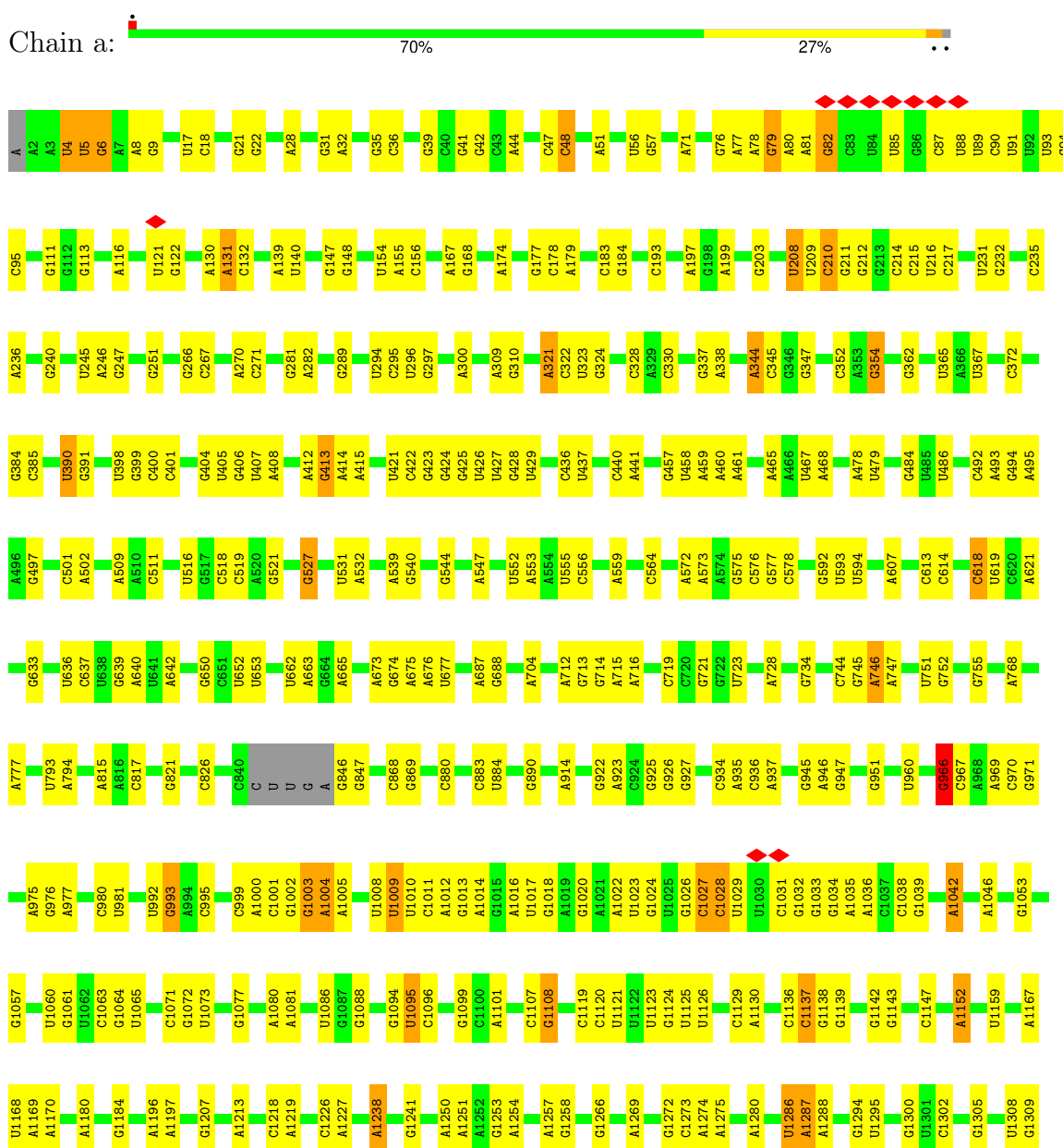
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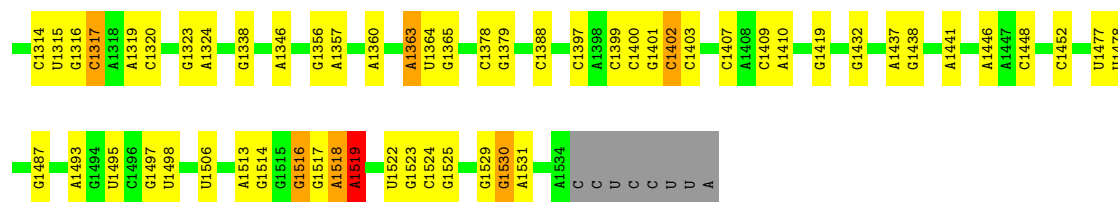
Mol	Chain	Residues	Atoms		AltConf
62	N	1	Total 1	O 1	0
62	8	1	Total 1	O 1	0

3 Residue-property plots

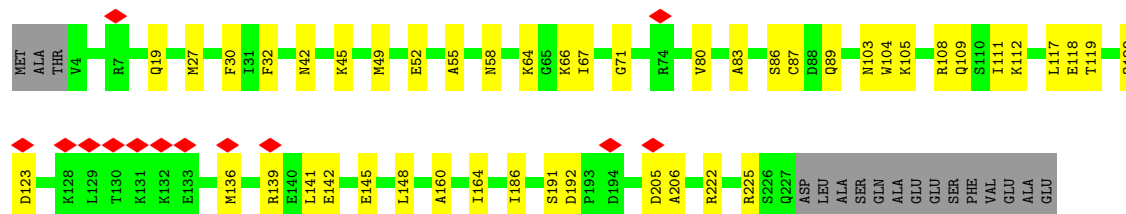
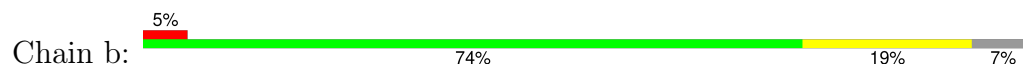
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S Ribosomal RNA

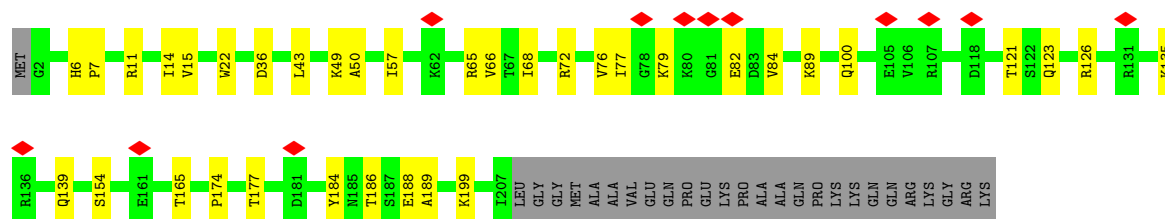




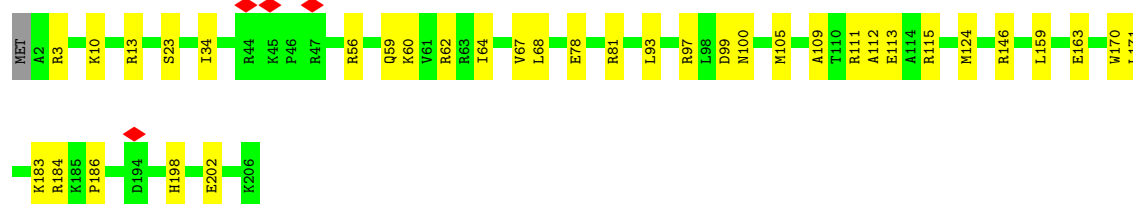
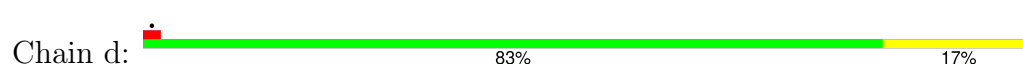
• Molecule 2: 30S ribosomal protein S2



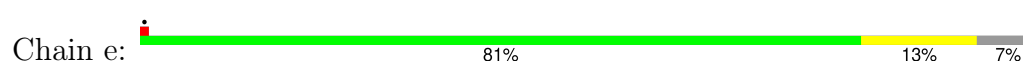
• Molecule 3: 30S ribosomal protein S3



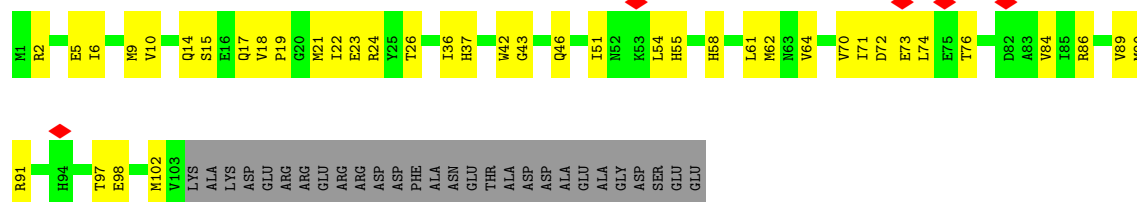
• Molecule 4: 30S ribosomal protein S4



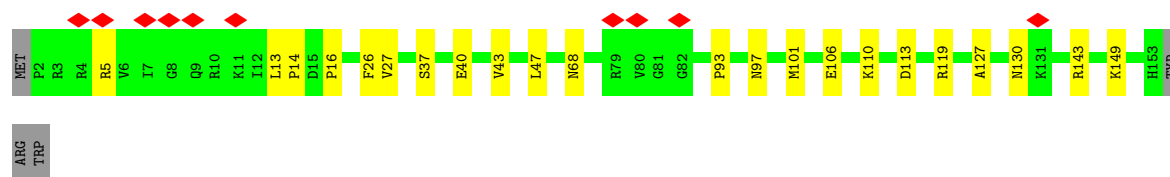
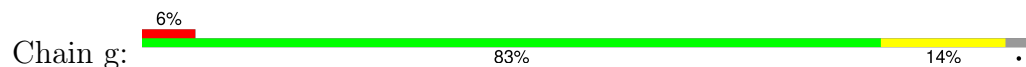
• Molecule 5: 30S ribosomal protein S5



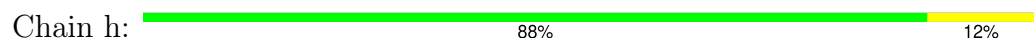
• Molecule 6: 30S ribosomal protein S6



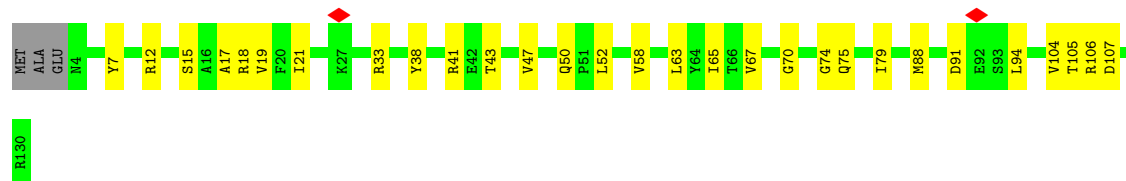
- Molecule 7: 30S ribosomal protein S7



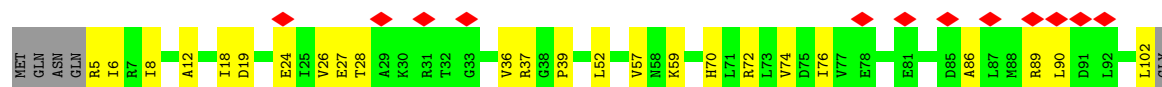
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

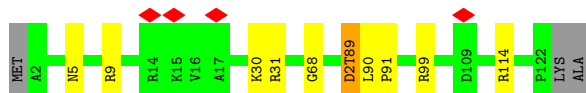
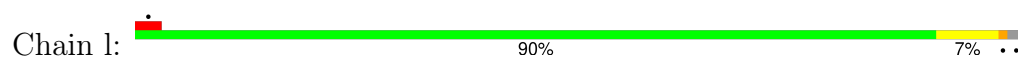


- Molecule 11: 30S ribosomal protein S11

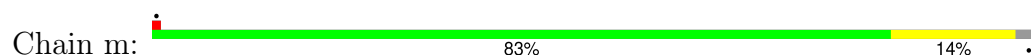




- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



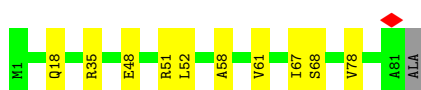
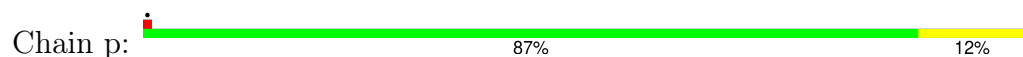
- Molecule 14: 30S ribosomal protein S14



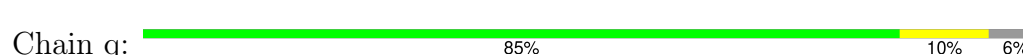
- Molecule 15: 30S ribosomal protein S15



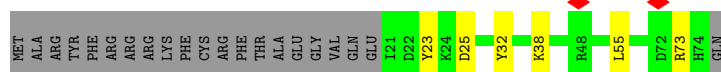
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



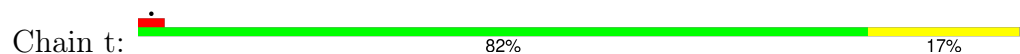
- Molecule 18: 30S ribosomal protein S18



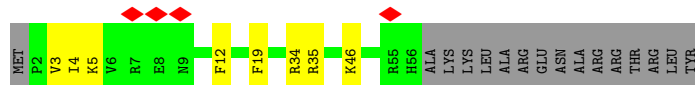
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



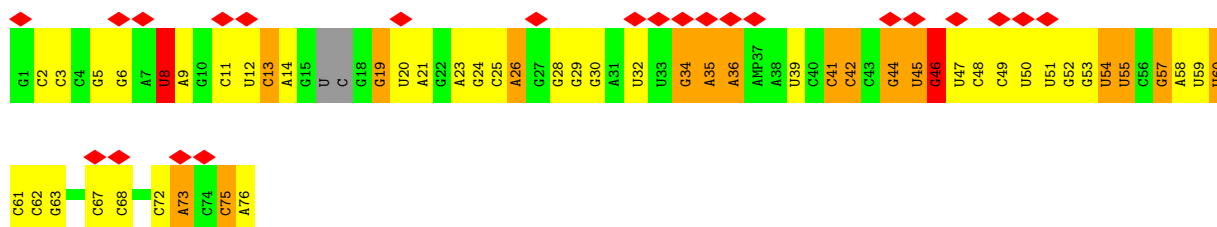
• Molecule 21: 30S ribosomal protein S21



• Molecule 22: P-site phenylalanyl-tRNA



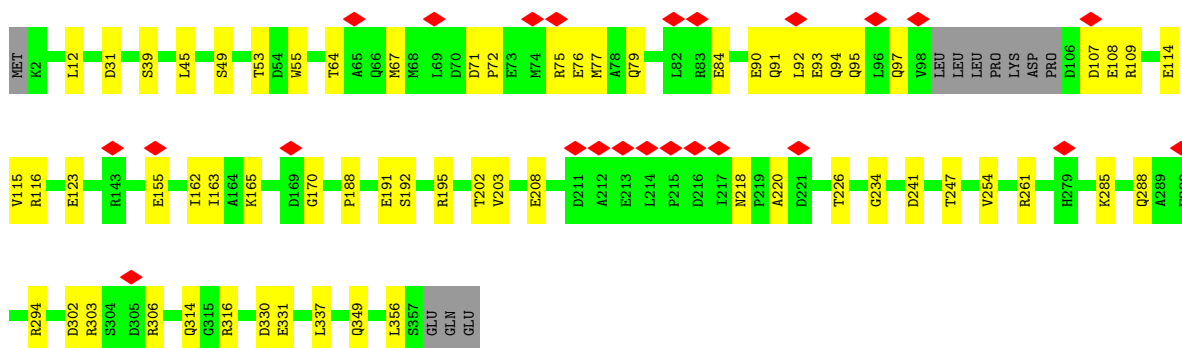
• Molecule 23: P-site phenylalanyl-tRNA



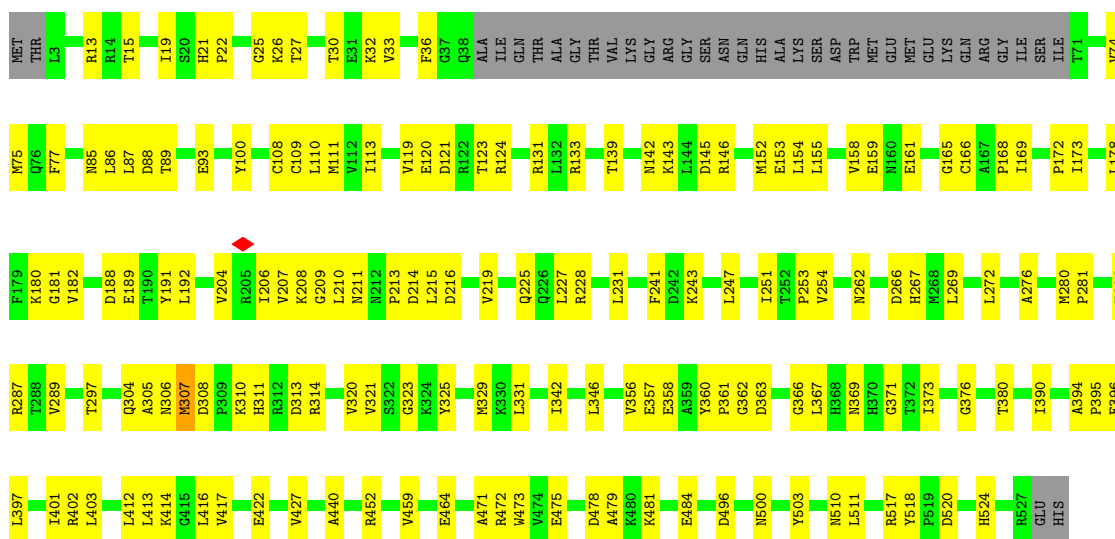
• Molecule 24: F-UAA mRNA



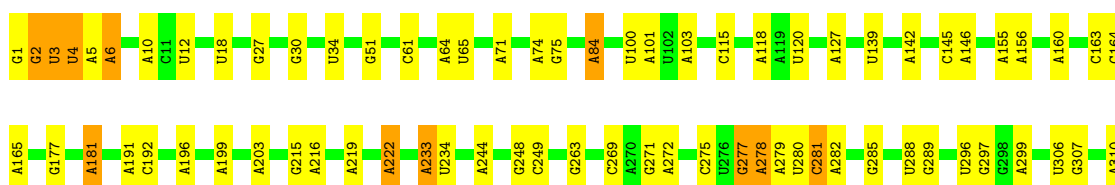
Chain w: 7% 79% 18% 5%



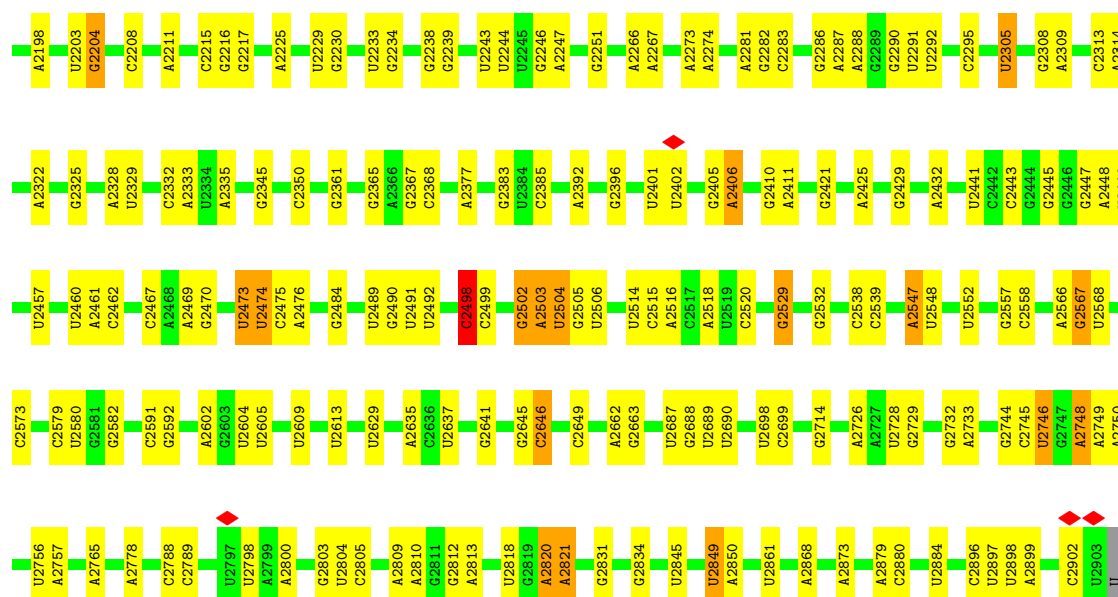
Chain v: 63% 30% 7%



Chain A: 72% 25%



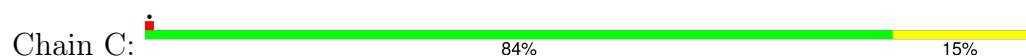




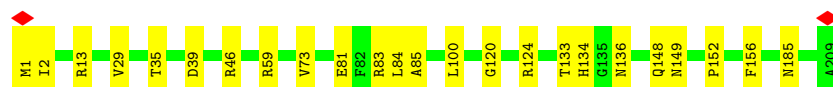
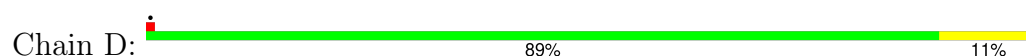
• Molecule 28: 5S Ribosomal RNA



• Molecule 29: 50S ribosomal protein L2

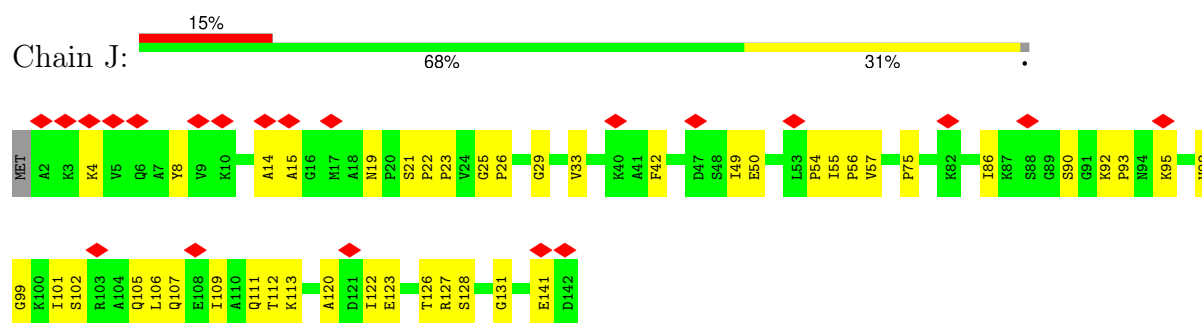


• Molecule 30: 50S ribosomal protein L3

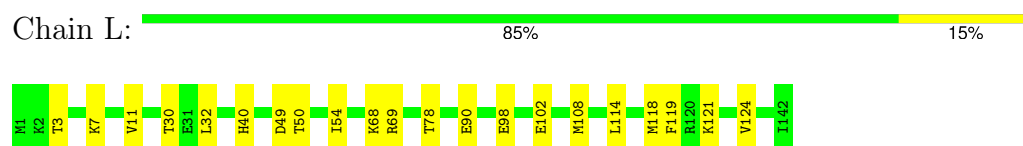


• Molecule 31: 50S ribosomal protein L4

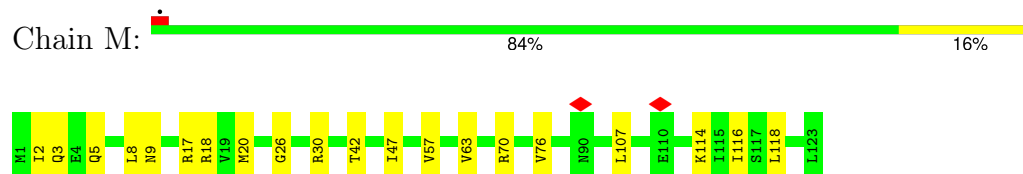




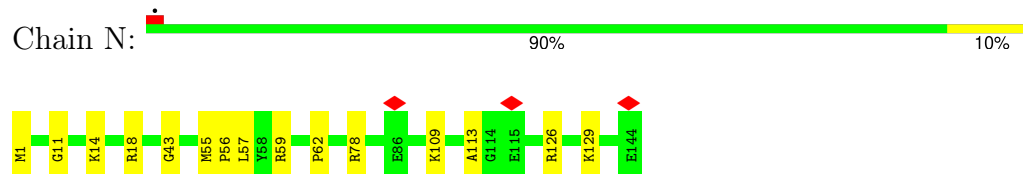
- Molecule 37: 50S ribosomal protein L13



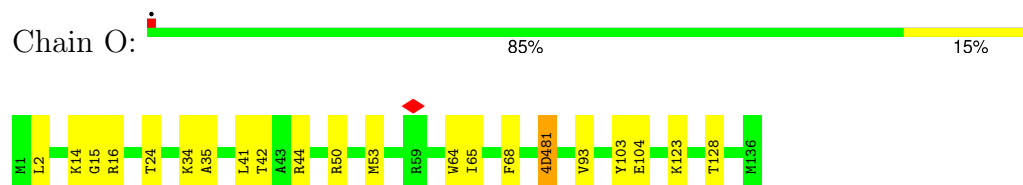
- Molecule 38: 50S ribosomal protein L14



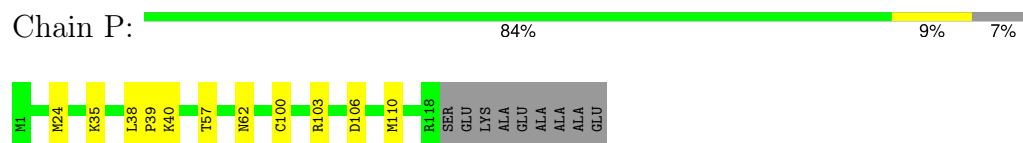
- Molecule 39: 50S ribosomal protein L15



- Molecule 40: 50S ribosomal protein L16



- Molecule 41: 50S ribosomal protein L17



- Molecule 42: 50S ribosomal protein L18

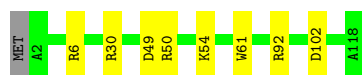




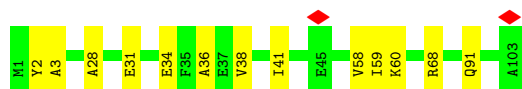
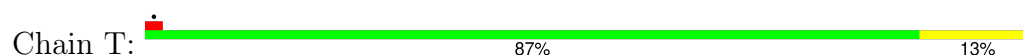
- Molecule 43: 50S ribosomal protein L19



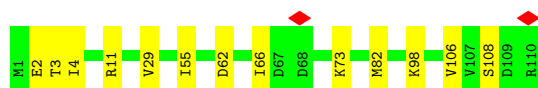
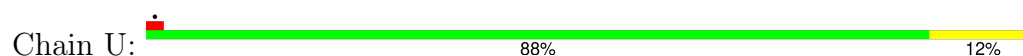
- Molecule 44: 50S ribosomal protein L20



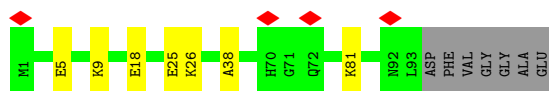
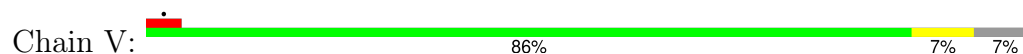
- Molecule 45: Ribosomal protein L21



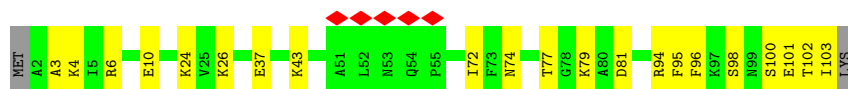
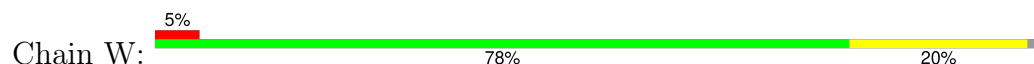
- Molecule 46: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L23



- Molecule 48: 50S ribosomal protein L24



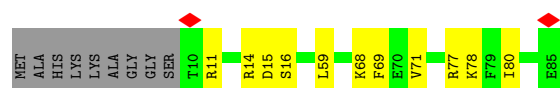
- Molecule 49: 50S ribosomal protein L25

Chain X:  83% 17%



- Molecule 50: 50S ribosomal protein L27

Chain Y:  76% 13% 11%



- Molecule 51: 50S ribosomal protein L28

Chain Z:  85% 14%



- Molecule 52: 50S ribosomal protein L29

Chain 1:  87% 10%



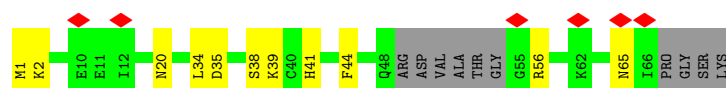
- Molecule 53: 50S ribosomal protein L30

Chain 2:  5% 90% 8%



- Molecule 54: 50S ribosomal protein L31

Chain 3:  9% 70% 16% 5%



- Molecule 55: 50S ribosomal protein L32

Chain 4:  88% 9%



- Molecule 56: 50S ribosomal protein L33

Chain 5:  87% 5% 7%



- Molecule 57: 50S ribosomal protein L34

Chain 6:  93% 7%



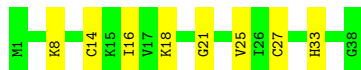
- Molecule 58: 50S ribosomal protein L35

Chain 7:  83% 15% .



