



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 03:39 am BST

PDB ID : 7OIF / pdb_00007oif
EMDB ID : EMD-12928
Title : CspA-27 cotranslational folding intermediate 2
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;
Novacek, J.; Valle, M.; Rodnina, M.V.
Deposited on : 2021-05-11
Resolution : 3.00 Å(reported)
Based on initial model : 6ORE

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

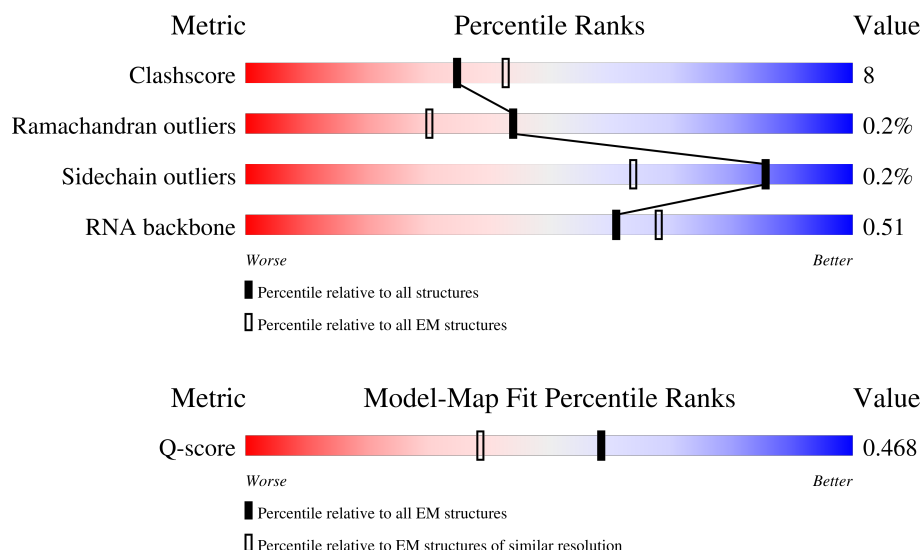
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	2903	
2	2	1534	
3	3	120	

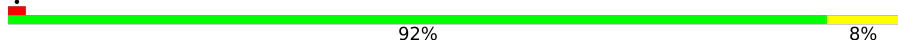
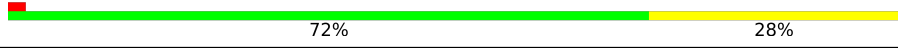
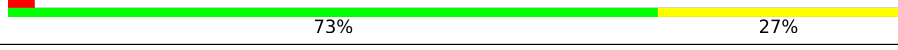
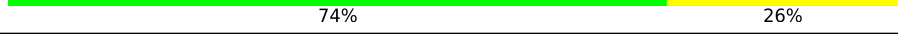
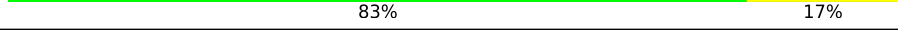
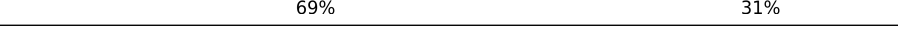
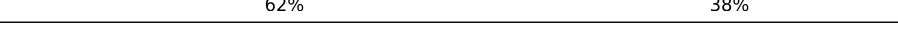
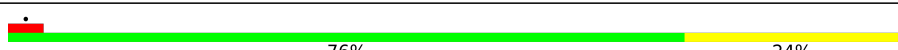
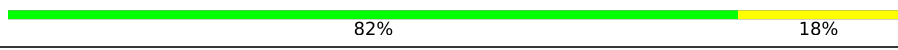
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Mol	Chain	Length	Quality of chain
4	4	6	100%
5	C	271	79% 21%
6	D	209	84% 14% .
7	E	201	84% 16%
8	F	177	64% 36%
9	G	175	78% 22%
10	H	149	58% 56% 42% .
11	I	142	85% 15%
12	J	123	85% 15%
13	K	144	79% 21%
14	L	136	86% 14%
15	M	119	82% 18%
16	N	116	76% 24%
17	O	114	83% 17%
18	P	117	87% 13%
19	Q	103	78% 20% ..
20	R	110	74% 26%
21	S	94	77% 22% .
22	T	103	74% 26%
23	U	94	79% 21%
24	V	80	6% 80% 19% .
25	W	77	83% 17%
26	X	62	87% 13%
27	Y	58	83% 17%
28	Z	66	6% 58% 41% .

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Mol	Chain	Length	Quality of chain
29	a	56	
30	b	52	
31	c	46	
32	d	64	
33	e	38	
34	f	225	
35	g	208	
36	h	205	
37	i	156	
38	j	104	
39	k	151	
40	l	129	
41	m	127	
42	n	99	
43	o	117	
44	p	123	
45	q	116	
46	r	100	
47	s	88	
48	t	82	
49	u	80	
50	v	66	
51	w	83	
52	x	86	
53	y	70	

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Mol	Chain	Length	Quality of chain
54	z	88	25% 48% 22% 6%
55	B	27	19% 26% 59% 11% •

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 145152 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S rRNA.

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

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	6	Total	C	N	O	P	0	0
			126	56	20	44	6		

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	80	Total	C	N	O	S	0	0
			601	370	121	109	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

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

- Molecule 35 is a protein called 30S ribosomal protein S3.

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

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

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

- Molecule 38 is a protein called 30S ribosomal protein S6.

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

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

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

- Molecule 43 is a protein called 30S ribosomal protein S11.

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

- Molecule 44 is a protein called 30S ribosomal protein S12.

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

- Molecule 45 is a protein called 30S ribosomal protein S13.

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

- Molecule 46 is a protein called 30S ribosomal protein S14.

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

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

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

- Molecule 51 is a protein called 30S ribosomal protein S19.

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

- Molecule 52 is a protein called 30S ribosomal protein S20.

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

- Molecule 53 is a protein called 30S ribosomal protein S21.

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

- Molecule 54 is a RNA chain called tRNA-Ser.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	88	Total	C	N	O	P	0	0
			1891	841	341	621	88		

- Molecule 55 is a protein called CspA transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	27	Total	C	N	O	S	0	0
			205	132	32	39	2		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	276	Total 276	Mg 276	0
56	2	119	Total 119	Mg 119	0
56	3	8	Total 8	Mg 8	0
56	4	1	Total 1	Mg 1	0
56	C	1	Total 1	Mg 1	0
56	D	2	Total 2	Mg 2	0
56	P	1	Total 1	Mg 1	0
56	T	1	Total 1	Mg 1	0
56	a	2	Total 2	Mg 2	0
56	h	1	Total 1	Mg 1	0
56	q	1	Total 1	Mg 1	0
56	r	1	Total 1	Mg 1	0
56	z	2	Total 2	Mg 2	0

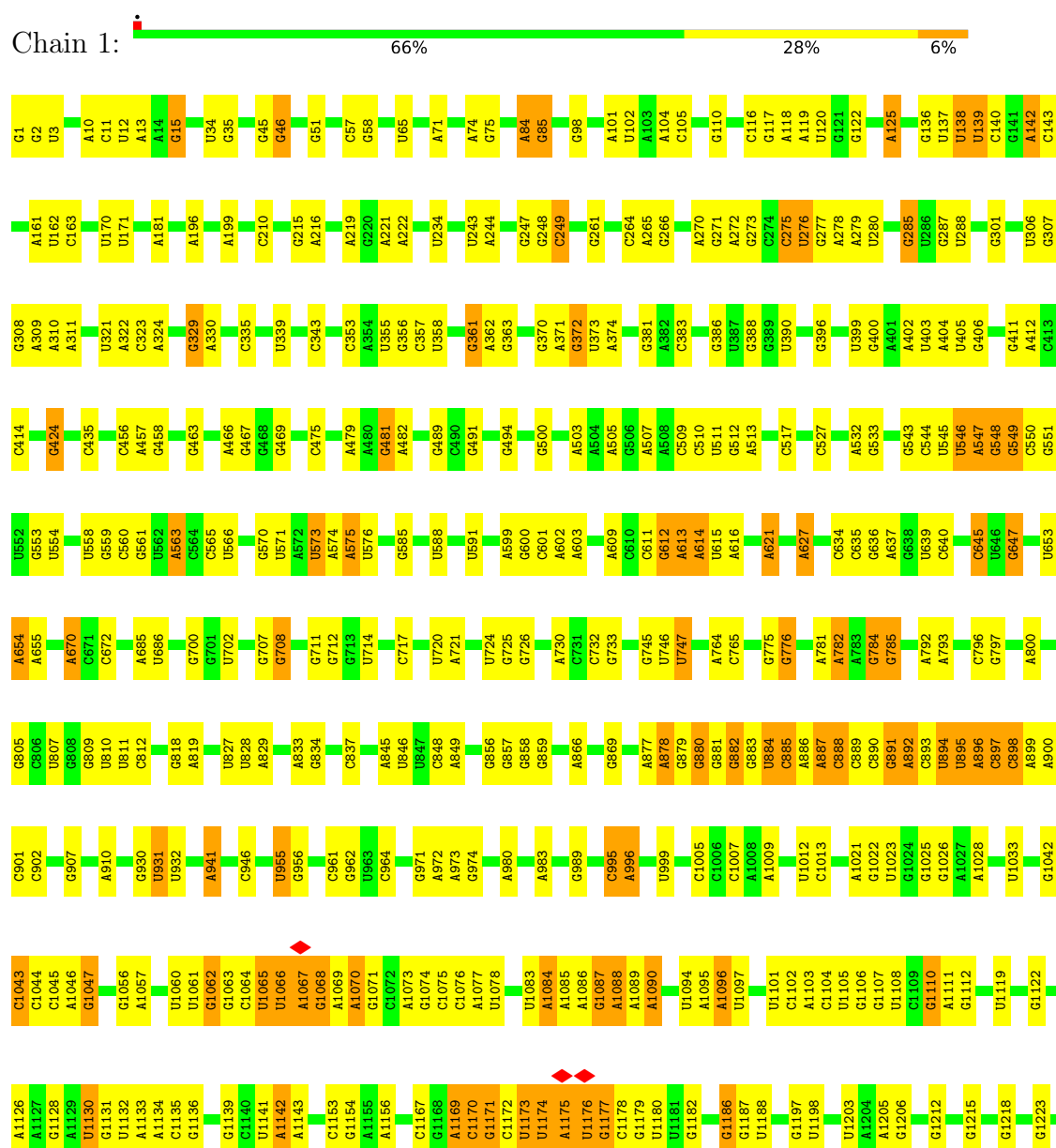
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total 1	Zn 1	0
57	e	1	Total 1	Zn 1	0

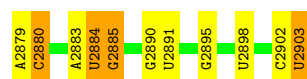
3 Residue-property plots

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

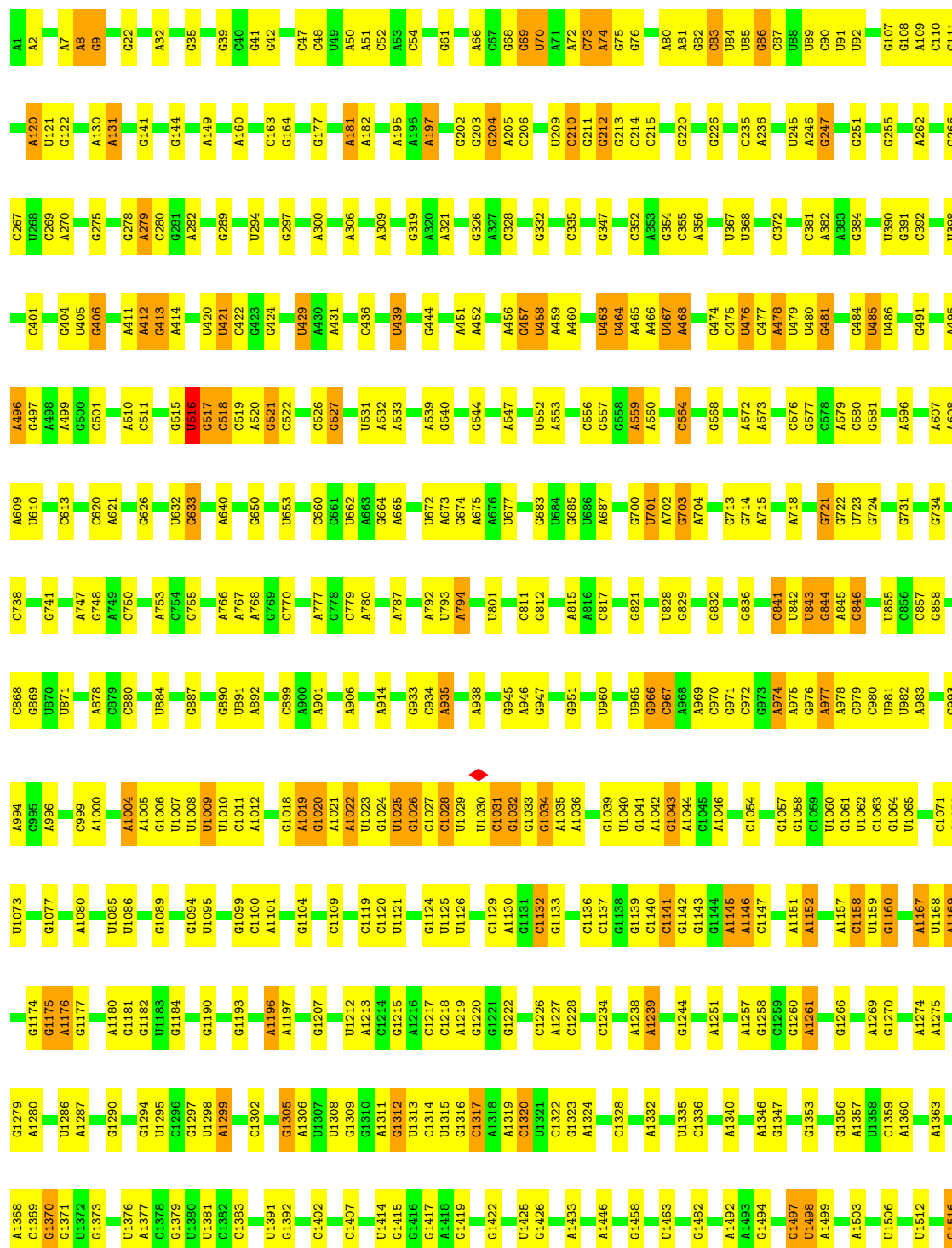
• Molecule 1: 23S rRNA







• Molecule 2: 16S rRNA





- Molecule 3: 5S rRNA

Chain 3: 77% 19%



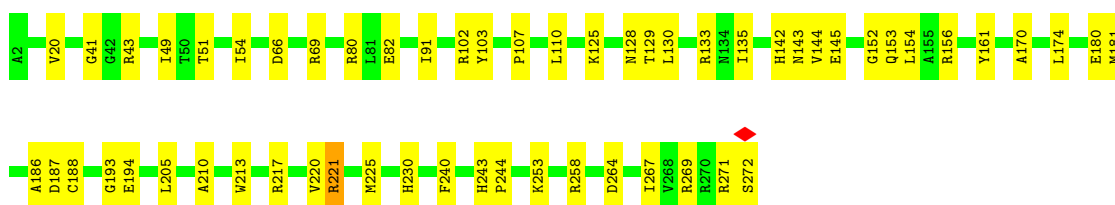
- Molecule 4: mRNA

Chain 4: 100%

There are no outlier residues recorded for this chain.