- Molecule 59: 50S ribosomal protein L36

Chain 8:  79% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	51.756	Depositor
Minimum map value	-35.316	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.043	Depositor
Recommended contour level	3.5	Depositor
Map size ($\text{\AA}$)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	a	0.13	0/36450	0.25	0/56856
2	b	0.13	0/1785	0.35	0/2404
3	c	0.11	0/1651	0.28	0/2225
4	d	0.13	0/1665	0.29	0/2227
5	e	0.13	0/1165	0.29	0/1568
6	f	0.14	0/858	0.40	0/1160
7	g	0.11	0/1206	0.28	0/1617
8	h	0.13	0/989	0.30	0/1326
9	i	0.12	0/1034	0.31	0/1375
10	j	0.12	0/796	0.33	0/1077
11	k	0.12	0/884	0.28	0/1191
12	l	0.14	0/945	0.31	0/1268
13	m	0.12	0/900	0.28	0/1204
14	n	0.13	0/817	0.32	0/1088
15	o	0.13	0/722	0.29	0/964
16	p	0.13	0/653	0.32	0/877
17	q	0.13	0/650	0.37	0/871
18	r	0.12	0/453	0.26	0/609
19	s	0.11	0/680	0.28	0/915
20	t	0.14	0/676	0.32	0/895
21	u	0.10	0/467	0.25	0/620
22	x	0.21	0/1651	0.24	0/2569
23	y	0.21	0/1605	0.31	0/2497
24	z	0.13	0/234	0.27	0/361
25	w	0.14	0/2788	0.33	0/3753
26	v	0.28	0/3971	0.48	0/5368
27	A	0.14	0/69147	0.26	0/107869
28	B	0.13	0/2876	0.27	0/4483
29	C	0.13	0/2121	0.29	0/2852
30	D	0.15	0/1576	0.30	0/2119
31	E	0.12	0/1571	0.26	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	F	0.12	0/1434	0.27	0/1926
33	G	0.13	0/1343	0.30	0/1816
34	H	0.09	0/290	0.30	0/392
35	I	0.15	0/997	0.41	0/1346
36	J	0.12	0/1042	0.39	0/1405
37	L	0.14	0/1152	0.26	0/1551
38	M	0.14	0/955	0.28	0/1279
39	N	0.13	0/1061	0.27	0/1412
40	O	0.13	0/1073	0.24	0/1433
41	P	0.14	0/958	0.30	0/1281
42	Q	0.11	0/902	0.29	0/1209
43	R	0.13	0/929	0.25	0/1242
44	S	0.14	0/960	0.22	0/1278
45	T	0.14	0/829	0.30	0/1107
46	U	0.13	0/864	0.25	0/1156
47	V	0.12	0/744	0.27	0/994
48	W	0.14	0/787	0.38	0/1051
49	X	0.14	0/766	0.33	0/1025
50	Y	0.13	0/589	0.31	0/779
51	Z	0.13	0/635	0.25	0/848
52	1	0.10	0/496	0.20	0/660
53	2	0.13	0/453	0.24	0/605
54	3	0.09	0/475	0.24	0/633
55	4	0.13	0/440	0.24	0/588
56	5	0.12	0/424	0.29	0/565
57	6	0.12	0/380	0.20	0/498
58	7	0.14	0/513	0.27	0/676
59	8	0.13	0/303	0.27	0/397
All	All	0.14	0/164780	0.28	0/245473

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	v	0	1
40	O	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	O	81	4D4	Mainchain
26	v	307	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32803	0	16528	236	0
2	b	1754	0	1782	30	0
3	c	1624	0	1696	21	0
4	d	1643	0	1707	27	0
5	e	1152	0	1196	16	0
6	f	839	0	833	28	0
7	g	1191	0	1245	16	0
8	h	979	0	1031	12	0
9	i	1022	0	1070	22	0
10	j	786	0	828	14	0
11	k	877	0	884	15	0
12	l	942	0	999	8	0
13	m	891	0	952	11	0
14	n	805	0	844	20	0
15	o	714	0	734	13	0
16	p	643	0	661	5	0
17	q	641	0	682	4	0
18	r	446	0	472	6	0
19	s	663	0	688	14	0
20	t	670	0	719	10	0
21	u	460	0	486	7	0
22	x	1632	0	838	16	0
23	y	1584	0	806	33	0
24	z	210	0	107	1	0
25	w	2750	0	2677	46	0
26	v	3898	0	3877	122	0
27	A	62252	0	31333	389	0
28	B	2572	0	1301	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	2082	0	2154	24	0
30	D	1566	0	1618	19	0
31	E	1552	0	1619	10	0
32	F	1410	0	1444	24	0
33	G	1323	0	1371	14	0
34	H	287	0	307	5	0
35	I	984	0	1014	34	0
36	J	1028	0	1079	30	0
37	L	1129	0	1162	16	0
38	M	946	0	1023	14	0
39	N	1052	0	1127	15	0
40	O	1075	0	1145	12	0
41	P	945	0	989	7	0
42	Q	892	0	923	5	0
43	R	917	0	962	3	0
44	S	947	0	1019	7	0
45	T	816	0	839	8	0
46	U	857	0	922	8	0
47	V	738	0	807	4	0
48	W	779	0	831	14	0
49	X	753	0	780	9	0
50	Y	582	0	599	6	0
51	Z	625	0	652	6	0
52	1	495	0	526	4	0
53	2	449	0	488	3	0
54	3	468	0	460	9	0
55	4	434	0	445	4	0
56	5	417	0	451	2	0
57	6	377	0	418	3	0
58	7	504	0	572	9	0
59	8	302	0	340	6	0
60	4	1	0	0	0	0
60	6	1	0	0	0	0
60	7	1	0	0	0	0
60	A	428	0	0	0	0
60	B	11	0	0	0	0
60	C	2	0	0	0	0
60	N	1	0	0	0	0
60	S	2	0	0	0	0
60	V	1	0	0	0	0
60	a	130	0	0	0	0
60	n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	x	2	0	0	0	0
61	3	1	0	0	0	0
61	8	1	0	0	0	0
62	8	1	0	0	0	0
62	A	122	0	0	1	0
62	B	5	0	0	0	0
62	C	1	0	0	0	0
62	N	1	0	0	0	0
62	a	23	0	0	0	0
62	y	1	0	0	0	0
62	z	1	0	0	0	0
All	All	153912	0	105062	1336	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 5.

All (1336) 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)
23:y:26:A:H61	23:y:44:G:H1	1.10	1.00
23:y:26:A:N6	23:y:44:G:H1	1.68	0.92
35:I:59:LEU:HD23	35:I:61:ARG:H	1.42	0.82
46:U:11:ARG:HH12	46:U:98:LYS:HB3	1.45	0.81
27:A:2131:U:H5'	27:A:2132:U:H5''	1.62	0.81
23:y:9:A:H1'	23:y:45:U:H2'	1.62	0.81
27:A:882:G:N3	27:A:896:A:N6	2.30	0.79
5:e:34:THR:HG22	5:e:52:LYS:HG2	1.65	0.79
2:b:67:ILE:HG12	2:b:89:GLN:HE21	1.48	0.78
26:v:173:ILE:HD11	26:v:180:LYS:HB2	1.66	0.77
26:v:119:VAL:HG11	26:v:161:GLU:HG3	1.66	0.77
30:D:133:THR:HG22	30:D:134:HIS:H	1.50	0.77
35:I:31:ARG:H	35:I:109:LYS:HD2	1.50	0.77
26:v:305:ALA:HA	26:v:314:ARG:HA	1.65	0.76
17:q:9:GLN:HE22	17:q:79:VAL:HG21	1.51	0.76
26:v:21:HIS:HD2	26:v:22:PRO:HD2	1.50	0.75
2:b:111:ILE:HD13	2:b:148:LEU:HD13	1.69	0.74
26:v:139:THR:OG1	26:v:253:PRO:O	2.05	0.73
41:P:35:LYS:NZ	41:P:100:CYS:SG	2.61	0.73
26:v:188:ASP:HB3	26:v:210:LEU:HD21	1.71	0.73
49:X:42:LEU:HD13	49:X:47:VAL:HG21	1.70	0.72
2:b:119:THR:O	2:b:123:ASP:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:5:ARG:HA	10:j:76:ILE:O	1.90	0.72
27:A:2134:A:H61	27:A:2156:G:H2'	1.54	0.72
50:Y:15:ASP:OD2	50:Y:16:SER:N	2.19	0.72
27:A:781:A:OP1	29:C:217:ARG:NH2	2.23	0.72
1:a:1147:C:O2	9:i:18:ARG:NH1	2.23	0.72
19:s:30:PRO:HA	19:s:48:THR:O	1.91	0.71
26:v:402:ARG:NE	26:v:464:GLU:OE2	2.23	0.71
31:E:97:ASN:HB2	31:E:100:MET:HG3	1.70	0.71
6:f:6:ILE:HG12	6:f:89:VAL:HG22	1.70	0.71
26:v:394:ALA:HB2	26:v:524:HIS:HB2	1.73	0.70
48:W:74:ASN:HD22	48:W:77:THR:HG22	1.55	0.70
20:t:10:ARG:HD3	20:t:13:GLN:HE21	1.56	0.70
27:A:2183:A:H2'	27:A:2184:A:C8	2.27	0.70
50:Y:11:ARG:O	50:Y:14:ARG:NH1	2.25	0.70
25:w:123:GLU:HG3	25:w:188:PRO:HB3	1.74	0.69
6:f:9:MET:SD	6:f:86:ARG:HB3	2.32	0.69
16:p:48:GLU:OE1	16:p:51:ARG:NH2	2.24	0.69
1:a:1266:G:N2	1:a:1269:A:OP2	2.24	0.69
8:h:15:ARG:NH1	8:h:75:ILE:O	2.26	0.69
1:a:673:A:H2'	1:a:674:G:C8	2.28	0.69
6:f:14:GLN:OE1	6:f:17:GLN:NE2	2.21	0.68
35:I:87:GLU:HB3	35:I:93:ALA:HB3	1.75	0.68
26:v:472:ARG:HG3	26:v:511:LEU:HD11	1.74	0.68
37:L:3:THR:HG21	44:S:61:TRP:HE1	1.56	0.68
36:J:102:SER:HA	36:J:141:GLU:HB3	1.76	0.68
26:v:21:HIS:CD2	26:v:22:PRO:HD2	2.27	0.68
27:A:1060:U:H4'	27:A:1062:G:H5''	1.76	0.68
1:a:427:U:OP1	4:d:13:ARG:NH2	2.27	0.68
27:A:475:C:O2	27:A:479:A:N6	2.26	0.68
35:I:117:LEU:HB3	35:I:120:ALA:HA	1.77	0.67
1:a:501:C:OP1	12:l:114:ARG:NH2	2.27	0.67
1:a:1009:U:H3	1:a:1020:G:H1	0.77	0.67
4:d:59:GLN:OE1	4:d:62:ARG:NH1	2.28	0.67
27:A:1779:U:OP2	27:A:1784:A:N6	2.26	0.67
1:a:78:A:H2'	1:a:79:G:C8	2.29	0.66
46:U:4:ILE:HG22	46:U:106:VAL:HG22	1.78	0.66
35:I:6:GLN:HA	35:I:9:GLN:HG3	1.77	0.66
4:d:99:ASP:OD2	4:d:100:ASN:N	2.29	0.66
9:i:12:ARG:NH1	9:i:107:ASP:OD1	2.29	0.66
27:A:1084:A:N3	27:A:1105:U:O2'	2.27	0.66
9:i:75:GLN:O	9:i:79:ILE:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:64:TRP:HB2	40:O:104:GLU:HB2	1.78	0.66
3:c:14:ILE:HG22	3:c:15:VAL:HG13	1.78	0.65
7:g:68:ASN:ND2	7:g:127:ALA:O	2.29	0.65
1:a:458:U:H2'	1:a:459:A:H8	1.61	0.65
9:i:106:ARG:NH1	9:i:107:ASP:O	2.29	0.65
13:m:3:ARG:HH12	32:F:110:ARG:HG2	1.62	0.65
1:a:1123:U:O3'	10:j:37:ARG:NH2	2.30	0.65
3:c:135:LYS:HE3	3:c:139:GLN:HE22	1.62	0.65
9:i:15:SER:HB3	9:i:70:GLY:HA3	1.79	0.64
27:A:411:G:OP2	27:A:2406:A:O2'	2.13	0.64
1:a:1013:G:N2	1:a:1016:A:OP2	2.27	0.64
29:C:29:PRO:HG2	29:C:34:LEU:HD11	1.79	0.64
5:e:36:LEU:HD22	5:e:134:ILE:HD13	1.79	0.64
27:A:511:U:H4'	27:A:1235:G:H4'	1.79	0.64
9:i:21:ILE:HG22	9:i:63:LEU:HG	1.78	0.64
27:A:1649:G:O2'	41:P:106:ASP:OD2	2.13	0.64
27:A:1153:C:OP1	44:S:92:ARG:NH2	2.31	0.64
1:a:999:C:N3	1:a:1042:A:N6	2.45	0.64
1:a:1363:A:O2'	1:a:1365:G:N7	2.29	0.64
27:A:219:A:N3	27:A:234:U:O2'	2.29	0.64
27:A:463:G:N2	27:A:466:A:OP2	2.24	0.64
26:v:26:LYS:NZ	26:v:88:ASP:OD2	2.31	0.64
27:A:1250:G:N7	39:N:18:ARG:NH2	2.45	0.64
27:A:2123:G:N2	27:A:2124:G:O6	2.31	0.64
4:d:183:LYS:HD2	4:d:184:ARG:HD2	1.78	0.64
1:a:1402:4OC:HM22	1:a:1403:C:H5'	1.79	0.63
2:b:86:SER:O	2:b:222:ARG:NH1	2.31	0.63
27:A:2100:G:H1	27:A:2189:U:H3	1.44	0.63
19:s:11:ILE:HD12	19:s:38:SER:HB3	1.79	0.63
19:s:50:ALA:HB1	19:s:57:HIS:HB3	1.79	0.63
27:A:1311:G:OP2	27:A:1311:G:N2	2.27	0.63
7:g:143:ARG:NE	23:y:41:C:OP1	2.31	0.63
26:v:320:VAL:HG23	26:v:361:PRO:HA	1.80	0.63
29:C:122:ALA:HB3	29:C:130:LEU:HD21	1.80	0.63
14:n:49:GLN:NE2	19:s:11:ILE:O	2.31	0.63
25:w:226:THR:HG22	25:w:241:ASP:HB3	1.81	0.63
27:A:2106:U:H2'	27:A:2107:G:C8	2.34	0.63
27:A:2120:G:H2'	27:A:2121:G:H8	1.64	0.63
29:C:35:GLU:HG2	29:C:36:LYS:H	1.62	0.63
15:o:47:LYS:O	15:o:53:ARG:NH2	2.31	0.63
25:w:285:LYS:HD3	25:w:288:GLN:HE21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1009:U:O2	1:a:1020:G:N2	2.22	0.63
3:c:57:ILE:HG12	3:c:66:VAL:HG12	1.80	0.63
27:A:2392:A:H2	39:N:55:MET:HE2	1.63	0.63
35:I:94:ARG:HG2	35:I:97:LYS:HE3	1.80	0.63
1:a:4:U:H2'	1:a:5:U:H5''	1.81	0.63
39:N:109:LYS:HG2	39:N:126:ARG:HB2	1.80	0.63
11:k:20:VAL:HG12	11:k:83:GLU:HB2	1.80	0.62
25:w:55:TRP:NE1	25:w:84:GLU:OE2	2.32	0.62
27:A:1315:C:O2'	27:A:1392:A:N3	2.32	0.62
48:W:10:GLU:OE1	48:W:24:LYS:NZ	2.31	0.62
4:d:202:GLU:OE1	5:e:112:ARG:NH1	2.29	0.62
27:A:2175:C:H2'	27:A:2176:A:H8	1.64	0.62
3:c:154:SER:HB3	3:c:165:THR:HG23	1.81	0.62
10:j:26:VAL:HG23	10:j:36:VAL:HG21	1.80	0.62
27:A:882:G:H22	27:A:894:U:H3	1.45	0.62
48:W:77:THR:OG1	48:W:79:LYS:NZ	2.30	0.62
3:c:22:TRP:NE1	3:c:36:ASP:OD2	2.31	0.62
26:v:211:ASN:OD1	26:v:228:ARG:NH1	2.32	0.62
25:w:188:PRO:HG2	25:w:191:GLU:HB2	1.82	0.62
27:A:1527:G:N1	27:A:1544:A:OP2	2.29	0.62
27:A:2189:U:H2'	27:A:2190:G:H8	1.65	0.62
1:a:77:A:H2'	1:a:78:A:C8	2.35	0.62
29:C:260:ASN:OD1	29:C:263:THR:OG1	2.17	0.62
23:y:11:C:H42	23:y:25:C:H42	1.47	0.62
27:A:1102:C:H2'	27:A:1103:A:H8	1.65	0.62
1:a:544:G:OP1	4:d:56:ARG:NH2	2.33	0.61
27:A:2365:G:N7	58:7:39:LYS:NZ	2.47	0.61
38:M:5:GLN:HG2	38:M:20:MET:HE3	1.81	0.61
27:A:1111:A:O2'	27:A:1112:G:OP1	2.18	0.61
27:A:2128:G:N3	27:A:2173:A:O2'	2.32	0.61
26:v:287:ARG:HH12	26:v:289:VAL:HG22	1.63	0.61
27:A:1665:A:H2	38:M:3:GLN:HE22	1.48	0.61
49:X:76:ASP:OD2	49:X:77:VAL:N	2.33	0.61
6:f:21:MET:HA	6:f:24:ARG:HE	1.65	0.61
52:1:10:SER:OG	52:1:13:GLU:OE1	2.17	0.61
40:O:15:GLY:O	40:O:16:ARG:NH1	2.34	0.61
1:a:751:U:OP1	15:o:17:ARG:NH2	2.34	0.61
27:A:1447:C:O2'	27:A:1544:A:N3	2.30	0.61
1:a:1038:C:N4	1:a:1039:G:O6	2.35	0.60
1:a:492:C:H2'	1:a:493:A:C8	2.37	0.60
14:n:38:ASP:OD2	54:3:65:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:18:ASP:OD1	15:o:19:ALA:N	2.34	0.60
23:y:28:G:H2'	23:y:29:G:C8	2.37	0.60
27:A:976:G:HO2'	27:A:1155:A:HO2'	1.45	0.60
27:A:2092:U:OP2	34:H:27:ARG:NH1	2.34	0.60
27:A:2498:OMC:HM22	27:A:2499:C:H5'	1.82	0.60
36:J:86:ILE:HD13	36:J:98:VAL:HG13	1.83	0.60
1:a:460:A:H2'	1:a:461:A:H8	1.67	0.60
1:a:1317:C:O5'	14:n:24:ARG:NH2	2.35	0.60
1:a:1530:G:O6	21:u:46:LYS:NZ	2.35	0.60
27:A:856:G:H2'	27:A:857:G:C8	2.37	0.60
41:P:57:THR:OG1	41:P:62:ASN:ND2	2.34	0.60
1:a:1073:U:O2'	2:b:105:LYS:NZ	2.35	0.60
13:m:71:ARG:O	13:m:75:MET:HG2	2.02	0.60
26:v:173:ILE:HA	26:v:227:LEU:HD12	1.83	0.60
26:v:342:ILE:HD13	26:v:367:LEU:HD22	1.83	0.60
1:a:1378:C:OP2	7:g:5:ARG:NH1	2.33	0.60
5:e:164:ILE:HA	8:h:114:ARG:HH12	1.67	0.60
26:v:119:VAL:O	26:v:120:GLU:HG2	2.02	0.60
27:A:538:A:H4'	37:L:7:LYS:HG2	1.84	0.60
27:A:546:U:H3'	27:A:547:A:H8	1.67	0.60
35:I:67:THR:HG21	35:I:75:ALA:HB2	1.84	0.60
26:v:108:CYS:SG	26:v:109:CYS:N	2.75	0.60
27:A:2100:G:O6	27:A:2189:U:O4	2.20	0.60
49:X:30:ILE:HD13	49:X:70:ILE:HD11	1.84	0.60
9:i:7:TYR:HE1	9:i:18:ARG:HB2	1.67	0.59
26:v:211:ASN:HA	26:v:228:ARG:HH22	1.66	0.59
26:v:111:MET:HE2	26:v:113:ILE:HG13	1.84	0.59
27:A:61:C:OP2	52:l:47:ARG:NH2	2.35	0.59
27:A:848:C:H2'	27:A:849:A:H8	1.66	0.59
1:a:744:C:H2'	1:a:745:G:H8	1.67	0.59
27:A:534:U:O2'	44:S:49:ASP:OD2	2.13	0.59
3:c:186:THR:HG22	3:c:199:LYS:HG2	1.84	0.59
12:l:68:GLY:O	12:l:99:ARG:NH1	2.33	0.59
32:F:108:VAL:HG11	32:F:176:PRO:HG3	1.84	0.59
27:A:2204:G:OP2	29:C:147:LYS:NZ	2.28	0.59
15:o:15:PHE:HE1	15:o:84:ARG:HD2	1.68	0.59
26:v:27:THR:O	26:v:30:THR:OG1	2.21	0.59
27:A:1417:C:HO2'	27:A:1587:G:HO2'	1.50	0.59
1:a:1077:G:N2	1:a:1080:A:OP2	2.33	0.59
1:a:1137:C:O2	1:a:1138:G:N2	2.35	0.59
27:A:886:A:N6	27:A:891:G:O6	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:G:22:GLN:NE2	33:G:38:ASN:O	2.35	0.59
1:a:674:G:H2'	1:a:675:A:H8	1.67	0.59
26:v:145:ASP:OD2	26:v:146:ARG:NH2	2.36	0.59
26:v:376:GLY:HA2	26:v:390:ILE:HD12	1.83	0.59
27:A:1223:G:OP1	45:T:68:ARG:NH1	2.36	0.59
17:q:17:MET:HE3	17:q:20:SER:HB3	1.84	0.59
23:y:73:A:H4'	23:y:73:A:OP1	2.03	0.59
25:w:108:GLU:N	25:w:108:GLU:OE2	2.36	0.59
22:x:26:A:H61	22:x:44:G:H1	1.49	0.58
23:y:34:G:H2'	23:y:35:A:C8	2.38	0.58
34:H:12:LEU:HD11	34:H:19:VAL:HG11	1.85	0.58
38:M:17:ARG:HE	38:M:47:ILE:HD11	1.68	0.58
6:f:15:SER:HA	6:f:18:VAL:HG23	1.85	0.58
22:x:17:C:H4'	22:x:18:G:H5''	1.85	0.58
1:a:76:G:H1	1:a:93:U:H3	1.51	0.58
26:v:225:GLN:HA	26:v:228:ARG:HD2	1.84	0.58
26:v:422:GLU:OE2	26:v:452:ARG:NH2	2.24	0.58
26:v:297:THR:HG22	26:v:380:THR:HG23	1.86	0.58
27:A:2140:G:N2	27:A:2151:U:O2'	2.36	0.58
26:v:142:ASN:OD1	26:v:143:LYS:N	2.36	0.58
27:A:881:G:O6	27:A:895:U:O4	2.21	0.58
35:I:25:ALA:HA	35:I:115:GLY:HA2	1.86	0.58
40:O:24:THR:O	40:O:34:LYS:NZ	2.36	0.58
47:V:38:ALA:O	47:V:81:LYS:NZ	2.36	0.58
1:a:82:G:H1'	1:a:87:C:H42	1.69	0.58
15:o:8:THR:HG23	15:o:31:LEU:HD11	1.86	0.58
27:A:2831:G:OP2	30:D:59:ARG:NH2	2.29	0.58
1:a:1071:C:H2'	1:a:1072:G:H8	1.68	0.58
22:x:36:A:O2'	25:w:155:GLU:OE2	2.22	0.58
27:A:833:A:H2'	27:A:834:G:H8	1.68	0.58
27:A:1536:C:H4'	27:A:1537:G:H5''	1.85	0.58
27:A:2377:A:O2'	42:Q:117:PHE:O	2.22	0.58
32:F:26:MET:O	32:F:30:ARG:NH1	2.36	0.58
32:F:95:ARG:HD2	54:3:1:MET:HE1	1.83	0.58
27:A:1417:C:O2'	27:A:1587:G:O2'	2.19	0.57
36:J:123:GLU:O	36:J:126:THR:OG1	2.21	0.57
1:a:178:C:H2'	1:a:179:A:H8	1.69	0.57
27:A:2728:U:HO2'	27:A:2729:G:H8	1.52	0.57
1:a:337:G:H2'	1:a:338:A:C8	2.39	0.57
1:a:1356:G:H2'	1:a:1357:A:C8	2.39	0.57
27:A:307:G:N1	27:A:310:A:OP2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:I:73:LYS:HB2	35:I:117:LEU:HB2	1.86	0.57
36:J:49:ILE:HG13	36:J:50:GLU:N	2.19	0.57
1:a:1088:G:H21	1:a:1167:A:H61	1.51	0.57
15:o:78:TYR:OH	15:o:89:ARG:O	2.22	0.57
27:A:2295:C:OP1	42:Q:10:ARG:NH1	2.38	0.57
34:H:1:MET:N	34:H:21:VAL:O	2.36	0.57
27:A:1392:A:N6	47:V:18:GLU:OE1	2.37	0.57
1:a:1027:C:N3	1:a:1028:C:N4	2.52	0.57
25:w:115:VAL:HG12	25:w:203:VAL:HG22	1.87	0.57
25:w:314:GLN:OE1	25:w:316:ARG:NH1	2.38	0.57
28:B:111:U:H2'	28:B:112:G:H8	1.69	0.57
40:O:42:THR:HG22	40:O:93:VAL:HG12	1.85	0.57
1:a:1218:C:H2'	1:a:1219:A:C8	2.40	0.57
26:v:173:ILE:HD12	26:v:219:VAL:HG11	1.87	0.57
1:a:458:U:H2'	1:a:459:A:C8	2.39	0.57
3:c:11:ARG:NH2	3:c:177:THR:O	2.37	0.57
26:v:19:ILE:HG22	26:v:89:THR:OG1	2.05	0.57
27:A:160:A:N3	27:A:2208:C:O2'	2.34	0.57
27:A:597:G:O2'	39:N:11:GLY:O	2.20	0.57
8:h:47:GLU:HG2	8:h:64:LYS:HB3	1.87	0.57
27:A:721:A:H2'	27:A:722:A:C8	2.40	0.57
3:c:43:LEU:HD13	3:c:68:ILE:HD11	1.87	0.56
1:a:337:G:H2'	1:a:338:A:H8	1.70	0.56
3:c:65:ARG:HE	3:c:100:GLN:HE21	1.52	0.56
36:J:86:ILE:HD11	36:J:99:GLY:HA3	1.86	0.56
7:g:113:ASP:HB2	7:g:119:ARG:HG2	1.88	0.56
11:k:35:THR:HG22	11:k:41:ALA:HA	1.86	0.56
26:v:13:ARG:NH1	26:v:363:ASP:OD2	2.37	0.56
27:A:675:A:OP1	31:E:58:LYS:NZ	2.36	0.56
27:A:2243:U:H2'	27:A:2244:U:C6	2.40	0.56
10:j:28:THR:HG21	10:j:90:LEU:HD22	1.87	0.56
27:A:700:G:O2'	27:A:1632:A:N3	2.38	0.56
1:a:77:A:H2'	1:a:78:A:H8	1.70	0.56
1:a:147:G:H2'	1:a:148:G:C8	2.40	0.56
22:x:23:A:H2'	22:x:24:G:C8	2.40	0.56
31:E:61:ARG:NH1	31:E:63:LYS:O	2.39	0.56
1:a:613:C:OP1	4:d:81:ARG:NH1	2.35	0.56
1:a:1152:A:OP1	10:j:70:HIS:ND1	2.32	0.56
30:D:46:ARG:NH1	30:D:85:ALA:O	2.38	0.56
27:A:617:G:OP1	31:E:102:ARG:NH1	2.38	0.56
42:Q:40:ILE:HG12	42:Q:47:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:113:VAL:HG12	18:r:73:ARG:HD3	1.88	0.56
1:a:1530:G:H2'	1:a:1531:A:H8	1.71	0.56
2:b:66:LYS:HA	2:b:89:GLN:HE22	1.71	0.56
11:k:97:ILE:HG22	21:u:12:PHE:HZ	1.70	0.56
27:A:1802:A:H2'	27:A:1803:A:C8	2.41	0.56
27:A:2229:U:H2'	27:A:2230:G:H8	1.72	0.56
36:J:90:SER:HB2	36:J:93:PRO:HG3	1.87	0.56
39:N:78:ARG:HG2	39:N:113:ALA:HB3	1.88	0.56
1:a:999:C:H2'	1:a:1000:A:H8	1.71	0.55
6:f:19:PRO:O	6:f:22:ILE:HB	2.06	0.55
27:A:2898:U:H2'	27:A:2899:A:H8	1.70	0.55
36:J:19:ASN:O	36:J:21:SER:N	2.39	0.55
38:M:9:ASN:OD1	38:M:18:ARG:NH1	2.40	0.55
44:S:102:ASP:OD2	45:T:2:TYR:OH	2.21	0.55
27:A:1059:G:N1	36:J:128:SER:OG	2.38	0.55
27:A:2185:U:H2'	27:A:2186:G:H8	1.71	0.55
27:A:18:U:OP1	44:S:30:ARG:NH2	2.40	0.55
23:y:75:C:H2'	27:A:2432:A:H1'	1.89	0.55
26:v:473:TRP:NE1	26:v:496:ASP:OD2	2.37	0.55
27:A:549:G:H2'	27:A:550:C:C6	2.42	0.55
31:E:108:ILE:HG23	39:N:1:MET:HE1	1.87	0.55
36:J:49:ILE:HG13	36:J:50:GLU:H	1.71	0.55
35:I:122:GLN:NE2	35:I:124:ASP:OD2	2.40	0.55
36:J:101:ILE:O	36:J:141:GLU:N	2.37	0.55
6:f:9:MET:HA	6:f:58:HIS:O	2.06	0.55
7:g:16:PRO:HG3	9:i:43:THR:HG22	1.89	0.55
25:w:107:ASP:OD1	25:w:109:ARG:NH1	2.40	0.55
27:A:115:C:HO2'	27:A:127:A:HO2'	1.54	0.55
27:A:476:G:N1	27:A:479:A:OP2	2.36	0.55
27:A:833:A:H2'	27:A:834:G:C8	2.42	0.55
13:m:3:ARG:O	13:m:57:ARG:NH1	2.39	0.55
23:y:26:A:N6	23:y:44:G:N1	2.35	0.55
26:v:369:ASN:HD22	26:v:373:ILE:HD12	1.70	0.55
35:I:77:VAL:HG21	35:I:82:ILE:HD13	1.89	0.55
23:y:35:A:H2'	23:y:36:A:C4	2.41	0.54
1:a:662:U:H2'	1:a:663:A:C8	2.43	0.54
11:k:29:ASN:OD1	11:k:30:THR:N	2.40	0.54
3:c:77:ILE:HA	3:c:84:VAL:HG23	1.88	0.54
23:y:28:G:H2'	23:y:29:G:H8	1.71	0.54
26:v:325:TYR:HA	26:v:329:MET:SD	2.48	0.54
27:A:1365:A:O2'	51:Z:11:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:145:GLU:HB2	29:C:188:CYS:HB3	1.90	0.54
1:a:673:A:H2'	1:a:674:G:H8	1.73	0.54
27:A:177:G:OP2	27:A:177:G:N2	2.31	0.54
27:A:549:G:H2'	27:A:550:C:H6	1.73	0.54
46:U:82:MET:HB2	46:U:98:LYS:HB2	1.90	0.54
49:X:51:GLN:OE1	49:X:57:TYR:OH	2.24	0.54
59:8:16:ILE:HD13	59:8:25:VAL:HG22	1.88	0.54
6:f:21:MET:HA	6:f:24:ARG:HH21	1.72	0.54
27:A:2332:C:OP1	50:Y:77:ARG:NH1	2.40	0.54
24:z:20:U:OP2	25:w:195:ARG:NH1	2.41	0.54
27:A:30:G:O2'	27:A:1214:A:N3	2.36	0.54
28:B:5:U:OP1	28:B:61:G:O2'	2.23	0.54
1:a:28:A:O2'	1:a:296:U:OP1	2.24	0.54
27:A:203:A:N7	62:A:3508:HOH:O	2.33	0.54
27:A:1193:G:OP1	39:N:14:LYS:NZ	2.37	0.54
27:A:2189:U:O2'	27:A:2190:G:OP1	2.23	0.54
1:a:714:G:H2'	1:a:715:A:C8	2.42	0.54
1:a:1356:G:H2'	1:a:1357:A:H8	1.73	0.54
4:d:170:TRP:CE2	4:d:186:PRO:HB3	2.43	0.54
18:r:32:TYR:CG	18:r:55:LEU:HD21	2.43	0.54
27:A:1386:C:H2'	27:A:1387:A:H8	1.73	0.54
1:a:1314:C:H2'	1:a:1315:U:C6	2.43	0.54
11:k:111:THR:HG23	21:u:3:VAL:HG22	1.90	0.54
27:A:1799:G:OP1	29:C:258:ARG:NH1	2.35	0.53
33:G:98:VAL:HG22	33:G:103:ILE:HG12	1.90	0.53
1:a:459:A:H2'	1:a:460:A:H8	1.73	0.53
23:y:52:G:H2'	23:y:53:G:H8	1.74	0.53
26:v:173:ILE:HG12	26:v:181:GLY:O	2.08	0.53
27:A:2071:A:H2'	27:A:2072:C:C6	2.43	0.53
32:F:147:ASP:OD1	32:F:148:ARG:N	2.42	0.53
42:Q:94:ARG:NH1	42:Q:97:PHE:O	2.40	0.53
1:a:21:G:H2'	1:a:22:G:H8	1.73	0.53
15:o:26:GLU:HG3	15:o:81:LEU:HD13	1.91	0.53
37:L:114:LEU:HG	37:L:118:MET:HE3	1.89	0.53
27:A:2557:G:H2'	27:A:2558:C:C6	2.44	0.53
33:G:127:THR:HG23	33:G:129:THR:H	1.73	0.53
59:8:18:LYS:HE2	59:8:21:GLY:HA2	1.90	0.53
1:a:981:U:O2'	14:n:61:ARG:NH1	2.41	0.53
6:f:36:ILE:HG12	6:f:64:VAL:HG12	1.89	0.53
26:v:287:ARG:NH1	26:v:289:VAL:HG22	2.22	0.53
27:A:414:C:H2'	27:A:415:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:17:U:H2'	1:a:18:C:C6	2.44	0.53
20:t:35:VAL:O	20:t:39:ILE:HD12	2.08	0.53
26:v:207:VAL:HG12	26:v:209:GLY:H	1.73	0.53
27:A:278:A:N6	27:A:362:A:N7	2.56	0.53
27:A:500:G:N1	27:A:503:A:OP2	2.41	0.53
27:A:1022:G:O6	37:L:68:LYS:NZ	2.35	0.53
27:A:2106:U:H2'	27:A:2107:G:H8	1.73	0.53
27:A:2502:G:H5''	27:A:2503:2MA:H5''	1.89	0.53
1:a:390:U:H2'	1:a:391:G:C8	2.44	0.53
26:v:32:LYS:HD2	26:v:262:ASN:ND2	2.24	0.53
27:A:1432:G:H2'	27:A:1433:A:C8	2.44	0.53
1:a:1287:A:H2'	1:a:1288:A:C8	2.43	0.53
19:s:11:ILE:HD11	19:s:15:LEU:HD22	1.91	0.53
35:I:24:SER:HB2	35:I:116:GLU:HG2	1.91	0.53
37:L:102:GLU:HB3	37:L:119:PHE:HZ	1.73	0.53
1:a:946:A:H2'	1:a:947:G:C8	2.44	0.52
1:a:1086:U:H3	1:a:1099:G:H22	1.55	0.52
10:j:19:ASP:OD1	10:j:72:ARG:NH1	2.40	0.52
27:A:1386:C:H2'	27:A:1387:A:C8	2.44	0.52
1:a:407:U:O2'	4:d:113:GLU:OE2	2.25	0.52
1:a:1522:U:H2'	1:a:1523:G:H8	1.75	0.52
5:e:165:LEU:O	8:h:114:ARG:NH2	2.42	0.52
27:A:1419:A:O2'	27:A:1421:G:N7	2.35	0.52
27:A:2246:G:H2'	27:A:2247:A:H8	1.74	0.52
22:x:23:A:H2'	22:x:24:G:H8	1.74	0.52
27:A:593:U:H2'	27:A:594:U:C6	2.44	0.52
27:A:1992:G:N2	27:A:1996:C:O2'	2.42	0.52
36:J:42:PHE:HE1	36:J:57:VAL:HG11	1.73	0.52
1:a:203:G:H1'	1:a:465:A:H61	1.73	0.52
9:i:65:ILE:HG21	9:i:79:ILE:HD12	1.91	0.52
23:y:51:U:O2	23:y:63:G:O6	2.26	0.52
26:v:75:MET:HE3	26:v:86:LEU:HD12	1.92	0.52
27:A:1443:U:H2'	27:A:1444:G:H8	1.73	0.52
51:Z:37:ARG:HG2	51:Z:46:PHE:HB3	1.92	0.52
1:a:555:U:H2'	1:a:556:C:C6	2.44	0.52
1:a:1314:C:H2'	1:a:1315:U:H6	1.74	0.52
15:o:6:GLU:O	15:o:10:LYS:HG2	2.09	0.52
54:3:35:ASP:N	54:3:35:ASP:OD1	2.43	0.52
1:a:1400:C:O2	25:w:192:SER:OG	2.27	0.52
19:s:41:PHE:H	19:s:44:MET:HE3	1.75	0.52
26:v:25:GLY:HA3	26:v:142:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:v:159:GLU:OE2	26:v:166:CYS:HB2	2.10	0.52
37:L:49:ASP:OD1	37:L:121:LYS:NZ	2.36	0.52
13:m:33:ILE:HD13	13:m:60:VAL:HG22	1.92	0.52
27:A:2291:U:H2'	27:A:2292:U:C6	2.44	0.52
1:a:1026:G:O2'	1:a:1027:C:OP1	2.25	0.52
27:A:1864:U:OP1	27:A:2410:G:O2'	2.26	0.52
28:B:7:G:O2'	42:Q:38:GLN:NE2	2.43	0.52
45:T:34:GLU:HG3	45:T:60:LYS:HG3	1.92	0.52
1:a:460:A:H2'	1:a:461:A:C8	2.44	0.52
1:a:1218:C:H2'	1:a:1219:A:H8	1.75	0.52
6:f:23:GLU:O	6:f:26:THR:HB	2.09	0.52
6:f:90:MET:HE1	18:r:23:TYR:CE1	2.45	0.52
27:A:1028:A:H2'	27:A:1029:A:C8	2.45	0.52
36:J:4:LYS:O	36:J:8:TYR:OH	2.23	0.52
25:w:303:ARG:O	25:w:306:ARG:NH1	2.43	0.51
27:A:714:U:O2'	27:A:716:A:N7	2.40	0.51
1:a:459:A:H2'	1:a:460:A:C8	2.44	0.51
27:A:299:A:N3	27:A:319:G:O2'	2.39	0.51
27:A:347:A:H2'	27:A:348:A:C8	2.45	0.51
27:A:644:A:H2'	27:A:645:C:O4'	2.10	0.51
27:A:2114:A:N3	27:A:2166:U:H2'	2.26	0.51
3:c:79:LYS:N	3:c:82:GLU:OE1	2.43	0.51
4:d:34:ILE:HD12	4:d:34:ILE:H	1.75	0.51
5:e:41:ASP:OD2	5:e:45:ARG:NH1	2.42	0.51
27:A:2246:G:H2'	27:A:2247:A:C8	2.45	0.51
32:F:131:GLY:HA2	32:F:153:ASP:HA	1.93	0.51
46:U:29:VAL:HB	46:U:55:ILE:HD11	1.92	0.51
1:a:82:G:H1'	1:a:87:C:N4	2.25	0.51
9:i:88:MET:HE1	9:i:104:VAL:HG13	1.93	0.51
11:k:83:GLU:HG2	11:k:109:ASN:HB2	1.92	0.51
27:A:1250:G:H5''	44:S:6:ARG:HD3	1.91	0.51
7:g:93:PRO:O	7:g:97:ASN:ND2	2.43	0.51
27:A:1433:A:H2'	27:A:1434:A:C8	2.45	0.51
1:a:713:G:H2'	1:a:714:G:C8	2.45	0.51
2:b:83:ALA:O	2:b:87:CYS:HB2	2.10	0.51
7:g:26:PHE:HD2	7:g:101:MET:HG2	1.75	0.51
8:h:18:GLN:HG2	8:h:63:LEU:HD13	1.92	0.51
27:A:956:G:O6	40:O:14:LYS:NZ	2.43	0.51
1:a:1360:A:OP2	14:n:75:ARG:NH2	2.44	0.51
3:c:49:LYS:O	3:c:72:ARG:NH2	2.43	0.51
1:a:1180:A:OP1	9:i:105:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:42:TRP:CE2	6:f:102:MET:HG3	2.45	0.51
27:A:881:G:N2	27:A:896:A:N7	2.59	0.51
27:A:1794:A:H2'	27:A:1795:C:C6	2.46	0.51
27:A:1:G:H2'	27:A:2:G:H8	1.75	0.51
27:A:2745:C:H2'	27:A:2746:U:C6	2.46	0.51
35:I:73:LYS:HB3	35:I:117:LEU:HD12	1.91	0.51
35:I:121:SER:OG	35:I:122:GLN:N	2.44	0.51
48:W:26:LYS:HE2	48:W:37:GLU:HG2	1.93	0.51
1:a:544:G:OP1	4:d:59:GLN:NE2	2.40	0.51
23:y:67:C:H2'	23:y:68:C:C6	2.46	0.51
26:v:518:TYR:O	26:v:520:ASP:N	2.43	0.51
27:A:244:A:OP2	58:7:8:ARG:NH2	2.40	0.51
27:A:547:A:H1'	27:A:548:G:C8	2.45	0.51
35:I:96:PHE:HE2	35:I:126:LEU:H	1.58	0.51
40:O:50:ARG:HD3	40:O:65:ILE:HD11	1.93	0.51
1:a:21:G:H2'	1:a:22:G:C8	2.46	0.50
2:b:30:PHE:HA	2:b:45:LYS:HD2	1.93	0.50
25:w:330:ASP:OD1	25:w:331:GLU:N	2.45	0.50
26:v:213:PRO:HA	26:v:216:ASP:HB2	1.94	0.50
1:a:539:A:H2'	1:a:540:G:C8	2.46	0.50
27:A:2135:A:H5''	27:A:2136:G:N7	2.26	0.50
1:a:408:A:O3'	4:d:23:SER:OG	2.29	0.50
1:a:1524:C:H2'	1:a:1525:G:H8	1.76	0.50
26:v:305:ALA:HB1	26:v:307:MET:HE2	1.92	0.50
27:A:191:A:H2'	27:A:192:C:C6	2.45	0.50
1:a:344:A:H5''	1:a:345:C:H5	1.76	0.50
1:a:674:G:H2'	1:a:675:A:C8	2.46	0.50
4:d:78:GLU:OE1	4:d:93:LEU:HD21	2.11	0.50
6:f:51:ILE:O	6:f:54:LEU:HG	2.11	0.50
26:v:243:LYS:HE2	26:v:247:LEU:HD21	1.93	0.50
29:C:95:LEU:HD13	29:C:101:ARG:HE	1.76	0.50
33:G:89:LEU:HD12	33:G:94:TYR:HB3	1.93	0.50
35:I:48:ALA:HB3	35:I:51:TYR:CE1	2.46	0.50
1:a:653:U:O4'	8:h:56:LYS:NZ	2.44	0.50
3:c:50:ALA:HB1	3:c:76:VAL:HG22	1.92	0.50
26:v:88:ASP:OD1	26:v:89:THR:N	2.45	0.50
26:v:396:GLU:N	26:v:396:GLU:OE1	2.44	0.50
27:A:1387:A:H5'	27:A:1469:A:H1'	1.92	0.50
27:A:2141:G:H2'	27:A:2142:A:C8	2.47	0.50
27:A:2184:A:H2'	27:A:2185:U:C6	2.46	0.50
27:A:2547:A:H2'	27:A:2548:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:309:A:O2'	1:a:607:A:N1	2.40	0.50
1:a:1073:U:O2	2:b:103:ASN:ND2	2.45	0.50
6:f:61:LEU:HD23	6:f:62:MET:N	2.26	0.50
27:A:580:U:H2'	27:A:581:C:C6	2.46	0.50
27:A:581:C:H2'	27:A:582:A:H8	1.76	0.50
27:A:742:A:H2'	27:A:743:A:C8	2.47	0.50
29:C:121:ASP:OD1	29:C:121:ASP:N	2.42	0.50
36:J:92:LYS:HB3	36:J:95:LYS:HB2	1.94	0.50
38:M:63:VAL:HG12	38:M:107:LEU:HD11	1.93	0.50
26:v:356:VAL:HG12	26:v:358:GLU:H	1.77	0.50
27:A:263:G:O2'	27:A:429:A:N3	2.45	0.50
27:A:1735:A:H2'	27:A:1736:U:C6	2.47	0.50
27:A:2120:G:H2'	27:A:2121:G:C8	2.44	0.50
27:A:2748:A:H5'	33:G:4:VAL:HG21	1.93	0.50
48:W:96:PHE:O	48:W:100:SER:HA	2.12	0.50
1:a:90:C:H2'	1:a:91:U:C6	2.47	0.50
23:y:19:G:N3	23:y:57:G:N2	2.59	0.50
27:A:711:G:H3'	27:A:712:G:H21	1.76	0.50
27:A:2328:A:H2'	27:A:2329:U:C6	2.46	0.50
35:I:17:GLU:HG3	35:I:53:ARG:HB2	1.93	0.50
39:N:56:PRO:HG2	39:N:59:ARG:HB2	1.94	0.50
27:A:414:C:H2'	27:A:415:A:C8	2.47	0.50
27:A:881:G:O6	27:A:895:U:C4	2.65	0.50
27:A:1438:U:H2'	27:A:1439:A:H8	1.76	0.50
10:j:6:ILE:HG22	10:j:102:LEU:HD13	1.93	0.49
22:x:74:C:H3'	25:w:261:ARG:HH22	1.76	0.49
27:A:2118:U:O2	27:A:2145:C:N4	2.45	0.49
27:A:2788:C:H2'	27:A:2789:C:C6	2.47	0.49
29:C:165:VAL:HG21	29:C:181:MET:HE3	1.94	0.49
1:a:1009:U:O4	1:a:1020:G:O6	2.29	0.49
1:a:1026:G:O6	1:a:1035:A:N1	2.45	0.49
26:v:478:ASP:OD1	26:v:479:ALA:N	2.45	0.49
27:A:1005:C:O2'	37:L:30:THR:HG21	2.11	0.49
28:B:16:G:N2	28:B:69:G:H1'	2.27	0.49
7:g:26:PHE:CD2	7:g:101:MET:HG2	2.47	0.49
26:v:133:ARG:HH11	26:v:133:ARG:HG2	1.76	0.49
27:A:627:A:OP1	39:N:78:ARG:NH2	2.33	0.49
49:X:4:ILE:HG12	49:X:50:MET:HE1	1.94	0.49
1:a:297:G:N2	1:a:300:A:OP2	2.37	0.49
1:a:999:C:H2'	1:a:1000:A:C8	2.46	0.49
4:d:159:LEU:O	4:d:163:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:46:GLN:HE22	6:f:55:HIS:HB3	1.77	0.49
27:A:645:C:H2'	27:A:647:G:C8	2.47	0.49
1:a:401:C:O2'	1:a:621:A:N3	2.37	0.49
2:b:67:ILE:HG22	2:b:160:ALA:HB3	1.93	0.49
2:b:191:SER:OG	2:b:192:ASP:N	2.46	0.49
5:e:156:LYS:NZ	8:h:73:GLU:OE2	2.46	0.49
27:A:351:C:H2'	27:A:352:A:H8	1.77	0.49
27:A:645:C:H2'	27:A:647:G:N7	2.27	0.49
30:D:1:MET:HE1	30:D:100:LEU:HD21	1.95	0.49
48:W:98:SER:OG	48:W:98:SER:O	2.28	0.49
1:a:1516:2MG:N2	1:a:1519:MA6:OP2	2.46	0.49
13:m:59:GLU:HA	13:m:62:LYS:NZ	2.27	0.49
15:o:18:ASP:HB3	15:o:21:ASP:HB2	1.94	0.49
17:q:25:ILE:HD13	17:q:44:LEU:HD12	1.94	0.49
25:w:64:THR:HA	25:w:67:MET:HE1	1.93	0.49
27:A:1:G:H2'	27:A:2:G:C8	2.48	0.49
27:A:639:U:H2'	27:A:640:C:C6	2.47	0.49
27:A:1416:G:O2'	27:A:1587:G:N2	2.46	0.49
1:a:131:A:H2'	1:a:132:C:C6	2.48	0.49
1:a:745:G:H2'	1:a:746:A:C8	2.47	0.49
25:w:247:THR:HG23	25:w:254:VAL:HG22	1.94	0.49
26:v:314:ARG:HH22	26:v:371:GLY:HA2	1.77	0.49
27:A:1361:G:H2'	27:A:1362:C:C6	2.48	0.49
27:A:2146:C:H4'	27:A:2147:A:C4	2.47	0.49
27:A:2637:U:OP1	30:D:83:ARG:NH1	2.46	0.49
27:A:2812:G:H2'	27:A:2813:A:C8	2.48	0.49
27:A:2850:A:N7	27:A:2868:A:O2'	2.39	0.49
4:d:60:LYS:O	4:d:64:ILE:HG13	2.12	0.49
23:y:51:U:H2'	23:y:52:G:C8	2.47	0.49
26:v:189:GLU:HG3	26:v:208:LYS:HG2	1.94	0.49
26:v:503:TYR:OH	26:v:510:ASN:OD1	2.23	0.49
27:A:713:G:H21	27:A:718:A:H62	1.60	0.49
1:a:413:G:O2'	1:a:428:G:N2	2.45	0.49
1:a:652:U:O4	1:a:752:G:O2'	2.25	0.49
6:f:26:THR:HG23	6:f:36:ILE:HD12	1.95	0.49
25:w:115:VAL:HG22	25:w:162:ILE:HG22	1.95	0.49
25:w:294:ARG:HH21	27:A:1915:3TD:H4'	1.78	0.49
27:A:1746:A:H2'	27:A:1747:U:C6	2.48	0.49
27:A:2820:A:O2'	27:A:2821:A:OP1	2.30	0.49
29:C:117:GLN:O	29:C:128:ASN:ND2	2.45	0.49
31:E:143:LEU:HD13	31:E:146:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:J:102:SER:OG	36:J:105:GLN:HB2	2.12	0.49
1:a:613:C:H2'	1:a:614:C:C6	2.48	0.49
27:A:576:U:H2'	27:A:577:G:C8	2.48	0.49
27:A:2191:A:H2'	27:A:2192:U:C6	2.48	0.49
32:F:142:ASP:N	32:F:142:ASP:OD1	2.42	0.49
45:T:3:ALA:HB3	45:T:59:ILE:HD11	1.95	0.49
53:2:11:ARG:HG2	53:2:11:ARG:HH11	1.78	0.49
1:a:1226:C:H2'	13:m:102:THR:HG22	1.95	0.48
9:i:17:ALA:HB2	9:i:67:VAL:HG23	1.94	0.48
20:t:60:ARG:O	20:t:64:LYS:HG2	2.13	0.48
26:v:189:GLU:HG2	26:v:206:ILE:HG22	1.94	0.48
27:A:636:G:N7	39:N:109:LYS:HE2	2.27	0.48
33:G:24:ILE:HD11	33:G:43:VAL:HG21	1.95	0.48
27:A:568:U:H1'	27:A:2030:6MZ:H9C1	1.94	0.48
27:A:1796:U:H2'	27:A:1797:G:H8	1.77	0.48
1:a:440:C:C2	1:a:441:A:C8	3.02	0.48
5:e:83:HIS:HE1	5:e:148:ASN:H	1.60	0.48
5:e:164:ILE:HG13	5:e:165:LEU:HD12	1.95	0.48
9:i:33:ARG:HH21	9:i:38:TYR:HA	1.77	0.48
14:n:37:SER:HB3	14:n:40:ASP:HB2	1.95	0.48
27:A:2177:C:H2'	27:A:2178:C:C6	2.47	0.48
4:d:67:VAL:HG22	4:d:97:ARG:NH1	2.28	0.48
49:X:26:PHE:HE2	49:X:89:ILE:HG13	1.79	0.48
1:a:404:G:OP2	4:d:115:ARG:NH2	2.46	0.48
1:a:552:U:C2	1:a:553:A:C8	3.01	0.48
1:a:1294:G:H2'	1:a:1295:U:C6	2.49	0.48
1:a:1323:G:H2'	1:a:1324:A:C8	2.48	0.48
4:d:105:MET:HG3	4:d:171:LEU:HD23	1.96	0.48
17:q:59:VAL:HG12	17:q:78:VAL:HA	1.96	0.48
22:x:76:A:H3'	25:w:234:GLY:HA3	1.96	0.48
27:A:277:G:H1'	27:A:278:A:C5	2.49	0.48
27:A:1704:C:H2'	27:A:1705:A:C8	2.49	0.48
29:C:71:LYS:NZ	29:C:100:GLU:OE1	2.41	0.48
39:N:62:PRO:HB2	58:7:30:ARG:HH21	1.78	0.48
1:a:1493:A:N6	25:w:302:ASP:OD1	2.46	0.48
5:e:88:VAL:HG22	5:e:93:ARG:HG3	1.96	0.48
6:f:10:VAL:HG22	6:f:58:HIS:HB3	1.95	0.48
27:A:1141:U:H4'	27:A:1142:A:O4'	2.13	0.48
27:A:2898:U:H2'	27:A:2899:A:C8	2.48	0.48
29:C:262:ARG:O	29:C:265:LYS:NZ	2.46	0.48
50:Y:59:LEU:HD12	50:Y:80:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:674:G:H21	11:k:118:HIS:HB2	1.77	0.48
1:a:746:A:H2'	1:a:747:A:C8	2.48	0.48
1:a:980:C:O2'	14:n:13:ARG:NH1	2.47	0.48
19:s:30:PRO:HB3	19:s:48:THR:HG22	1.96	0.48
19:s:52:HIS:CD2	19:s:54:GLY:H	2.31	0.48
20:t:24:ARG:HA	20:t:27:MET:HG3	1.95	0.48
23:y:25:C:O2'	23:y:26:A:H8	1.97	0.48
25:w:95:GLN:O	25:w:349:GLN:HG2	2.13	0.48
27:A:282:A:N6	27:A:359:G:O6	2.46	0.48
27:A:2155:U:H2'	27:A:2156:G:O4'	2.13	0.48
27:A:2281:A:O2'	27:A:2282:G:H5'	2.14	0.48
40:O:35:ALA:HA	40:O:128:THR:HG22	1.95	0.48
47:V:5:GLU:OE2	47:V:9:LYS:NZ	2.41	0.48
1:a:31:G:O2'	1:a:48:C:N4	2.47	0.48
22:x:51:U:H2'	22:x:52:G:H8	1.78	0.48
26:v:228:ARG:O	26:v:231:LEU:N	2.45	0.48
26:v:308:ASP:O	26:v:310:LYS:N	2.47	0.48
27:A:1645:G:H5''	27:A:1646:C:H5'	1.96	0.48
27:A:2635:A:O2'	30:D:81:GLU:OE1	2.31	0.48
27:A:2646:C:OP2	27:A:2732:G:O2'	2.31	0.48
1:a:578:C:O2'	1:a:728:A:N3	2.42	0.48
6:f:10:VAL:HG12	6:f:84:VAL:HA	1.95	0.48
11:k:67:ALA:HB2	11:k:96:THR:HG23	1.96	0.48
14:n:34:VAL:O	14:n:41:ARG:NH2	2.46	0.48
27:A:1441:G:H2'	27:A:1442:U:C6	2.48	0.48
27:A:1590:A:H2'	27:A:1591:A:C8	2.48	0.48
27:A:1771:C:H2'	27:A:1772:A:H8	1.79	0.48
33:G:52:PHE:HZ	33:G:72:LEU:HD22	1.78	0.48
34:H:9:VAL:HG22	34:H:11:ASN:H	1.78	0.48
35:I:12:VAL:HA	35:I:15:VAL:HG22	1.95	0.48
41:P:103:ARG:HH21	41:P:110:MET:HE1	1.79	0.48
1:a:235:C:H2'	1:a:236:A:H8	1.78	0.48
1:a:1130:A:OP1	9:i:18:ARG:NH2	2.47	0.48
26:v:33:VAL:HG21	26:v:86:LEU:HD11	1.95	0.48
26:v:100:TYR:CE2	26:v:133:ARG:HD2	2.49	0.48
26:v:360:TYR:O	26:v:362:GLY:N	2.42	0.48
27:A:570:G:H2'	27:A:2030:6MZ:N7	2.28	0.48
27:A:2405:G:O2'	27:A:2411:A:N6	2.47	0.48
29:C:84:ASP:OD2	29:C:87:ARG:NE	2.42	0.48
1:a:1001:C:H2'	1:a:1002:G:C8	2.49	0.47
1:a:1250:A:H2'	1:a:1251:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1253:G:H2'	1:a:1254:A:H8	1.78	0.47
1:a:1524:C:H2'	1:a:1525:G:C8	2.49	0.47
2:b:55:ALA:HA	2:b:58:ASN:ND2	2.29	0.47
15:o:36:ILE:O	15:o:40:GLN:HG2	2.13	0.47
25:w:90:GLU:O	25:w:93:GLU:HG3	2.14	0.47
25:w:337:LEU:HD23	25:w:337:LEU:H	1.79	0.47
26:v:314:ARG:NH2	26:v:371:GLY:HA2	2.29	0.47
26:v:416:LEU:HG	26:v:427:VAL:HG21	1.95	0.47
27:A:1597:A:H5''	27:A:1598:A:H5'	1.95	0.47
35:I:87:GLU:HG2	35:I:95:LEU:HB2	1.96	0.47
38:M:76:VAL:HG22	43:R:73:VAL:HB	1.95	0.47
44:S:50:ARG:O	44:S:54:LYS:NZ	2.46	0.47
53:2:23:THR:HG23	53:2:47:MET:HB2	1.96	0.47
26:v:369:ASN:ND2	26:v:373:ILE:HD12	2.29	0.47
27:A:1288:G:OP2	27:A:1288:G:N2	2.39	0.47
31:E:165:HIS:CE1	31:E:166:LYS:HE3	2.49	0.47
45:T:36:ALA:HA	45:T:58:VAL:HG23	1.96	0.47
3:c:123:GLN:HG2	3:c:126:ARG:HH21	1.79	0.47
6:f:5:GLU:OE2	18:r:23:TYR:OH	2.31	0.47
27:A:1064:C:H5'	27:A:1065:U:O5'	2.14	0.47
30:D:39:ASP:N	30:D:39:ASP:OD1	2.46	0.47
36:J:25:GLY:O	36:J:29:GLY:N	2.47	0.47
54:3:41:HIS:HB3	54:3:44:PHE:HD1	1.79	0.47
27:A:1469:A:H2'	27:A:1470:A:C8	2.50	0.47
27:A:1796:U:H2'	27:A:1797:G:C8	2.50	0.47
27:A:2421:G:N7	58:7:31:HIS:NE2	2.62	0.47
1:a:712:A:H2'	1:a:713:G:C8	2.48	0.47
1:a:1129:C:H4'	9:i:18:ARG:HH22	1.79	0.47
27:A:2025:C:H2'	27:A:2026:U:C6	2.49	0.47
1:a:216:U:H2'	1:a:217:C:C6	2.49	0.47
14:n:47:LYS:O	14:n:50:THR:OG1	2.30	0.47
26:v:311:HIS:NE2	26:v:313:ASP:OD1	2.47	0.47
27:A:1704:C:H2'	27:A:1705:A:H8	1.79	0.47
27:A:1733:G:H2'	27:A:1734:G:H8	1.80	0.47
27:A:2127:G:H21	27:A:2173:A:H1'	1.80	0.47
1:a:407:U:H5''	4:d:112:ALA:HB1	1.96	0.47
1:a:457:G:H2'	1:a:458:U:C6	2.49	0.47
1:a:946:A:H2'	1:a:947:G:H8	1.78	0.47
16:p:52:LEU:HD12	16:p:78:VAL:HG21	1.95	0.47
26:v:191:TYR:CE1	26:v:206:ILE:HG23	2.50	0.47
26:v:323:GLY:O	26:v:361:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:v:401:ILE:HG21	26:v:412:LEU:HD11	1.97	0.47
27:A:145:C:H2'	27:A:146:A:C8	2.49	0.47
27:A:581:C:H2'	27:A:582:A:C8	2.50	0.47
27:A:742:A:H2'	27:A:743:A:H8	1.79	0.47
27:A:881:G:N2	27:A:896:A:H62	2.13	0.47
27:A:2467:C:O2	40:O:123:LYS:NZ	2.48	0.47
27:A:2473:U:O2'	27:A:2474:U:OP1	2.30	0.47
38:M:70:ARG:HG2	38:M:76:VAL:HG12	1.96	0.47
1:a:826:C:O2	8:h:16:ASN:ND2	2.48	0.47
1:a:922:G:H2'	1:a:923:A:C8	2.50	0.47
30:D:1:MET:SD	30:D:2:ILE:N	2.88	0.47
36:J:127:ARG:O	36:J:131:GLY:N	2.37	0.47
1:a:945:G:C2	1:a:946:A:C8	3.03	0.47
1:a:1011:C:H2'	1:a:1012:A:H8	1.80	0.47
27:A:1682:G:H2'	27:A:1683:U:C6	2.49	0.47
27:A:1869:G:N2	27:A:1872:A:OP2	2.47	0.47
27:A:1954:G:O2'	27:A:1956:U:O4	2.29	0.47
27:A:2514:U:H2'	27:A:2515:C:C6	2.49	0.47
33:G:17:VAL:HG12	33:G:26:ILE:HG22	1.97	0.47
45:T:28:ALA:HB3	45:T:31:GLU:HG2	1.97	0.47
15:o:25:THR:HG21	15:o:70:LEU:HB2	1.97	0.47
23:y:9:A:H5'	23:y:46:G7M:H22	1.80	0.47
25:w:49:SER:O	25:w:53:THR:HG23	2.15	0.47
25:w:72:PRO:O	25:w:75:ARG:NH1	2.39	0.47
26:v:77:PHE:CG	26:v:77:PHE:O	2.68	0.47
27:A:827:U:H4'	27:A:828:U:C5	2.50	0.47
27:A:1263:U:O2'	55:4:8:PRO:HD2	2.15	0.47
1:a:5:U:H4'	1:a:6:G:H5'	1.97	0.46
7:g:27:VAL:HG22	7:g:43:VAL:HG11	1.97	0.46
14:n:3:LYS:HG3	14:n:6:MET:HE1	1.97	0.46
25:w:330:ASP:OD1	25:w:331:GLU:HG3	2.15	0.46
26:v:272:LEU:HD12	26:v:276:ALA:HB2	1.96	0.46
26:v:475:GLU:OE2	26:v:500:ASN:ND2	2.44	0.46
27:A:721:A:H2'	27:A:722:A:H8	1.79	0.46
48:W:3:ALA:O	48:W:6:ARG:NE	2.47	0.46
1:a:501:C:H2'	1:a:502:A:H8	1.80	0.46
26:v:111:MET:HE3	26:v:111:MET:HB2	1.79	0.46
27:A:27:G:N2	27:A:512:G:H1'	2.29	0.46
27:A:832:U:H2'	27:A:833:A:H8	1.80	0.46
27:A:1771:C:H2'	27:A:1772:A:C8	2.51	0.46
32:F:29:PRO:HB2	32:F:169:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:J:14:ALA:HA	36:J:54:PRO:HA	1.97	0.46
41:P:24:MET:HE1	41:P:40:LYS:HB3	1.97	0.46
1:a:745:G:O2'	1:a:746:A:H5'	2.14	0.46
27:A:2146:C:O2'	27:A:2147:A:N7	2.46	0.46
27:A:2849:U:H4'	27:A:2868:A:C2	2.50	0.46
32:F:175:PHE:CD1	32:F:176:PRO:HD2	2.50	0.46
36:J:56:PRO:HD3	36:J:75:PRO:HD3	1.98	0.46
46:U:3:THR:OG1	46:U:62:ASP:OD2	2.33	0.46
1:a:1124:G:N2	1:a:1125:U:O4	2.43	0.46
22:x:66:U:H2'	22:x:67:C:C6	2.50	0.46
27:A:1059:G:H1'	36:J:113:LYS:HD3	1.98	0.46