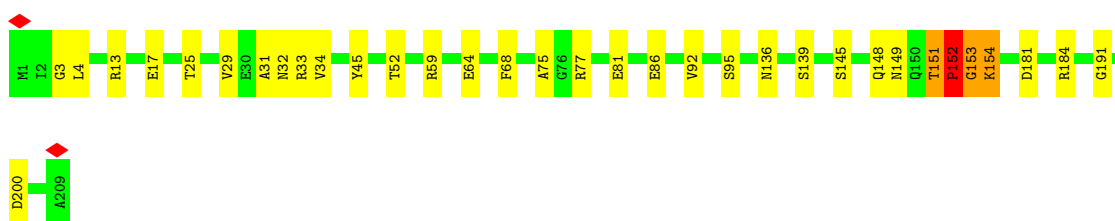
- Molecule 5: 50S ribosomal protein L2

Chain C: 79% 21%



- Molecule 6: 50S ribosomal protein L3

Chain D: 84% 14%



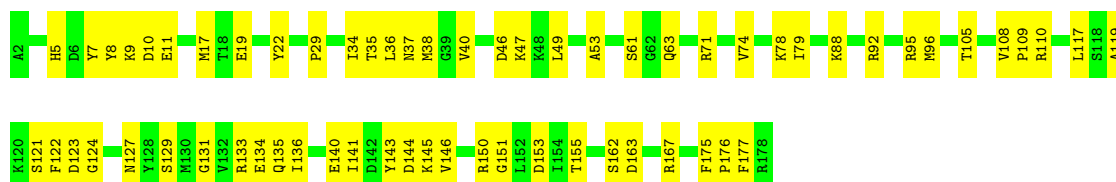
- Molecule 7: 50S ribosomal protein L4

Chain E: 84% 16%

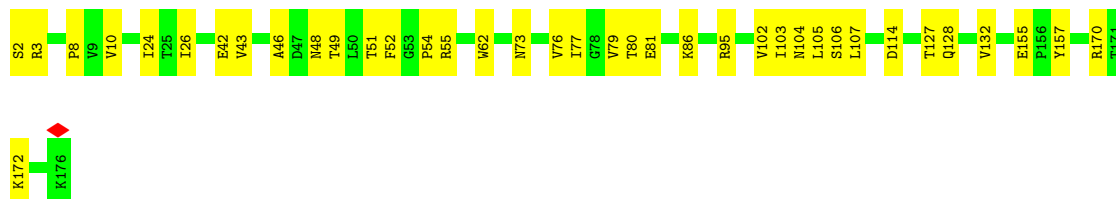
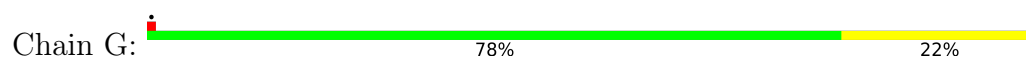


- Molecule 8: 50S ribosomal protein L5

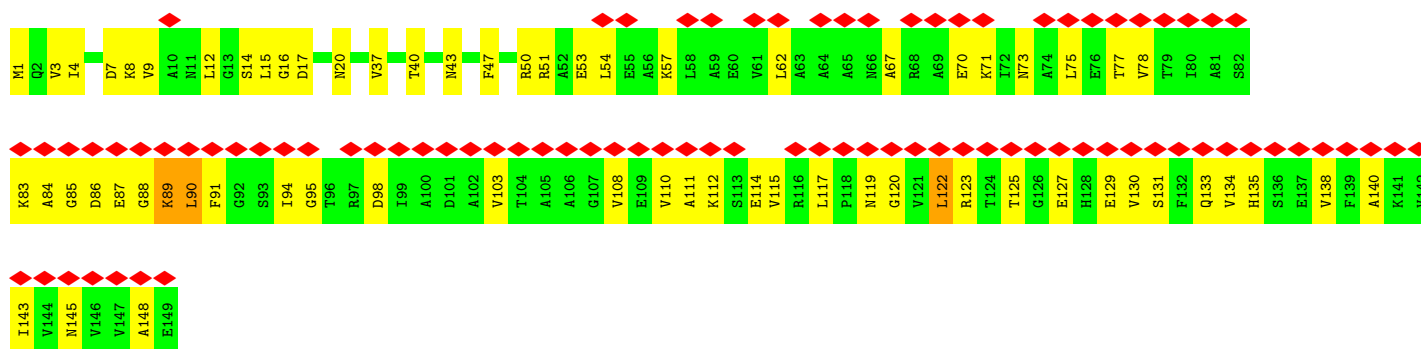
Chain F: 64% 36%



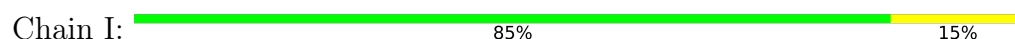
• Molecule 9: 50S ribosomal protein L6



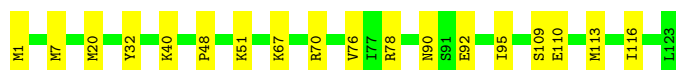
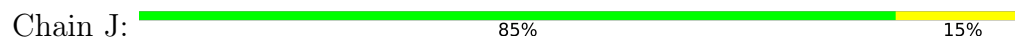
• Molecule 10: 50S ribosomal protein L9



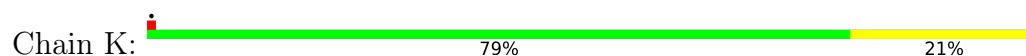
• Molecule 11: 50S ribosomal protein L13



• Molecule 12: 50S ribosomal protein L14

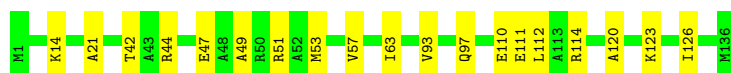
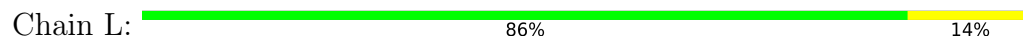


• Molecule 13: 50S ribosomal protein L15

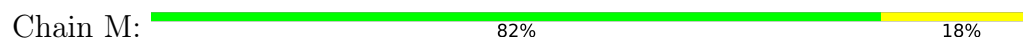




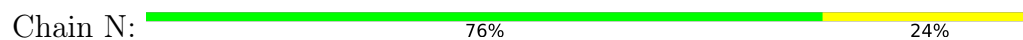
- Molecule 14: 50S ribosomal protein L16



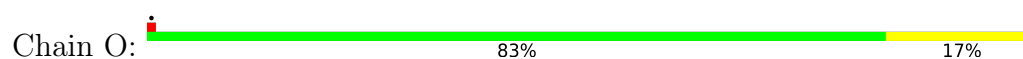
- Molecule 15: 50S ribosomal protein L17



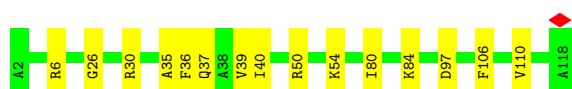
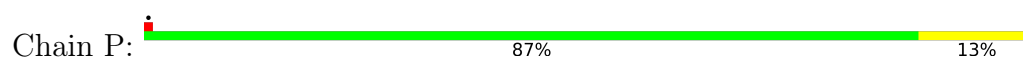
- Molecule 16: 50S ribosomal protein L18



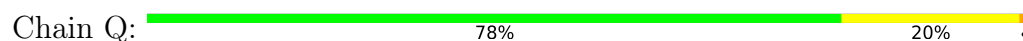
- Molecule 17: 50S ribosomal protein L19



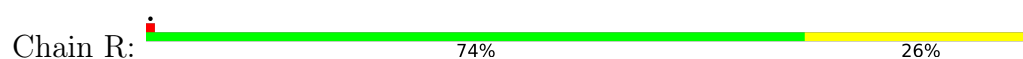
- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21



- Molecule 20: 50S ribosomal protein L22





- Molecule 21: 50S ribosomal protein L23

Chain S: 77% 22%



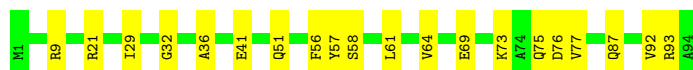
- Molecule 22: 50S ribosomal protein L24

Chain T: 74% 26%



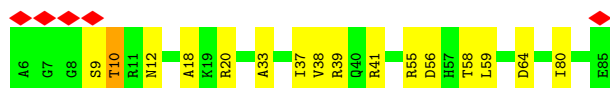
- Molecule 23: 50S ribosomal protein L25

Chain U: 79% 21%



- Molecule 24: 50S ribosomal protein L27

Chain V: 6% 80% 19%



- Molecule 25: 50S ribosomal protein L28

Chain W: 83% 17%



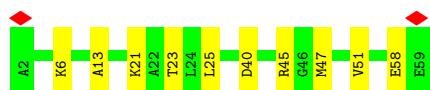
- Molecule 26: 50S ribosomal protein L29

Chain X: 87% 13%



- Molecule 27: 50S ribosomal protein L30

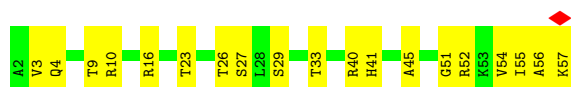
Chain Y: 83% 17%



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



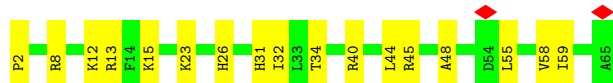
- Molecule 30: 50S ribosomal protein L33



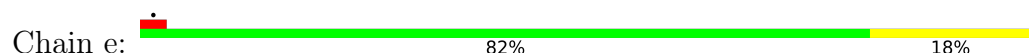
- Molecule 31: 50S ribosomal protein L34



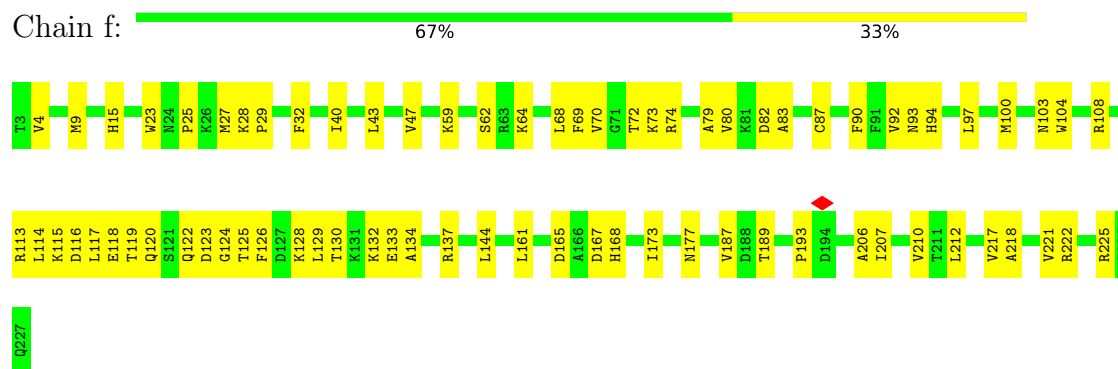
- Molecule 32: 50S ribosomal protein L35



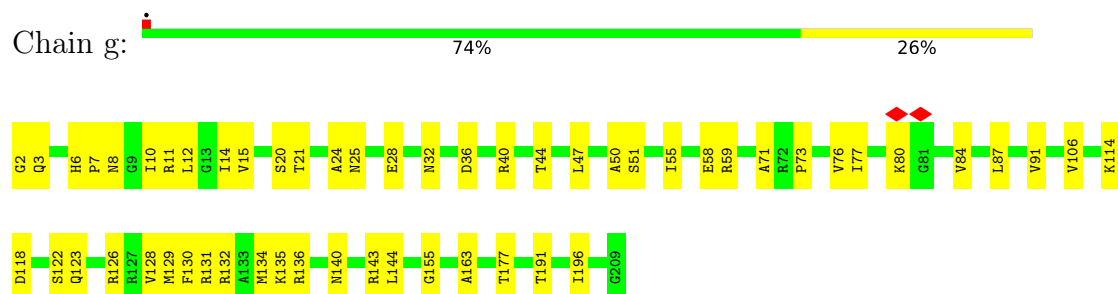
- Molecule 33: 50S ribosomal protein L36



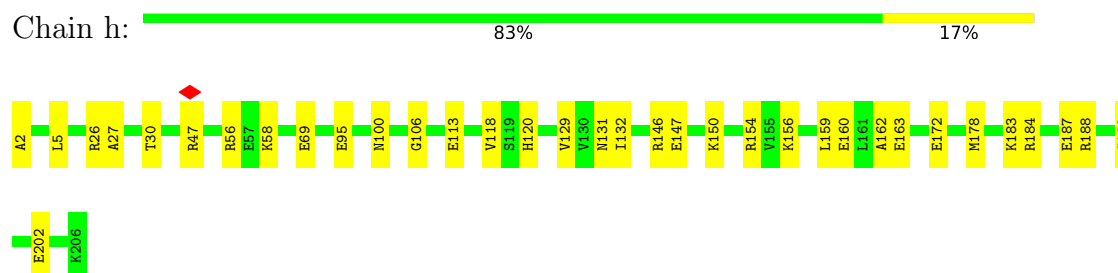
- Molecule 34: 30S ribosomal protein S2



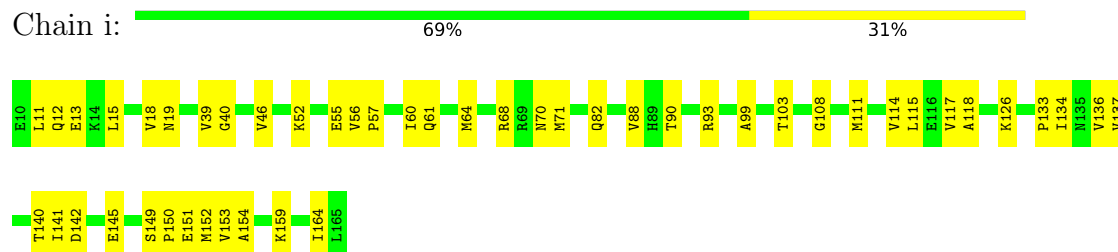
• Molecule 35: 30S ribosomal protein S3



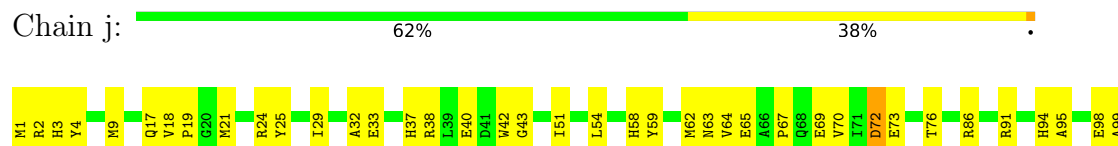
• Molecule 36: 30S ribosomal protein S4



• Molecule 37: 30S ribosomal protein S5



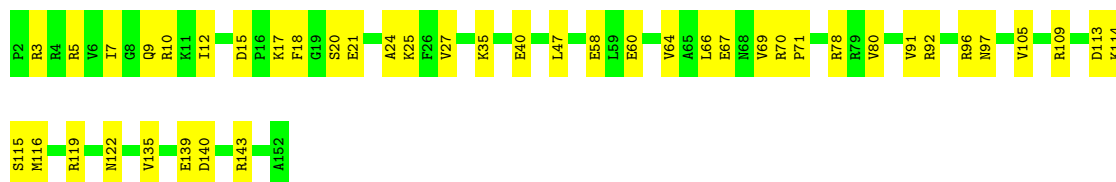
• Molecule 38: 30S ribosomal protein S6





- Molecule 39: 30S ribosomal protein S7

Chain k: 72% 28%



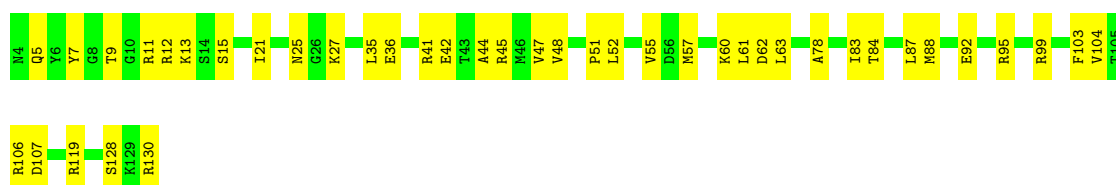
- Molecule 40: 30S ribosomal protein S8

Chain l: 78% 22%



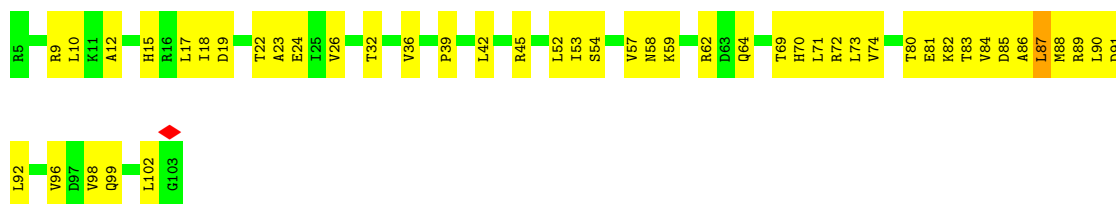
- Molecule 41: 30S ribosomal protein S9

Chain m: 68% 32%



- Molecule 42: 30S ribosomal protein S10

Chain n: 53% 46%



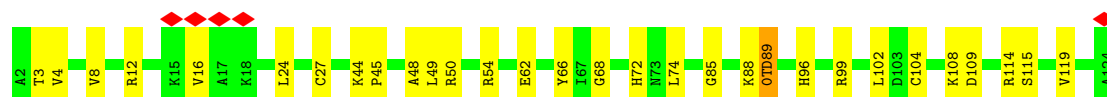
- Molecule 43: 30S ribosomal protein S11