27:A:1506:U:H2'	27:A:1507:C:C6	2.50	0.46
27:A:2687:U:H2'	27:A:2688:G:O4'	2.16	0.46
29:C:258:ARG:HD2	29:C:270:ARG:HH12	1.79	0.46
1:a:208:U:H2'	1:a:210:C:H1'	1.97	0.46
13:m:59:GLU:HA	13:m:62:LYS:HZ3	1.80	0.46
27:A:1570:A:H2'	27:A:1571:A:C8	2.50	0.46
30:D:152:PRO:HG3	30:D:156:PHE:CZ	2.50	0.46
32:F:105:THR:HA	54:3:38:SER:HB3	1.97	0.46
35:I:42:ARG:HH22	35:I:50:VAL:HG22	1.81	0.46
1:a:154:U:H2'	1:a:155:A:H8	1.80	0.46
1:a:1000:A:H2'	1:a:1001:C:C6	2.50	0.46
1:a:1004:A:H2'	1:a:1005:A:O4'	2.16	0.46
14:n:46:LEU:HB3	19:s:13:LEU:HD13	1.97	0.46
27:A:671:C:OP1	39:N:43:GLY:N	2.46	0.46
28:B:52:A:HO2'	28:B:53:A:H8	1.62	0.46
31:E:61:ARG:HH12	31:E:64:GLY:HA3	1.81	0.46
35:I:103:ASN:HA	35:I:107:GLU:HB3	1.95	0.46
1:a:1071:C:H2'	1:a:1072:G:C8	2.49	0.46
1:a:1401:G:H2'	1:a:1402:4OC:O4'	2.15	0.46
7:g:13:LEU:HD23	7:g:14:PRO:O	2.15	0.46
14:n:88:ALA:HB1	14:n:96:LEU:HD22	1.98	0.46
26:v:155:LEU:O	26:v:158:VAL:HG12	2.16	0.46
27:A:249:C:O2	58:7:12:LYS:NZ	2.49	0.46
27:A:2099:U:O2	27:A:2190:G:N2	2.46	0.46
59:8:14:CYS:SG	59:8:27:CYS:HB3	2.56	0.46
1:a:1120:C:H2'	1:a:1121:U:H6	1.81	0.46
26:v:173:ILE:HG22	26:v:227:LEU:CD1	2.46	0.46
27:A:191:A:H2'	27:A:192:C:H6	1.81	0.46
27:A:1724:G:O6	27:A:1737:G:N2	2.48	0.46
27:A:2216:G:H2'	27:A:2217:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2233:U:H2'	27:A:2234:G:C8	2.51	0.46
27:A:2641:G:H5''	37:L:78:THR:HB	1.96	0.46
36:J:109:ILE:O	36:J:112:THR:OG1	2.19	0.46
50:Y:71:VAL:HG22	50:Y:78:LYS:HG2	1.98	0.46
1:a:1014:A:C2	1:a:1219:A:H1'	2.51	0.46
27:A:1326:U:H2'	27:A:1327:A:H8	1.80	0.46
27:A:1443:U:H2'	27:A:1444:G:C8	2.50	0.46
27:A:1808:A:H3'	27:A:1809:A:C8	2.50	0.46
27:A:2111:U:O4'	27:A:2118:U:O2'	2.29	0.46
34:H:25:TYR:HE1	34:H:29:PHE:HD2	1.63	0.46
57:6:31:LEU:HD22	57:6:42:LEU:HD13	1.98	0.46
1:a:113:G:H1'	1:a:354:G:H5'	1.98	0.46
1:a:639:G:O6	1:a:640:A:N6	2.49	0.46
1:a:1169:A:H2'	1:a:1170:A:C8	2.50	0.46
2:b:164:ILE:HA	2:b:186:ILE:HG22	1.98	0.46
26:v:517:ARG:HG3	26:v:518:TYR:CD2	2.51	0.46
27:A:1410:G:H2'	27:A:1411:U:C6	2.51	0.46
32:F:147:ASP:OD1	32:F:150:ARG:NH2	2.49	0.46
37:L:32:LEU:HD22	37:L:54:ILE:HG21	1.97	0.46
38:M:17:ARG:NE	38:M:47:ILE:HD11	2.30	0.46
1:a:193:C:H4'	20:t:56:PRO:HG3	1.98	0.45
1:a:1238:A:H2	1:a:1241:G:N3	2.13	0.45
9:i:52:LEU:HD13	9:i:58:VAL:HA	1.98	0.45
15:o:15:PHE:HZ	15:o:81:LEU:HD12	1.81	0.45
25:w:165:LYS:HZ1	25:w:208:GLU:HG3	1.80	0.45
26:v:109:CYS:SG	26:v:110:LEU:N	2.89	0.45
26:v:131:ARG:HA	26:v:131:ARG:HD2	1.80	0.45
27:A:1434:A:H2'	27:A:1435:G:H8	1.81	0.45
27:A:1669:A:H5'	38:M:5:GLN:HE22	1.82	0.45
27:A:2834:G:H2'	27:A:2879:A:H61	1.81	0.45
29:C:201:MET:HG3	29:C:202:LEU:HD22	1.97	0.45
51:Z:43:GLU:OE1	51:Z:45:ARG:NE	2.49	0.45
1:a:1308:U:H2'	1:a:1309:G:H8	1.81	0.45
26:v:36:PHE:CZ	26:v:266:ASP:HB3	2.51	0.45
27:A:1405:U:H2'	27:A:1406:U:C6	2.51	0.45
27:A:2103:C:H2'	27:A:2104:C:C6	2.51	0.45
37:L:69:ARG:HG3	37:L:90:GLU:HG3	1.98	0.45
1:a:362:G:N2	1:a:365:U:OP2	2.49	0.45
1:a:1253:G:H2'	1:a:1254:A:C8	2.51	0.45
11:k:64:GLN:HG3	11:k:99:ALA:HB2	1.98	0.45
23:y:35:A:H8	23:y:35:A:OP2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:y:55:PSU:N3	23:y:58:A:OP2	2.49	0.45
28:B:41:G:O6	32:F:69:LYS:NZ	2.49	0.45
33:G:22:GLN:HE21	33:G:39:ASP:HA	1.81	0.45
48:W:4:LYS:O	48:W:94:ARG:NH1	2.42	0.45
1:a:216:U:H2'	1:a:217:C:H6	1.80	0.45
20:t:35:VAL:HG11	20:t:79:LEU:HD13	1.98	0.45
23:y:23:A:H2'	23:y:24:G:C8	2.51	0.45
25:w:12:LEU:HG	25:w:45:LEU:HD13	1.97	0.45
26:v:241:PHE:HB3	26:v:251:ILE:HG21	1.98	0.45
46:U:2:GLU:HG2	46:U:108:SER:OG	2.17	0.45
1:a:636:U:H2'	1:a:637:C:C6	2.51	0.45
1:a:1142:G:C2	1:a:1143:G:H1'	2.52	0.45
2:b:117:LEU:HB3	2:b:141:LEU:HD13	1.99	0.45
13:m:77:ILE:HG22	13:m:81:MET:HE2	1.98	0.45
16:p:18:GLN:OE1	16:p:35:ARG:HD2	2.16	0.45
26:v:243:LYS:O	26:v:247:LEU:HD23	2.17	0.45
27:A:351:C:H2'	27:A:352:A:C8	2.51	0.45
27:A:358:U:N3	27:A:359:G:N7	2.65	0.45
27:A:885:C:H2'	27:A:886:A:C8	2.51	0.45
27:A:2591:C:H2'	27:A:2592:G:H8	1.82	0.45
1:a:155:A:H2'	1:a:156:C:C6	2.51	0.45
1:a:519:C:O5'	25:w:306:ARG:NH2	2.46	0.45
1:a:1319:A:O2'	1:a:1323:G:N7	2.45	0.45
4:d:109:ALA:HB3	4:d:113:GLU:HG3	1.98	0.45
6:f:71:ILE:HA	6:f:74:LEU:HD12	1.99	0.45
26:v:191:TYR:HE1	26:v:206:ILE:HG23	1.82	0.45
27:A:2144:G:N2	27:A:2146:C:O2'	2.50	0.45
38:M:2:ILE:HD12	38:M:8:LEU:HD21	1.98	0.45
1:a:745:G:H2'	1:a:746:A:H8	1.80	0.45
1:a:993:G:O2'	1:a:995:C:N4	2.44	0.45
26:v:32:LYS:HD2	26:v:262:ASN:HD22	1.81	0.45
27:A:288:U:H2'	27:A:289:G:H8	1.82	0.45
27:A:703:U:H2'	27:A:704:G:O4'	2.17	0.45
27:A:1607:C:N4	27:A:1622:G:OP2	2.37	0.45
27:A:2020:A:H5'	55:4:9:THR:HG21	1.98	0.45
36:J:111:GLN:CD	36:J:111:GLN:H	2.25	0.45
38:M:107:LEU:HB2	38:M:116:ILE:HD11	1.98	0.45
41:P:103:ARG:HE	41:P:110:MET:HE2	1.80	0.45
55:4:31:ASP:OD1	55:4:32:LYS:N	2.49	0.45
2:b:49:MET:HA	2:b:52:GLU:CD	2.41	0.45
2:b:109:GLN:N	2:b:109:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:v:214:ASP:OD1	26:v:215:LEU:N	2.48	0.45
26:v:412:LEU:HD12	26:v:459:VAL:HG11	1.99	0.45
32:F:103:LEU:HA	32:F:107:ALA:HB3	1.99	0.45
48:W:96:PHE:N	48:W:101:GLU:O	2.44	0.45
51:Z:32:ASN:OD1	51:Z:34:HIS:NE2	2.49	0.45
1:a:89:U:H2'	1:a:90:C:C6	2.51	0.45
1:a:951:G:HO2'	1:a:970:C:HO2'	1.63	0.45
1:a:1119:C:H2'	1:a:1120:C:H6	1.82	0.45
27:A:1469:A:H2'	27:A:1470:A:H8	1.82	0.45
1:a:1530:G:H2'	1:a:1531:A:C8	2.52	0.45
26:v:169:ILE:HD13	26:v:241:PHE:HE1	1.82	0.45
26:v:346:LEU:HD23	26:v:346:LEU:H	1.82	0.45
31:E:149:ILE:HB	31:E:188:MET:HG2	1.99	0.45
1:a:235:C:H2'	1:a:236:A:C8	2.52	0.44
1:a:309:A:H2'	1:a:310:G:H8	1.82	0.44
1:a:555:U:H2'	1:a:556:C:H6	1.82	0.44
10:j:86:ALA:HA	10:j:89:ARG:HG2	1.99	0.44
26:v:192:LEU:HB2	26:v:204:VAL:HG11	1.99	0.44
27:A:64:A:H2'	27:A:65:U:C6	2.52	0.44
27:A:582:A:H2'	27:A:583:G:H8	1.82	0.44
27:A:2139:U:H2'	27:A:2140:G:C8	2.52	0.44
41:P:38:LEU:HB3	41:P:39:PRO:HD3	1.99	0.44
56:5:25:LYS:NZ	56:5:30:LYS:O	2.49	0.44
4:d:10:LYS:HE3	4:d:10:LYS:HB2	1.77	0.44
7:g:68:ASN:OD1	7:g:130:ASN:ND2	2.50	0.44
10:j:52:LEU:O	14:n:81:ARG:NH1	2.47	0.44
27:A:574:A:N6	27:A:2034:U:OP1	2.51	0.44
27:A:2467:C:OP1	59:8:8:LYS:NZ	2.49	0.44
30:D:133:THR:HG22	30:D:134:HIS:N	2.27	0.44
46:U:55:ILE:HG23	46:U:66:ILE:HD12	1.99	0.44
58:7:62:LEU:HB3	58:7:65:ALA:HB3	1.99	0.44
1:a:1063:C:OP2	1:a:1064:G:O2'	2.33	0.44
21:u:34:ARG:HE	21:u:35:ARG:HG3	1.83	0.44
29:C:145:GLU:HG2	29:C:151:GLY:C	2.42	0.44
1:a:642:A:N7	8:h:107:SER:HA	2.33	0.44
1:a:1002:G:C2	1:a:1003:G:H1'	2.52	0.44
4:d:124:MET:HE3	4:d:146:ARG:HB2	1.99	0.44
14:n:64:CYS:HB3	14:n:68:GLY:H	1.82	0.44
26:v:111:MET:SD	26:v:139:THR:HG22	2.57	0.44
26:v:331:LEU:HD22	26:v:342:ILE:HD12	1.99	0.44
27:A:3:U:H2'	27:A:4:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2141:G:H2'	27:A:2142:A:H8	1.81	0.44
35:I:15:VAL:HA	35:I:18:VAL:HG12	2.00	0.44
35:I:80:THR:O	35:I:82:ILE:HG23	2.16	0.44
1:a:880:C:OP1	12:l:9:ARG:NH1	2.51	0.44
6:f:46:GLN:NE2	6:f:55:HIS:HB3	2.33	0.44
9:i:12:ARG:HG2	9:i:74:GLY:HA2	2.00	0.44
27:A:2579:C:O2'	30:D:136:ASN:OD1	2.35	0.44
28:B:14:U:OP2	28:B:70:C:O2'	2.35	0.44
36:J:22:PRO:N	36:J:23:PRO:HD2	2.33	0.44
1:a:1081:A:N7	5:e:52:LYS:NZ	2.65	0.44
3:c:65:ARG:HE	3:c:100:GLN:NE2	2.14	0.44
5:e:153:VAL:HA	5:e:156:LYS:HG2	2.00	0.44
6:f:43:GLY:HA2	6:f:58:HIS:CE1	2.53	0.44
8:h:87:LYS:HG3	8:h:125:ILE:HD11	1.99	0.44
23:y:8:4SU:H2'	23:y:13:C:H41	1.83	0.44
23:y:26:A:N6	23:y:44:G:C6	2.84	0.44
26:v:395:PRO:HB2	26:v:440:ALA:H	1.83	0.44
27:A:2154:A:H2'	27:A:2155:U:C6	2.53	0.44
27:A:2286:G:H1	56:5:23:THR:HG21	1.82	0.44
29:C:185:GLU:HG3	29:C:187:ASP:H	1.82	0.44
1:a:80:A:H2'	1:a:81:A:C2	2.52	0.44
1:a:246:A:C2	1:a:282:A:C5	3.05	0.44
1:a:1107:C:C4	1:a:1108:G:C8	3.06	0.44
1:a:1495:U:O2'	27:A:1919:A:N1	2.42	0.44
10:j:39:PRO:HA	10:j:74:VAL:HG12	1.99	0.44
26:v:280:MET:HB2	26:v:281:PRO:HD2	1.98	0.44
27:A:636:G:OP1	39:N:129:LYS:NZ	2.40	0.44
54:3:34:LEU:HD23	54:3:34:LEU:H	1.83	0.44
1:a:35:G:H2'	1:a:36:C:C6	2.52	0.44
1:a:210:C:O3'	1:a:211:G:N2	2.51	0.44
27:A:222:A:C2	27:A:233:A:H5''	2.52	0.44
27:A:1385:A:O2'	27:A:1396:U:O2	2.36	0.44
27:A:1752:C:H2'	27:A:1753:G:C8	2.52	0.44
27:A:2191:A:O2'	27:A:2192:U:OP1	2.30	0.44
1:a:719:C:H1'	18:r:38:LYS:HB3	2.00	0.44
5:e:69:ARG:O	5:e:69:ARG:HG2	2.18	0.44
11:k:109:ASN:HD21	21:u:5:LYS:HG3	1.83	0.44
12:l:5:ASN:O	12:l:9:ARG:HG3	2.18	0.44
26:v:139:THR:OG1	26:v:254:VAL:HA	2.17	0.44
27:A:363:G:H2'	27:A:364:C:H6	1.83	0.44
27:A:848:C:H2'	27:A:849:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1046:A:H61	35:I:8:LYS:NZ	2.16	0.44
27:A:1571:A:H2'	27:A:1572:A:H8	1.83	0.44
27:A:2804:U:H2'	27:A:2805:C:H6	1.83	0.44
30:D:35:THR:HG22	30:D:73:VAL:HG21	2.00	0.44
33:G:72:LEU:O	33:G:75:MET:HG2	2.18	0.44
1:a:1286:U:H2'	1:a:1287:A:H5'	1.98	0.43
23:y:19:G:O4'	23:y:57:G:N2	2.51	0.43
27:A:155:A:H2'	27:A:156:A:C8	2.53	0.43
27:A:832:U:H2'	27:A:833:A:C8	2.53	0.43
27:A:1790:C:H2'	27:A:1791:A:C8	2.53	0.43
27:A:1856:U:H2'	27:A:1857:G:O4'	2.18	0.43
27:A:2037:A:H2'	27:A:2038:G:C8	2.53	0.43
1:a:715:A:H2'	1:a:716:A:C8	2.52	0.43
1:a:744:C:H2'	1:a:745:G:C8	2.49	0.43
1:a:1060:U:H2'	1:a:1061:G:H8	1.83	0.43
2:b:136:MET:O	2:b:139:ARG:N	2.52	0.43
4:d:111:ARG:O	4:d:115:ARG:HG2	2.18	0.43
26:v:165:GLY:O	26:v:251:ILE:HA	2.18	0.43
27:A:373:U:H2'	27:A:374:A:H8	1.82	0.43
27:A:1013:C:H2'	27:A:1014:A:H8	1.83	0.43
27:A:1032:A:OP1	59:8:8:LYS:HG2	2.18	0.43
27:A:2099:U:H2'	27:A:2100:G:H8	1.82	0.43
31:E:146:VAL:HG12	31:E:167:VAL:HG12	1.99	0.43
1:a:1273:C:H2'	1:a:1274:A:O4'	2.18	0.43
22:x:51:U:H2'	22:x:52:G:C8	2.54	0.43
26:v:402:ARG:HE	26:v:464:GLU:CD	2.25	0.43
27:A:871:U:H2'	27:A:872:U:C6	2.53	0.43
2:b:67:ILE:H	2:b:89:GLN:NE2	2.16	0.43
11:k:109:ASN:HD22	21:u:5:LYS:HA	1.84	0.43
13:m:88:GLY:O	13:m:92:ARG:HG3	2.17	0.43
23:y:9:A:H4'	23:y:46:G7M:OP2	2.18	0.43
26:v:413:LEU:HD12	26:v:413:LEU:HA	1.74	0.43
26:v:481:LYS:O	26:v:484:GLU:HG3	2.18	0.43
27:A:306:U:H2'	27:A:307:G:O4'	2.18	0.43
27:A:1425:G:H2'	27:A:1426:G:C8	2.53	0.43
27:A:1571:A:H2'	27:A:1572:A:C8	2.54	0.43
27:A:2074:U:H2'	27:A:2075:U:C6	2.53	0.43
1:a:1088:G:N2	1:a:1167:A:H61	2.14	0.43
6:f:72:ASP:O	6:f:76:THR:HG23	2.17	0.43
26:v:297:THR:O	26:v:321:VAL:HG12	2.18	0.43
26:v:414:LYS:C	26:v:416:LEU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:359:G:H2'	27:A:360:U:C6	2.54	0.43
35:I:116:GLU:OE1	35:I:118:ILE:HG13	2.19	0.43
54:3:20:ASN:ND2	54:3:39:LYS:HG3	2.33	0.43
1:a:154:U:H2'	1:a:155:A:C8	2.54	0.43
20:t:39:ILE:HG23	20:t:86:LEU:HD21	1.99	0.43
26:v:123:THR:O	26:v:123:THR:HG22	2.18	0.43
26:v:178:LEU:H	26:v:178:LEU:HD23	1.82	0.43
27:A:1111:A:HO2'	27:A:1112:G:P	2.38	0.43
27:A:1720:U:H2'	27:A:1721:G:O4'	2.19	0.43
27:A:1853:A:H2'	27:A:1854:A:C8	2.54	0.43
27:A:2142:A:H2'	27:A:2143:C:C6	2.53	0.43
27:A:2233:U:H2'	27:A:2234:G:H8	1.83	0.43
28:B:111:U:H2'	28:B:112:G:C8	2.52	0.43
59:8:27:CYS:SG	59:8:33:HIS:HB2	2.58	0.43
2:b:64:LYS:HA	2:b:225:ARG:HH12	1.84	0.43
7:g:149:LYS:HB2	7:g:149:LYS:HE3	1.79	0.43
10:j:24:GLU:O	10:j:27:GLU:HG3	2.19	0.43
19:s:67:VAL:O	54:3:56:ARG:NH2	2.41	0.43
23:y:50:U:H2'	23:y:51:U:O4'	2.18	0.43
25:w:93:GLU:O	25:w:97:GLN:HG2	2.19	0.43
27:A:784:G:H5'	27:A:785:G:OP1	2.19	0.43
40:O:2:LEU:HD12	40:O:68:PHE:CE1	2.53	0.43
1:a:390:U:H2'	1:a:391:G:H8	1.81	0.43
14:n:26:GLU:OE2	14:n:27:LEU:HD12	2.18	0.43
22:x:15:G:N2	22:x:21:A:N3	2.67	0.43
22:x:47:U:O2'	22:x:48:C:OP1	2.32	0.43
26:v:93:GLU:N	26:v:93:GLU:OE1	2.52	0.43
27:A:1107:G:H4'	35:I:80:THR:HA	2.00	0.43
27:A:2215:C:H2'	27:A:2216:G:H8	1.84	0.43
1:a:1011:C:H2'	1:a:1012:A:C8	2.54	0.43
3:c:89:LYS:HB2	3:c:89:LYS:HE3	1.87	0.43
23:y:2:C:H2'	23:y:3:C:C6	2.53	0.43
27:A:365:U:H2'	27:A:366:C:H6	1.84	0.43
27:A:876:C:H2'	27:A:877:A:O4'	2.18	0.43
27:A:1794:A:H2'	27:A:1795:C:H6	1.82	0.43
27:A:2139:U:H2'	27:A:2140:G:H8	1.84	0.43
35:I:42:ARG:NH1	36:J:120:ALA:HA	2.33	0.43
47:V:25:GLU:OE1	47:V:26:LYS:NZ	2.52	0.43
51:Z:39:TRP:HE1	51:Z:41:GLU:CD	2.27	0.43
52:1:27:ASN:O	52:1:31:GLN:HG3	2.19	0.43
1:a:636:U:H2'	1:a:637:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:676:A:H2'	1:a:677:U:H6	1.84	0.43
1:a:936:C:C4	1:a:937:A:N7	2.87	0.43
1:a:1017:U:H2'	1:a:1018:G:H8	1.83	0.43
4:d:198:HIS:O	4:d:202:GLU:HG3	2.19	0.43
7:g:37:SER:O	7:g:40:GLU:HG2	2.18	0.43
10:j:8:ILE:HB	10:j:74:VAL:HG22	2.01	0.43
23:y:61:C:H2'	23:y:62:C:C6	2.54	0.43
26:v:74:VAL:HG12	26:v:87:LEU:HD13	2.01	0.43
26:v:266:ASP:OD1	26:v:267:HIS:N	2.51	0.43
26:v:403:LEU:HD23	26:v:403:LEU:H	1.83	0.43
27:A:1434:A:H2'	27:A:1435:G:C8	2.54	0.43
27:A:2266:A:H4'	27:A:2267:A:N3	2.33	0.43
36:J:21:SER:HB3	36:J:23:PRO:HD2	2.01	0.43
36:J:55:ILE:HG13	36:J:55:ILE:O	2.19	0.43
39:N:62:PRO:HG2	58:7:25:LYS:HD3	2.00	0.43
1:a:167:A:N6	1:a:168:G:O6	2.52	0.42
1:a:966:2MG:N2	22:x:34:G:H5'	2.34	0.42
2:b:87:CYS:O	2:b:89:GLN:HG2	2.19	0.42
6:f:70:VAL:HA	6:f:73:GLU:OE2	2.19	0.42
22:x:26:A:N6	22:x:44:G:H1	2.13	0.42
23:y:49:C:H2'	23:y:50:U:C6	2.53	0.42
26:v:168:PRO:HA	26:v:254:VAL:CG2	2.49	0.42
27:A:624:C:O2'	27:A:657:U:OP1	2.34	0.42
27:A:1028:A:H2'	27:A:1029:A:H8	1.83	0.42
27:A:1198:U:H2'	27:A:1199:U:H6	1.84	0.42
1:a:642:A:C8	8:h:107:SER:HA	2.54	0.42
1:a:768:A:H4'	1:a:1523:G:N2	2.35	0.42
2:b:32:PHE:HB2	2:b:42:ASN:HB2	2.01	0.42
7:g:106:GLU:HG3	7:g:110:LYS:HE3	2.00	0.42
26:v:152:MET:SD	26:v:153:GLU:N	2.92	0.42
27:A:1138:G:N3	37:L:108:MET:HE2	2.34	0.42
32:F:127:ASN:HB2	32:F:156:ILE:O	2.20	0.42
35:I:51:TYR:CE2	35:I:89:PRO:HD3	2.55	0.42
1:a:41:G:H2'	1:a:42:G:H8	1.83	0.42
1:a:501:C:H2'	1:a:502:A:C8	2.54	0.42
1:a:593:U:H2'	1:a:594:U:C6	2.54	0.42
26:v:269:LEU:HD23	26:v:269:LEU:HA	1.89	0.42
26:v:471:ALA:O	26:v:472:ARG:HG2	2.20	0.42
27:A:1159:U:C2	27:A:1160:G:C8	3.07	0.42
27:A:1673:G:O6	30:D:134:HIS:HD2	2.02	0.42
28:B:106:G:H2'	28:B:107:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D:120:GLY:O	30:D:124:ARG:HB2	2.19	0.42
1:a:399:G:H2'	1:a:400:C:C6	2.55	0.42
1:a:405:U:O4	4:d:3:ARG:N	2.50	0.42
1:a:1026:G:C2	1:a:1027:C:C2	3.07	0.42
1:a:1409:C:H2'	1:a:1410:A:H8	1.84	0.42
2:b:118:GLU:OE2	2:b:122:GLN:NE2	2.53	0.42
27:A:64:A:H2'	27:A:65:U:H6	1.83	0.42
27:A:353:C:H2'	27:A:354:A:C8	2.53	0.42
27:A:419:U:H2'	27:A:420:C:H6	1.85	0.42
27:A:851:C:H2'	27:A:852:U:C6	2.54	0.42
27:A:2014:A:H2'	27:A:2015:A:C8	2.54	0.42
27:A:2070:A:H2'	27:A:2071:A:H8	1.84	0.42
27:A:2187:U:H2'	27:A:2188:U:C6	2.54	0.42
27:A:2532:G:N2	27:A:2663:G:O2'	2.52	0.42
30:D:2:ILE:HD11	30:D:84:LEU:HD12	2.00	0.42
1:a:214:C:H2'	1:a:215:C:H6	1.84	0.42
1:a:1060:U:OP1	14:n:85:ARG:NH2	2.52	0.42
2:b:205:ASP:OD1	2:b:206:ALA:N	2.52	0.42
15:o:48:LYS:HA	15:o:48:LYS:HD3	1.79	0.42
25:w:76:GLU:HG2	25:w:77:MET:N	2.33	0.42
27:A:813:U:H2'	27:A:814:C:C6	2.55	0.42
27:A:2191:A:HO2'	27:A:2192:U:P	2.42	0.42
27:A:2243:U:H2'	27:A:2244:U:H6	1.84	0.42
27:A:2591:C:H2'	27:A:2592:G:C8	2.55	0.42
35:I:18:VAL:HB	35:I:86:MET:HE3	2.01	0.42
37:L:11:VAL:HG11	37:L:50:THR:HG22	2.01	0.42
37:L:40:HIS:H	37:L:40:HIS:CD2	2.37	0.42
48:W:72:ILE:HD13	48:W:103:ILE:HD13	2.01	0.42
1:a:1315:U:H2'	1:a:1316:G:O4'	2.20	0.42
9:i:19:VAL:HG23	9:i:65:ILE:HG12	2.02	0.42
9:i:47:VAL:HA	9:i:50:GLN:HG3	2.01	0.42
13:m:107:ARG:NH1	13:m:111:GLY:O	2.53	0.42
25:w:76:GLU:O	25:w:79:GLN:HG3	2.20	0.42
26:v:121:ASP:HA	26:v:124:ARG:NH1	2.35	0.42
27:A:458:G:C8	57:6:37:LYS:HG2	2.55	0.42
27:A:2489:U:H2'	27:A:2490:G:O4'	2.19	0.42
27:A:2645:G:OP2	27:A:2645:G:N2	2.34	0.42
32:F:101:GLU:HG3	32:F:102:ARG:N	2.35	0.42
32:F:126:GLY:O	32:F:158:THR:OG1	2.37	0.42
32:F:128:TYR:CE2	32:F:130:MET:HB3	2.55	0.42
49:X:24:ASN:ND2	49:X:45:ASP:OD2	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Y:68:LYS:NZ	50:Y:69:PHE:O	2.47	0.42
1:a:687:A:C2	1:a:704:A:C5	3.08	0.42
1:a:1022:A:H2'	1:a:1023:U:O4'	2.19	0.42
2:b:19:GLN:N	2:b:19:GLN:OE1	2.53	0.42
6:f:2:ARG:HE	6:f:91:ARG:HH21	1.67	0.42
12:l:30:LYS:HD2	12:l:30:LYS:HA	1.88	0.42
14:n:49:GLN:HE22	19:s:12:ASP:HA	1.85	0.42
14:n:83:LYS:HA	14:n:83:LYS:HD3	1.70	0.42
23:y:58:A:H2	23:y:60:U:H2'	1.85	0.42
27:A:3:U:H2'	27:A:4:U:H6	1.83	0.42
27:A:5:A:H2'	27:A:6:A:H8	1.84	0.42
27:A:1198:U:C2	27:A:1199:U:C5	3.08	0.42
27:A:1433:A:H2'	27:A:1434:A:H8	1.82	0.42
27:A:2484:G:OP1	40:O:44:ARG:HD2	2.20	0.42
35:l:3:LEU:HD23	35:l:3:LEU:H	1.83	0.42
37:L:102:GLU:HG2	37:L:124:VAL:HG21	2.01	0.42
40:O:41:LEU:HD23	40:O:41:LEU:HA	1.94	0.42
1:a:111:G:H1	1:a:330:C:H42	1.68	0.42
1:a:1316:G:N1	1:a:1319:A:OP2	2.50	0.42
2:b:142:GLU:HA	2:b:145:GLU:HG2	2.02	0.42
12:l:31:ARG:HE	12:l:31:ARG:HB3	1.69	0.42
27:A:288:U:H2'	27:A:289:G:C8	2.55	0.42
27:A:438:G:H2'	27:A:439:A:C8	2.55	0.42
27:A:1295:C:C2	27:A:1296:G:C8	3.07	0.42
32:F:46:ASP:HB3	32:F:49:LEU:HD23	2.01	0.42
36:J:122:ILE:HD12	36:J:122:ILE:H	1.84	0.42
37:L:98:GLU:O	37:L:102:GLU:HG3	2.19	0.42
57:6:42:LEU:HD23	57:6:42:LEU:HA	1.92	0.42
1:a:56:U:H2'	1:a:57:G:H8	1.85	0.42
1:a:323:U:H2'	1:a:324:G:O4'	2.20	0.42
1:a:1125:U:O2'	1:a:1126:U:O5'	2.33	0.42
1:a:1518:MA6:O5'	1:a:1518:MA6:H8	2.20	0.42
9:i:91:ASP:HB3	9:i:94:LEU:HD23	2.01	0.42
10:j:12:ALA:HB3	10:j:18:ILE:HB	2.02	0.42
11:k:122:ARG:HA	11:k:123:PRO:HD3	1.92	0.42
23:y:52:G:H2'	23:y:53:G:C8	2.53	0.42
25:w:116:ARG:HG3	25:w:202:THR:OG1	2.20	0.42
26:v:15:THR:HG22	26:v:85:ASN:HB2	2.01	0.42
27:A:2:G:H2'	27:A:3:U:C6	2.54	0.42
27:A:296:U:H2'	27:A:297:G:H8	1.85	0.42
27:A:1045:C:H1'	27:A:1047:G:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1883:U:H2'	27:A:1884:G:O4'	2.20	0.42
27:A:2081:U:H2'	27:A:2082:A:H8	1.85	0.42
27:A:2146:C:H4'	27:A:2147:A:C5	2.55	0.42
32:F:58:ALA:HB2	32:F:65:PRO:HD3	2.02	0.42
1:a:1057:G:O2'	3:c:188:GLU:OE2	2.21	0.42
2:b:112:LYS:HA	2:b:112:LYS:HD2	1.79	0.42
5:e:151:GLU:OE2	5:e:151:GLU:N	2.49	0.42
26:v:154:LEU:C	26:v:154:LEU:HD23	2.44	0.42
26:v:304:GLN:HE22	26:v:306:ASN:HB3	1.85	0.42
26:v:346:LEU:HD23	26:v:366:GLY:O	2.19	0.42
27:A:2273:A:H2'	27:A:2274:A:C8	2.55	0.42
27:A:2728:U:O2'	27:A:2729:G:H8	2.01	0.42
27:A:2845:U:H5''	43:R:52:ASN:O	2.20	0.42
32:F:122:PHE:HE2	32:F:167:ARG:HB2	1.84	0.42
1:a:1088:G:H21	1:a:1167:A:N6	2.14	0.41
16:p:67:ILE:HG22	16:p:68:SER:O	2.20	0.41
26:v:357:GLU:N	26:v:357:GLU:OE1	2.53	0.41
27:A:2529:G:H4'	33:G:175:LYS:HD3	2.02	0.41
27:A:2820:A:N3	27:A:2820:A:H2'	2.35	0.41
36:J:22:PRO:HA	36:J:26:PRO:HD2	2.02	0.41
51:Z:6:GLN:O	51:Z:74:ARG:NH2	2.53	0.41
1:a:231:U:H2'	1:a:232:G:H8	1.85	0.41
1:a:883:C:O2'	1:a:884:U:H5'	2.20	0.41
5:e:65:GLU:OE2	5:e:68:ARG:NH2	2.53	0.41
19:s:11:ILE:HB	19:s:41:PHE:HE2	1.84	0.41
26:v:305:ALA:O	26:v:307:MET:HG2	2.20	0.41
27:A:365:U:H2'	27:A:366:C:C6	2.55	0.41
27:A:728:G:H4'	29:C:13:ARG:HD3	2.02	0.41
27:A:859:G:O2'	27:A:916:G:O6	2.28	0.41
27:A:1224:U:H2'	27:A:1225:G:C8	2.55	0.41
27:A:2052:A:H4'	30:D:148:GLN:O	2.19	0.41
27:A:2367:G:C2	27:A:2368:C:C5	3.08	0.41
27:A:2662:A:H2'	27:A:2663:G:O4'	2.19	0.41
28:B:114:C:H2'	28:B:115:A:H8	1.85	0.41
36:J:92:LYS:HB3	36:J:95:LYS:HE2	2.01	0.41
48:W:81:ASP:OD1	48:W:98:SER:OG	2.37	0.41
58:7:8:ARG:HA	58:7:8:ARG:HD2	1.86	0.41
25:w:31:ASP:N	25:w:31:ASP:OD1	2.49	0.41
25:w:91:GLN:NE2	25:w:95:GLN:HG2	2.36	0.41
26:v:414:LYS:HA	26:v:417:VAL:HG12	2.03	0.41
27:A:1198:U:H2'	27:A:1199:U:C6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1605:C:N4	27:A:1606:C:H41	2.18	0.41
33:G:33:LEU:HD12	33:G:79:VAL:HG23	2.01	0.41
35:I:116:GLU:C	35:I:117:LEU:HD23	2.46	0.41
38:M:26:GLY:HA3	38:M:30:ARG:HH11	1.85	0.41
1:a:321:A:H2'	1:a:322:C:C6	2.55	0.41
1:a:436:C:H2'	1:a:437:U:C6	2.56	0.41
6:f:18:VAL:HG11	6:f:58:HIS:CE1	2.56	0.41
6:f:37:HIS:HB3	6:f:97:THR:OG1	2.19	0.41
26:v:397:LEU:O	26:v:397:LEU:HD23	2.21	0.41
27:A:675:A:N3	27:A:2443:C:O2'	2.49	0.41
27:A:1532:A:N6	27:A:1540:G:O6	2.53	0.41
29:C:30:PHE:HD2	29:C:33:LEU:HD12	1.85	0.41
33:G:28:GLY:HA3	33:G:79:VAL:CG1	2.51	0.41
1:a:139:A:H2'	1:a:140:U:C6	2.56	0.41
1:a:398:U:H2'	1:a:399:G:H8	1.85	0.41
4:d:62:ARG:HH21	4:d:68:LEU:HA	1.85	0.41
10:j:52:LEU:HD21	10:j:59:LYS:HD2	2.01	0.41
12:l:90:LEU:HA	12:l:91:PRO:HD3	1.95	0.41
14:n:52:PRO:O	14:n:55:SER:OG	2.33	0.41
26:v:121:ASP:HA	26:v:124:ARG:HH12	1.85	0.41
27:A:419:U:H2'	27:A:420:C:C6	2.56	0.41
27:A:1038:G:H2'	27:A:1039:A:C8	2.56	0.41
27:A:1542:U:H2'	27:A:1543:G:O4'	2.20	0.41
1:a:270:A:H2'	1:a:271:C:C6	2.56	0.41
1:a:868:C:H2'	1:a:869:G:O4'	2.21	0.41
1:a:1272:G:H2'	1:a:1273:C:C6	2.56	0.41
5:e:15:LEU:HD12	5:e:37:THR:HG22	2.02	0.41
9:i:41:ARG:NH1	9:i:43:THR:OG1	2.54	0.41
19:s:41:PHE:O	19:s:44:MET:HG2	2.21	0.41
27:A:967:U:H2'	27:A:968:C:C6	2.56	0.41
27:A:2462:C:H1'	27:A:2491:U:O4	2.21	0.41
30:D:13:ARG:HD2	43:R:56:HIS:ND1	2.36	0.41
35:I:45:GLY:HA2	35:I:49:GLY:O	2.20	0.41
37:L:49:ASP:CG	37:L:121:LYS:HZ3	2.24	0.41
1:a:8:A:N6	4:d:202:GLU:O	2.53	0.41
1:a:155:A:H2'	1:a:156:C:H6	1.85	0.41
1:a:294:U:H2'	1:a:295:C:C6	2.56	0.41
1:a:384:G:H2'	1:a:385:C:H6	1.85	0.41
1:a:1513:A:H2'	1:a:1514:G:C8	2.56	0.41
16:p:58:ALA:HA	16:p:61:VAL:HG12	2.03	0.41
21:u:4:ILE:HG13	21:u:19:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:w:91:GLN:O	25:w:94:GLN:HG3	2.20	0.41
27:A:181:A:H1'	27:A:435:C:H5'	2.02	0.41
27:A:593:U:H2'	27:A:594:U:H6	1.85	0.41
27:A:1281:G:H2'	27:A:1282:U:C6	2.56	0.41
27:A:2070:A:H2'	27:A:2071:A:C8	2.55	0.41
28:B:48:U:H2'	28:B:49:C:C6	2.55	0.41
32:F:36:LEU:HD22	32:F:154:ILE:HG12	2.02	0.41
35:I:68:PRO:HA	35:I:72:LEU:HD11	2.02	0.41
38:M:114:LYS:HE2	38:M:118:LEU:HD11	2.02	0.41
1:a:1000:A:H2'	1:a:1001:C:H6	1.85	0.41
2:b:55:ALA:HA	2:b:58:ASN:HD21	1.85	0.41
13:m:86:TYR:O	13:m:90:ARG:HG2	2.20	0.41
25:w:114:GLU:HB3	25:w:163:ILE:HG23	2.03	0.41
26:v:360:TYR:N	26:v:363:ASP:OD2	2.45	0.41
26:v:472:ARG:HD3	26:v:524:HIS:HB3	2.03	0.41
27:A:1102:C:C2	27:A:1103:A:C8	3.09	0.41
27:A:1196:C:C2	27:A:1197:G:C8	3.09	0.41
27:A:2020:A:H62	55:4:6:ASN:ND2	2.19	0.41
27:A:2305:U:C2	32:F:151:GLY:HA3	2.56	0.41
27:A:2313:C:H2'	27:A:2314:A:H8	1.86	0.41
29:C:16:VAL:HG22	29:C:206:GLY:HA3	2.03	0.41
29:C:75:PRO:HG2	29:C:97:LYS:HG3	2.03	0.41
53:2:40:ASP:OD1	53:2:45:ARG:NE	2.40	0.41
1:a:425:G:H2'	1:a:426:U:C6	2.56	0.41
1:a:618:C:H5''	1:a:619:U:H5''	2.03	0.41
1:a:1001:C:H2'	1:a:1002:G:H8	1.84	0.41
1:a:1095:U:H2'	1:a:1096:C:C6	2.56	0.41
1:a:1518:MA6:H92	1:a:1519:MA6:N6	2.35	0.41
3:c:174:PRO:HB2	3:c:177:THR:HG22	2.03	0.41
7:g:47:LEU:HD23	7:g:47:LEU:HA	1.88	0.41
20:t:81:ALA:O	20:t:85:LYS:HG3	2.21	0.41
23:y:28:G:H1	23:y:42:C:H42	1.69	0.41
25:w:108:GLU:HB2	25:w:170:GLY:HA2	2.01	0.41
27:A:27:G:H22	27:A:512:G:H1'	1.86	0.41
27:A:155:A:H2'	27:A:156:A:H8	1.85	0.41
27:A:993:G:H1'	45:T:91:GLN:HE21	1.85	0.41
27:A:1036:G:C6	27:A:1120:G:C6	3.09	0.41
27:A:1563:U:H2'	27:A:1564:C:C6	2.56	0.41
27:A:1575:C:H2'	27:A:1576:U:C6	2.56	0.41
27:A:1928:A:H2'	27:A:1929:G:O4'	2.21	0.41
27:A:2039:U:H2'	27:A:2040:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:2290:G:H2'	27:A:2291:U:C6	2.56	0.41
27:A:2515:C:H2'	27:A:2516:A:H8	1.85	0.41
27:A:2567:G:H2'	27:A:2568:U:C6	2.56	0.41
27:A:2809:A:H2'	27:A:2810:A:C8	2.56	0.41
36:J:106:LEU:HD12	36:J:107:GLN:N	2.36	0.41
39:N:57:LEU:HD22	58:7:54:ASP:HB3	2.03	0.41
46:U:73:LYS:HB3	46:U:73:LYS:HE2	1.84	0.41
1:a:846:G:H2'	1:a:847:G:C8	2.56	0.41
1:a:1437:A:H2'	1:a:1438:G:H8	1.86	0.41
11:k:45:ALA:HB3	11:k:70:CYS:HB2	2.03	0.41
20:t:43:ASP:OD1	20:t:44:LYS:N	2.54	0.41
25:w:218:ASN:HD21	25:w:220:ALA:HB3	1.86	0.41
26:v:168:PRO:HA	26:v:254:VAL:HG22	2.02	0.41
27:A:480:A:O2'	48:W:43:LYS:O	2.39	0.41
27:A:2189:U:HO2'	27:A:2190:G:P	2.42	0.41
45:T:38:VAL:HG11	45:T:41:ILE:HG13	2.03	0.41
49:X:43:ASP:OD1	49:X:43:ASP:N	2.52	0.41
19:s:45:ILE:HD12	19:s:64:ASP:HA	2.03	0.40
27:A:145:C:H2'	27:A:146:A:H8	1.85	0.40
27:A:279:A:H2'	27:A:280:U:O4'	2.22	0.40
27:A:987:C:H2'	27:A:988:A:O4'	2.21	0.40
27:A:1387:A:H2'	27:A:1388:G:H8	1.86	0.40
27:A:1636:U:H2'	27:A:1637:A:C8	2.56	0.40
27:A:1790:C:H2'	27:A:1791:A:N7	2.36	0.40
27:A:2460:U:C2	27:A:2461:A:C8	3.09	0.40
27:A:2896:C:H2'	27:A:2897:U:H6	1.86	0.40
1:a:1319:A:C8	1:a:1323:G:C6	3.09	0.40
1:a:1477:U:H2'	1:a:1478:U:C6	2.56	0.40
2:b:27:MET:HB2	2:b:30:PHE:HD2	1.87	0.40
2:b:71:GLY:HA3	2:b:80:VAL:HG21	2.03	0.40
8:h:13:ARG:HD2	8:h:27:MET:HE2	2.03	0.40
9:i:88:MET:CE	9:i:104:VAL:HG22	2.51	0.40
25:w:92:LEU:HD12	25:w:93:GLU:N	2.36	0.40
26:v:25:GLY:HA3	26:v:142:ASN:HD22	1.86	0.40
26:v:172:PRO:HA	26:v:182:VAL:HG22	2.03	0.40
26:v:286:THR:OG1	26:v:287:ARG:N	2.55	0.40
27:A:281:C:N4	27:A:282:A:H62	2.20	0.40
27:A:513:A:H5'	27:A:1216:G:O2'	2.21	0.40
27:A:981:A:OP2	27:A:982:C:N4	2.47	0.40
27:A:1000:A:H2'	27:A:1001:A:C8	2.55	0.40
27:A:1670:C:O2	30:D:134:HIS:HE1	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1889:A:H2'	27:A:1890:A:C8	2.56	0.40
29:C:21:ASN:HB3	29:C:24:LEU:HG	2.02	0.40
36:J:15:ALA:HB2	36:J:55:ILE:HG12	2.03	0.40
48:W:95:PHE:HA	48:W:102:THR:HA	2.04	0.40
6:f:98:GLU:N	6:f:98:GLU:OE1	2.54	0.40
25:w:356:LEU:HD23	25:w:356:LEU:HA	1.95	0.40
27:A:84:A:OP1	48:W:6:ARG:NH2	2.54	0.40
27:A:1019:U:OP1	27:A:1035:U:O2'	2.34	0.40
27:A:2185:U:H2'	27:A:2186:G:C8	2.53	0.40
27:A:2698:U:H2'	27:A:2699:C:C6	2.56	0.40
28:B:42:C:C6	32:F:66:LEU:HB2	2.55	0.40
52:1:19:LEU:HD23	52:1:19:LEU:HA	1.89	0.40
1:a:592:G:H2'	1:a:593:U:C6	2.57	0.40
1:a:1010:U:H2'	1:a:1011:C:H6	1.86	0.40
1:a:1119:C:H2'	1:a:1120:C:C6	2.56	0.40
3:c:7:PRO:HD2	3:c:184:TYR:CD2	2.57	0.40
7:g:68:ASN:HD21	7:g:130:ASN:CG	2.29	0.40
11:k:25:ALA:O	11:k:88:GLY:HA3	2.21	0.40
18:r:25:ASP:OD1	18:r:25:ASP:N	2.46	0.40
20:t:79:LEU:HD23	20:t:79:LEU:HA	1.90	0.40
25:w:114:GLU:HA	25:w:162:ILE:O	2.21	0.40
26:v:169:ILE:HD12	26:v:169:ILE:HA	1.87	0.40
27:A:1112:G:H2'	27:A:1113:U:C6	2.57	0.40
27:A:2030:6MZ:C2	27:A:2499:C:H5''	2.51	0.40
27:A:2803:G:H2'	27:A:2804:U:C6	2.56	0.40
30:D:29:VAL:O	30:D:185:ASN:HB3	2.22	0.40
32:F:117:LEU:HD13	32:F:176:PRO:HG2	2.04	0.40
40:O:53:MET:HE1	40:O:103:TYR:CD2	2.57	0.40
1:a:925:G:C2	1:a:927:G:C8	3.10	0.40
2:b:104:TRP:HE1	2:b:108:ARG:NH2	2.19	0.40
3:c:6:HIS:HB3	14:n:89:MET:HE3	2.03	0.40
3:c:121:THR:HG23	3:c:189:ALA:HB2	2.03	0.40
12:l:89:D2T:OD1	12:l:89:D2T:N	2.53	0.40
22:x:50:U:H2'	22:x:51:U:C6	2.57	0.40
22:x:74:C:H3'	25:w:261:ARG:NH2	2.36	0.40
25:w:39:SER:OG	27:A:1067:A:O2'	2.25	0.40
25:w:71:ASP:N	25:w:71:ASP:OD1	2.55	0.40
27:A:697:G:H2'	27:A:698:C:C6	2.57	0.40
28:B:40:U:C6	54:3:2:LYS:HE3	2.57	0.40
33:G:133:LEU:HB3	33:G:141:ILE:HD11	2.02	0.40
35:I:40:GLU:OE2	35:I:102:ALA:HB1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:M:42:THR:HG22	38:M:57:VAL:HG22	2.04	0.40
49:X:64:VAL:HG13	49:X:64:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
3	c	204/233 (88%)	199 (98%)	5 (2%)	0	100	100
4	d	203/206 (98%)	203 (100%)	0	0	100	100
5	e	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
6	f	101/131 (77%)	97 (96%)	4 (4%)	0	100	100
7	g	150/156 (96%)	140 (93%)	10 (7%)	0	100	100
8	h	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	i	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
10	j	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	41
11	k	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
12	l	118/124 (95%)	112 (95%)	6 (5%)	0	100	100
13	m	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	p	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
17	q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
18	r	52/75 (69%)	51 (98%)	1 (2%)	0	100	100
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	t	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	u	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
25	w	345/360 (96%)	318 (92%)	27 (8%)	0	100	100
26	v	489/529 (92%)	425 (87%)	64 (13%)	0	100	100
29	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
30	D	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	24	57
31	E	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
32	F	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
33	G	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
34	H	37/149 (25%)	31 (84%)	6 (16%)	0	100	100
35	I	129/165 (78%)	102 (79%)	27 (21%)	0	100	100
36	J	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	18	49
37	L	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
38	M	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
39	N	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
40	O	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
41	P	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
42	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	R	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
44	S	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
45	T	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
46	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	V	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
48	W	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
49	X	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
50	Y	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
51	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
52	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
53	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
54	3	56/70 (80%)	56 (100%)	0	0	100	100
55	4	53/57 (93%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	5	49/55 (89%)	49 (100%)	0	0	100	100
57	6	44/46 (96%)	44 (100%)	0	0	100	100
58	7	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7	30
59	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	6546/7082 (92%)	6242 (95%)	300 (5%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	57	VAL
30	D	149	ASN
36	J	33	VAL
58	7	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	186/199 (94%)	186 (100%)	0	100	100
3	c	170/190 (90%)	170 (100%)	0	100	100
4	d	172/173 (99%)	172 (100%)	0	100	100
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	90 (100%)	0	100	100
7	g	125/129 (97%)	125 (100%)	0	100	100
8	h	104/105 (99%)	104 (100%)	0	100	100
9	i	105/107 (98%)	105 (100%)	0	100	100
10	j	86/90 (96%)	86 (100%)	0	100	100
11	k	89/98 (91%)	89 (100%)	0	100	100
12	l	101/103 (98%)	101 (100%)	0	100	100
13	m	93/96 (97%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	73/78 (94%)	73 (100%)	0	100	100
18	r	47/65 (72%)	47 (100%)	0	100	100
19	s	72/79 (91%)	72 (100%)	0	100	100
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	48/61 (79%)	48 (100%)	0	100	100
25	w	289/300 (96%)	289 (100%)	0	100	100
26	v	422/453 (93%)	422 (100%)	0	100	100
29	C	216/218 (99%)	216 (100%)	0	100	100
30	D	163/163 (100%)	163 (100%)	0	100	100
31	E	165/165 (100%)	165 (100%)	0	100	100
32	F	148/150 (99%)	148 (100%)	0	100	100
33	G	137/138 (99%)	137 (100%)	0	100	100
34	H	30/114 (26%)	30 (100%)	0	100	100
35	I	99/123 (80%)	99 (100%)	0	100	100
36	J	108/110 (98%)	108 (100%)	0	100	100
37	L	116/116 (100%)	116 (100%)	0	100	100
38	M	104/104 (100%)	104 (100%)	0	100	100
39	N	103/103 (100%)	103 (100%)	0	100	100
40	O	107/107 (100%)	107 (100%)	0	100	100
41	P	98/103 (95%)	98 (100%)	0	100	100
42	Q	86/87 (99%)	86 (100%)	0	100	100
43	R	99/100 (99%)	99 (100%)	0	100	100
44	S	89/90 (99%)	89 (100%)	0	100	100
45	T	84/84 (100%)	84 (100%)	0	100	100
46	U	93/93 (100%)	93 (100%)	0	100	100
47	V	80/84 (95%)	80 (100%)	0	100	100
48	W	83/85 (98%)	83 (100%)	0	100	100
49	X	78/78 (100%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Y	58/63 (92%)	58 (100%)	0	100	100
51	Z	67/68 (98%)	67 (100%)	0	100	100
52	1	54/55 (98%)	54 (100%)	0	100	100
53	2	48/49 (98%)	48 (100%)	0	100	100
54	3	53/62 (86%)	53 (100%)	0	100	100
55	4	46/48 (96%)	46 (100%)	0	100	100
56	5	46/49 (94%)	46 (100%)	0	100	100
57	6	38/38 (100%)	38 (100%)	0	100	100
58	7	51/52 (98%)	51 (100%)	0	100	100
59	8	34/34 (100%)	34 (100%)	0	100	100
All	All	5461/5789 (94%)	5461 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	HIS
2	b	42	ASN
2	b	89	GLN
3	c	3	GLN
3	c	25	ASN
3	c	100	GLN
3	c	123	GLN
3	c	139	GLN
3	c	140	ASN
4	d	36	GLN
4	d	74	ASN
4	d	131	ASN
4	d	140	ASN
5	e	12	GLN
5	e	19	ASN
5	e	70	ASN
6	f	46	GLN
6	f	58	HIS
7	g	68	ASN
7	g	122	ASN
7	g	130	ASN