Chain o: 74% 26%



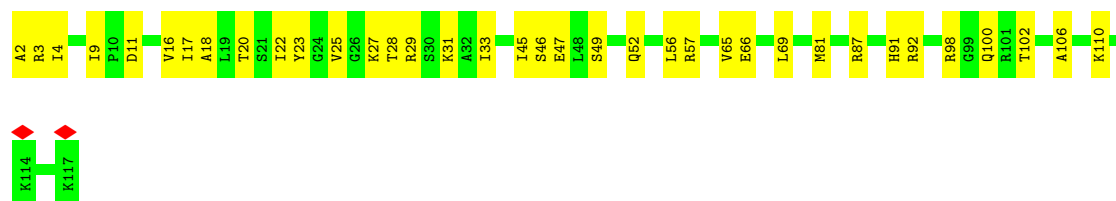
- Molecule 44: 30S ribosomal protein S12

Chain p:  76% 24%



- Molecule 45: 30S ribosomal protein S13

Chain q:  69% 31%



- Molecule 46: 30S ribosomal protein S14

Chain r:  77% 23%



- Molecule 47: 30S ribosomal protein S15

Chain s:  83% 17%



- Molecule 48: 30S ribosomal protein S16

Chain t:  85% 15%



- Molecule 49: 30S ribosomal protein S17

Chain u:  66% 34%

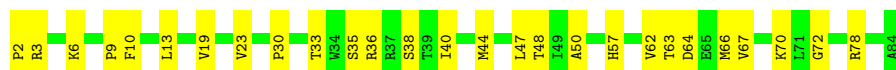


- Molecule 50: 30S ribosomal protein S18

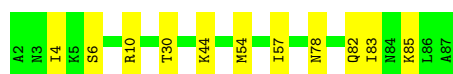
Chain v:  82% 18%



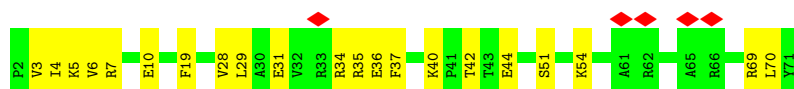
- Molecule 51: 30S ribosomal protein S19



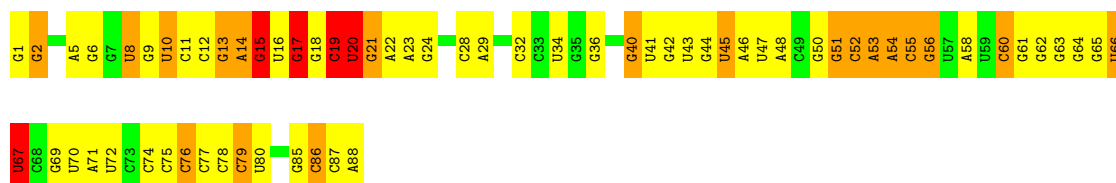
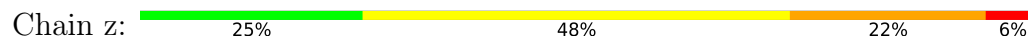
- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21



- Molecule 54: tRNA-Ser



- Molecule 55: CspA transcriptional activator



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.042	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 2MA, UR3, 1MG, 5MU, 0TD, PSU, OMG, 5MC, G7M, 6MZ, MA6, MG, OMU, 4OC, FME, 3TD, ZN, OMC