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Mol	Chain	Res	Type
8	h	16	ASN
8	h	18	GLN
8	h	38	ASN
8	h	67	GLN
9	i	110	GLN
9	i	126	GLN
11	k	109	ASN
12	l	46	ASN
12	l	96	HIS
13	m	105	ASN
14	n	66	GLN
15	o	51	HIS
16	p	29	ASN
17	q	9	GLN
18	r	74	HIS
19	s	14	HIS
19	s	52	HIS
20	t	13	GLN
20	t	21	ASN
21	u	9	ASN
25	w	57	GLN
25	w	66	GLN
25	w	110	ASN
25	w	156	HIS
25	w	263	GLN
25	w	288	GLN
25	w	296	ASN
26	v	21	HIS
26	v	92	HIS
26	v	225	GLN
26	v	369	ASN
29	C	25	HIS
29	C	58	HIS
29	C	70	ASN
29	C	86	ASN
29	C	143	ASN
30	D	49	GLN
30	D	134	HIS
31	E	62	GLN
31	E	97	ASN
31	E	165	HIS
33	G	22	GLN

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Mol	Chain	Res	Type
33	G	73	ASN
33	G	88	GLN
33	G	128	GLN
36	J	31	GLN
36	J	105	GLN
37	L	40	HIS
37	L	76	HIS
38	M	3	GLN
39	N	54	GLN
39	N	104	GLN
40	O	13	HIS
41	P	16	HIS
41	P	23	ASN
41	P	62	ASN
42	Q	29	HIS
42	Q	38	GLN
43	R	10	GLN
43	R	12	GLN
43	R	66	ASN
44	S	72	ASN
45	T	6	GLN
45	T	89	HIS
45	T	91	GLN
46	U	7	HIS
46	U	40	ASN
46	U	57	ASN
48	W	53	ASN
48	W	74	ASN
49	X	49	ASN
50	Y	50	ASN
51	Z	17	ASN
52	1	36	GLN
52	1	45	GLN
52	1	58	ASN
54	3	41	HIS
54	3	61	ASN
55	4	6	ASN
57	6	6	GLN
58	7	28	ASN
59	8	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1542 (98%)	178 (11%)	0
22	x	75/76 (98%)	16 (21%)	0
23	y	70/76 (92%)	29 (41%)	0
24	z	9/21 (42%)	2 (22%)	0
27	A	2897/2904 (99%)	342 (11%)	16 (0%)
28	B	119/120 (99%)	11 (9%)	2 (1%)
All	All	4696/4739 (99%)	578 (12%)	18 (0%)

All (578) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	32	A
1	a	39	G
1	a	44	A
1	a	47	C
1	a	48	C
1	a	51	A
1	a	71	A
1	a	79	G
1	a	82	G
1	a	85	U
1	a	88	U
1	a	94	G
1	a	95	C
1	a	116	A
1	a	121	U
1	a	122	G
1	a	130	A
1	a	131	A
1	a	174	A
1	a	177	G
1	a	183	C
1	a	184	G
1	a	197	A
1	a	199	A
1	a	208	U
1	a	209	U
1	a	210	C
1	a	212	G

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Mol	Chain	Res	Type
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	321	A
1	a	328	C
1	a	344	A
1	a	347	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	372	C
1	a	390	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	415	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	467	U
1	a	468	A
1	a	478	A
1	a	479	U
1	a	484	G
1	a	486	U
1	a	494	G
1	a	495	A
1	a	497	G
1	a	509	A
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	531	U

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Mol	Chain	Res	Type
1	a	532	A
1	a	547	A
1	a	559	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	618	C
1	a	633	G
1	a	650	G
1	a	665	A
1	a	688	G
1	a	721	G
1	a	723	U
1	a	734	G
1	a	746	A
1	a	755	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	821	G
1	a	890	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	966	2MG
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	1003	G
1	a	1004	A
1	a	1008	U

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Mol	Chain	Res	Type
1	a	1009	U
1	a	1024	G
1	a	1027	C
1	a	1028	C
1	a	1029	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1036	A
1	a	1042	A
1	a	1046	A
1	a	1053	G
1	a	1065	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1108	G
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1152	A
1	a	1159	U
1	a	1168	U
1	a	1184	G
1	a	1196	A
1	a	1197	A
1	a	1213	A
1	a	1227	A
1	a	1238	A
1	a	1257	A
1	a	1258	G
1	a	1275	A
1	a	1280	A
1	a	1286	U
1	a	1287	A
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1338	G

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Mol	Chain	Res	Type
1	a	1346	A
1	a	1363	A
1	a	1364	U
1	a	1379	G
1	a	1388	C
1	a	1397	C
1	a	1399	C
1	a	1419	G
1	a	1432	G
1	a	1441	A
1	a	1446	A
1	a	1448	C
1	a	1452	C
1	a	1487	G
1	a	1497	G
1	a	1506	U
1	a	1517	G
1	a	1519	MA6
1	a	1529	G
1	a	1530	G
22	x	12	U
22	x	13	C
22	x	16	U
22	x	17	C
22	x	19	G
22	x	20	U
22	x	22	G
22	x	37	MIA
22	x	38	A
22	x	44	G
22	x	45	U
22	x	47	U
22	x	48	C
22	x	49	C
22	x	55	PSU
22	x	76	A
23	y	5	G
23	y	6	G
23	y	8	4SU
23	y	12	U
23	y	13	C
23	y	14	A

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Mol	Chain	Res	Type
23	y	19	G
23	y	20	U
23	y	21	A
23	y	26	A
23	y	30	G
23	y	34	G
23	y	35	A
23	y	36	A
23	y	41	C
23	y	42	C
23	y	44	G
23	y	45	U
23	y	46	G7M
23	y	47	U
23	y	48	C
23	y	54	5MU
23	y	57	G
23	y	59	U
23	y	60	U
23	y	72	C
23	y	73	A
23	y	75	C
23	y	76	A
24	z	12	A
24	z	20	U
27	A	2	G
27	A	4	U
27	A	6	A
27	A	10	A
27	A	12	U
27	A	34	U
27	A	51	G
27	A	71	A
27	A	74	A
27	A	75	G
27	A	84	A
27	A	100	U
27	A	101	A
27	A	103	A
27	A	118	A
27	A	120	U
27	A	139	U

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Mol	Chain	Res	Type
27	A	142	A
27	A	163	C
27	A	164	C
27	A	165	A
27	A	181	A
27	A	196	A
27	A	199	A
27	A	215	G
27	A	216	A
27	A	222	A
27	A	233	A
27	A	248	G
27	A	269	C
27	A	271	G
27	A	272	A
27	A	275	C
27	A	278	A
27	A	281	C
27	A	285	G
27	A	311	A
27	A	329	G
27	A	330	A
27	A	362	A
27	A	367	G
27	A	386	G
27	A	396	G
27	A	404	A
27	A	411	G
27	A	412	A
27	A	428	A
27	A	481	G
27	A	491	G
27	A	505	A
27	A	509	C
27	A	512	G
27	A	530	G
27	A	532	A
27	A	544	C
27	A	545	U
27	A	546	U
27	A	547	A
27	A	549	G