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	1	0.83	0/69286	0.56	7/108087 (0.0%)
2	2	0.73	0/36590	0.52	0/57074
3	3	0.72	0/2872	0.50	0/4478
4	4	0.65	0/139	0.48	0/214
5	C	1.12	1/2121 (0.0%)	0.72	0/2852
6	D	1.11	0/1586	0.71	1/2134 (0.0%)
7	E	1.02	0/1571	0.70	0/2113
8	F	0.78	0/1434	0.70	0/1926
9	G	0.71	0/1333	0.65	0/1805
10	H	0.53	0/1122	0.91	0/1515
11	I	1.09	0/1152	0.68	0/1551
12	J	1.06	0/955	0.69	0/1279
13	K	1.10	0/1062	0.73	0/1413
14	L	1.05	0/1093	0.67	0/1460
15	M	1.14	0/964	0.76	0/1289
16	N	0.91	0/902	0.74	0/1209
17	O	1.04	0/929	0.66	0/1242
18	P	1.19	0/960	0.78	0/1278
19	Q	1.00	0/829	0.71	2/1107 (0.2%)
20	R	1.11	0/864	0.71	0/1156
21	S	0.98	0/752	0.65	0/1005
22	T	0.83	0/796	0.63	0/1062
23	U	0.93	0/766	0.70	0/1025
24	V	1.06	0/608	0.66	0/804
25	W	1.04	0/635	0.70	0/848
26	X	0.88	0/502	0.74	0/667
27	Y	1.08	0/452	0.67	0/605
28	Z	0.67	1/531 (0.2%)	0.80	2/709 (0.3%)
29	a	1.06	0/450	0.68	0/599
30	b	0.87	0/433	0.62	0/576
31	c	1.20	0/380	0.76	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	1.16	0/513	0.77	0/676
33	e	1.08	0/303	0.66	0/397
34	f	0.68	0/1791	0.73	0/2413
35	g	0.85	0/1663	0.71	0/2241
36	h	0.84	0/1665	0.69	0/2227
37	i	0.97	0/1165	0.76	0/1568
38	j	0.76	0/867	0.75	0/1171
39	k	0.74	0/1195	0.72	0/1602
40	l	0.95	0/989	0.69	0/1326
41	m	0.83	0/1034	0.79	0/1375
42	n	0.75	0/800	0.75	0/1082
43	o	0.83	0/893	0.69	0/1205
44	p	0.95	0/960	0.72	0/1286
45	q	0.82	0/909	0.75	0/1215
46	r	0.89	0/817	0.72	0/1088
47	s	0.90	0/722	0.71	0/964
48	t	0.93	0/659	0.69	0/884
49	u	0.80	0/657	0.64	0/881
50	v	0.87	0/553	0.72	0/743
51	w	0.75	0/680	0.69	0/915
52	x	0.90	0/675	0.78	0/895
53	y	0.69	0/597	0.71	0/792
54	z	0.66	2/2062 (0.1%)	0.65	7/3208 (0.2%)
55	B	0.64	0/200	1.15	2/267 (0.7%)
All	All	0.84	4/156438 (0.0%)	0.60	21/234001 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	20	U	C5-C6	6.33	1.46	1.34
54	z	20	U	C2-N3	5.39	1.48	1.37
28	Z	6	HIS	C-N	5.37	1.40	1.33
5	C	221	ARG	CB-CG	-5.07	1.37	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	67	U	O5'-P-OP1	-9.70	78.89	108.00
1	1	2512	C	C5'-C4'-C3'	7.62	127.43	116.00
54	z	19	C	OP2-P-O3'	-7.56	85.32	108.00
28	Z	6	HIS	CA-C-N	7.15	127.08	120.21
28	Z	6	HIS	C-N-CA	7.15	127.08	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	708	G	O3'-P-O5'	-7.12	93.32	104.00
54	z	8	U	O5'-P-OP1	-6.89	87.31	108.00
55	B	4	LYS	N-CA-C	-6.86	104.38	112.89
55	B	12	PHE	N-CA-C	-6.69	104.74	113.17
54	z	19	C	OP1-P-O3'	-6.13	89.61	108.00
1	1	2122	U	C4'-C3'-O3'	-6.05	103.92	113.00
1	1	2118	U	C2'-C3'-O3'	-5.99	100.52	109.50
54	z	15	G	C1'-C2'-O2'	5.99	117.38	108.40
54	z	67	U	C2'-C3'-O3'	-5.75	105.07	113.70
1	1	2512	C	O5'-C5'-C4'	5.40	119.60	111.50
1	1	980	A	N9-C1'-C2'	5.35	120.03	112.00
6	D	152	PRO	CA-N-CD	-5.20	104.72	112.00
1	1	1871	A	O4'-C1'-N9	5.18	115.97	108.20
19	Q	52	PRO	CA-C-N	5.10	131.28	121.54
19	Q	52	PRO	C-N-CA	5.10	131.28	121.54
54	z	8	U	O3'-P-O5'	-5.10	96.35	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31365	573	0
2	2	32929	0	16586	320	0
3	3	2569	0	1301	17	0
4	4	126	0	65	0	0
5	C	2082	0	2154	39	0
6	D	1565	0	1616	30	0
7	E	1552	0	1619	27	0
8	F	1410	0	1444	57	0
9	G	1313	0	1358	23	0
10	H	1111	0	1148	60	0
11	I	1129	0	1162	16	0
12	J	946	0	1023	17	0
13	K	1053	0	1129	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	1074	0	1157	13	0
15	M	951	0	994	19	0
16	N	892	0	923	19	0
17	O	917	0	962	14	0
18	P	947	0	1019	10	0
19	Q	816	0	839	23	0
20	R	857	0	922	20	0
21	S	746	0	811	16	0
22	T	788	0	843	20	0
23	U	753	0	780	13	0
24	V	601	0	615	13	0
25	W	625	0	652	11	0
26	X	501	0	531	5	0
27	Y	448	0	488	6	0
28	Z	522	0	520	25	0
29	a	444	0	458	13	0
30	b	426	0	464	3	0
31	c	377	0	418	11	0
32	d	504	0	572	13	0
33	e	302	0	340	5	0
34	f	1760	0	1787	64	0
35	g	1636	0	1710	40	0
36	h	1643	0	1707	31	0
37	i	1152	0	1196	36	0
38	j	848	0	846	37	0
39	k	1181	0	1238	38	0
40	l	979	0	1031	23	0
41	m	1022	0	1070	33	0
42	n	790	0	831	37	0
43	o	877	0	887	24	0
44	p	957	0	1017	24	0
45	q	900	0	965	31	0
46	r	805	0	844	25	0
47	s	714	0	734	12	0
48	t	649	0	666	8	0
49	u	648	0	691	20	0
50	v	544	0	560	9	0
51	w	663	0	688	23	0
52	x	669	0	719	8	0
53	y	589	0	629	18	0
54	z	1891	0	955	63	0
55	B	205	0	195	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1	276	0	0	0	0
56	2	119	0	0	0	0
56	3	8	0	0	0	0
56	4	1	0	0	0	0
56	C	1	0	0	0	0
56	D	2	0	0	0	0
56	P	1	0	0	0	0
56	T	1	0	0	0	0
56	a	2	0	0	0	0
56	h	1	0	0	0	0
56	q	1	0	0	0	0
56	r	1	0	0	0	0
56	z	2	0	0	0	0
57	Z	1	0	0	0	0
57	e	1	0	0	0	0
All	All	145152	0	97244	1854	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1854) 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)
6:D:151:THR:HG23	6:D:152:PRO:HD3	1.27	1.15
55:B:2:SER:HA	55:B:5:MET:HB3	1.41	1.03
1:1:1068:G:N2	1:1:1095:A:N3	2.10	0.99
42:n:57:VAL:O	42:n:58:ASN:ND2	1.98	0.97
55:B:2:SER:HA	55:B:5:MET:CB	1.96	0.94
20:R:69:LEU:HD22	20:R:107:VAL:HG22	1.50	0.93
1:1:1172:C:O2'	1:1:1173:U:O4'	1.88	0.91
54:z:17:OMG:HM23	54:z:69:G:H21	1.36	0.91
1:1:2107:G:H8	1:1:2107:G:H5''	1.36	0.89
37:i:151:GLU:OE1	37:i:151:GLU:N	2.06	0.89
45:q:9:ILE:HG23	45:q:18:ALA:HB1	1.55	0.88
1:1:2571:U:O2'	6:D:151:THR:HG21	1.74	0.88
2:2:626:G:O3'	48:t:51:ARG:NH1	2.07	0.88
1:1:1754:A:N1	1:1:2716:C:O2'	2.08	0.87
1:1:2530:A:N7	9:G:172:LYS:NZ	2.23	0.87
2:2:979:C:O2	46:r:59:ARG:NH2	2.08	0.87
1:1:621:A:OP2	13:K:99:ASN:ND2	2.08	0.86
55:B:2:SER:CA	55:B:5:MET:HB3	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1364:G:OP2	25:W:2:SER:N	2.08	0.86
1:1:2100:G:O6	1:1:2189:U:N3	2.09	0.86
41:m:42:GLU:OE2	41:m:45:ARG:NH1	2.08	0.86
1:1:1450:G:N2	1:1:1452:G:O6	2.09	0.86
2:2:878:A:OP1	40:l:80:ARG:NH1	2.09	0.86
41:m:25:ASN:OD1	41:m:27:LYS:NZ	2.09	0.85
2:2:1005:A:N6	2:2:1024:G:O2'	2.10	0.85
2:2:683:G:N2	43:o:39:GLY:O	2.10	0.84
38:j:17:GLN:OE1	38:j:17:GLN:N	2.10	0.84
1:1:2102:G:O6	1:1:2187:U:C4	2.32	0.82
2:2:1376:U:OP2	39:k:25:LYS:NZ	2.13	0.82
1:1:2305:U:O2'	8:F:133:ARG:NH1	2.12	0.82
1:1:2127:G:O2'	1:1:2128:G:O4'	1.98	0.81
46:r:41:ARG:NH2	51:w:6:LYS:O	2.13	0.81
54:z:17:OMG:CM2	54:z:69:G:H21	1.94	0.81
1:1:1223:G:OP1	19:Q:68:ARG:NH2	2.13	0.81
1:1:1779:U:OP2	1:1:1784:A:N6	2.13	0.81
2:2:1145:A:O2'	2:2:1146:A:OP2	1.98	0.81
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.14	0.81
39:k:67:GLU:OE1	39:k:70:ARG:NH1	2.15	0.80
45:q:16:VAL:O	45:q:20:THR:HG23	1.81	0.80
2:2:1261:A:N6	2:2:1274:A:O2'	2.14	0.80
38:j:51:ILE:O	38:j:54:LEU:HD23	1.82	0.80
1:1:565:C:N4	1:1:576:U:O4	2.16	0.79
2:2:1028:C:O2	2:2:1033:G:N1	2.16	0.79
50:v:22:ASP:OD1	50:v:25:ASP:N	2.15	0.79
1:1:1582:C:O2'	1:1:1585:C:N3	2.13	0.78
2:2:1193:G:O6	35:g:3:GLN:NE2	2.16	0.78
2:2:1167:A:O2'	2:2:1169:A:N7	2.15	0.78
35:g:40:ARG:NH1	35:g:55:ILE:O	2.17	0.78
2:2:1006:G:N2	2:2:1023:U:O2	2.16	0.78
1:1:1169:A:N6	1:1:1180:U:O4	2.17	0.78
36:h:184:ARG:NH1	36:h:187:GLU:OE1	2.17	0.77
1:1:889:C:OP1	54:z:52:C:N4	2.17	0.77
39:k:116:MET:HA	39:k:119:ARG:HE	1.50	0.77
38:j:69:GLU:OE1	38:j:69:GLU:N	2.16	0.77
2:2:1377:A:OP1	39:k:92:ARG:NH1	2.18	0.76
8:F:117:LEU:N	8:F:177:PHE:O	2.18	0.76
1:1:563:A:N3	18:P:37:GLN:NE2	2.34	0.76
12:J:51:LYS:NZ	12:J:95:ILE:O	2.19	0.76
1:1:891:G:O2'	1:1:892:A:OP1	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:938:A:N3	2:2:1376:U:O2'	2.18	0.76
1:1:1007:C:OP1	11:I:37:ARG:NH2	2.19	0.75
1:1:1203:U:N3	1:1:1242:U:O4	2.18	0.75
1:1:2469:A:N6	1:1:2481:G:O2'	2.19	0.75
1:1:585:G:N7	18:P:6:ARG:NH1	2.34	0.75
34:f:119:THR:O	34:f:124:GLY:N	2.17	0.75
41:m:84:THR:HG21	41:m:103:PHE:HB3	1.69	0.75
55:B:2:SER:C	55:B:5:MET:HB3	2.11	0.75
10:H:84:ALA:HB1	10:H:90:LEU:HD12	1.68	0.74
1:1:2753:A:O2'	33:e:15:LYS:NZ	2.20	0.74
1:1:475:C:O2	1:1:479:A:N6	2.21	0.74
1:1:1028:A:OP2	1:1:1126:A:N6	2.20	0.74
1:1:1047:G:HO2'	1:1:1110:G:H1	1.34	0.74
2:2:1168:U:O2'	2:2:1169:A:OP1	2.05	0.74
8:F:8:TYR:OH	8:F:29:PRO:O	2.06	0.73
41:m:106:ARG:NH1	41:m:107:ASP:O	2.21	0.73
1:1:2125:G:H2'	1:1:2173:A:H61	1.51	0.73
1:1:482:A:OP1	22:T:47:LYS:NZ	2.19	0.73
20:R:2:GLU:N	20:R:2:GLU:OE1	2.22	0.73
47:s:78:TYR:OH	47:s:89:ARG:O	2.06	0.73
35:g:77:ILE:HA	35:g:84:VAL:HG23	1.72	0.72
54:z:70:U:O2'	54:z:72:U:OP2	2.07	0.72
1:1:1475:G:O2'	1:1:1514:G:O6	2.08	0.72
10:H:1:MET:N	10:H:20:ASN:OD1	2.17	0.71
3:3:51:G:OP1	16:N:63:LYS:NZ	2.22	0.71
54:z:21:G:N2	54:z:58:A:N7	2.37	0.71
9:G:2:SER:OG	9:G:3:ARG:N	2.23	0.71
53:y:31:GLU:OE2	53:y:34:ARG:NH2	2.24	0.71
24:V:33:ALA:N	24:V:64:ASP:OD1	2.24	0.71
38:j:32:ALA:CB	38:j:70:VAL:HG11	2.20	0.71
1:1:301:G:OP2	22:T:82:ARG:NH1	2.23	0.71
41:m:62:ASP:C	41:m:63:LEU:HD12	2.16	0.71
1:1:1652:A:OP1	15:M:8:ARG:NH2	2.22	0.71
2:2:1060:U:H5''	42:n:53:ILE:HD12	1.71	0.71
6:D:136:ASN:OD1	6:D:139:SER:OG	2.09	0.71
34:f:73:LYS:NZ	34:f:165:ASP:OD2	2.24	0.71
34:f:115:LYS:O	34:f:119:THR:HG23	1.90	0.71
2:2:981:U:OP1	46:r:9:ARG:NH1	2.24	0.70
51:w:33:THR:HG22	51:w:35:SER:H	1.55	0.70
1:1:2171:A:O2'	1:1:2173:A:OP1	2.10	0.70
5:C:142:HIS:ND1	5:C:193:GLY:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:40:ARG:O	35:g:44:THR:HG23	1.90	0.70
2:2:1533:C:O2'	2:2:1534:A:OP1	2.10	0.70
2:2:980:C:O2'	46:r:13:ARG:NH1	2.25	0.70
18:P:97:ASP:OD2	19:Q:13:ARG:NH1	2.25	0.70
2:2:1290:G:OP1	39:k:35:LYS:NZ	2.24	0.70
44:p:48:ALA:C	44:p:49:LEU:HD12	2.17	0.70
47:s:4:SER:O	47:s:8:THR:HG23	1.92	0.70
1:1:956:G:O6	14:L:14:LYS:NZ	2.23	0.70
1:1:2885:G:O6	29:a:40:ARG:NH2	2.25	0.70
10:H:4:ILE:HD12	10:H:17:ASP:C	2.17	0.70
20:R:25:ARG:NH1	20:R:74:ILE:O	2.24	0.69
28:Z:35:ASP:OD2	45:q:57:ARG:NE	2.25	0.69
2:2:107:G:N7	52:x:10:ARG:NH2	2.40	0.69
2:2:620:C:C2	36:h:132:ILE:HD13	2.27	0.69
55:B:1:FME:HB2	55:B:4:LYS:HB2	1.74	0.69
2:2:1031:C:O3'	2:2:1032:G:N2	2.25	0.69
21:S:69:ARG:NH2	21:S:72:GLN:O	2.25	0.69
2:2:1298:U:OP2	39:k:114:LYS:NZ	2.24	0.69
37:i:136:VAL:O	37:i:140:THR:HG23	1.93	0.69
2:2:412:A:H62	2:2:431:A:H61	1.41	0.69
42:n:24:GLU:OE2	42:n:90:LEU:HD11	1.92	0.69
1:1:2122:U:OP2	1:1:2122:U:H6	1.76	0.69