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Mol	Chain	Res	Type
27	A	563	A
27	A	573	U
27	A	575	A
27	A	603	A
27	A	615	U
27	A	627	A
27	A	637	A
27	A	645	C
27	A	647	G
27	A	654	A
27	A	655	A
27	A	686	U
27	A	709	U
27	A	710	U
27	A	717	C
27	A	719	C
27	A	730	A
27	A	740	C
27	A	747	5MU
27	A	764	A
27	A	775	G
27	A	776	G
27	A	782	A
27	A	784	G
27	A	785	G
27	A	805	G
27	A	812	C
27	A	827	U
27	A	828	U
27	A	830	G
27	A	845	A
27	A	846	U
27	A	859	G
27	A	890	C
27	A	891	G
27	A	893	C
27	A	895	U
27	A	896	A
27	A	897	C
27	A	900	A
27	A	910	A
27	A	915	C

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Mol	Chain	Res	Type
27	A	927	A
27	A	946	C
27	A	961	C
27	A	974	G
27	A	983	A
27	A	990	A
27	A	996	A
27	A	1009	A
27	A	1012	U
27	A	1013	C
27	A	1022	G
27	A	1026	G
27	A	1032	A
27	A	1033	U
27	A	1039	A
27	A	1046	A
27	A	1047	G
27	A	1059	G
27	A	1060	U
27	A	1061	U
27	A	1062	G
27	A	1063	G
27	A	1064	C
27	A	1065	U
27	A	1066	U
27	A	1067	A
27	A	1068	G
27	A	1070	A
27	A	1071	G
27	A	1084	A
27	A	1085	A
27	A	1088	A
27	A	1090	A
27	A	1104	C
27	A	1106	G
27	A	1111	A
27	A	1112	G
27	A	1132	U
27	A	1135	C
27	A	1142	A
27	A	1170	C
27	A	1212	G

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Mol	Chain	Res	Type
27	A	1253	A
27	A	1255	U
27	A	1256	G
27	A	1271	G
27	A	1272	A
27	A	1273	U
27	A	1288	G
27	A	1300	G
27	A	1301	A
27	A	1329	U
27	A	1365	A
27	A	1379	U
27	A	1383	A
27	A	1395	A
27	A	1416	G
27	A	1428	C
27	A	1452	G
27	A	1482	G
27	A	1493	C
27	A	1508	A
27	A	1509	A
27	A	1510	G
27	A	1515	A
27	A	1524	G
27	A	1534	U
27	A	1535	A
27	A	1536	C
27	A	1537	G
27	A	1539	U
27	A	1554	U
27	A	1569	A
27	A	1578	U
27	A	1583	A
27	A	1584	U
27	A	1585	C
27	A	1606	C
27	A	1608	A
27	A	1626	A
27	A	1647	U
27	A	1648	U
27	A	1674	G
27	A	1675	C

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Mol	Chain	Res	Type
27	A	1676	A
27	A	1715	G
27	A	1729	U
27	A	1730	C
27	A	1732	C
27	A	1733	G
27	A	1738	G
27	A	1758	U
27	A	1764	C
27	A	1773	A
27	A	1800	C
27	A	1801	A
27	A	1808	A
27	A	1816	C
27	A	1829	A
27	A	1848	A
27	A	1858	A
27	A	1872	A
27	A	1906	G
27	A	1913	A
27	A	1914	C
27	A	1929	G
27	A	1930	G
27	A	1936	A
27	A	1937	A
27	A	1955	U
27	A	1963	U
27	A	1964	G
27	A	1967	C
27	A	1970	A
27	A	1971	U
27	A	1972	G
27	A	1991	U
27	A	1993	U
27	A	2021	C
27	A	2023	C
27	A	2031	A
27	A	2033	A
27	A	2036	C
27	A	2043	C
27	A	2055	C
27	A	2056	G

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Mol	Chain	Res	Type
27	A	2060	A
27	A	2061	G
27	A	2062	A
27	A	2069	G7M
27	A	2093	G
27	A	2108	A
27	A	2110	G
27	A	2111	U
27	A	2112	G
27	A	2113	U
27	A	2115	G
27	A	2116	G
27	A	2118	U
27	A	2119	A
27	A	2120	G
27	A	2131	U
27	A	2132	U
27	A	2133	G
27	A	2136	G
27	A	2138	G
27	A	2145	C
27	A	2146	C
27	A	2157	G
27	A	2159	G
27	A	2162	G
27	A	2167	U
27	A	2170	A
27	A	2172	U
27	A	2173	A
27	A	2179	C
27	A	2182	U
27	A	2189	U
27	A	2190	G
27	A	2192	U
27	A	2198	A
27	A	2203	U
27	A	2204	G
27	A	2211	A
27	A	2225	A
27	A	2238	G
27	A	2239	G
27	A	2283	C

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Mol	Chain	Res	Type
27	A	2287	A
27	A	2288	A
27	A	2305	U
27	A	2308	G
27	A	2309	A
27	A	2322	A
27	A	2325	G
27	A	2333	A
27	A	2335	A
27	A	2345	G
27	A	2350	C
27	A	2361	G
27	A	2383	G
27	A	2385	C
27	A	2396	G
27	A	2401	U
27	A	2402	U
27	A	2406	A
27	A	2425	A
27	A	2429	G
27	A	2441	U
27	A	2447	G
27	A	2448	A
27	A	2469	A
27	A	2470	G
27	A	2474	U
27	A	2475	C
27	A	2476	A
27	A	2492	U
27	A	2498	OMC
27	A	2502	G
27	A	2504	PSU
27	A	2505	G
27	A	2506	U
27	A	2518	A
27	A	2520	C
27	A	2529	G
27	A	2539	C
27	A	2547	A
27	A	2566	A
27	A	2567	G
27	A	2573	C

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Mol	Chain	Res	Type
27	A	2582	G
27	A	2602	A
27	A	2609	U
27	A	2613	U
27	A	2629	U
27	A	2646	C
27	A	2649	C
27	A	2689	U
27	A	2690	U
27	A	2714	G
27	A	2726	A
27	A	2733	A
27	A	2744	G
27	A	2746	U
27	A	2748	A
27	A	2749	A
27	A	2750	A
27	A	2757	A
27	A	2765	A
27	A	2778	A
27	A	2798	U
27	A	2800	A
27	A	2818	U
27	A	2820	A
27	A	2821	A
27	A	2849	U
27	A	2861	U
27	A	2873	A
27	A	2880	C
27	A	2884	U
27	A	2902	C
28	B	4	C
28	B	24	G
28	B	35	C
28	B	41	G
28	B	44	G
28	B	45	A
28	B	56	G
28	B	67	G
28	B	89	U
28	B	91	C
28	B	109	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	A	3	U
27	A	271	G
27	A	277	G
27	A	784	G
27	A	1002	G
27	A	1026	G
27	A	1031	G
27	A	1111	A
27	A	1328	A
27	A	1583	A
27	A	1847	A
27	A	2189	U
27	A	2191	A
27	A	2473	U
27	A	2538	C
27	A	2756	U
28	B	3	C
28	B	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	a	527	1	23,26,27	1.54	3 (13%)	34,39,42	1.77	5 (14%)
11	IAS	k	119	11	6,7,8	0.95	0	3,8,10	1.51	1 (33%)
1	4OC	a	1402	60,1	20,23,24	0.75	0	25,32,35	0.96	1 (4%)
40	4D4	O	81	40	9,11,12	2.54	2 (22%)	7,13,15	0.95	1 (14%)
27	PSU	A	2580	27	18,21,22	1.42	3 (16%)	21,30,33	2.07	4 (19%)
27	3TD	A	1915	60,27	19,22,23	4.21	7 (36%)	23,32,35	1.81	3 (13%)
40	MS6	O	82	40	5,7,8	0.52	0	2,7,9	1.27	0
27	PSU	A	1911	27	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMU	A	2552	27	19,22,23	1.24	3 (15%)	25,31,34	1.84	5 (20%)
27	PSU	A	2457	27	18,21,22	1.38	3 (16%)	21,30,33	2.11	5 (23%)
1	5MC	a	967	1	19,22,23	1.60	3 (15%)	26,32,35	1.11	2 (7%)
1	PSU	a	516	1	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
30	MEQ	D	150	30	8,9,10	0.51	0	5,10,12	0.14	0
27	OMC	A	2498	60,27	19,22,23	0.80	0	25,31,34	0.90	1 (4%)
27	2MG	A	2445	60,27	23,26,27	1.24	4 (17%)	33,38,41	2.22	7 (21%)
27	PSU	A	746	60,27	18,21,22	1.37	3 (16%)	21,30,33	2.01	4 (19%)
23	PSU	y	32	23	18,21,22	1.35	2 (11%)	21,30,33	2.04	5 (23%)
27	5MU	A	747	27	19,22,23	1.40	6 (31%)	27,32,35	2.08	6 (22%)
27	G7M	A	2069	27	23,26,27	1.54	3 (13%)	34,39,42	1.71	5 (14%)
23	4SU	y	8	23	18,21,22	1.86	5 (27%)	25,30,33	2.43	5 (20%)
1	2MG	a	1207	1	23,26,27	1.26	4 (17%)	33,38,41	2.22	7 (21%)
1	MA6	a	1518	1	23,26,27	1.47	4 (17%)	33,38,41	2.43	13 (39%)
27	PSU	A	955	27	18,21,22	1.41	3 (16%)	21,30,33	2.03	3 (14%)
27	2MA	A	2503	27	22,25,26	1.48	4 (18%)	32,37,40	2.29	9 (28%)
22	PSU	x	32	22	18,21,22	1.38	3 (16%)	21,30,33	1.98	3 (14%)
27	PSU	A	1917	27	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
27	5MU	A	1939	27	19,22,23	1.38	5 (26%)	27,32,35	2.16	6 (22%)
1	2MG	a	1516	1	23,26,27	1.23	3 (13%)	33,38,41	2.24	8 (24%)
22	MIA	x	37	22	28,31,32	2.35	6 (21%)	38,44,47	2.81	14 (36%)
27	2MG	A	1835	27	23,26,27	1.25	4 (17%)	33,38,41	2.24	7 (21%)
27	OMG	A	2251	60,27,22	23,26,27	1.18	3 (13%)	32,38,41	2.02	6 (18%)
27	PSU	A	2604	27	18,21,22	1.39	3 (16%)	21,30,33	2.01	4 (19%)
1	5MC	a	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.10	3 (11%)
27	6MZ	A	2030	27	22,25,26	1.46	4 (18%)	29,36,39	2.26	10 (34%)
22	PSU	x	39	22	18,21,22	1.36	2 (11%)	21,30,33	2.10	4 (19%)
1	UR3	a	1498	1	19,22,23	0.94	0	26,32,35	1.73	3 (11%)
27	PSU	A	2504	27	18,21,22	1.39	2 (11%)	21,30,33	2.05	4 (19%)
12	D2T	l	89	12	8,9,10	2.32	1 (12%)	6,11,13	2.49	2 (33%)
22	5MU	x	54	22	19,22,23	1.34	4 (21%)	27,32,35	2.17	8 (29%)
23	PSU	y	39	23	18,21,22	1.37	2 (11%)	21,30,33	2.06	5 (23%)
27	PSU	A	2605	27	18,21,22	1.35	3 (16%)	21,30,33	2.06	4 (19%)
1	2MG	a	966	1	23,26,27	1.28	4 (17%)	33,38,41	2.21	8 (24%)
22	G7M	x	46	22	23,26,27	2.39	5 (21%)	34,39,42	3.03	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	G7M	y	46	23	23,26,27	2.38	5 (21%)	34,39,42	3.00	10 (29%)
1	MA6	a	1519	1	23,26,27	1.48	4 (17%)	33,38,41	2.44	13 (39%)
23	PSU	y	55	23	18,21,22	1.36	2 (11%)	21,30,33	2.06	3 (14%)
27	H2U	A	2449	27	18,21,22	1.15	3 (16%)	19,30,33	0.79	0
27	5MC	A	1962	60,27	19,22,23	1.49	3 (15%)	26,32,35	1.10	2 (7%)
23	5MU	y	54	23	19,22,23	1.40	5 (26%)	27,32,35	2.20	6 (22%)
22	4SU	x	8	22	18,21,22	1.90	4 (22%)	25,30,33	2.07	4 (16%)
27	6MZ	A	1618	27	22,25,26	1.46	4 (18%)	29,36,39	2.21	9 (31%)
22	PSU	x	55	22	18,21,22	1.38	2 (11%)	21,30,33	2.10	4 (19%)
27	1MG	A	745	27	23,26,27	1.19	3 (13%)	33,39,42	1.75	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
11	IAS	k	119	11	-	0/7/7/8	-
1	4OC	a	1402	60,1	-	3/9/29/30	0/2/2/2
40	4D4	O	81	40	-	7/11/12/14	-
27	PSU	A	2580	27	-	0/7/25/26	0/2/2/2
27	3TD	A	1915	60,27	-	0/7/25/26	0/2/2/2
40	MS6	O	82	40	-	2/4/6/8	-
27	PSU	A	1911	27	-	0/7/25/26	0/2/2/2
27	OMU	A	2552	27	-	0/9/27/28	0/2/2/2
27	PSU	A	2457	27	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
30	MEQ	D	150	30	-	2/8/9/11	-
27	OMC	A	2498	60,27	-	2/9/27/28	0/2/2/2
27	2MG	A	2445	60,27	-	0/9/27/28	0/3/3/3
27	PSU	A	746	60,27	-	4/7/25/26	0/2/2/2
23	PSU	y	32	23	-	0/7/25/26	0/2/2/2
27	5MU	A	747	27	-	0/7/25/26	0/2/2/2
27	G7M	A	2069	27	-	0/7/25/26	0/3/3/3
23	4SU	y	8	23	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PSU	A	955	27	-	0/7/25/26	0/2/2/2
27	2MA	A	2503	27	-	0/7/25/26	0/3/3/3
22	PSU	x	32	22	-	0/7/25/26	0/2/2/2
27	PSU	A	1917	27	-	1/7/25/26	0/2/2/2
27	5MU	A	1939	27	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
22	MIA	x	37	22	-	5/15/33/34	0/3/3/3
27	2MG	A	1835	27	-	0/9/27/28	0/3/3/3
27	OMG	A	2251	60,27,22	-	0/9/27/28	0/3/3/3
27	PSU	A	2604	27	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
27	6MZ	A	2030	27	-	2/9/27/28	0/3/3/3
22	PSU	x	39	22	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
27	PSU	A	2504	27	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	1/7/12/14	-
22	5MU	x	54	22	-	0/7/25/26	0/2/2/2
23	PSU	y	39	23	-	1/7/25/26	0/2/2/2
27	PSU	A	2605	27	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/9/27/28	0/3/3/3
22	G7M	x	46	22	-	0/7/25/26	0/3/3/3
23	G7M	y	46	23	-	4/7/25/26	0/3/3/3
1	MA6	a	1519	1	-	5/11/29/30	0/3/3/3
23	PSU	y	55	23	-	3/7/25/26	0/2/2/2
27	H2U	A	2449	27	-	0/7/38/39	0/2/2/2
27	5MC	A	1962	60,27	-	0/7/25/26	0/2/2/2
23	5MU	y	54	23	-	2/7/25/26	0/2/2/2
22	4SU	x	8	22	-	0/7/25/26	0/2/2/2
27	6MZ	A	1618	27	-	0/9/27/28	0/3/3/3
22	PSU	x	55	22	-	3/7/25/26	0/2/2/2
27	1MG	A	745	27	-	0/7/25/26	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1915	3TD	C6-C5	12.58	1.49	1.35
27	A	1915	3TD	C2-N1	9.69	1.49	1.37
22	x	46	G7M	C8-N7	7.80	1.46	1.33
23	y	46	G7M	C8-N7	7.65	1.46	1.33
22	x	37	MIA	C2-S10	-7.35	1.69	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	x	37	MIA	C13-C14	6.83	1.52	1.32
40	O	81	4D4	CZ-NE	6.24	1.45	1.33
12	l	89	D2T	CB-CA	-5.88	1.52	1.54
27	A	1915	3TD	C6-N1	5.86	1.45	1.36
1	a	967	5MC	C5-C4	5.75	1.48	1.44
1	a	1407	5MC	C5-C4	5.44	1.48	1.44
27	A	1962	5MC	C5-C4	5.26	1.48	1.44
23	y	8	4SU	C4-S4	-5.17	1.59	1.68
27	A	2069	G7M	C5-N7	-4.98	1.33	1.39
27	A	1915	3TD	C2-N3	4.97	1.49	1.38
22	x	8	4SU	C4-S4	-4.94	1.60	1.68
1	a	527	G7M	C5-N7	-4.89	1.33	1.39
22	x	46	G7M	C5-N7	-4.76	1.33	1.39
23	y	46	G7M	C5-N7	-4.70	1.33	1.39
22	x	37	MIA	C5-C4	4.59	1.47	1.39
1	a	1518	MA6	C5-C4	4.56	1.47	1.39
27	A	1618	6MZ	C5-C4	4.54	1.47	1.39
1	a	1519	MA6	C5-C4	4.51	1.47	1.39
27	A	2503	2MA	C5-C4	4.46	1.47	1.39
27	A	2030	6MZ	C5-C4	4.43	1.47	1.39
23	y	46	G7M	C8-N9	4.18	1.47	1.35
22	x	46	G7M	C8-N9	4.11	1.46	1.35
23	y	46	G7M	C5-C4	3.80	1.47	1.38
22	x	8	4SU	C4-N3	-3.78	1.33	1.37
22	x	46	G7M	C5-C4	3.65	1.47	1.38
23	y	8	4SU	C4-N3	-3.43	1.34	1.37
23	y	55	PSU	C6-C5	3.38	1.39	1.35
23	y	32	PSU	C6-C5	3.38	1.39	1.35
23	y	39	PSU	C6-C5	3.35	1.39	1.35
27	A	1917	PSU	C6-C5	3.32	1.39	1.35
27	A	1911	PSU	C6-C5	3.30	1.38	1.35
22	x	55	PSU	C6-C5	3.24	1.38	1.35
1	a	527	G7M	C5-C4	3.22	1.46	1.38
27	A	745	1MG	C5-C4	3.22	1.47	1.38
27	A	955	PSU	C6-C5	3.20	1.38	1.35
1	a	966	2MG	C5-C4	3.16	1.47	1.38
27	A	2504	PSU	C6-C5	3.14	1.38	1.35
22	x	39	PSU	C6-C5	3.11	1.38	1.35
27	A	2069	G7M	C5-C4	3.09	1.46	1.38
22	x	32	PSU	C6-C5	3.09	1.38	1.35
27	A	2580	PSU	C6-C5	3.08	1.38	1.35
1	a	1207	2MG	C5-C4	3.08	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	O	81	4D4	CZ-NH1	3.06	1.45	1.34
27	A	746	PSU	C6-C5	3.06	1.38	1.35
27	A	2604	PSU	C6-C5	3.05	1.38	1.35
1	a	516	PSU	C6-C5	3.05	1.38	1.35
27	A	2251	OMG	C5-C4	3.04	1.47	1.38
27	A	1835	2MG	C5-C4	3.02	1.47	1.38
1	a	1516	2MG	C5-C4	3.00	1.47	1.38
27	A	2449	H2U	C2-N3	-2.98	1.32	1.38
27	A	2445	2MG	C5-C4	2.98	1.46	1.38
27	A	2457	PSU	C6-C5	2.86	1.38	1.35
22	x	8	4SU	C5-C4	-2.86	1.39	1.42
27	A	2552	OMU	C4-N3	-2.83	1.33	1.38
27	A	2604	PSU	C4-N3	-2.82	1.33	1.38
27	A	2605	PSU	C6-C5	2.81	1.38	1.35
1	a	1519	MA6	C5-C6	2.80	1.48	1.41
27	A	955	PSU	C4-N3	-2.78	1.33	1.38
27	A	746	PSU	C4-N3	-2.78	1.33	1.38
27	A	2504	PSU	C4-N3	-2.78	1.33	1.38
27	A	2457	PSU	C4-N3	-2.76	1.33	1.38
27	A	2605	PSU	C4-N3	-2.75	1.33	1.38
22	x	32	PSU	C4-N3	-2.75	1.33	1.38
23	y	54	5MU	C6-C5	2.75	1.39	1.34
27	A	747	5MU	C6-C5	2.75	1.39	1.34
27	A	1915	3TD	C4-N3	2.74	1.46	1.40
1	a	967	5MC	C6-C5	2.74	1.39	1.34
27	A	2030	6MZ	C5-C6	2.74	1.48	1.41
27	A	747	5MU	C4-N3	-2.73	1.33	1.38
27	A	1911	PSU	C4-N3	-2.72	1.33	1.38
27	A	1618	6MZ	C5-C6	2.72	1.48	1.41
27	A	1939	5MU	C4-N3	-2.70	1.33	1.38
27	A	2580	PSU	C4-N3	-2.70	1.33	1.38
22	x	55	PSU	C4-N3	-2.69	1.33	1.38
27	A	1917	PSU	C4-N3	-2.68	1.33	1.38
22	x	39	PSU	C4-N3	-2.68	1.33	1.38
1	a	516	PSU	C4-N3	-2.67	1.33	1.38
27	A	2503	2MA	C5-C6	2.67	1.48	1.41
27	A	2449	H2U	C4-N3	-2.66	1.33	1.37
1	a	1518	MA6	C5-C6	2.66	1.48	1.41
23	y	8	4SU	C5-C4	-2.65	1.39	1.42
1	a	1407	5MC	C6-C5	2.64	1.38	1.34
27	A	1835	2MG	C6-N1	-2.62	1.34	1.38
23	y	39	PSU	C4-N3	-2.61	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1962	5MC	C6-C5	2.61	1.38	1.34
1	a	966	2MG	C6-N1	-2.61	1.34	1.38
27	A	1915	3TD	O2-C2	-2.60	1.18	1.23
22	x	37	MIA	C5-C6	2.59	1.48	1.41
1	a	1207	2MG	C6-N1	-2.58	1.34	1.38
27	A	1939	5MU	C6-C5	2.58	1.38	1.34
22	x	54	5MU	C4-N3	-2.57	1.34	1.38
27	A	2445	2MG	C6-N1	-2.56	1.34	1.38
23	y	55	PSU	C4-N3	-2.56	1.34	1.38
23	y	32	PSU	C4-N3	-2.55	1.34	1.38
27	A	2069	G7M	C6-N1	-2.52	1.34	1.38
27	A	2251	OMG	C6-N1	-2.52	1.34	1.38
23	y	54	5MU	C4-N3	-2.51	1.34	1.38
1	a	527	G7M	C6-N1	-2.50	1.34	1.38
22	x	54	5MU	C6-C5	2.48	1.38	1.34
22	x	37	MIA	C5-N7	-2.48	1.34	1.39
1	a	1516	2MG	C6-N1	-2.44	1.34	1.38
22	x	8	4SU	C2-N3	-2.43	1.33	1.38
27	A	1939	5MU	C6-N1	-2.41	1.33	1.38
23	y	54	5MU	C4-C5	2.40	1.48	1.44
27	A	2552	OMU	C2-N3	-2.39	1.33	1.38
22	x	54	5MU	C6-N1	-2.39	1.33	1.38
23	y	46	G7M	C6-N1	-2.39	1.34	1.38
1	a	1518	MA6	C5-N7	-2.38	1.34	1.39
22	x	46	G7M	C6-N1	-2.38	1.34	1.38
27	A	747	5MU	C6-N1	-2.36	1.34	1.38
27	A	2503	2MA	C5-N7	-2.36	1.34	1.39
27	A	2030	6MZ	C5-N7	-2.33	1.34	1.39
23	y	54	5MU	C6-N1	-2.33	1.34	1.38
27	A	2449	H2U	C2-N1	-2.32	1.32	1.35
1	a	1519	MA6	C5-N7	-2.31	1.34	1.39
1	a	1407	5MC	C6-N1	-2.31	1.34	1.38
27	A	1962	5MC	C6-N1	-2.30	1.34	1.38
27	A	2503	2MA	C8-N7	2.30	1.36	1.31
1	a	966	2MG	C5-N7	-2.29	1.34	1.39
27	A	745	1MG	C2-N1	2.28	1.41	1.37
1	a	1519	MA6	C8-N7	2.28	1.36	1.31
27	A	1618	6MZ	C5-N7	-2.28	1.34	1.39
1	a	967	5MC	C6-N1	-2.27	1.34	1.38
1	a	966	2MG	C2-N3	2.25	1.36	1.32
27	A	2445	2MG	C5-N7	-2.23	1.34	1.39
27	A	2580	PSU	O4'-C1'	-2.23	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1618	6MZ	C8-N7	2.23	1.36	1.31
27	A	2030	6MZ	C8-N7	2.22	1.36	1.31
27	A	1939	5MU	C2-N3	-2.22	1.34	1.38
23	y	54	5MU	C2-N1	2.22	1.41	1.38
27	A	1939	5MU	C4-C5	2.21	1.48	1.44
27	A	1835	2MG	C5-N7	-2.21	1.34	1.39
27	A	2251	OMG	C5-N7	-2.19	1.34	1.39
27	A	745	1MG	C5-N7	-2.19	1.34	1.39
1	a	1518	MA6	C8-N7	2.18	1.35	1.31
27	A	747	5MU	C2-N3	-2.18	1.34	1.38
22	x	54	5MU	C2-N1	2.18	1.41	1.38
1	a	1207	2MG	C2-N3	2.17	1.36	1.32
22	x	37	MIA	C8-N7	2.15	1.35	1.31
27	A	1915	3TD	O4-C4	-2.14	1.18	1.23
27	A	747	5MU	C4-C5	2.14	1.48	1.44
23	y	8	4SU	C2-N3	-2.13	1.34	1.38
27	A	955	PSU	C2-N3	-2.11	1.34	1.37
1	a	1207	2MG	C5-N7	-2.10	1.34	1.39
27	A	746	PSU	C2-N3	-2.09	1.34	1.37
27	A	1835	2MG	C2-N3	2.09	1.35	1.32
27	A	2604	PSU	C2-N3	-2.07	1.34	1.37
27	A	2552	OMU	C5-C4	-2.06	1.39	1.43
1	a	1516	2MG	C5-N7	-2.06	1.34	1.39
23	y	8	4SU	C2-N1	2.05	1.41	1.38
27	A	2605	PSU	C2-N3	-2.05	1.34	1.37
22	x	32	PSU	C2-N3	-2.05	1.34	1.37
27	A	2457	PSU	C2-N3	-2.05	1.34	1.37
27	A	2445	2MG	C2-N3	2.03	1.35	1.32
27	A	747	5MU	C2-N1	2.01	1.41	1.38