2:2:544:G:OP1	36:h:56:ARG:NH2	2.22	0.69
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.75	0.69
2:2:1006:G:H22	2:2:1023:U:H2'	1.58	0.69
1:1:1534:U:O2'	1:1:1537:G:O6	2.11	0.69
2:2:1152:A:OP1	42:n:70:HIS:ND1	2.26	0.69
2:2:974:A:OP1	46:r:69:ARG:NH1	2.26	0.68
28:Z:51:VAL:HG23	28:Z:52:ALA:H	1.57	0.68
1:1:571:U:C5	1:1:2030:6MZ:H9	2.28	0.68
6:D:181:ASP:OD2	6:D:184:ARG:NH2	2.26	0.68
1:1:2508:G:H1	1:1:2580:PSU:HN3	1.39	0.68
34:f:129:LEU:HD21	34:f:134:ALA:HB2	1.75	0.68
38:j:38:ARG:NH2	38:j:63:ASN:OD1	2.25	0.68
41:m:128:SER:OG	41:m:130:ARG:OXT	2.09	0.68
1:1:219:A:N3	1:1:234:U:O2'	2.27	0.68
18:P:50:ARG:O	18:P:54:LYS:NZ	2.26	0.68
1:1:2107:G:H5''	1:1:2107:G:C8	2.25	0.68
2:2:1006:G:C2	2:2:1023:U:O2	2.46	0.68
2:2:35:G:N3	44:p:115:SER:OG	2.25	0.68
5:C:180:GLU:OE2	5:C:267:ILE:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:611:C:C2'	1:1:612:G:H5'	2.24	0.68
2:2:673:A:O3'	38:j:86:ARG:NH2	2.27	0.68
2:2:1126:U:O4	42:n:9:ARG:NH1	2.27	0.68
11:I:49:ASP:OD1	11:I:121:LYS:NZ	2.26	0.68
1:1:138:U:O2'	1:1:139:U:O2	2.10	0.67
1:1:2683:C:O2	12:J:70:ARG:NH2	2.27	0.67
34:f:207:ILE:H	34:f:207:ILE:HD12	1.59	0.67
54:z:14:A:H3'	54:z:15:G:H5''	1.76	0.67
1:1:2831:G:OP2	6:D:59:ARG:NH1	2.22	0.67
2:2:356:A:N3	2:2:368:U:O2'	2.27	0.67
38:j:2:ARG:HE	38:j:91:ARG:HH12	1.41	0.67
53:y:4:ILE:HD12	53:y:19:PHE:HD1	1.59	0.67
1:1:2483:C:N3	14:L:123:LYS:NZ	2.42	0.67
2:2:1222:G:OP2	2:2:1322:C:N4	2.27	0.67
15:M:24:MET:SD	15:M:44:LEU:HD22	2.34	0.67
8:F:46:ASP:OD1	8:F:47:LYS:N	2.28	0.67
54:z:9:G:O2'	54:z:10:U:OP1	2.11	0.67
1:1:13:A:O2'	1:1:15:G:O6	2.13	0.66
1:1:500:G:N1	1:1:503:A:OP2	2.28	0.66
48:t:18:GLN:OE1	48:t:35:ARG:NE	2.24	0.66
44:p:99:ARG:NE	44:p:104:CYS:SG	2.67	0.66
1:1:65:U:O2'	1:1:456:C:N3	2.27	0.66
1:1:1069:A:O2'	1:1:1074:G:N1	2.29	0.66
2:2:401:C:O2'	2:2:621:A:N3	2.27	0.66
15:M:59:SER:OG	15:M:62:ASN:OD1	2.09	0.66
17:O:14:LYS:HE2	17:O:77:HIS:HA	1.77	0.66
7:E:1:MET:HB3	7:E:14:VAL:HG23	1.76	0.66
19:Q:44:GLY:O	19:Q:45:GLU:HG3	1.95	0.66
1:1:1668:A:O2'	1:1:1674:G:N7	2.22	0.66
7:E:2:GLU:OE2	7:E:13:THR:OG1	2.13	0.66
19:Q:51:VAL:HB	19:Q:52:PRO:HD3	1.77	0.66
34:f:217:VAL:O	34:f:221:VAL:HG13	1.95	0.66
54:z:21:G:N2	54:z:58:A:H62	1.93	0.66
1:1:627:A:OP1	13:K:78:ARG:NH1	2.26	0.66
2:2:464:U:N3	2:2:467:U:OP2	2.26	0.66
41:m:92:GLU:OE2	41:m:95:ARG:NE	2.26	0.66
1:1:1266:G:OP1	29:a:16:ARG:NE	2.25	0.65
16:N:111:ARG:NH2	16:N:117:PHE:OXT	2.29	0.65
40:l:5:ASP:OD2	40:l:77:ARG:NH1	2.28	0.65
1:1:2194:U:H2'	1:1:2195:U:C6	2.32	0.65
2:2:738:C:OP1	38:j:4:TYR:OH	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B:2:SER:HA	55:B:5:MET:HB2	1.78	0.65
48:t:44:SER:N	48:t:47:GLU:OE2	2.25	0.65
2:2:1320:C:N3	51:w:36:ARG:NH1	2.44	0.65
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.77	0.65
35:g:32:ASN:OD1	35:g:59:ARG:NH1	2.30	0.65
1:1:309:A:N3	1:1:329:G:O2'	2.30	0.65
1:1:1068:G:O2'	1:1:1070:A:N6	2.29	0.65
2:2:1317:C:OP2	46:r:28:LYS:NZ	2.27	0.65
41:m:12:ARG:HG3	41:m:13:LYS:H	1.62	0.65
42:n:87:LEU:HD12	42:n:88:MET:N	2.12	0.65
55:B:12:PHE:CD1	55:B:12:PHE:O	2.49	0.65
1:1:402:A:H2'	1:1:403:U:H5'	1.79	0.65
2:2:890:G:O2'	2:2:906:A:N6	2.30	0.65
21:S:93:LEU:HD23	21:S:94:ASP:N	2.11	0.65
28:Z:58:ASP:OD1	28:Z:59:ARG:N	2.30	0.65
54:z:51:G:H22	54:z:53:A:H5'	1.62	0.65
1:1:517:C:OP2	29:a:10:ARG:NH2	2.30	0.64
2:2:855:U:OP2	2:2:871:U:N3	2.29	0.64
42:n:80:THR:OG1	42:n:83:THR:OG1	2.09	0.64
1:1:1066:U:N3	1:1:1069:A:OP2	2.30	0.64
1:1:895:U:O2'	1:1:896:A:O4'	2.15	0.64
1:1:2021:C:OP1	29:a:9:THR:HG21	1.97	0.64
1:1:2902:C:H3'	1:1:2903:U:H5''	1.79	0.64
6:D:151:THR:HG23	6:D:152:PRO:CD	2.18	0.64
2:2:1145:A:O2'	2:2:1146:A:P	2.56	0.64
2:2:1317:C:OP1	46:r:24:ARG:NH2	2.28	0.64
35:g:47:LEU:HD12	35:g:47:LEU:N	2.13	0.64
1:1:2125:G:C2'	1:1:2173:A:H61	2.11	0.64
1:1:2278:A:OP2	24:V:12:ASN:ND2	2.30	0.64
1:1:2312:U:O2	8:F:37:ASN:ND2	2.30	0.64
35:g:25:ASN:N	35:g:28:GLU:OE2	2.31	0.64
1:1:125:A:H2	31:c:9:VAL:HG12	1.63	0.64
1:1:125:A:OP2	31:c:19:ARG:NH2	2.30	0.64
22:T:72:ILE:HD12	22:T:83:VAL:HG21	1.79	0.64
39:k:66:LEU:HD21	39:k:97:ASN:OD1	1.97	0.64
41:m:36:GLU:OE1	41:m:45:ARG:NH1	2.31	0.64
37:i:57:PRO:HA	37:i:60:ILE:HG12	1.80	0.64
2:2:411:A:OP1	36:h:26:ARG:NH1	2.30	0.64
1:1:1083:U:O2'	1:1:1085:A:OP2	2.11	0.64
1:1:1901:A:OP2	5:C:253:LYS:NZ	2.31	0.64
6:D:152:PRO:O	6:D:154:LYS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:324:A:OP2	1:1:1205:A:N6	2.32	0.63
34:f:114:LEU:C	34:f:114:LEU:HD23	2.23	0.63
2:2:109:A:H5'	2:2:110:C:H5	1.63	0.63
2:2:501:C:OP1	44:p:114:ARG:NH2	2.30	0.63
54:z:17:OMG:HM23	54:z:69:G:N2	2.10	0.63
1:1:1870:C:H6	1:1:1870:C:OP1	1.82	0.63
5:C:125:LYS:HG2	5:C:128:ASN:OD1	1.97	0.63
1:1:611:C:H2'	1:1:612:G:H5'	1.79	0.63
21:S:6:ARG:NH1	21:S:37:ASP:OD1	2.32	0.63
38:j:38:ARG:NH1	38:j:98:GLU:O	2.31	0.63
55:B:2:SER:O	55:B:5:MET:HB3	1.98	0.63
2:2:1309:G:OP2	45:q:98:ARG:NE	2.30	0.63
6:D:25:THR:OG1	6:D:191:GLY:O	2.15	0.63
8:F:95:ARG:HH12	28:Z:1:MET:HE1	1.64	0.63
21:S:11:LEU:O	26:X:29:ARG:NH1	2.29	0.63
17:O:34:GLU:OE1	17:O:34:GLU:N	2.32	0.63
1:1:2258:C:O2'	1:1:2427:C:OP2	2.16	0.63
37:i:55:GLU:HG3	37:i:57:PRO:HD2	1.80	0.63
14:L:49:ALA:HB1	14:L:120:ALA:HB1	1.81	0.62
1:1:2146:C:O2'	1:1:2147:A:O5'	2.15	0.62
10:H:15:LEU:C	10:H:15:LEU:HD23	2.24	0.62
1:1:2162:G:H5''	1:1:2173:A:H5''	1.81	0.62
16:N:94:ARG:NH2	16:N:97:PHE:O	2.32	0.62
10:H:90:LEU:HD21	10:H:123:ARG:O	1.99	0.62
21:S:65:GLY:N	21:S:79:ASP:OD1	2.30	0.62
44:p:48:ALA:O	44:p:49:LEU:HD12	2.00	0.62
44:p:68:GLY:O	44:p:99:ARG:NH1	2.32	0.62
55:B:22:THR:O	55:B:24:ASP:N	2.31	0.62
22:T:74:ASN:ND2	22:T:81:ASP:OD2	2.31	0.62
35:g:20:SER:OG	35:g:40:ARG:NH2	2.32	0.62
1:1:1364:G:N7	25:W:2:SER:OG	2.32	0.62
1:1:2159:G:H2'	1:1:2160:C:C6	2.35	0.62
1:1:2249:U:N3	1:1:2253:G:OP2	2.30	0.62
34:f:130:THR:HG23	34:f:133:GLU:HB3	1.82	0.62
36:h:188:ARG:NH1	36:h:192:SER:O	2.28	0.62
8:F:134:GLU:HG2	8:F:136:ILE:HD12	1.79	0.62
34:f:87:CYS:O	34:f:225:ARG:NH1	2.33	0.62
40:l:83:LEU:HD23	40:l:83:LEU:C	2.25	0.62
53:y:70:LEU:HD23	53:y:70:LEU:H	1.64	0.61
1:1:811:U:H2'	13:K:21:ARG:HA	1.82	0.61
1:1:1789:A:OP2	5:C:221:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:24:THR:HG23	31:c:27:GLY:H	1.64	0.61
35:g:51:SER:HB2	35:g:71:ALA:HB3	1.82	0.61
1:1:2102:G:C6	1:1:2187:U:N3	2.67	0.61
2:2:662:U:O2'	2:2:836:G:OP1	2.18	0.61
11:I:114:LEU:HG	11:I:118:MET:HE3	1.83	0.61
34:f:206:ALA:O	34:f:210:VAL:HG13	2.00	0.61
36:h:47:ARG:NE	36:h:47:ARG:HA	2.15	0.61
38:j:72:ASP:OD1	38:j:73:GLU:N	2.33	0.61
39:k:15:ASP:OD1	39:k:20:SER:N	2.32	0.61
1:1:1087:G:H1	1:1:1102:C:H42	1.48	0.61
2:2:405:U:O4	36:h:2:ALA:N	2.34	0.61
5:C:258:ARG:NH1	5:C:264:ASP:OD1	2.31	0.61
26:X:49:ASP:OD1	26:X:52:ARG:NH2	2.33	0.61
2:2:664:G:H22	2:2:741:G:H1	1.48	0.61
2:2:2:A:N3	2:2:613:C:O2'	2.31	0.61
2:2:933:G:O6	39:k:3:ARG:NH2	2.32	0.61
35:g:14:ILE:HG22	35:g:15:VAL:HG13	1.83	0.61
1:1:1056:G:O2'	1:1:1103:A:N6	2.33	0.61
37:i:154:ALA:HA	37:i:164:ILE:HD11	1.83	0.61
39:k:113:ASP:OD2	39:k:122:ASN:ND2	2.34	0.61
1:1:307:G:N1	1:1:310:A:OP2	2.31	0.61
10:H:67:ALA:O	10:H:70:GLU:HG3	2.01	0.61
21:S:8:LEU:CD2	21:S:50:LEU:HD21	2.30	0.61
37:i:39:VAL:HG12	37:i:40:GLY:N	2.16	0.61
35:g:155:GLY:O	35:g:196:ILE:HG12	2.00	0.61
1:1:1042:G:O2'	1:1:1043:C:H5''	2.00	0.60
7:E:176:ASP:OD1	7:E:179:SER:OG	2.13	0.60
40:l:77:ARG:NE	40:l:79:SER:O	2.34	0.60
32:d:15:LYS:HB2	32:d:23:LYS:HE2	1.84	0.60
2:2:1340:A:HO2'	54:z:32:C:HO2'	1.50	0.60
38:j:18:VAL:HG21	38:j:58:HIS:CD2	2.36	0.60
38:j:69:GLU:O	38:j:72:ASP:OD1	2.19	0.60
1:1:894:U:O2'	1:1:895:U:P	2.59	0.60
10:H:85:GLY:HA2	10:H:125:THR:OG1	2.01	0.60
2:2:297:G:N2	2:2:300:A:OP2	2.32	0.60
35:g:24:ALA:HB1	35:g:28:GLU:HG2	1.83	0.60
1:1:1915:3TD:H2'	1:1:1916:A:O4'	2.02	0.60
36:h:58:LYS:NZ	36:h:69:GLU:OE1	2.28	0.60
1:1:545:U:O2'	1:1:546:U:O3'	2.19	0.60
1:1:2316:G:H2'	1:1:2317:A:H8	1.67	0.60
1:1:1244:A:O2'	7:E:29:HIS:NE2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:280:C:N4	49:u:41:THR:OG1	2.34	0.60
2:2:811:C:O2'	2:2:901:A:N1	2.35	0.60
10:H:114:GLU:OE2	10:H:133:GLN:C	2.45	0.60
42:n:81:GLU:N	42:n:81:GLU:OE1	2.29	0.59
48:t:51:ARG:C	48:t:52:LEU:HD12	2.27	0.59
1:1:511:U:H2'	1:1:512:G:H5'	1.83	0.59
1:1:2848:G:O2'	1:1:2867:G:N2	2.31	0.59
38:j:2:ARG:HE	38:j:91:ARG:NH1	2.00	0.59
1:1:2902:C:C3'	1:1:2903:U:H5''	2.32	0.59
19:Q:52:PRO:HD2	19:Q:53:PHE:H	1.68	0.59
10:H:7:ASP:OD1	10:H:8:LYS:N	2.36	0.59
2:2:1119:C:OP2	41:m:11:ARG:NH1	2.36	0.59
19:Q:38:VAL:HG13	19:Q:54:VAL:HB	1.85	0.59
22:T:7:ARG:O	22:T:25:VAL:HB	2.02	0.59
50:v:14:THR:HG21	50:v:48:ARG:HE	1.67	0.59
10:H:70:GLU:HG2	10:H:138:VAL:HG11	1.85	0.59
45:q:16:VAL:HG23	45:q:17:ILE:HD12	1.85	0.59
1:1:1914:C:H2'	1:1:1915:3TD:O4	2.02	0.59
1:1:321:U:O3'	7:E:162:ARG:NH1	2.32	0.58
1:1:1028:A:N3	1:1:2486:C:O2'	2.25	0.58
1:1:2457:PSU:HN3	1:1:2494:G:H1	1.49	0.58
36:h:27:ALA:O	36:h:30:THR:OG1	2.21	0.58
1:1:636:G:N7	13:K:109:LYS:HE2	2.18	0.58
2:2:1004:A:H2'	2:2:1005:A:O4'	2.04	0.58
38:j:1:MET:HE3	38:j:67:PRO:HD3	1.85	0.58
15:M:38:LEU:HB3	15:M:39:PRO:HD3	1.84	0.58
52:x:82:GLN:O	52:x:85:LYS:HG3	2.03	0.58
1:1:355:U:H2'	1:1:356:G:H8	1.67	0.58
6:D:151:THR:CG2	6:D:152:PRO:HD3	2.17	0.58
39:k:69:VAL:HG12	39:k:135:VAL:HG12	1.85	0.58
1:1:275:C:N3	1:1:362:A:N6	2.51	0.58
8:F:162:SER:OG	8:F:163:ASP:N	2.36	0.58
40:l:30:SER:O	40:l:34:VAL:HG23	2.02	0.58
8:F:63:GLN:HA	28:Z:6:HIS:ND1	2.18	0.58
10:H:9:VAL:HB	10:H:12:LEU:HD21	1.84	0.58
19:Q:55:ASP:OD1	19:Q:55:ASP:N	2.37	0.58
1:1:2052:A:O2'	6:D:148:GLN:O	2.21	0.58
1:1:2305:U:O3'	8:F:133:ARG:NH1	2.36	0.58
39:k:12:ILE:HG23	39:k:21:GLU:OE1	2.04	0.58
40:l:96:MET:SD	40:l:130:ALA:HB1	2.44	0.58
1:1:573:U:O2'	1:1:575:A:OP1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:40:GLU:OE1	41:m:41:ARG:NH2	2.36	0.58
43:o:19:GLY:C	43:o:82:LEU:HD12	2.29	0.58
1:1:2655:G:O2'	1:1:2664:G:O6	2.15	0.58
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.36	0.58
23:U:9:ARG:HG2	23:U:41:GLU:CG	2.34	0.58
34:f:118:GLU:O	34:f:122:GLN:HG3	2.03	0.58
43:o:13:ARG:HE	43:o:14:LYS:N	2.01	0.58
38:j:32:ALA:HB2	38:j:70:VAL:HG11	1.85	0.58
41:m:51:PRO:O	41:m:55:VAL:HG22	2.03	0.58
41:m:130:ARG:NH1	54:z:34:U:OP2	2.34	0.58
49:u:76:VAL:HG23	49:u:77:ARG:HG2	1.85	0.58
2:2:496:A:H2'	2:2:496:A:N3	2.18	0.57
8:F:121:SER:OG	8:F:129:SER:O	2.18	0.57
21:S:8:LEU:HD21	21:S:50:LEU:HD21	1.85	0.57
38:j:42:TRP:CE3	38:j:102:MET:HE2	2.39	0.57
42:n:19:ASP:HA	42:n:22:THR:HG22	1.86	0.57
54:z:44:G:O2'	54:z:45:U:OP1	2.21	0.57
1:1:2128:G:C2	1:1:2173:A:O2'	2.56	0.57
10:H:86:ASP:OD1	10:H:87:GLU:N	2.37	0.57
10:H:95:GLY:N	10:H:98:ASP:OD2	2.37	0.57
1:1:280:U:O4	1:1:361:G:N2	2.37	0.57
42:n:86:ALA:HA	42:n:89:ARG:HG2	1.87	0.57
16:N:15:ARG:NH2	16:N:95:SER:OG	2.38	0.57
1:1:1067:A:O2'	1:1:1068:G:O4'	2.22	0.57
2:2:294:U:OP1	2:2:610:U:O2'	2.20	0.57
50:v:37:GLY:O	50:v:63:ARG:NH2	2.36	0.57
1:1:2305:U:N3	8:F:151:GLY:O	2.38	0.57
2:2:1266:G:N2	2:2:1269:A:OP2	2.32	0.57
23:U:75:GLN:HB2	23:U:92:VAL:HG23	1.87	0.57
30:b:13:SER:HA	30:b:49:TYR:CD1	2.40	0.57
1:1:1078:U:O2'	1:1:1088:A:OP1	2.13	0.57
7:E:117:ARG:NH2	7:E:183:PHE:O	2.36	0.57
10:H:67:ALA:O	10:H:71:LYS:HG3	2.04	0.57
22:T:86:ARG:NH2	22:T:102:THR:OG1	2.38	0.57
1:1:891:G:HO2'	1:1:892:A:P	2.28	0.56
51:w:50:ALA:HB1	51:w:57:HIS:HB3	1.86	0.56
1:1:2808:G:O2'	1:1:2890:G:O6	2.20	0.56
19:Q:52:PRO:CD	19:Q:53:PHE:H	2.18	0.56
20:R:13:SER:O	20:R:17:VAL:HG23	2.04	0.56
22:T:79:LYS:HG2	22:T:80:ALA:H	1.68	0.56
24:V:37:ILE:HG22	24:V:38:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2107:G:H8	1:1:2107:G:C5'	2.15	0.56
1:1:2116:G:O2'	1:1:2117:A:OP1	2.21	0.56
1:1:2636:C:O2'	6:D:45:TYR:OH	2.24	0.56
2:2:1004:A:O2'	2:2:1036:A:N1	2.31	0.56
8:F:140:GLU:OE2	28:Z:26:SER:OG	2.22	0.56
20:R:83:LYS:HD2	20:R:95:ARG:HD3	1.87	0.56
37:i:99:ALA:HB1	37:i:103:THR:HG21	1.88	0.56
1:1:1341:G:OP2	1:1:1394:U:O2'	2.18	0.56
1:1:2646:C:OP2	1:1:2732:G:O2'	2.23	0.56
2:2:1359:C:OP2	46:r:75:ARG:NE	2.38	0.56
28:Z:16:CYS:SG	28:Z:17:SER:N	2.79	0.56
2:2:1130:A:O2'	41:m:5:GLN:NE2	2.39	0.56
34:f:82:ASP:OD1	34:f:83:ALA:N	2.38	0.56
35:g:21:THR:HG22	35:g:21:THR:O	2.06	0.56
2:2:1176:A:H2'	2:2:1177:G:C8	2.41	0.56
2:2:1305:G:H21	2:2:1332:A:H2	1.53	0.56
35:g:114:LYS:NZ	35:g:118:ASP:OD2	2.33	0.56
1:1:2305:U:HO2'	8:F:133:ARG:HH11	1.52	0.56
1:1:2445:2MG:OP1	7:E:69:ARG:NH1	2.29	0.56
2:2:935:A:O2'	2:2:1383:C:N3	2.36	0.56
29:a:23:THR:O	29:a:23:THR:HG23	2.06	0.56
1:1:782:A:N7	5:C:220:VAL:HG21	2.21	0.56
1:1:1527:G:N1	1:1:1544:A:OP2	2.36	0.56
1:1:2304:G:H22	1:1:2312:U:H3	1.53	0.56
2:2:404:G:O6	36:h:2:ALA:N	2.39	0.56
2:2:1251:A:N3	2:2:1369:C:O2'	2.36	0.56
42:n:84:VAL:HG13	42:n:85:ASP:N	2.21	0.56
1:1:2128:G:H21	1:1:2174:C:H5'	1.71	0.56
1:1:2831:G:N2	1:1:2884:U:OP2	2.39	0.56
2:2:1043:G:H2'	2:2:1044:A:C8	2.41	0.56
2:2:1160:G:H22	2:2:1176:A:H2	1.52	0.56
15:M:54:LEU:HD11	15:M:62:ASN:HD22	1.70	0.56
34:f:59:LYS:O	34:f:62:SER:OG	2.19	0.56
45:q:23:TYR:CE1	45:q:69:LEU:HD23	2.41	0.56
1:1:1584:U:H5'	1:1:1585:C:C6	2.41	0.55
1:1:2122:U:OP1	1:1:2169:A:O2'	2.25	0.55
19:Q:29:THR:O	19:Q:29:THR:HG22	2.07	0.55
28:Z:5:ILE:HG13	28:Z:6:HIS:HD2	1.71	0.55
28:Z:57:VAL:HG23	51:w:64:ASP:OD1	2.06	0.55
1:1:2123:G:H2'	1:1:2124:G:C8	2.41	0.55
21:S:3:ARG:NH2	21:S:5:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:115:SER:O	39:k:119:ARG:HD3	2.06	0.55
1:l:714:U:OP2	47:s:88:ARG:NH1	2.37	0.55
51:w:64:ASP:O	51:w:67:VAL:HG23	2.06	0.55
1:l:2377:A:O2'	16:N:117:PHE:O	2.11	0.55
40:l:55:THR:HG23	40:l:56:LYS:H	1.71	0.55
40:l:55:THR:HG23	40:l:56:LYS:N	2.21	0.55
54:z:52:C:H4'	54:z:53:A:OP1	2.05	0.55
1:l:370:G:O2'	1:l:424:G:OP1	2.25	0.55
1:l:1315:C:O2'	1:l:1392:A:N3	2.39	0.55
1:l:2102:G:O6	1:l:2187:U:O4	2.23	0.55
2:2:564:C:OP1	44:p:12:ARG:NH1	2.39	0.55
2:2:842:U:H2'	2:2:844:G:H21	1.71	0.55
9:G:10:VAL:HA	9:G:49:THR:HG22	1.88	0.55
52:x:4:ILE:HG22	52:x:6:SER:H	1.72	0.55
54:z:66:5MU:C2'	54:z:67:U:H5'	2.37	0.55
23:U:32:GLY:O	23:U:93:ARG:NH1	2.40	0.55
34:f:128:LYS:HD2	34:f:128:LYS:O	2.07	0.55
14:L:47:GLU:OE2	14:L:51:ARG:NE	2.35	0.55
39:k:71:PRO:O	39:k:96:ARG:HG2	2.06	0.55
53:y:51:SER:O	53:y:54:LYS:HG2	2.07	0.55
28:Z:37:CYS:SG	28:Z:39:LYS:HB3	2.47	0.55
38:j:2:ARG:HB3	38:j:91:ARG:HH12	1.72	0.55
1:l:2402:U:O2'	1:l:2403:C:H5''	2.06	0.55
5:C:269:ARG:NH2	5:C:272:SER:OG	2.41	0.55
31:c:35:ARG:HG3	31:c:42:LEU:HD11	1.89	0.55
40:l:54:ASP:OD1	40:l:54:ASP:N	2.37	0.55
42:n:26:VAL:HG13	42:n:36:VAL:HG21	1.89	0.55
55:B:3:GLY:O	55:B:6:THR:HB	2.07	0.55
1:l:85:G:OP2	22:T:7:ARG:HB2	2.07	0.54
1:l:2092:U:N3	1:l:2226:C:OP2	2.33	0.54
2:2:9:G:OP2	37:i:126:LYS:NZ	2.27	0.54
2:2:770:C:O2'	2:2:899:C:N3	2.36	0.54
6:D:4:LEU:HD23	6:D:29:VAL:HG11	1.89	0.54
10:H:8:LYS:HA	10:H:14:SER:HA	1.89	0.54
7:E:77:ILE:HG22	7:E:77:ILE:O	2.07	0.54
10:H:4:ILE:HD12	10:H:17:ASP:O	2.07	0.54
49:u:26:GLU:O	49:u:26:GLU:HG2	2.07	0.54
1:l:700:G:O2'	1:l:1632:A:N3	2.38	0.54
1:l:1528:A:C5	1:l:1529:G:H1'	2.43	0.54
10:H:83:LYS:O	10:H:83:LYS:HD2	2.08	0.54
19:Q:27:ILE:O	19:Q:66:HIS:NE2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:8:LYS:HG2	30:b:24:THR:HG22	1.90	0.54
54:z:53:A:OP2	54:z:54:A:H5'	2.07	0.54
1:1:1383:A:N3	1:1:1405:U:O2'	2.39	0.54
6:D:77:ARG:NH1	6:D:200:ASP:OD1	2.37	0.54
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.88	0.54
20:R:95:ARG:HH11	20:R:95:ARG:HG3	1.73	0.54
23:U:51:GLN:OE1	23:U:57:TYR:OH	2.24	0.54
1:1:2108:A:H62	1:1:2178:C:N4	2.06	0.54
2:2:406:G:H5'	36:h:5:LEU:HD22	1.88	0.54
2:2:675:A:H1'	43:o:118:HIS:CD2	2.43	0.54
6:D:13:ARG:NH1	17:O:75:GLN:OE1	2.33	0.54
37:i:12:GLN:HG3	37:i:117:VAL:HG12	1.90	0.54
55:B:11:TRP:HA	55:B:14:ALA:HB3	1.88	0.54
2:2:1340:A:O2'	54:z:32:C:O2'	2.17	0.54
2:2:1533:C:O2'	2:2:1534:A:P	2.66	0.54
5:C:43:ARG:NH2	5:C:49:ILE:HD11	2.23	0.54
24:V:59:LEU:CD1	24:V:80:ILE:HD12	2.38	0.54
38:j:62:MET:HG2	38:j:64:VAL:HG23	1.89	0.54
1:1:2111:U:O2'	1:1:2115:G:N2	2.33	0.54
2:2:1031:C:O2'	2:2:1033:G:N7	2.41	0.54
42:n:102:LEU:C	42:n:102:LEU:HD23	2.33	0.54
44:p:16:VAL:O	44:p:16:VAL:HG13	2.08	0.54
45:q:100:GLN:OE1	45:q:100:GLN:N	2.40	0.54
2:2:1168:U:HO2'	2:2:1169:A:P	2.31	0.54
2:2:1218:C:H2'	2:2:1219:A:C8	2.43	0.54
10:H:51:ARG:HA	10:H:54:LEU:HB3	1.89	0.54
14:L:110:GLU:O	14:L:114:ARG:HG2	2.08	0.54
34:f:93:ASN:OD1	34:f:94:HIS:N	2.40	0.54
37:i:133:PRO:HA	37:i:136:VAL:HG12	1.90	0.54
39:k:135:VAL:O	39:k:139:GLU:HG2	2.07	0.54
53:y:3:VAL:HG23	53:y:3:VAL:O	2.06	0.54
55:B:15:ASP:OD1	55:B:16:LYS:N	2.41	0.54
1:1:1870:C:OP1	1:1:1870:C:C6	2.61	0.53
6:D:34:VAL:HB	6:D:92:VAL:O	2.07	0.53
1:1:402:A:H2'	1:1:403:U:C5'	2.38	0.53
1:1:1779:U:H5	1:1:1784:A:N7	2.06	0.53
1:1:2140:G:H2'	1:1:2141:G:O4'	2.08	0.53
1:1:2192:U:H2'	1:1:2193:G:O4'	2.08	0.53
1:1:2294:G:OP1	16:N:10:ARG:HD3	2.09	0.53
2:2:1073:U:O2	34:f:103:ASN:ND2	2.40	0.53
10:H:86:ASP:OD2	38:j:17:GLN:NE2	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:45:ALA:O	29:a:57:LYS:NZ	2.31	0.53
54:z:12:C:H2'	54:z:13:G:C8	2.42	0.53
54:z:20:U:O2'	54:z:71:A:N7	2.41	0.53
1:1:388:G:O6	1:1:390:U:O2'	2.13	0.53
1:1:880:G:C2	1:1:881:G:C8	2.96	0.53
1:1:1068:G:H22	1:1:1095:A:H1'	1.73	0.53
2:2:841:C:H2'	2:2:843:U:H5'	1.91	0.53
21:S:93:LEU:HD23	21:S:94:ASP:C	2.33	0.53
29:a:52:ARG:NH2	29:a:54:VAL:HG12	2.22	0.53
39:k:66:LEU:HD23	39:k:70:ARG:NH2	2.22	0.53
5:C:205:LEU:N	5:C:205:LEU:HD12	2.24	0.53
35:g:36:ASP:OD1	35:g:59:ARG:NH2	2.41	0.53
41:m:60:LYS:HB3	41:m:61:LEU:HD12	1.90	0.53
50:v:19:GLN:N	50:v:19:GLN:OE1	2.41	0.53
53:y:7:ARG:N	53:y:10:GLU:OE1	2.36	0.53
1:1:279:A:N6	1:1:361:G:H1'	2.22	0.53
2:2:1360:A:OP2	46:r:75:ARG:NH2	2.41	0.53
46:r:10:GLU:O	46:r:14:VAL:HG23	2.09	0.53
1:1:599:A:O2'	1:1:600:G:H5'	2.09	0.53
1:1:1818:U:O2'	5:C:153:GLN:O	2.23	0.53
8:F:144:ASP:OD1	8:F:145:LYS:N	2.42	0.53
10:H:85:GLY:CA	10:H:125:THR:OG1	2.57	0.53
1:1:2189:U:C2	1:1:2190:G:C8	2.97	0.53
10:H:15:LEU:HD23	10:H:16:GLY:N	2.24	0.53
20:R:86:MET:SD	20:R:87:PRO:HD2	2.49	0.53
1:1:714:U:OP2	47:s:88:ARG:NH2	2.42	0.53
5:C:161:TYR:HB3	5:C:194:GLU:HG2	1.91	0.53
2:2:685:G:N1	2:2:704:A:OP2	2.40	0.53
2:2:1220:G:P	46:r:53:ARG:HH12	2.32	0.53
10:H:54:LEU:HA	10:H:57:LYS:HE2	1.91	0.53
27:Y:47:MET:O	27:Y:51:VAL:HG22	2.09	0.53
54:z:9:G:N2	54:z:13:G:H1	2.07	0.53
1:1:402:A:C2'	1:1:403:U:H5'	2.39	0.52
1:1:1722:A:H2'	1:1:1723:G:O4'	2.09	0.52
2:2:1039:G:H2'	2:2:1040:U:C6	2.45	0.52
2:2:1129:C:O2	2:2:1130:A:N6	2.36	0.52
1:1:356:G:C6	1:1:357:C:C4	2.97	0.52
1:1:1590:A:H2'	1:1:1591:A:C8	2.44	0.52
1:1:2308:G:O6	1:1:2311:A:N7	2.43	0.52
34:f:4:VAL:HG21	34:f:212:LEU:HD21	1.91	0.52
35:g:129:MET:SD	35:g:132:ARG:NH2	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:673:A:H2'	2:2:674:G:C8	2.44	0.52
28:Z:59:ARG:O	28:Z:63:ARG:HG3	2.08	0.52
51:w:36:ARG:NH2	51:w:72:GLY:O	2.42	0.52
53:y:28:VAL:HG23	53:y:29:LEU:N	2.24	0.52
1:1:672:C:OP2	13:K:42:SER:OG	2.24	0.52
2:2:1527:U:OP2	53:y:42:THR:HG22	2.09	0.52
15:M:47:VAL:O	15:M:51:LEU:HD23	2.09	0.52
22:T:86:ARG:NH1	22:T:100:SER:O	2.40	0.52
39:k:24:ALA:HA	39:k:27:VAL:HG22	1.90	0.52
47:s:21:ASP:OD1	47:s:22:THR:N	2.42	0.52
54:z:1:G:O2'	54:z:2:G:P	2.67	0.52
1:1:887:A:O2'	1:1:888:C:O5'	2.26	0.52
1:1:2102:G:C2	1:1:2188:U:C2	2.98	0.52
1:1:2128:G:N3	1:1:2173:A:O2'	2.38	0.52
1:1:2148:G:H2'	1:1:2149:U:C6	2.44	0.52
44:p:24:LEU:HD23	44:p:27:CYS:O	2.09	0.52
46:r:42:TRP:O	46:r:46:LEU:HD23	2.09	0.52
54:z:69:G:C2'	54:z:70:U:H5'	2.39	0.52
1:1:1827:U:OP2	5:C:221:ARG:NE	2.41	0.52
2:2:109:A:H5'	2:2:110:C:C5	2.44	0.52
2:2:1100:C:OP1	53:y:69:ARG:NH1	2.43	0.52
2:2:1309:G:OP2	45:q:98:ARG:NH2	2.39	0.52
8:F:34:ILE:HD12	8:F:96:MET:HG3	1.92	0.52
19:Q:29:THR:HG23	19:Q:65:ALA:HA	1.92	0.52
1:1:2640:G:OP1	11:I:95:ARG:NH2	2.40	0.52
2:2:131:A:O2'	2:2:262:A:N3	2.40	0.52
2:2:946:A:H2'	2:2:947:G:C8	2.43	0.52
2:2:1168:U:O2'	2:2:1169:A:C5'	2.58	0.52
42:n:42:LEU:HB2	42:n:71:LEU:HB3	1.92	0.52
44:p:85:GLY:O	44:p:96:HIS:ND1	2.43	0.52
1:1:400:G:N7	25:W:57:ARG:NH1	2.58	0.52