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	x	37	MIA	C12-C13-C14	-8.54	111.67	127.01
22	x	37	MIA	C5-C4-N3	-8.32	118.42	127.18
27	A	2503	2MA	C5-C4-N3	-8.11	118.64	127.18
22	x	46	G7M	CN7-N7-C8	-7.94	112.77	124.79
23	y	46	G7M	CN7-N7-C8	-7.89	112.84	124.79
23	y	8	4SU	C4-N3-C2	-7.58	120.05	127.31
27	A	1835	2MG	C2-N3-C4	7.35	121.19	112.00
1	a	1207	2MG	C2-N3-C4	7.26	121.09	112.00
27	A	2445	2MG	C2-N3-C4	7.23	121.04	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1516	2MG	C2-N3-C4	7.21	121.02	112.00
1	a	966	2MG	C2-N3-C4	7.10	120.88	112.00
1	a	1498	UR3	C4-N3-C2	-6.93	119.00	124.58
22	x	46	G7M	N9-C8-N7	-6.91	95.70	112.48
22	x	46	G7M	C8-N7-C5	6.69	116.15	107.78
23	y	46	G7M	N9-C8-N7	-6.68	96.27	112.48
22	x	37	MIA	N3-C4-N9	6.57	135.33	126.99
27	A	2457	PSU	N1-C2-N3	6.55	122.08	115.17
22	x	55	PSU	N1-C2-N3	6.54	122.06	115.17
22	x	39	PSU	N1-C2-N3	6.50	122.03	115.17
23	y	46	G7M	N9-C4-N3	6.47	138.90	125.95
23	y	46	G7M	C8-N7-C5	6.45	115.84	107.78
27	A	955	PSU	N1-C2-N3	6.43	121.95	115.17
27	A	1911	PSU	N1-C2-N3	6.41	121.93	115.17
27	A	746	PSU	N1-C2-N3	6.41	121.93	115.17
1	a	966	2MG	C5-C4-N3	-6.41	118.19	128.39
27	A	2580	PSU	N1-C2-N3	6.41	121.93	115.17
27	A	2504	PSU	N1-C2-N3	6.39	121.91	115.17
23	y	55	PSU	N1-C2-N3	6.38	121.89	115.17
23	y	39	PSU	N1-C2-N3	6.37	121.89	115.17
27	A	1835	2MG	C5-C4-N3	-6.36	118.27	128.39
27	A	2251	OMG	C5-C4-N3	-6.33	118.32	128.39
27	A	1917	PSU	N1-C2-N3	6.32	121.84	115.17
23	y	32	PSU	N1-C2-N3	6.31	121.83	115.17
1	a	516	PSU	N1-C2-N3	6.30	121.81	115.17
22	x	46	G7M	N9-C4-N3	6.28	138.52	125.95
27	A	2604	PSU	N1-C2-N3	6.28	121.79	115.17
27	A	2605	PSU	N1-C2-N3	6.24	121.75	115.17
1	a	1207	2MG	C5-C4-N3	-6.24	118.45	128.39
27	A	2503	2MA	N3-C4-N9	6.24	134.91	126.99
23	y	8	4SU	C5-C4-N3	6.22	120.53	114.75
27	A	2445	2MG	C5-C4-N3	-6.19	118.54	128.39
22	x	32	PSU	N1-C2-N3	6.17	121.67	115.17
1	a	1516	2MG	C5-C4-N3	-6.01	118.83	128.39
22	x	8	4SU	C4-N3-C2	-6.00	121.56	127.31
27	A	1618	6MZ	C5-C4-N3	-5.94	118.54	126.72
27	A	2030	6MZ	C5-C4-N3	-5.91	118.58	126.72
1	a	1518	MA6	C5-C4-N3	-5.89	118.61	126.72
1	a	1519	MA6	C5-C4-N3	-5.77	118.78	126.72
27	A	1915	3TD	N1-C2-N3	5.76	120.31	116.13
1	a	527	G7M	N9-C4-N3	5.66	137.26	125.95
23	y	46	G7M	C5-C4-N3	-5.63	117.51	128.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	745	1MG	C5-C4-N3	-5.60	119.48	128.39
1	a	527	G7M	C5-C4-N3	-5.55	117.67	128.15
22	x	8	4SU	C5-C4-N3	5.54	119.91	114.75
23	y	54	5MU	C4-N3-C2	-5.48	120.15	127.34
22	x	46	G7M	C5-C4-N3	-5.47	117.81	128.15
27	A	1939	5MU	C4-N3-C2	-5.33	120.35	127.34
27	A	2069	G7M	N9-C4-N3	5.29	136.53	125.95
27	A	2069	G7M	C5-C4-N3	-5.23	118.27	128.15
23	y	54	5MU	N3-C2-N1	5.21	121.68	114.89
27	A	2251	OMG	C2-N3-C4	5.18	121.23	112.30
22	x	54	5MU	C4-N3-C2	-5.11	120.64	127.34
27	A	747	5MU	N3-C2-N1	5.08	121.51	114.89
27	A	747	5MU	C4-N3-C2	-5.07	120.69	127.34
27	A	1939	5MU	N3-C2-N1	5.04	121.45	114.89
27	A	2552	OMU	C4-N3-C2	-5.00	120.41	126.61
1	a	966	2MG	N9-C4-N3	4.79	135.54	125.95
27	A	1835	2MG	N9-C4-N3	4.79	135.53	125.95
22	x	54	5MU	N3-C2-N1	4.79	121.12	114.89
1	a	527	G7M	C2-N3-C4	4.78	120.54	112.30
1	a	1518	MA6	N3-C4-N9	4.71	135.18	127.17
27	A	2251	OMG	N9-C4-N3	4.71	135.36	125.95
1	a	1519	MA6	C10-N6-C6	-4.67	108.64	120.52
27	A	2069	G7M	C2-N3-C4	4.67	120.34	112.30
22	x	54	5MU	O4-C4-C5	-4.62	119.63	124.92
27	A	1618	6MZ	N3-C4-N9	4.60	134.99	127.17
1	a	1207	2MG	N9-C4-N3	4.58	135.10	125.95
27	A	1939	5MU	C5-C4-N3	4.56	119.28	115.32
22	x	54	5MU	C5-C4-N3	4.56	119.28	115.32
27	A	2030	6MZ	N3-C4-N9	4.55	134.90	127.17
23	y	46	G7M	C2-N3-C4	4.54	120.12	112.30
23	y	54	5MU	C5-C4-N3	4.53	119.26	115.32
27	A	2445	2MG	N9-C4-N3	4.50	134.95	125.95
23	y	8	4SU	N3-C2-N1	4.48	120.72	114.89
1	a	1518	MA6	C10-N6-C6	-4.46	109.18	120.52
27	A	2552	OMU	N3-C2-N1	4.44	120.67	114.89
1	a	1519	MA6	C9-N6-C6	-4.43	109.25	120.52
22	x	46	G7M	C2-N3-C4	4.41	119.90	112.30
27	A	745	1MG	C2-N3-C4	4.40	121.87	111.98
22	x	46	G7M	C8-N9-C4	4.34	117.84	107.09
1	a	1519	MA6	N3-C4-N9	4.33	134.52	127.17
22	x	39	PSU	C4-N3-C2	-4.32	120.42	126.37
27	A	2605	PSU	C4-N3-C2	-4.32	120.42	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	747	5MU	C5-C4-N3	4.31	119.07	115.32
12	l	89	D2T	CB1-SB-CB	4.29	110.07	102.36
27	A	1915	3TD	C4-N3-C2	-4.25	120.11	124.61
1	a	1516	2MG	N9-C4-N3	4.25	134.45	125.95
27	A	746	PSU	C4-N3-C2	-4.24	120.53	126.37
27	A	2457	PSU	C4-N3-C2	-4.23	120.54	126.37
27	A	745	1MG	N9-C4-N3	4.22	134.39	125.95
23	y	39	PSU	C4-N3-C2	-4.21	120.58	126.37
23	y	46	G7M	C8-N9-C4	4.16	117.38	107.09
27	A	2504	PSU	C4-N3-C2	-4.14	120.66	126.37
1	a	1518	MA6	C9-N6-C6	-4.14	109.98	120.52
23	y	8	4SU	C5-C4-S4	-4.13	119.58	124.31
27	A	1911	PSU	C4-N3-C2	-4.11	120.71	126.37
1	a	1519	MA6	C2-N1-C6	4.11	121.87	111.83
22	x	55	PSU	O2-C2-N1	-4.10	118.56	122.79
23	y	55	PSU	C4-N3-C2	-4.09	120.73	126.37
1	a	516	PSU	C4-N3-C2	-4.09	120.74	126.37
23	y	32	PSU	C4-N3-C2	-4.09	120.74	126.37
22	x	55	PSU	C4-N3-C2	-4.08	120.75	126.37
27	A	747	5MU	O4-C4-C5	-4.07	120.26	124.92
23	y	54	5MU	O4-C4-C5	-4.07	120.26	124.92
27	A	2580	PSU	C4-N3-C2	-4.04	120.81	126.37
27	A	1939	5MU	O4-C4-C5	-4.02	120.32	124.92
1	a	1518	MA6	C2-N1-C6	4.01	121.63	111.83
27	A	955	PSU	C4-N3-C2	-4.00	120.86	126.37
27	A	2604	PSU	C4-N3-C2	-4.00	120.86	126.37
22	x	32	PSU	C4-N3-C2	-3.95	120.93	126.37
22	x	37	MIA	C16-C14-C13	-3.92	110.90	122.66
27	A	2552	OMU	C5-C4-N3	3.90	120.26	114.80
27	A	1939	5MU	C5-C6-N1	-3.88	119.10	123.31
1	a	1518	MA6	N1-C6-N6	3.85	121.55	116.86
22	x	46	G7M	C1'-N9-C8	-3.84	113.76	126.74
23	y	46	G7M	C1'-N9-C8	-3.83	113.81	126.74
1	a	516	PSU	O2-C2-N1	-3.80	118.87	122.79
27	A	2457	PSU	O2-C2-N1	-3.80	118.87	122.79
27	A	1618	6MZ	C2-N3-C4	3.79	121.10	111.83
27	A	1917	PSU	C4-N3-C2	-3.77	121.17	126.37
23	y	32	PSU	O2-C2-N1	-3.75	118.92	122.79
1	a	1519	MA6	C4-C5-N7	-3.75	106.29	110.58
23	y	55	PSU	O2-C2-N1	-3.75	118.92	122.79
27	A	2030	6MZ	C4-C5-N7	-3.74	106.30	110.58
27	A	1917	PSU	O2-C2-N1	-3.73	118.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2030	6MZ	C2-N3-C4	3.73	120.94	111.83
22	x	8	4SU	N3-C2-N1	3.73	119.74	114.89
27	A	2030	6MZ	C9-N6-C6	-3.71	119.41	122.85
22	x	37	MIA	C15-C14-C13	-3.71	111.52	122.66
1	a	1519	MA6	C2-N3-C4	3.71	120.89	111.83
22	x	39	PSU	O2-C2-N1	-3.70	118.97	122.79
27	A	2504	PSU	O2-C2-N1	-3.70	118.98	122.79
22	x	37	MIA	C11-S10-C2	-3.68	99.49	102.25
27	A	2580	PSU	O2-C2-N1	-3.68	119.00	122.79
1	a	1518	MA6	C2-N3-C4	3.68	120.81	111.83
23	y	54	5MU	C5-C6-N1	-3.67	119.33	123.31
27	A	1911	PSU	O2-C2-N1	-3.66	119.02	122.79
27	A	2030	6MZ	C6-C5-N7	3.65	136.41	132.43
23	y	46	G7M	CN7-N7-C5	3.62	131.31	126.80
23	y	39	PSU	O2-C2-N1	-3.61	119.06	122.79
27	A	1618	6MZ	C4-C5-N7	-3.60	106.47	110.58
27	A	1618	6MZ	C6-C5-N7	3.58	136.33	132.43
27	A	2605	PSU	O2-C2-N1	-3.57	119.10	122.79
27	A	2604	PSU	O2-C2-N1	-3.56	119.12	122.79
1	a	1516	2MG	C6-C5-N7	3.53	136.71	130.29
22	x	8	4SU	C5-C4-S4	-3.52	120.28	124.31
27	A	2503	2MA	C4-C5-N7	-3.49	106.60	110.58
27	A	747	5MU	C5-C6-N1	-3.47	119.55	123.31
22	x	32	PSU	O2-C2-N1	-3.45	119.23	122.79
22	x	46	G7M	CN7-N7-C5	3.44	131.09	126.80
22	x	37	MIA	C2-N3-C4	3.43	121.28	112.29
27	A	746	PSU	O2-C2-N1	-3.41	119.27	122.79
22	x	37	MIA	C4-C5-N7	-3.38	106.72	110.58
1	a	967	5MC	C5-C6-N1	-3.36	119.67	123.31
27	A	955	PSU	O2-C2-N1	-3.35	119.33	122.79
1	a	1518	MA6	C4-C5-N7	-3.28	106.83	110.58
27	A	1618	6MZ	N1-C2-N3	-3.28	123.62	128.58
27	A	2445	2MG	C6-C5-N7	3.26	136.22	130.29
1	a	1207	2MG	C6-C5-N7	3.25	136.20	130.29
1	a	1519	MA6	N1-C2-N3	-3.24	123.67	128.58
12	l	89	D2T	OD2-CG-CB	3.24	120.16	113.15
1	a	1498	UR3	C5-C4-N3	3.22	119.28	115.04
27	A	1962	5MC	C5-C6-N1	-3.18	119.86	123.31
27	A	2030	6MZ	N1-C2-N3	-3.15	123.82	128.58
27	A	2251	OMG	C6-C5-N7	3.15	136.02	130.29
22	x	54	5MU	C5-C6-N1	-3.13	119.91	123.31
1	a	1518	MA6	N1-C2-N3	-3.13	123.84	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1407	5MC	C5-C6-N1	-3.11	119.94	123.31
27	A	1835	2MG	C6-C5-N7	3.00	135.74	130.29
27	A	1618	6MZ	C9-N6-C6	-2.98	120.08	122.85
27	A	2552	OMU	O4-C4-C5	-2.98	120.02	125.16
1	a	1519	MA6	N1-C6-N6	2.92	120.41	116.86
1	a	1518	MA6	C5-C6-N6	-2.89	120.76	125.33
1	a	966	2MG	C6-C5-N7	2.88	135.53	130.29
22	x	37	MIA	C6-C5-N7	2.87	135.55	132.43
27	A	2503	2MA	N6-C6-N1	2.87	120.89	117.03
23	y	54	5MU	O2-C2-N1	-2.86	119.07	122.80
27	A	1939	5MU	O2-C2-N1	-2.83	119.11	122.80
1	a	1407	5MC	C5-C4-N3	-2.79	118.89	121.75
27	A	2503	2MA	C2-N1-C6	2.79	122.38	118.10
1	a	1516	2MG	C4-C5-N7	-2.76	106.30	110.67
1	a	967	5MC	C5-C4-N3	-2.70	118.98	121.75
27	A	2030	6MZ	C5-N7-C8	2.70	107.69	103.45
27	A	2030	6MZ	C4-N9-C8	2.69	108.56	105.74
1	a	1519	MA6	C10-N6-C9	-2.68	107.58	116.18
27	A	1962	5MC	C5-C4-N3	-2.68	119.01	121.75
1	a	1519	MA6	C5-N7-C8	2.64	107.60	103.45
1	a	1516	2MG	N1-C2-N2	2.64	119.25	116.56
27	A	2445	2MG	C4-C5-N7	-2.63	106.51	110.67
1	a	1207	2MG	C4-C5-N7	-2.61	106.53	110.67
27	A	745	1MG	C4-C5-N7	-2.59	106.56	110.67
27	A	2503	2MA	C4-N9-C8	2.58	108.45	105.74
23	y	46	G7M	O6-C6-C5	-2.58	122.26	128.01
27	A	1618	6MZ	C5-N7-C8	2.57	107.48	103.45
27	A	1618	6MZ	C4-N9-C8	2.56	108.43	105.74
27	A	2503	2MA	C5-N7-C8	2.55	107.45	103.45
27	A	745	1MG	C6-C5-N7	2.54	135.00	129.36
22	x	46	G7M	O6-C6-C5	-2.54	122.35	128.01
1	a	1518	MA6	C4-N9-C8	2.53	108.39	105.74
27	A	2251	OMG	C4-C5-N7	-2.52	106.68	110.67
11	k	119	IAS	OD1-CG-CB	-2.51	118.08	125.38
27	A	747	5MU	O2-C2-N1	-2.49	119.56	122.80
22	x	37	MIA	C5-N7-C8	2.48	107.35	103.45
22	x	37	MIA	C4-N9-C8	2.47	108.33	105.74
27	A	2552	OMU	O2-C2-N1	-2.46	119.60	122.80
1	a	527	G7M	O6-C6-C5	-2.45	122.54	128.01
27	A	2069	G7M	O6-C6-C5	-2.44	122.56	128.01
23	y	8	4SU	O2-C2-N1	-2.43	119.63	122.80
1	a	966	2MG	C4-C5-N7	-2.43	106.81	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	C4-N9-C8	2.43	108.29	105.74
27	A	1835	2MG	C4-C5-N7	-2.41	106.86	110.67
27	A	2580	PSU	O4'-C1'-C2'	2.39	108.46	105.15
22	x	54	5MU	C1'-N1-C2	2.38	121.86	117.59
1	a	1518	MA6	C5-N7-C8	2.37	107.18	103.45
1	a	516	PSU	O4'-C1'-C2'	2.34	108.39	105.15
22	x	37	MIA	N6-C6-N1	2.32	121.45	118.33
27	A	1915	3TD	C6-C5-C4	2.30	119.74	118.19
1	a	1402	4OC	C6-C5-C4	2.28	119.75	117.00
22	x	54	5MU	C1'-N1-C6	-2.27	117.41	121.15
27	A	2457	PSU	O4'-C1'-C2'	2.27	108.30	105.15
27	A	2498	OMC	O2-C2-N3	-2.26	118.76	122.33
22	x	37	MIA	N3-C2-N1	-2.25	122.89	127.00
22	x	54	5MU	O2-C2-N1	-2.25	119.87	122.80
22	x	39	PSU	C5-C6-N1	-2.23	119.05	122.14
1	a	1518	MA6	C10-N6-C9	-2.21	109.09	116.18
1	a	527	G7M	C5-C6-N1	2.19	116.37	111.84
27	A	746	PSU	C5-C6-N1	-2.18	119.11	122.14
27	A	2503	2MA	C6-C5-N7	2.18	136.29	132.09
22	x	37	MIA	C2-N1-C6	2.16	121.64	117.54
27	A	1835	2MG	O6-C6-C5	-2.15	120.85	126.53
27	A	2445	2MG	N1-C2-N2	2.15	118.76	116.56
27	A	2251	OMG	O6-C6-C5	-2.14	120.89	126.53
23	y	39	PSU	C5-C6-N1	-2.14	119.17	122.14
27	A	2030	6MZ	N9-C8-N7	-2.13	110.92	113.94
27	A	2069	G7M	C5-C6-N1	2.13	116.23	111.84
1	a	1519	MA6	C5-C6-N6	-2.13	121.97	125.33
1	a	1516	2MG	O6-C6-C5	-2.12	120.94	126.53
1	a	966	2MG	C2-N1-C6	-2.12	121.99	124.55
1	a	1516	2MG	N2-C2-N3	-2.12	117.81	120.51
1	a	1207	2MG	N1-C2-N2	2.11	118.72	116.56
27	A	2504	PSU	C5-C6-N1	-2.11	119.21	122.14
1	a	966	2MG	O6-C6-C5	-2.11	120.97	126.53
27	A	1835	2MG	N1-C2-N2	2.09	118.69	116.56
1	a	966	2MG	CM2-N2-C2	-2.09	119.16	123.65
23	y	32	PSU	O4'-C1'-C2'	2.08	108.03	105.15
27	A	2445	2MG	O6-C6-C5	-2.07	121.07	126.53
1	a	1498	UR3	C3U-N3-C4	2.06	120.72	117.87
1	a	1207	2MG	O6-C6-C5	-2.06	121.10	126.53
27	A	2605	PSU	O4'-C1'-C2'	2.05	107.99	105.15
40	O	81	4D4	O-C-CA	-2.05	119.50	124.77
27	A	1917	PSU	O4'-C1'-C2'	2.04	107.98	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	2604	PSU	C5-C6-N1	-2.04	119.31	122.14
23	y	32	PSU	C5-C6-N1	-2.04	119.31	122.14
27	A	2503	2MA	N9-C8-N7	-2.04	111.05	113.94
27	A	1911	PSU	C5-C6-N1	-2.03	119.32	122.14
27	A	2457	PSU	C5-C6-N1	-2.01	119.35	122.14
22	x	55	PSU	C5-C6-N1	-2.01	119.35	122.14
23	y	39	PSU	O4'-C1'-C2'	2.01	107.93	105.15
1	a	1407	5MC	O2-C2-N3	-2.00	119.17	122.33

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	966	2MG	N1-C2-N2-CM2
1	a	966	2MG	N3-C2-N2-CM2
1	a	1518	MA6	C5-C6-N6-C9
1	a	1519	MA6	O4'-C4'-C5'-O5'
1	a	1519	MA6	C5-C6-N6-C9
22	x	37	MIA	N6-C12-C13-C14
22	x	37	MIA	C12-C13-C14-C15
22	x	37	MIA	C12-C13-C14-C16
40	O	81	4D4	C-CA-CB-OB
40	O	81	4D4	C-CA-CB-CG
40	O	81	4D4	N-CA-CB-OB
40	O	81	4D4	N-CA-CB-CG
40	O	81	4D4	OB-CB-CG-CD
23	y	46	G7M	C4'-C5'-O5'-P
23	y	54	5MU	C3'-C4'-C5'-O5'
23	y	54	5MU	O4'-C4'-C5'-O5'
23	y	55	PSU	C2'-C1'-C5-C4
27	A	746	PSU	C2'-C1'-C5-C4
27	A	746	PSU	O4'-C1'-C5-C4
27	A	746	PSU	C2'-C1'-C5-C6
40	O	82	MS6	CA-CB-CG-SD
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	527	G7M	C3'-C4'-C5'-O5'
1	a	1402	4OC	O4'-C4'-C5'-O5'
22	x	37	MIA	O4'-C4'-C5'-O5'
22	x	37	MIA	C3'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C9
1	a	1519	MA6	C3'-C4'-C5'-O5'
30	D	150	MEQ	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
30	D	150	MEQ	OE1-CD-CG-CB
22	x	55	PSU	C3'-C4'-C5'-O5'
22	x	55	PSU	O4'-C4'-C5'-O5'
27	A	2030	6MZ	O4'-C4'-C5'-O5'
22	x	55	PSU	C4'-C5'-O5'-P
1	a	1402	4OC	C3'-C4'-C5'-O5'
40	O	82	MS6	CB-CG-SD-CE
23	y	46	G7M	C3'-C4'-C5'-O5'
12	l	89	D2T	CG-CB-SB-CB1
27	A	2030	6MZ	C3'-C4'-C5'-O5'
1	a	1518	MA6	N1-C6-N6-C9
40	O	81	4D4	CA-CB-CG-CD
27	A	2498	OMC	O4'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C2'-O2'-CM2
27	A	2498	OMC	C3'-C2'-O2'-CM2
23	y	39	PSU	O4'-C1'-C5-C4
23	y	55	PSU	O4'-C1'-C5-C4
23	y	55	PSU	C4'-C5'-O5'-P
1	a	1519	MA6	C5-C6-N6-C10
23	y	46	G7M	C2'-C1'-N9-C8
27	A	746	PSU	O4'-C1'-C5-C6
27	A	1917	PSU	C3'-C4'-C5'-O5'
40	O	81	4D4	O-C-CA-CB
23	y	46	G7M	C2'-C1'-N9-C4

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1402	4OC	2	0
27	A	1915	3TD	1	0
27	A	2498	OMC	1	0
23	y	8	4SU	1	0
1	a	1518	MA6	2	0
27	A	2503	2MA	1	0
1	a	1516	2MG	1	0
27	A	2030	6MZ	3	0
12	l	89	D2T	1	0
1	a	966	2MG	1	0
23	y	46	G7M	2	0
1	a	1519	MA6	2	0
23	y	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 583 ligands modelled in this entry, 583 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

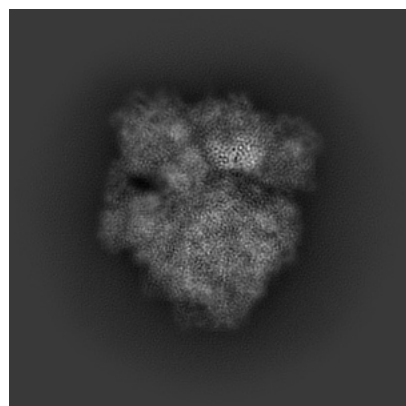
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29620. These allow visual inspection of the internal detail of the map and identification of artifacts.

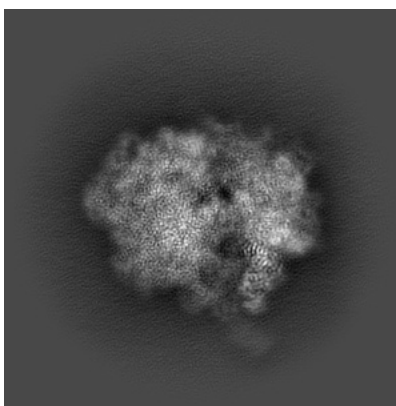
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

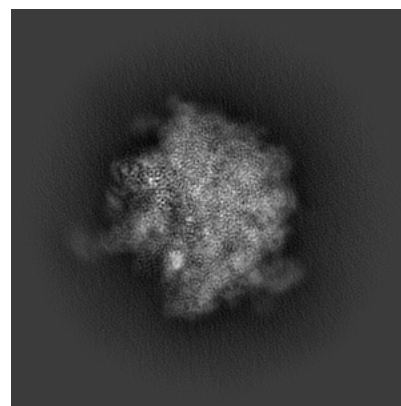
6.1.1 Primary map



X

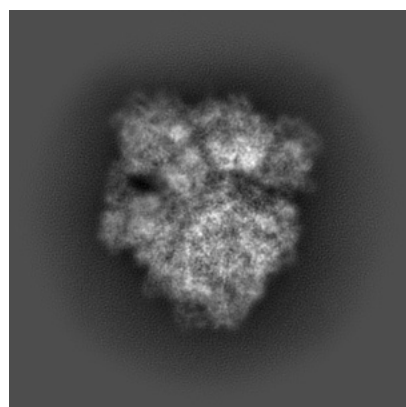


Y

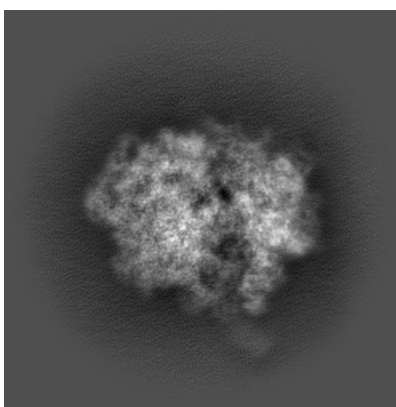


Z

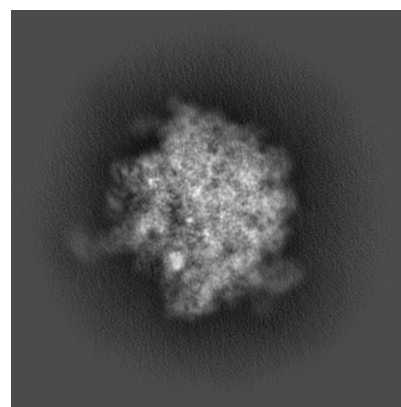
6.1.2 Raw map



X



Y

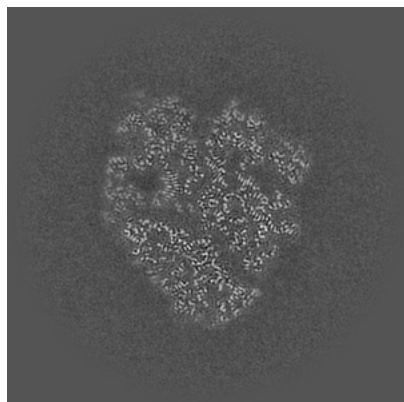


Z

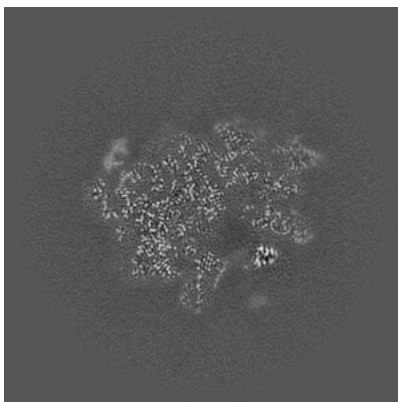
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

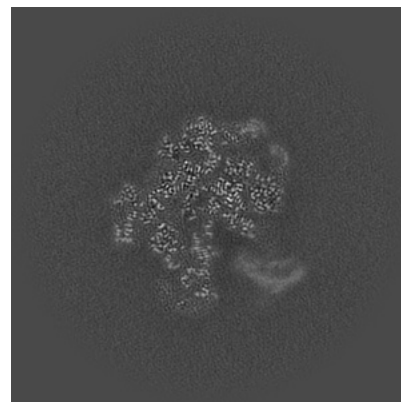
6.2.1 Primary map



X Index: 256

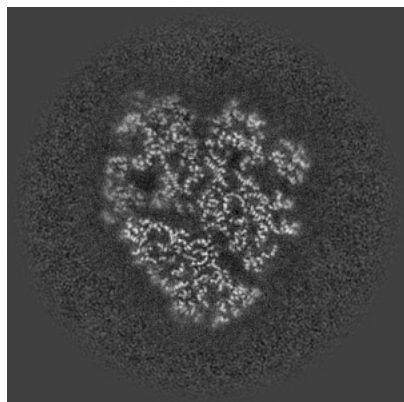


Y Index: 256

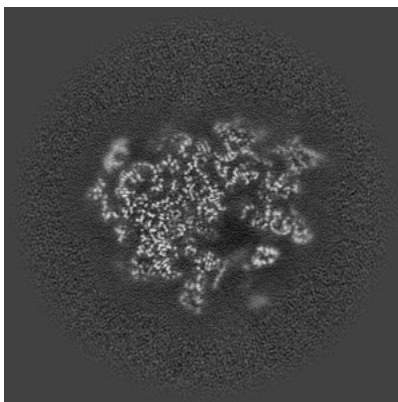


Z Index: 256

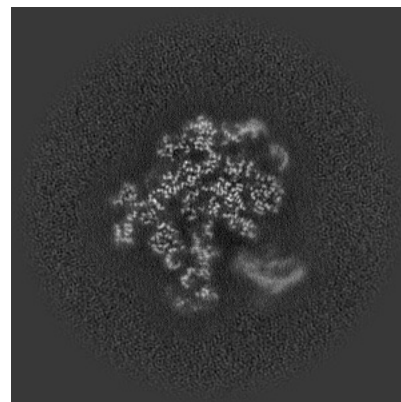
6.2.2 Raw map



X Index: 256



Y Index: 256

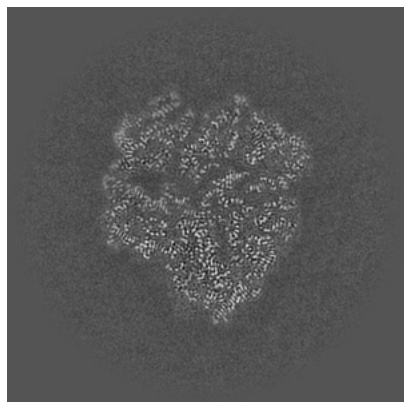


Z Index: 256

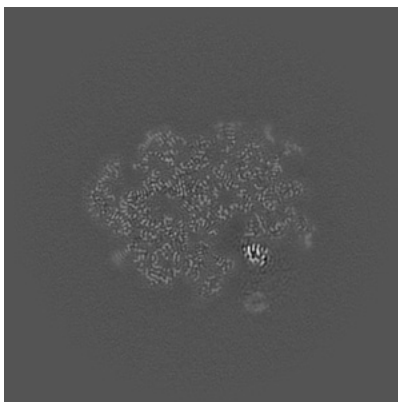
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

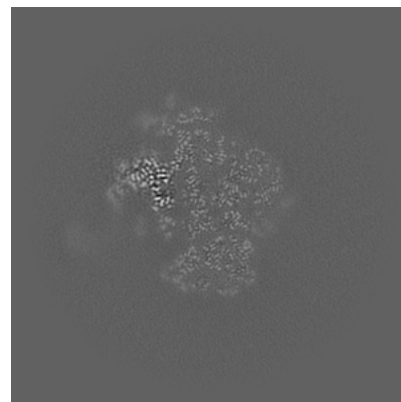
6.3.1 Primary map



X Index: 246

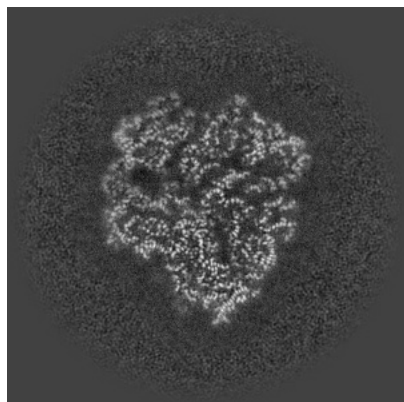


Y Index: 272

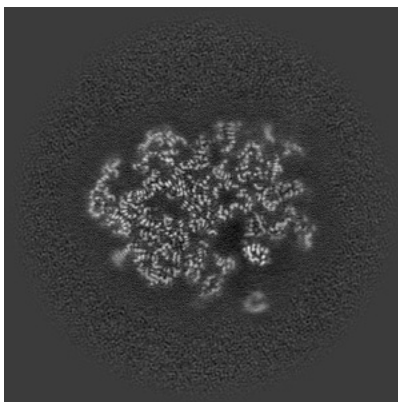


Z Index: 328

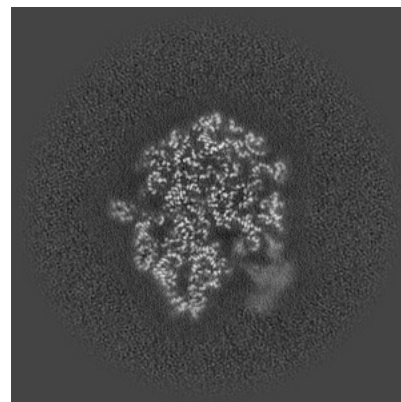
6.3.2 Raw map



X Index: 247



Y Index: 272

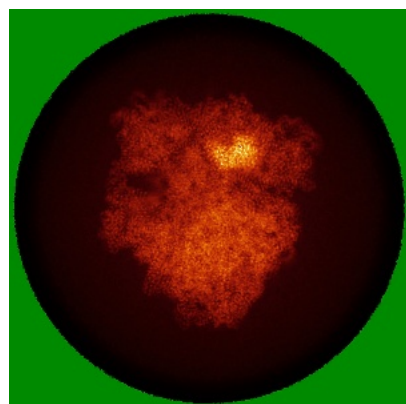


Z Index: 231

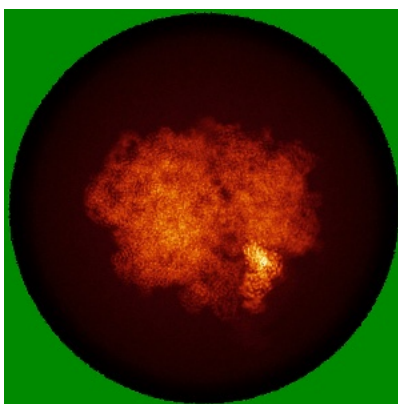
The images above show the largest variance slices of the map in three orthogonal directions.