1:1:1075:C:H2'	1:1:1076:C:C6	2.44	0.52
1:1:1105:U:H2'	1:1:1106:G:H8	1.74	0.52
2:2:90:C:O2'	2:2:91:U:H5'	2.10	0.52
2:2:1147:C:O2'	41:m:7:TYR:OH	2.19	0.52
7:E:48:THR:O	7:E:52:VAL:HG23	2.10	0.52
16:N:27:VAL:HG21	16:N:40:ILE:HD12	1.91	0.52
20:R:72:THR:HG21	20:R:108:SER:OG	2.10	0.52
20:R:83:LYS:HG2	20:R:97:LEU:HD13	1.91	0.52
34:f:130:THR:HG23	34:f:133:GLU:CB	2.40	0.52
1:1:372:G:O2'	1:1:400:G:O6	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:527:C:O2'	1:1:2779:U:O2'	2.25	0.52
1:1:1870:C:O2'	1:1:1871:A:O4'	2.26	0.52
1:1:2051:A:N6	1:1:2614:A:O2'	2.37	0.52
37:i:56:VAL:HB	37:i:57:PRO:HD3	1.91	0.52
38:j:86:ARG:NH1	50:v:64:TYR:O	2.43	0.52
54:z:9:G:H22	54:z:13:G:H22	1.57	0.52
1:1:2611:C:O4'	55:B:21:ILE:HG21	2.09	0.52
19:Q:52:PRO:O	19:Q:53:PHE:CG	2.63	0.52
36:h:47:ARG:HG2	36:h:47:ARG:HH11	1.75	0.52
54:z:12:C:H2'	54:z:13:G:O4'	2.11	0.52
9:G:80:THR:HG23	9:G:81:GLU:HG3	1.92	0.51
22:T:38:GLY:N	22:T:62:GLU:OE2	2.43	0.51
36:h:146:ARG:CG	36:h:147:GLU:N	2.73	0.51
54:z:44:G:C2'	54:z:45:U:OP1	2.57	0.51
54:z:78:C:C2'	54:z:79:C:H5'	2.40	0.51
1:1:635:C:H2'	1:1:636:G:O4'	2.11	0.51
1:1:807:U:OP1	13:K:36:LYS:HE2	2.10	0.51
1:1:1086:A:O2'	1:1:1103:A:N6	2.39	0.51
1:1:2107:G:C8	1:1:2107:G:C5'	2.91	0.51
2:2:8:A:N6	36:h:202:GLU:O	2.37	0.51
5:C:20:VAL:HG23	5:C:20:VAL:O	2.11	0.51
9:G:26:ILE:HG22	9:G:79:VAL:HG21	1.92	0.51
13:K:27:LEU:HD22	13:K:27:LEU:N	2.25	0.51
22:T:99:ASN:C	22:T:99:ASN:OD1	2.53	0.51
54:z:1:G:O2'	54:z:2:G:O5'	2.28	0.51
1:1:1170:C:N4	1:1:1171:G:O6	2.43	0.51
1:1:1278:C:O2'	15:M:27:SER:OG	2.24	0.51
2:2:685:G:N2	2:2:704:A:OP2	2.42	0.51
49:u:17:MET:HG3	49:u:20:SER:HB2	1.91	0.51
1:1:1090:A:N1	1:1:1102:C:C2	2.79	0.51
1:1:1171:G:C6	1:1:1172:C:C4	2.98	0.51
1:1:1798:U:OP2	5:C:271:ARG:NH2	2.44	0.51
1:1:2178:C:H2'	1:1:2179:C:C5	2.46	0.51
2:2:933:G:N7	39:k:3:ARG:NE	2.51	0.51
11:I:77:HIS:CE1	11:I:80:HIS:O	2.64	0.51
1:1:12:U:H2'	1:1:13:A:H5'	1.91	0.51
1:1:1980:G:O2'	1:1:1982:U:OP2	2.24	0.51
1:1:2161:C:O2'	1:1:2173:A:H4'	2.10	0.51
17:O:71:GLU:OE2	17:O:101:ARG:NE	2.44	0.51
34:f:133:GLU:O	34:f:137:ARG:HG2	2.10	0.51
43:o:60:PRO:HD3	43:o:91:PRO:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B:1:FME:O	55:B:5:MET:N	2.41	0.51
1:1:639:U:H2'	1:1:640:C:C6	2.45	0.51
2:2:496:A:O2'	2:2:497:G:C8	2.64	0.51
2:2:580:C:H2'	2:2:581:G:O4'	2.11	0.51
2:2:766:A:OP2	2:2:812:G:N2	2.43	0.51
3:3:1:U:O2'	3:3:2:G:H8	1.93	0.51
12:J:78:ARG:NH2	17:O:71:GLU:OE1	2.36	0.51
1:1:707:G:H2'	1:1:708:G:O4'	2.11	0.51
1:1:878:A:N7	1:1:899:A:H2	2.08	0.51
2:2:1141:C:HO2'	2:2:1142:G:H8	1.59	0.51
2:2:1311:A:OP1	28:Z:59:ARG:NH1	2.44	0.51
7:E:176:ASP:OD1	7:E:176:ASP:N	2.43	0.51
36:h:95:GLU:HA	36:h:100:ASN:HD22	1.76	0.51
45:q:25:VAL:HG12	45:q:29:ARG:HD2	1.93	0.51
1:1:891:G:O2'	1:1:892:A:P	2.69	0.51
1:1:1172:C:H2'	1:1:1173:U:C2	2.46	0.51
2:2:1132:C:H2'	2:2:1133:G:C8	2.46	0.51
14:L:21:ALA:HB2	14:L:97:GLN:HB2	1.93	0.51
44:p:4:VAL:O	44:p:8:VAL:HG23	2.11	0.51
47:s:21:ASP:O	47:s:23:GLY:N	2.44	0.51
1:1:1370:C:H2'	1:1:1371:G:O4'	2.11	0.51
1:1:2104:C:H41	1:1:2185:U:H3	1.58	0.51
2:2:335:C:O2'	2:2:1433:A:N3	2.38	0.51
2:2:1320:C:OP2	51:w:70:LYS:NZ	2.43	0.51
10:H:84:ALA:O	10:H:148:ALA:HA	2.11	0.51
10:H:86:ASP:O	10:H:89:LYS:HD2	2.10	0.51
38:j:21:MET:HG2	38:j:24:ARG:HH21	1.76	0.51
54:z:65:G:C4	54:z:66:5MU:H73	2.46	0.51
1:1:510:C:C2'	1:1:511:U:H5'	2.41	0.51
1:1:1818:U:OP2	5:C:156:ARG:NE	2.44	0.51
1:1:2050:C:H2'	1:1:2051:A:O4'	2.11	0.51
2:2:1007:U:H2'	2:2:1008:U:H6	1.75	0.51
6:D:33:ARG:NH1	6:D:75:ALA:O	2.44	0.51
34:f:207:ILE:O	34:f:210:VAL:HG22	2.10	0.51
43:o:107:ILE:HG23	53:y:6:VAL:HG21	1.92	0.51
1:1:548:G:H3'	1:1:549:G:O4'	2.11	0.50
1:1:2519:U:O4'	1:1:2542:A:N6	2.44	0.50
2:2:202:G:O2'	2:2:468:A:H8	1.94	0.50
2:2:559:A:H4'	2:2:560:A:H3'	1.92	0.50
13:K:124:GLY:C	13:K:125:LEU:HD12	2.35	0.50
1:1:463:G:N2	1:1:466:A:OP2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:639:U:H2'	1:1:640:C:H6	1.76	0.50
1:1:2532:G:O2'	1:1:2657:A:N1	2.44	0.50
10:H:77:THR:HA	10:H:143:ILE:O	2.10	0.50
13:K:123:ARG:NE	13:K:143:GLU:OE2	2.35	0.50
22:T:36:VAL:CG1	22:T:39:ILE:HD12	2.41	0.50
37:i:159:LYS:NZ	40:l:42:GLU:O	2.37	0.50
51:w:35:SER:OG	51:w:38:SER:OG	2.23	0.50
1:1:653:U:H5	1:1:654:A:H62	1.59	0.50
1:1:732:C:H2'	1:1:733:G:O4'	2.10	0.50
1:1:856:G:H2'	1:1:857:G:C8	2.46	0.50
1:1:1328:A:H2'	1:1:1330:C:C5	2.45	0.50
2:2:108:G:H5'	2:2:109:A:H5''	1.91	0.50
2:2:1061:G:OP2	35:g:2:GLY:O	2.29	0.50
2:2:1222:G:H5''	51:w:78:ARG:HD2	1.93	0.50
35:g:73:PRO:HA	35:g:76:VAL:HG22	1.92	0.50
1:1:1074:G:C2	1:1:1075:C:N4	2.80	0.50
8:F:143:TYR:O	8:F:146:VAL:HG13	2.11	0.50
10:H:94:ILE:HG13	10:H:94:ILE:O	2.11	0.50
21:S:6:ARG:O	21:S:10:VAL:HG23	2.11	0.50
34:f:114:LEU:HD12	34:f:144:LEU:C	2.37	0.50
38:j:3:HIS:ND1	38:j:95:ALA:N	2.60	0.50
43:o:13:ARG:HE	43:o:14:LYS:H	1.57	0.50
1:1:1588:G:C2	1:1:1589:U:C4	2.99	0.50
2:2:197:A:N1	2:2:220:G:O2'	2.44	0.50
8:F:17:MET:SD	8:F:22:TYR:HB2	2.51	0.50
40:l:90:ASP:OD1	40:l:90:ASP:N	2.39	0.50
1:1:897:C:H2'	1:1:898:C:O4'	2.10	0.50
2:2:69:G:H2'	2:2:70:U:C6	2.47	0.50
2:2:1234:C:OP1	41:m:119:ARG:NH2	2.45	0.50
13:K:70:LYS:O	13:K:74:THR:HG23	2.11	0.50
31:c:31:LEU:HD22	31:c:42:LEU:HD21	1.92	0.50
37:i:137:VAL:O	37:i:141:ILE:HG12	2.12	0.50
39:k:40:GLU:OE1	41:m:41:ARG:NH1	2.45	0.50
1:1:84:A:N1	1:1:98:G:O2'	2.40	0.50
1:1:613:A:H4'	1:1:614:A:OP1	2.12	0.50
1:1:810:U:N3	13:K:29:LYS:O	2.45	0.50
1:1:894:U:O2'	1:1:895:U:O5'	2.28	0.50
1:1:1358:G:C8	1:1:1371:G:O6	2.65	0.50
1:1:2113:U:N3	1:1:2114:A:N7	2.60	0.50
2:2:82:G:H1	2:2:86:G:N2	2.09	0.50
2:2:412:A:H62	2:2:431:A:N6	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1347:G:O2'	2:2:1373:G:O6	2.20	0.50
42:n:17:LEU:CD2	42:n:96:VAL:HG23	2.42	0.50
1:1:323:C:H2'	7:E:163:ASN:OD1	2.11	0.50
1:1:2100:G:O6	1:1:2189:U:C4	2.65	0.50
2:2:90:C:H2'	2:2:91:U:H6	1.76	0.50
41:m:44:ALA:HA	41:m:47:VAL:HG22	1.93	0.50
2:2:1168:U:H3'	2:2:1169:A:H5'	1.94	0.50
10:H:51:ARG:HG3	10:H:54:LEU:HD23	1.93	0.50
16:N:70:ALA:O	16:N:74:VAL:HG23	2.12	0.50
47:s:21:ASP:O	47:s:22:THR:HG22	2.12	0.50
1:1:2584:U:H2'	1:1:2585:U:C2	2.46	0.49
2:2:411:A:P	36:h:26:ARG:HH12	2.34	0.49
34:f:27:MET:HG3	34:f:189:THR:HA	1.94	0.49
1:1:1722:A:O2'	1:1:1723:G:H5'	2.13	0.49
2:2:213:G:C8	2:2:214:C:C5	2.99	0.49
2:2:983:A:OP1	46:r:6:MET:HE1	2.12	0.49
35:g:80:LYS:HD3	35:g:80:LYS:N	2.27	0.49
45:q:23:TYR:HB3	45:q:66:GLU:HG3	1.94	0.49
49:u:60:GLU:O	49:u:76:VAL:HG22	2.12	0.49
1:1:2106:U:H2'	1:1:2107:G:C8	2.47	0.49
1:1:2127:G:O2'	1:1:2128:G:O5'	2.30	0.49
1:1:2885:G:O6	29:a:29:SER:OG	2.30	0.49
7:E:23:PHE:CE1	13:K:1:MET:SD	3.06	0.49
10:H:114:GLU:CD	10:H:134:VAL:HA	2.37	0.49
13:K:19:LEU:HD12	13:K:19:LEU:N	2.27	0.49
51:w:40:ILE:HD12	51:w:66:MET:O	2.12	0.49
2:2:945:G:C2	2:2:946:A:C8	3.00	0.49
2:2:1145:A:C2'	2:2:1146:A:OP2	2.59	0.49
20:R:73:LYS:HB2	20:R:106:VAL:HB	1.94	0.49
22:T:94:ARG:HB3	22:T:103:ILE:HD12	1.94	0.49
38:j:9:MET:HG2	38:j:59:TYR:CE1	2.48	0.49
50:v:74:HIS:CG	50:v:74:HIS:O	2.66	0.49
51:w:63:THR:HG22	51:w:64:ASP:N	2.27	0.49
2:2:1181:G:O2'	2:2:1182:G:N7	2.40	0.49
1:1:574:A:N6	1:1:2034:U:OP1	2.42	0.49
1:1:931:U:N3	1:1:1167:C:O2	2.45	0.49
1:1:1378:A:O2'	1:1:1380:G:N7	2.46	0.49
42:n:15:HIS:HA	42:n:18:ILE:HG22	1.94	0.49
47:s:5:THR:O	47:s:8:THR:OG1	2.25	0.49
8:F:35:THR:C	8:F:36:LEU:HD12	2.38	0.49
8:F:122:PHE:O	8:F:123:ASP:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:155:GLU:HG2	9:G:157:TYR:H	1.78	0.49
19:Q:45:GLU:OE1	19:Q:45:GLU:O	2.31	0.49
20:R:82:MET:HG3	20:R:98:LYS:HB2	1.93	0.49
34:f:23:TRP:CZ3	34:f:25:PRO:HA	2.47	0.49
35:g:140:ASN:O	35:g:144:LEU:HD23	2.12	0.49
43:o:109:ASN:OD1	53:y:5:LYS:HA	2.13	0.49
1:1:829:A:N7	1:1:2247:A:O2'	2.46	0.49
1:1:1590:A:H2'	1:1:1591:A:H8	1.77	0.49
2:2:73:C:H2'	2:2:74:A:H5'	1.94	0.49
2:2:999:C:N3	2:2:1042:A:N6	2.60	0.49
42:n:92:LEU:HD13	42:n:96:VAL:HB	1.94	0.49
1:1:285:G:C6	1:1:356:G:C6	3.00	0.49
1:1:878:A:H3'	1:1:879:G:H8	1.77	0.49
1:1:1664:A:H2	12:J:1:MET:HE1	1.78	0.49
1:1:2195:U:O2'	1:1:2196:C:H5'	2.13	0.49
1:1:2795:C:H2'	1:1:2796:U:C6	2.47	0.49
34:f:218:ALA:HA	34:f:221:VAL:HG22	1.94	0.49
1:1:1954:G:O2'	1:1:1956:U:O4	2.23	0.49
1:1:2101:A:H2'	1:1:2102:G:O4'	2.12	0.49
1:1:2189:U:H1'	1:1:2190:G:C8	2.48	0.49
2:2:279:A:H5''	2:2:280:C:H3'	1.94	0.49
2:2:475:C:H2'	2:2:476:U:C6	2.48	0.49
3:3:31:C:O5'	3:3:31:C:H6	1.96	0.49
32:d:26:HIS:CE1	32:d:48:ALA:HB2	2.48	0.49
38:j:9:MET:HE3	38:j:59:TYR:CE1	2.48	0.49
1:1:137:U:H2'	1:1:138:U:H5'	1.94	0.48
1:1:458:G:O2'	1:1:469:G:O6	2.28	0.48
1:1:566:U:O2'	1:1:809:G:OP2	2.27	0.48
1:1:2144:G:H1'	1:1:2147:A:H62	1.78	0.48
1:1:2387:U:OP1	24:V:55:ARG:NH2	2.30	0.48
2:2:1239:A:H62	2:2:1299:A:N6	2.11	0.48
9:G:24:ILE:HD11	9:G:43:VAL:HG11	1.95	0.48
20:R:70:LYS:N	20:R:108:SER:O	2.46	0.48
34:f:68:LEU:HB3	34:f:161:LEU:HD12	1.95	0.48
42:n:32:THR:O	42:n:82:LYS:NZ	2.29	0.48
48:t:46:LYS:N	48:t:46:LYS:HD2	2.28	0.48
54:z:54:A:C2'	54:z:55:C:O4'	2.61	0.48
54:z:55:C:H2'	54:z:56:G:H8	1.77	0.48
1:1:137:U:C2'	1:1:138:U:H5'	2.42	0.48
1:1:1754:A:O2'	17:O:103:ARG:NH2	2.47	0.48
1:1:2314:A:OP1	8:F:88:LYS:NZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:203:G:O2'	2:2:465:A:N1	2.46	0.48
2:2:516:PSU:H4'	2:2:517:G:OP1	2.12	0.48
2:2:842:U:C2'	2:2:844:G:H21	2.27	0.48
15:M:65:LEU:O	15:M:69:ARG:HG3	2.13	0.48
38:j:43:GLY:HA2	38:j:58:HIS:CE1	2.48	0.48
39:k:5:ARG:NH1	39:k:7:ILE:HG22	2.28	0.48
40:l:11:LEU:HD22	40:l:75:ILE:HD11	1.94	0.48
48:t:6:LEU:HD23	48:t:17:TYR:CG	2.48	0.48
51:w:30:PRO:HA	51:w:48:THR:O	2.13	0.48
1:1:1870:C:O2'	1:1:1871:A:C5'	2.61	0.48
1:1:2364:C:H2'	1:1:2365:G:O4'	2.13	0.48
1:1:2780:G:OP2	11:I:120:ARG:NE	2.38	0.48
8:F:40:VAL:HG12	8:F:40:VAL:O	2.12	0.48
37:i:88:VAL:HG12	37:i:93:ARG:HG3	1.95	0.48
38:j:37:HIS:NE2	38:j:65:GLU:HB2	2.28	0.48
39:k:47:LEU:HD23	39:k:58:GLU:HB3	1.95	0.48
39:k:78:ARG:HG2	39:k:80:VAL:HG23	1.96	0.48
2:2:255:G:P	49:u:71:LYS:HZ3	2.36	0.48
8:F:135:GLN:CG	8:F:141:ILE:HD13	2.43	0.48