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

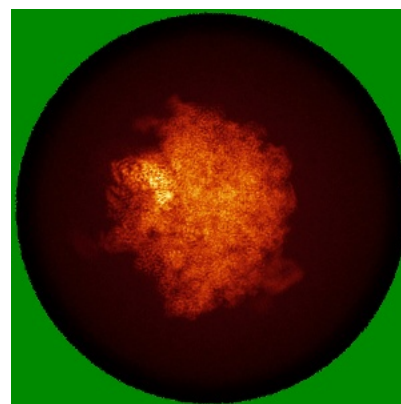
6.4.1 Primary map



X

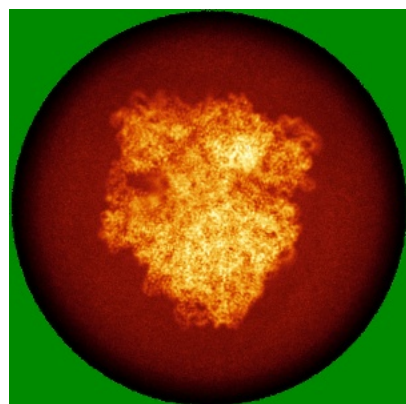


Y

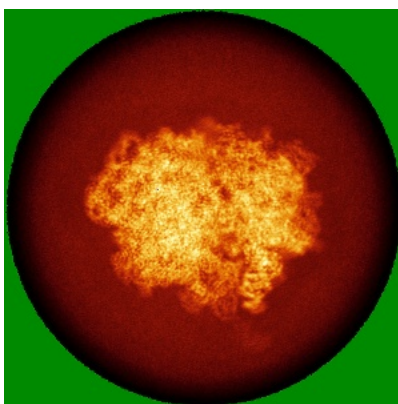


Z

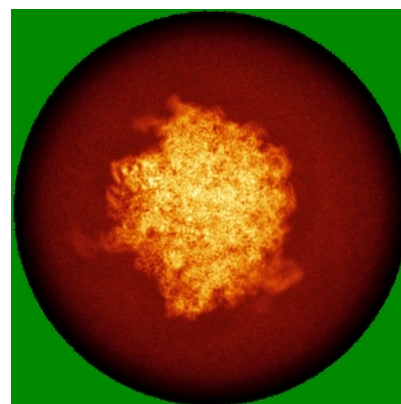
6.4.2 Raw map



X



Y

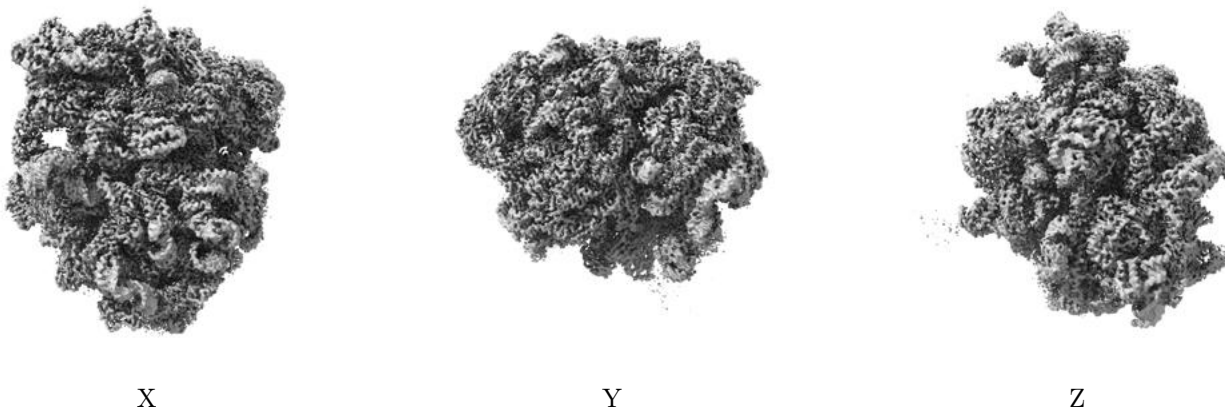


Z

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.

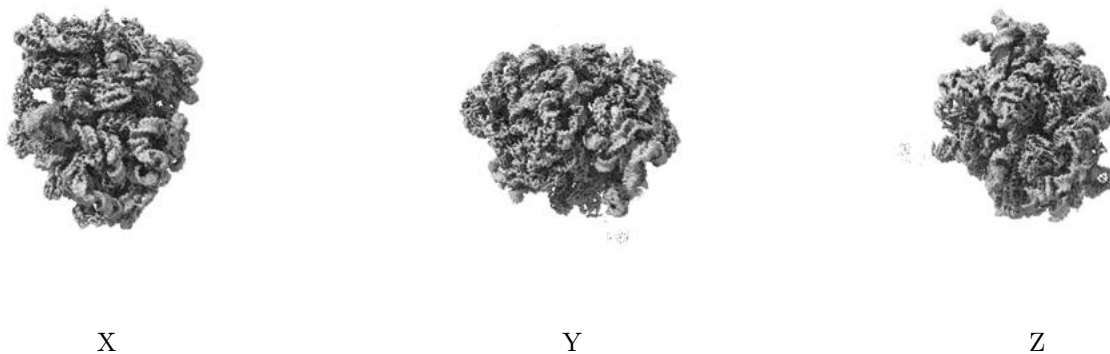
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

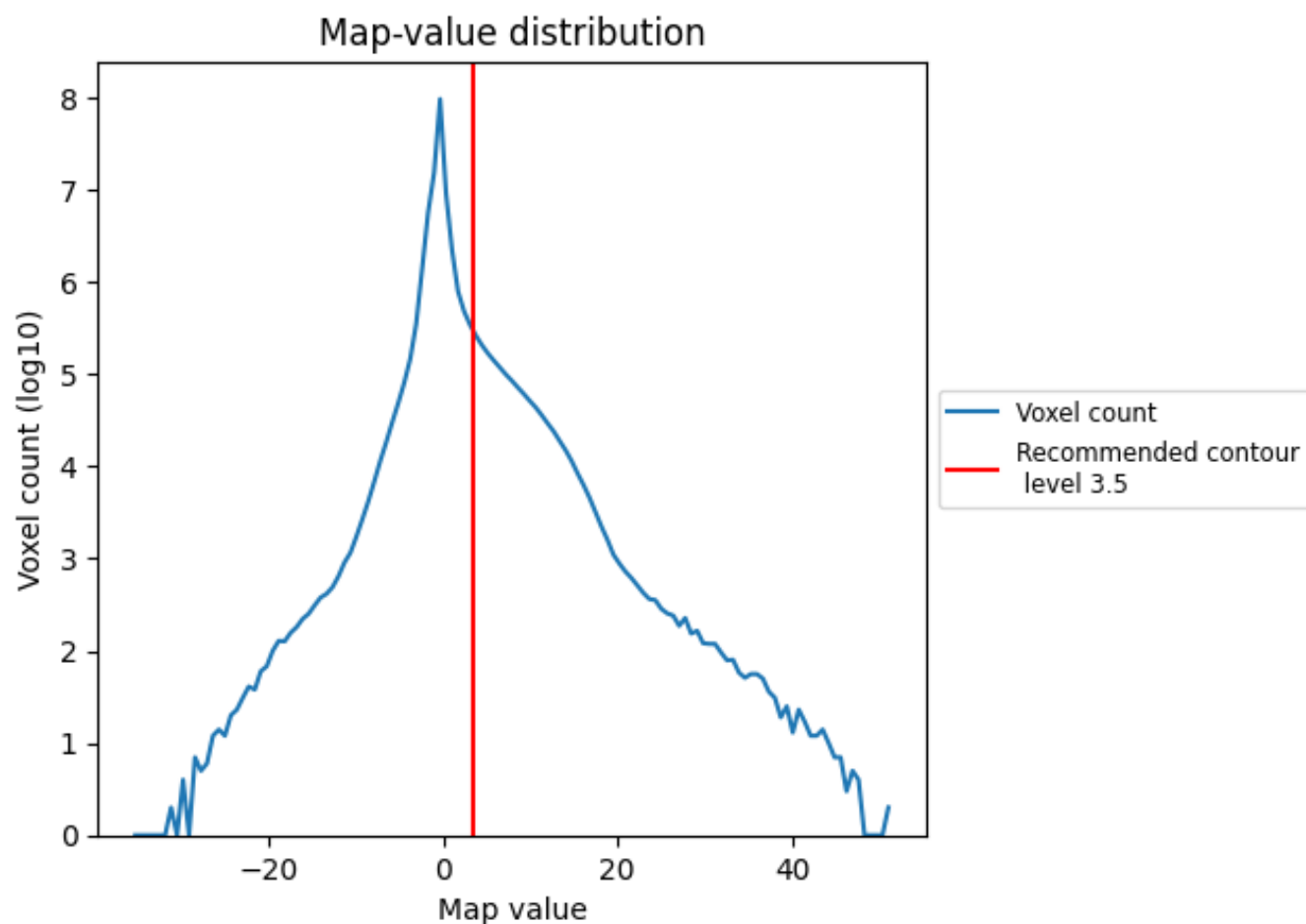
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

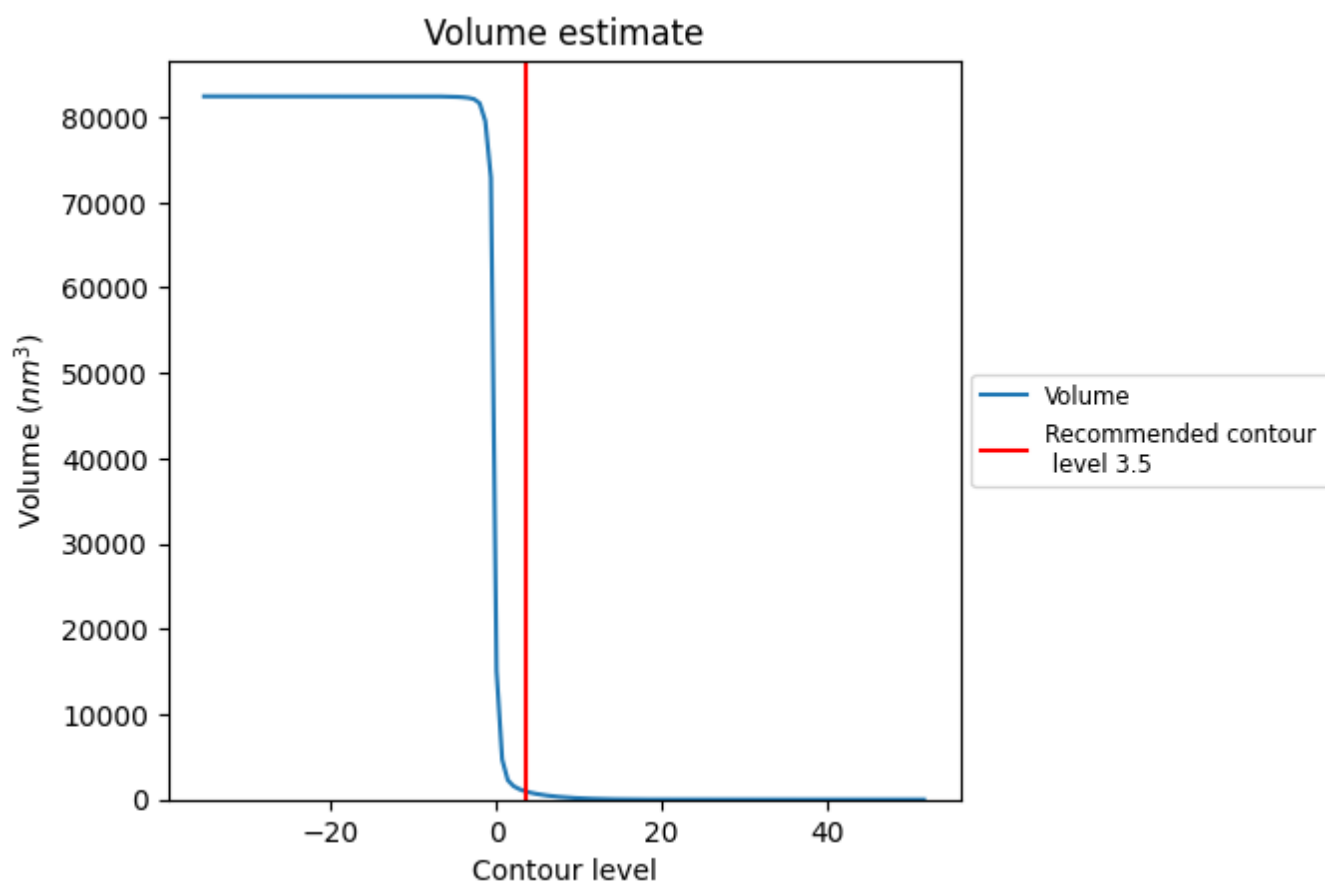
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

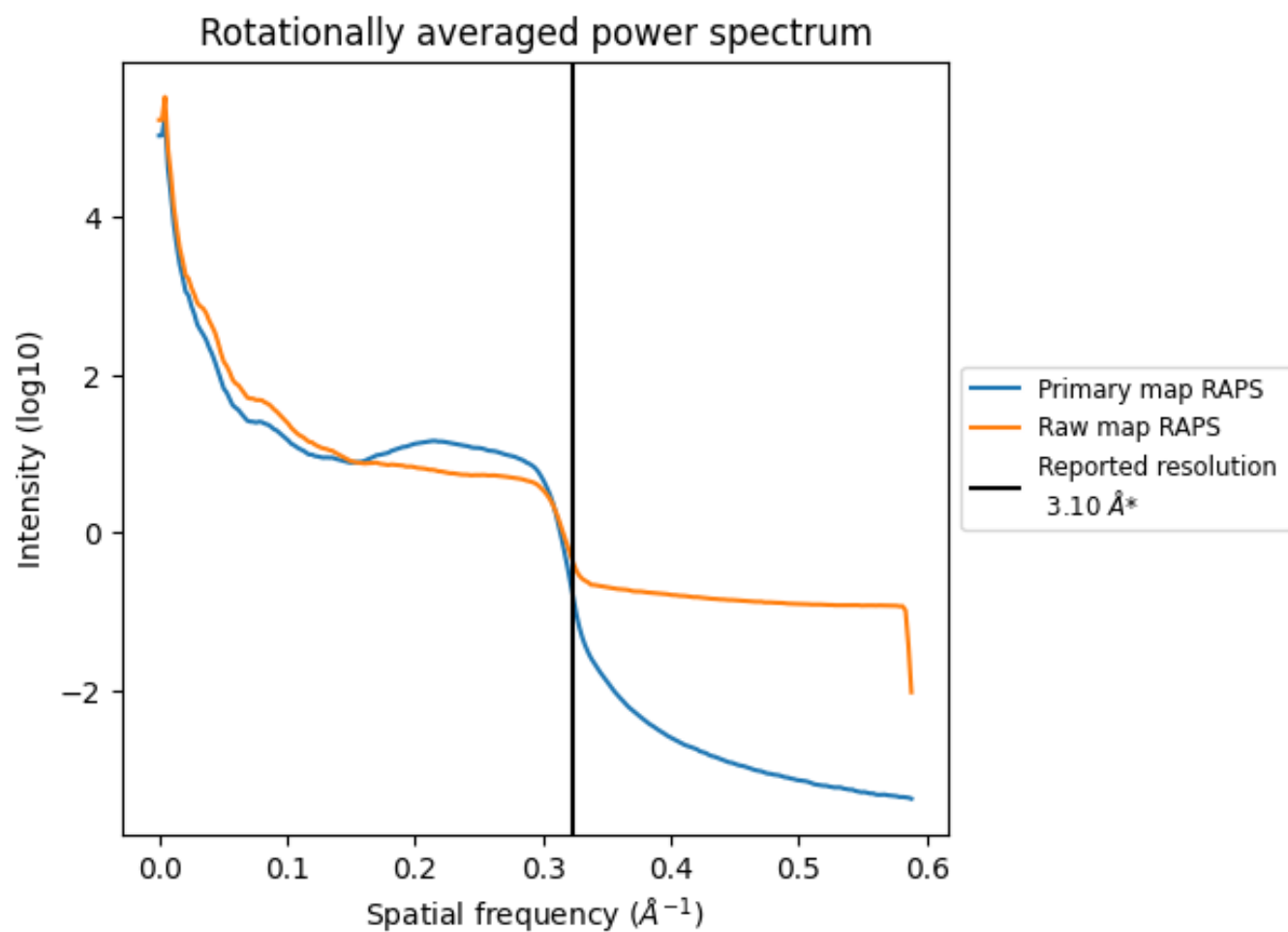
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 983 nm^3 ; this corresponds to an approximate mass of 888 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

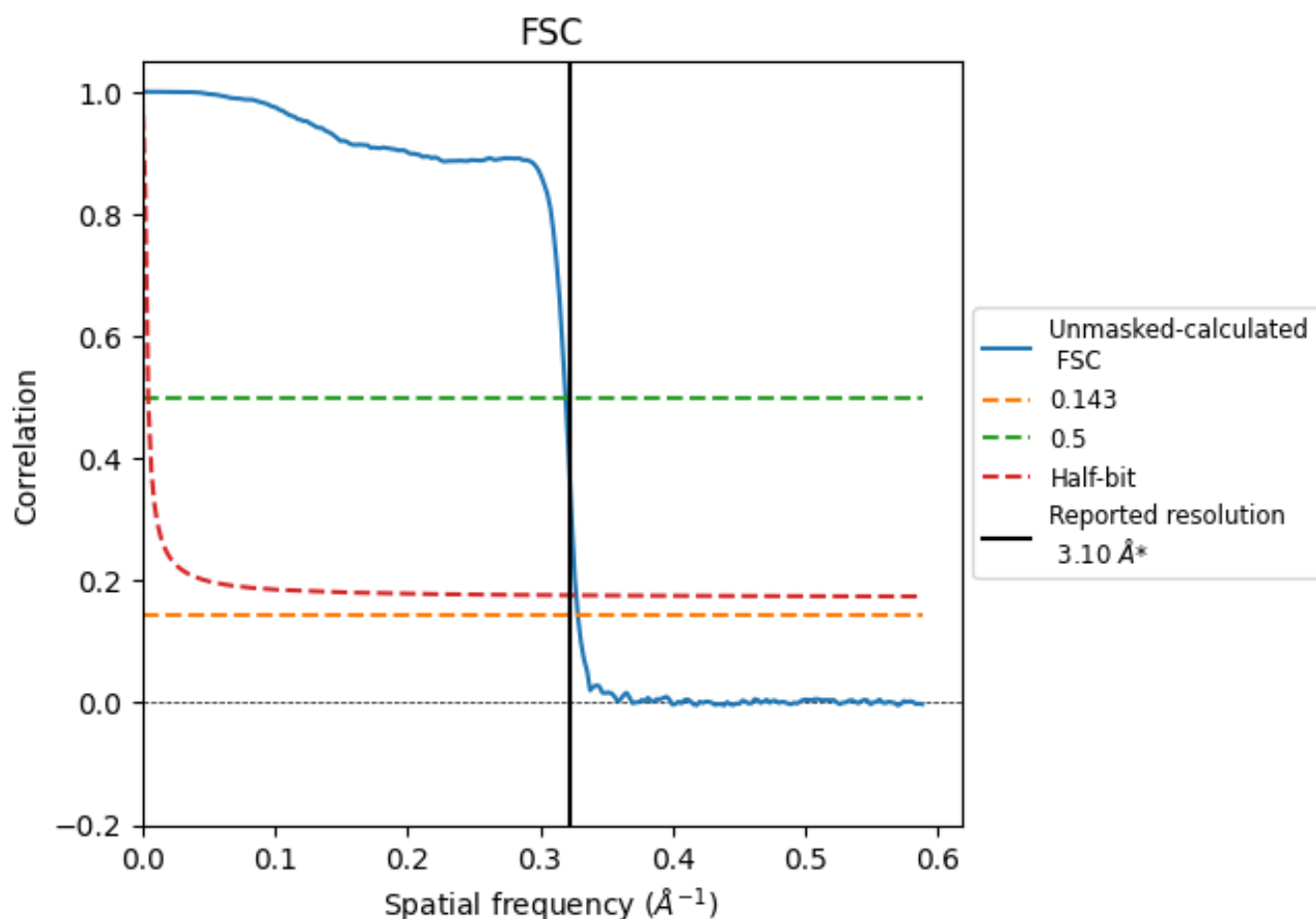


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

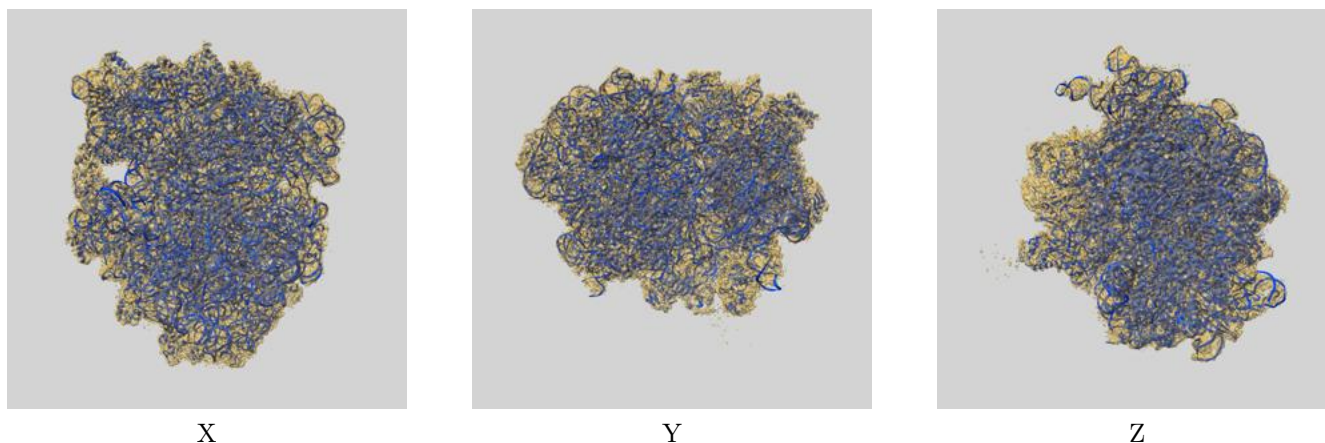
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.13	3.06

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

9 Map-model fit [i](#)

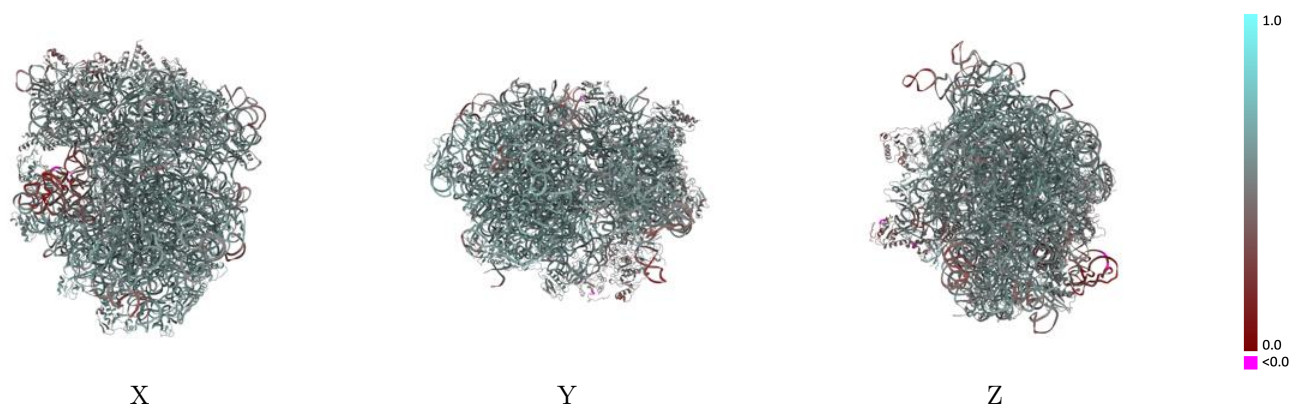
This section contains information regarding the fit between EMDB map EMD-29620 and PDB model 8FZD. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



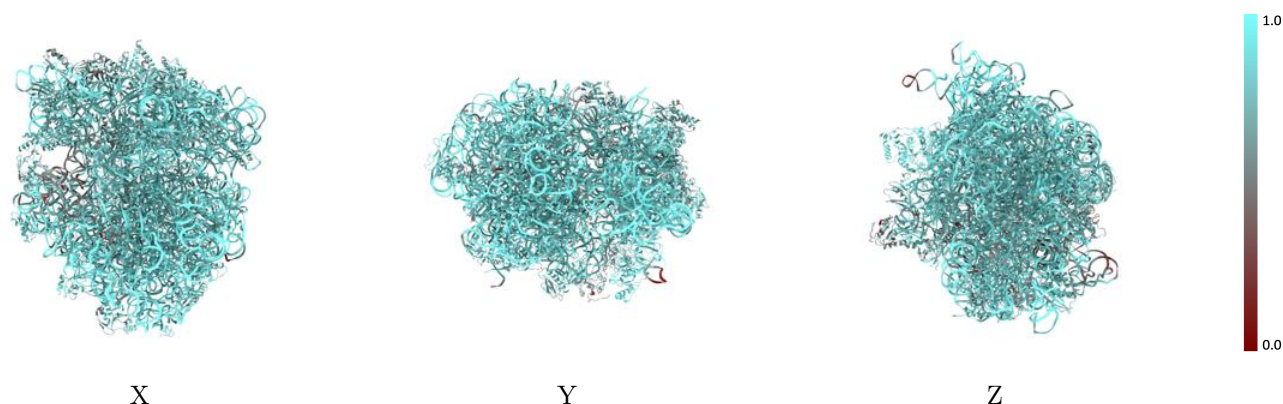
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



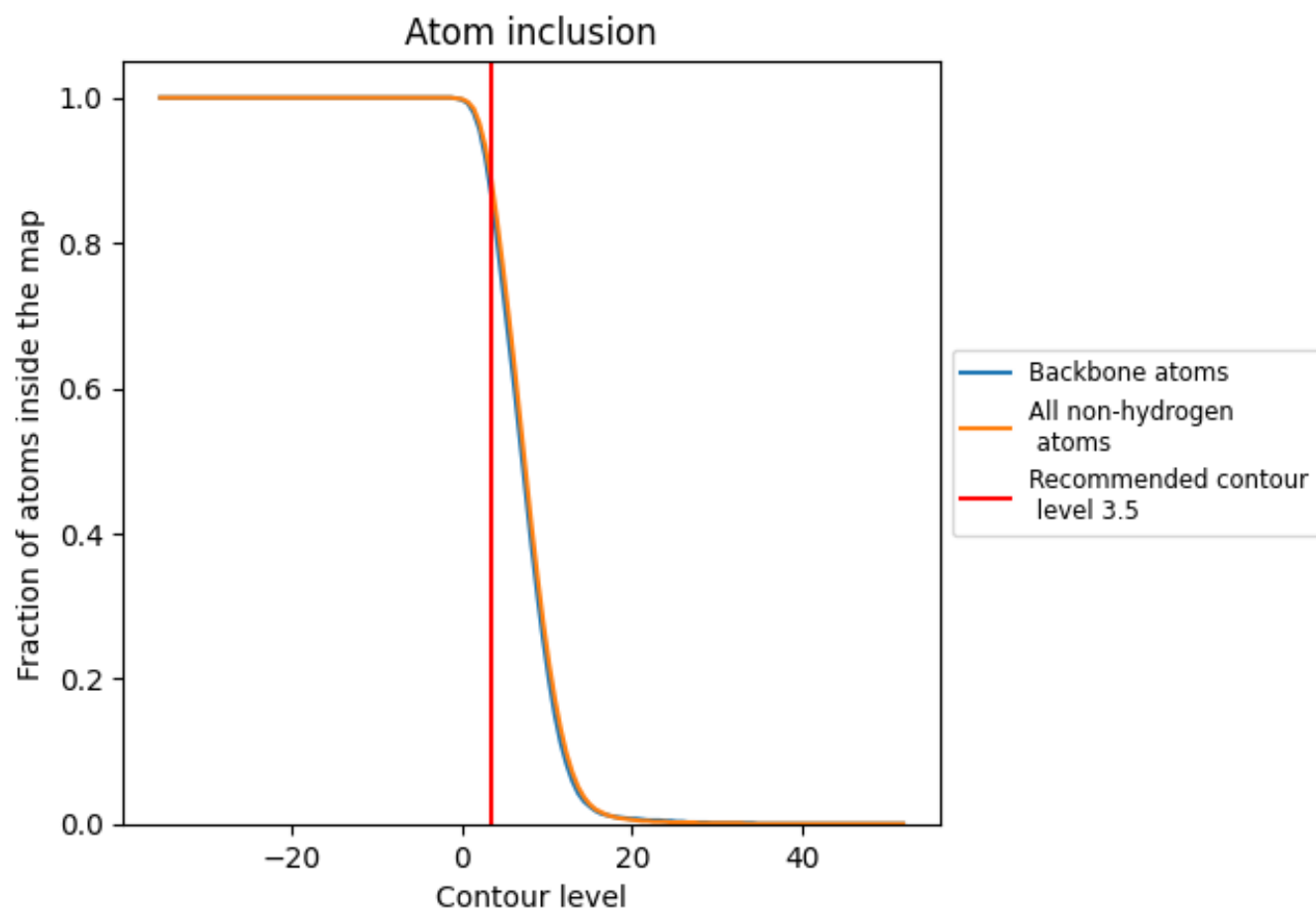
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 89% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.5520
1	 0.8340	 0.5670
2	 0.8560	 0.5900
3	 0.7060	 0.5050
4	 0.9190	 0.6070
5	 0.8410	 0.5610
6	 0.9040	 0.6070
7	 0.9130	 0.6120
8	 0.8940	 0.5950
A	 0.9330	 0.5640
B	 0.9130	 0.5530
C	 0.8710	 0.5980
D	 0.8820	 0.5930
E	 0.8550	 0.5830
F	 0.8050	 0.5490
G	 0.7900	 0.5390
H	 0.2150	 0.4510
I	 0.5320	 0.3520
J	 0.6590	 0.3980
L	 0.8880	 0.5970
M	 0.8280	 0.5960
N	 0.8800	 0.5900
O	 0.8690	 0.5940
P	 0.9260	 0.6090
Q	 0.8700	 0.5740
R	 0.8540	 0.5910
S	 0.9300	 0.6090
T	 0.8850	 0.5890
U	 0.8720	 0.5910
V	 0.8200	 0.5790
W	 0.8270	 0.5620
X	 0.8390	 0.5750
Y	 0.8850	 0.6010
Z	 0.8690	 0.5840
a	 0.9270	 0.5510



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Chain	Atom inclusion	Q-score
b	 0.7200	 0.4860
c	 0.7100	 0.5260
d	 0.8010	 0.5090
e	 0.8270	 0.5600
f	 0.7620	 0.5020
g	 0.7250	 0.5020
h	 0.8320	 0.5630
i	 0.8070	 0.5270
j	 0.6850	 0.4780
k	 0.8170	 0.5430
l	 0.8280	 0.5820
m	 0.7920	 0.5340
n	 0.7970	 0.5290
o	 0.7880	 0.5400
p	 0.8360	 0.5520
q	 0.8060	 0.5670
r	 0.7990	 0.5540
s	 0.8050	 0.5240
t	 0.8240	 0.5480
u	 0.6540	 0.4970
v	 0.9420	 0.4950
w	 0.7530	 0.5250
x	 0.8870	 0.5570
y	 0.4930	 0.3010
z	 0.8430	 0.5640