10:H:115:VAL:HG22	10:H:117:LEU:HD11	1.95	0.48
28:Z:44:PHE:CD2	28:Z:45:THR:HG23	2.48	0.48
28:Z:58:ASP:OD1	28:Z:58:ASP:C	2.57	0.48
40:l:93:PRO:O	40:l:117:ARG:NH2	2.47	0.48
1:1:381:G:OP1	25:W:18:ARG:NH2	2.40	0.48
1:1:2134:A:O2'	1:1:2159:G:O2'	2.30	0.48
26:X:32:ALA:HB2	26:X:37:LEU:HD23	1.95	0.48
28:Z:51:VAL:HG23	28:Z:52:ALA:N	2.26	0.48
1:1:724:U:H2'	1:1:725:G:O4'	2.14	0.48
1:1:784:G:O2'	1:1:785:G:O5'	2.24	0.48
1:1:1342:A:O2'	1:1:1344:U:OP2	2.20	0.48
1:1:1469:A:H2'	1:1:1470:A:C8	2.48	0.48
2:2:880:C:OP2	44:p:3:THR:HG21	2.13	0.48
6:D:31:ALA:HB1	6:D:95:SER:OG	2.13	0.48
13:K:61:LEU:O	32:d:13:ARG:NE	2.32	0.48
16:N:43:ASN:OD1	16:N:45:SER:OG	2.22	0.48
19:Q:93:PHE:C	19:Q:93:PHE:CD1	2.92	0.48
35:g:6:HIS:HB3	46:r:89:MET:SD	2.53	0.48
40:l:7:ILE:O	40:l:11:LEU:HG	2.13	0.48
44:p:72:HIS:HB2	44:p:74:LEU:HD23	1.95	0.48
45:q:2:ALA:O	45:q:9:ILE:N	2.46	0.48
52:x:44:LYS:HE3	52:x:83:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1056:G:O2'	1:1:1086:A:O2'	2.30	0.48
2:2:459:A:H2'	2:2:460:A:C8	2.49	0.48
5:C:41:GLY:O	5:C:43:ARG:NH1	2.46	0.48
45:q:27:LYS:O	45:q:31:LYS:HG3	2.13	0.48
1:1:810:U:C2	13:K:29:LYS:O	2.66	0.48
1:1:1141:U:H4'	1:1:1142:A:O4'	2.14	0.48
1:1:1521:G:OP2	1:1:1522:A:O2'	2.28	0.48
1:1:2305:U:O2	8:F:151:GLY:HA3	2.14	0.48
8:F:53:ALA:HB2	8:F:150:ARG:HE	1.78	0.48
37:i:70:ASN:CG	37:i:70:ASN:O	2.55	0.48
37:i:149:SER:H	37:i:152:MET:CE	2.27	0.48
38:j:1:MET:CE	38:j:67:PRO:HD3	2.44	0.48
48:t:69:ASP:OD1	48:t:69:ASP:N	2.38	0.48
1:1:11:C:H2'	1:1:12:U:H5'	1.96	0.48
1:1:588:U:O4	1:1:670:A:H1'	2.14	0.48
1:1:1056:G:HO2'	1:1:1103:A:H61	1.60	0.48
1:1:2512:C:O5'	1:1:2512:C:H6	1.97	0.48
2:2:89:U:H2'	2:2:90:C:C6	2.49	0.48
2:2:475:C:H2'	2:2:476:U:H6	1.79	0.48
2:2:779:C:H2'	2:2:780:A:O4'	2.13	0.48
3:3:43:C:H5''	28:Z:1:MET:HA	1.96	0.48
8:F:19:GLU:CG	8:F:19:GLU:O	2.61	0.48
23:U:36:ALA:O	23:U:93:ARG:NH2	2.43	0.48
31:c:42:LEU:HD23	31:c:43:THR:HG23	1.96	0.48
32:d:55:LEU:CD2	32:d:59:ILE:HD11	2.44	0.48
35:g:123:GLN:HB3	35:g:128:VAL:CG2	2.43	0.48
45:q:9:ILE:CG2	45:q:18:ALA:HB1	2.35	0.48
1:1:287:G:H2'	1:1:288:U:C6	2.48	0.48
1:1:601:C:H2'	1:1:602:A:O4'	2.14	0.48
1:1:1143:A:OP1	11:I:27:ARG:NH2	2.44	0.48
1:1:2134:A:O2'	1:1:2159:G:C2'	2.61	0.48
1:1:2305:U:H5''	8:F:131:GLY:HA3	1.94	0.48
10:H:87:GLU:OE2	38:j:17:GLN:HB3	2.13	0.48
31:c:31:LEU:HD22	31:c:42:LEU:CD2	2.43	0.48
34:f:68:LEU:HD12	34:f:90:PHE:O	2.14	0.48
35:g:140:ASN:OD1	35:g:143:ARG:NH1	2.46	0.48
40:l:55:THR:HG23	40:l:56:LYS:HG2	1.95	0.48
48:t:19:VAL:HG22	48:t:37:GLY:C	2.39	0.48
1:1:388:G:N7	1:1:390:U:H2'	2.29	0.47
1:1:2122:U:OP2	1:1:2122:U:C6	2.62	0.47
2:2:515:G:H3'	2:2:516:PSU:O4	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:106:PHE:O	18:P:110:VAL:HG23	2.14	0.47
37:i:13:GLU:OE2	37:i:68:ARG:NH1	2.47	0.47
40:l:5:ASP:CG	40:l:77:ARG:HH12	2.21	0.47
44:p:54:ARG:HD2	44:p:62:GLU:HG2	1.96	0.47
49:u:68:SER:OG	49:u:69:LYS:N	2.47	0.47
1:1:818:G:N1	1:1:1188:U:OP2	2.32	0.47
1:1:1068:G:HO2'	1:1:1070:A:N6	2.12	0.47
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.49	0.47
8:F:53:ALA:CB	8:F:150:ARG:HE	2.27	0.47
34:f:119:THR:HA	34:f:123:ASP:OD1	2.13	0.47
1:1:57:C:H2'	1:1:58:G:O4'	2.15	0.47
1:1:2188:U:O4	1:1:2189:U:C4	2.67	0.47
2:2:1009:U:O2	2:2:1021:A:C2	2.67	0.47
21:S:33:LYS:HG3	21:S:80:TRP:CE3	2.50	0.47
28:Z:53:THR:HG23	28:Z:54:GLY:N	2.29	0.47
35:g:123:GLN:HB3	35:g:128:VAL:HG21	1.96	0.47
35:g:155:GLY:HA2	35:g:163:ALA:HB1	1.97	0.47
40:l:87:LYS:HG3	40:l:125:ILE:HD11	1.96	0.47
1:1:645:C:H2'	1:1:647:G:C8	2.49	0.47
1:1:2070:A:H2'	1:1:2071:A:O4'	2.15	0.47
3:3:48:U:P	16:N:30:ARG:HH22	2.37	0.47
10:H:12:LEU:HD23	10:H:12:LEU:H	1.78	0.47
10:H:119:ASN:OD1	10:H:120:GLY:N	2.47	0.47
16:N:53:THR:HB	16:N:65:THR:HB	1.96	0.47
36:h:146:ARG:HG3	36:h:147:GLU:H	1.80	0.47
41:m:41:ARG:O	41:m:45:ARG:HG3	2.14	0.47
46:r:50:THR:HG22	51:w:13:LEU:HD13	1.96	0.47
47:s:26:GLU:HG3	47:s:81:LEU:HD22	1.97	0.47
1:1:170:U:H2'	1:1:171:U:C6	2.50	0.47
1:1:210:C:OP1	31:c:29:GLN:NE2	2.48	0.47
1:1:244:A:OP2	32:d:8:ARG:NH2	2.40	0.47
1:1:1103:A:OP2	1:1:1104:C:N4	2.47	0.47
1:1:1539:U:H2'	1:1:1540:G:H8	1.78	0.47
1:1:2029:G:N1	1:1:2033:A:OP2	2.39	0.47
1:1:2484:G:OP1	14:L:44:ARG:NH1	2.43	0.47
1:1:2804:U:H2'	1:1:2805:C:C6	2.49	0.47
2:2:713:G:H2'	2:2:714:G:C8	2.49	0.47
2:2:1004:A:C8	2:2:1025:U:H1'	2.50	0.47
2:2:1319:A:O2'	2:2:1323:G:N7	2.44	0.47
5:C:133:ARG:NE	5:C:187:ASP:OD1	2.44	0.47
8:F:105:THR:HG21	28:Z:22:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:99:ARG:HE	44:p:104:CYS:HG	1.61	0.47
45:q:46:SER:C	45:q:47:GLU:HG3	2.39	0.47
1:1:469:G:O6	31:c:37:LYS:HE2	2.15	0.47
1:1:613:A:O4'	1:1:614:A:C8	2.67	0.47
25:W:54:LYS:O	25:W:58:VAL:HG23	2.14	0.47
34:f:9:MET:HE1	34:f:47:VAL:HA	1.96	0.47
36:h:146:ARG:CG	36:h:147:GLU:H	2.28	0.47
37:i:150:PRO:HA	37:i:153:VAL:HG22	1.95	0.47
1:1:1869:G:H21	1:1:1872:A:H62	1.61	0.47
2:2:9:G:H5'	37:i:108:GLY:HA3	1.97	0.47
2:2:526:C:OP2	44:p:88:LYS:HE3	2.14	0.47
2:2:1086:U:H3	2:2:1099:G:H22	1.63	0.47
2:2:1168:U:O2'	2:2:1169:A:H5''	2.14	0.47
2:2:1168:U:C3'	2:2:1169:A:H5'	2.44	0.47
3:3:2:G:H2'	3:3:3:C:C6	2.49	0.47
6:D:3:GLY:C	6:D:4:LEU:HD12	2.40	0.47
16:N:31:THR:O	16:N:102:ARG:NH1	2.40	0.47
16:N:47:VAL:C	16:N:48:LEU:HD22	2.40	0.47
23:U:58:SER:O	23:U:73:LYS:NZ	2.48	0.47
39:k:91:VAL:HG12	39:k:96:ARG:HG3	1.97	0.47
40:l:75:ILE:HG23	40:l:75:ILE:O	2.14	0.47
41:m:35:LEU:HD21	41:m:48:VAL:HG21	1.97	0.47
43:o:70:CYS:O	43:o:74:VAL:HG22	2.15	0.47
54:z:12:C:C2'	54:z:13:G:O5'	2.63	0.47
54:z:15:G:H1'	54:z:20:U:O4	2.15	0.47
1:1:894:U:H1'	1:1:895:U:OP1	2.15	0.47
1:1:2297:A:N1	1:1:2321:U:H5	2.13	0.47
2:2:858:G:O6	2:2:869:G:C8	2.68	0.47
2:2:1370:G:C2	2:2:1371:G:C8	3.03	0.47
8:F:134:GLU:CG	8:F:136:ILE:HD12	2.45	0.47
18:P:97:ASP:OD2	19:Q:13:ARG:CZ	2.62	0.47
34:f:130:THR:HG23	34:f:130:THR:O	2.15	0.47
50:v:25:ASP:O	50:v:29:LEU:HD13	2.15	0.47
51:w:3:ARG:NH1	51:w:9:PRO:O	2.47	0.47
1:1:558:U:OP1	11:I:113:PRO:HD2	2.15	0.47
28:Z:41:HIS:ND1	28:Z:43:PHE:HB2	2.30	0.47
43:o:34:ILE:HG12	43:o:70:CYS:SG	2.54	0.47
45:q:4:ILE:CG1	45:q:9:ILE:HD12	2.45	0.47
46:r:50:THR:CG2	51:w:13:LEU:HD13	2.45	0.47
52:x:54:MET:O	52:x:54:MET:HG2	2.14	0.47
55:B:21:ILE:O	55:B:21:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:720:U:H2'	1:1:721:A:C8	2.50	0.47
1:1:964:C:O2'	1:1:2273:A:N3	2.48	0.47
1:1:1722:A:N6	1:1:1738:G:H1'	2.30	0.47
1:1:2350:C:OP2	32:d:45:ARG:NH2	2.48	0.47
1:1:2561:U:O3'	12:J:40:LYS:NZ	2.44	0.47
1:1:2849:U:N3	1:1:2867:G:O4'	2.48	0.47
2:2:110:C:H2'	2:2:111:G:O4'	2.15	0.47
2:2:951:G:HO2'	2:2:970:C:HO2'	1.59	0.47
5:C:66:ASP:OD2	5:C:102:ARG:NH1	2.48	0.47
13:K:132:ARG:HG3	13:K:142:ILE:HD12	1.96	0.47
25:W:43:GLU:OE1	25:W:45:ARG:NH1	2.48	0.47
34:f:64:LYS:N	34:f:64:LYS:HD2	2.30	0.47
46:r:14:VAL:O	46:r:18:ASP:OD2	2.32	0.47
1:1:116:C:H2'	1:1:117:G:O4'	2.15	0.46
2:2:521:G:N7	44:p:50:ARG:NH2	2.62	0.46
2:2:1147:C:H4'	41:m:7:TYR:CE2	2.50	0.46
2:2:1356:G:H2'	2:2:1357:A:C8	2.50	0.46
8:F:47:LYS:HE2	8:F:47:LYS:HA	1.97	0.46
34:f:32:PHE:N	34:f:40:ILE:O	2.38	0.46
36:h:172:GLU:HB2	36:h:183:LYS:HD2	1.97	0.46
41:m:130:ARG:HD2	54:z:36:G:OP1	2.15	0.46
42:n:52:LEU:HD23	42:n:62:ARG:HG2	1.97	0.46
1:1:1096:A:H2'	1:1:1097:U:O4'	2.15	0.46
1:1:1545:A:H2'	1:1:1546:G:O4'	2.16	0.46
1:1:1775:U:O4	1:1:1789:A:H2	1.98	0.46
2:2:1080:A:OP1	37:i:52:LYS:NZ	2.47	0.46
2:2:1168:U:O2'	2:2:1169:A:P	2.73	0.46
10:H:40:THR:OG1	10:H:43:ASN:OD1	2.26	0.46
23:U:21:ARG:HE	23:U:87:GLN:HA	1.79	0.46
35:g:7:PRO:HA	35:g:10:ILE:HG22	1.97	0.46
37:i:149:SER:H	37:i:152:MET:HE2	1.80	0.46
1:1:2511:U:O4	1:1:2575:C:N3	2.49	0.46
2:2:411:A:P	36:h:26:ARG:NH1	2.88	0.46
2:2:868:C:H2'	2:2:869:G:O4'	2.15	0.46
2:2:1005:A:H3'	2:2:1006:G:H8	1.80	0.46
2:2:1018:G:H2'	2:2:1019:A:O4'	2.15	0.46
2:2:1160:G:OP1	34:f:132:LYS:NZ	2.48	0.46
3:3:1:U:O2'	3:3:2:G:O4'	2.33	0.46
10:H:129:GLU:OE1	10:H:129:GLU:N	2.48	0.46
16:N:4:LYS:O	16:N:8:ILE:HG13	2.15	0.46
39:k:69:VAL:CG1	39:k:135:VAL:HG12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:23:TYR:CD1	45:q:69:LEU:HD23	2.51	0.46
49:u:7:THR:HG21	49:u:60:GLU:OE2	2.16	0.46
54:z:10:U:C2	54:z:11:C:C5	3.04	0.46
1:1:776:G:N7	1:1:793:A:O2'	2.39	0.46
1:1:2126:A:N1	1:1:2163:A:OP1	2.48	0.46
2:2:214:C:H2'	2:2:215:C:H6	1.80	0.46
2:2:608:A:H2'	2:2:609:A:O4'	2.15	0.46
2:2:792:A:O2'	2:2:794:A:N7	2.45	0.46
6:D:17:GLU:OE1	6:D:17:GLU:N	2.42	0.46
9:G:43:VAL:HG23	9:G:52:PHE:CE1	2.50	0.46
10:H:75:LEU:H	10:H:75:LEU:HD12	1.80	0.46
10:H:90:LEU:HD21	10:H:123:ARG:C	2.40	0.46
45:q:81:MET:SD	45:q:92:ARG:HB3	2.55	0.46
49:u:26:GLU:OE1	49:u:26:GLU:N	2.48	0.46
1:1:781:A:OP1	5:C:217:ARG:NH2	2.44	0.46
1:1:1231:U:H2'	1:1:1232:G:H8	1.80	0.46
1:1:2102:G:N1	1:1:2187:U:N3	2.64	0.46
1:1:2147:A:N6	1:1:2148:G:H21	2.14	0.46
2:2:209:U:H3'	2:2:210:C:O2	2.15	0.46
2:2:451:A:H4'	2:2:452:A:O4'	2.15	0.46
6:D:153:GLY:O	6:D:154:LYS:HB3	2.15	0.46
27:Y:13:ALA:O	27:Y:21:LYS:HE2	2.15	0.46
37:i:159:LYS:NZ	40:l:43:GLU:HA	2.31	0.46
1:1:362:A:C4	1:1:363:G:C8	3.04	0.46
1:1:1062:G:C6	1:1:1063:G:C6	3.04	0.46
1:1:1094:U:O2'	1:1:1096:A:N7	2.48	0.46
1:1:1870:C:H2'	1:1:1871:A:C8	2.50	0.46
2:2:1328:C:H5''	45:q:28:THR:HG21	1.97	0.46
9:G:76:VAL:O	9:G:80:THR:HG22	2.15	0.46
12:J:76:VAL:HG12	17:O:73:VAL:HB	1.98	0.46
20:R:31:GLN:O	20:R:35:ILE:HG13	2.15	0.46
27:Y:6:LYS:HB2	27:Y:58:GLU:HB3	1.97	0.46
38:j:72:ASP:O	38:j:76:THR:HG23	2.16	0.46
1:1:357:C:C2	1:1:358:U:C5	3.03	0.46
1:1:1062:G:H2'	1:1:1063:G:C8	2.51	0.46
1:1:1069:A:N1	1:1:1096:A:H5'	2.30	0.46
1:1:1588:G:N1	1:1:1589:U:O4	2.48	0.46
1:1:2193:G:C6	1:1:2194:U:C4	3.03	0.46
1:1:2233:U:H2'	1:1:2234:G:C8	2.51	0.46
1:1:2512:C:H1'	6:D:145:SER:O	2.15	0.46
29:a:26:THR:OG1	29:a:27:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:k:105:VAL:O	39:k:109:ARG:HG3	2.16	0.46
43:o:64:GLN:O	43:o:68:GLU:HG3	2.15	0.46
54:z:16:U:O2'	54:z:17:OMG:H5''	2.16	0.46
1:1:1808:A:H3'	1:1:1809:A:C8	2.51	0.46
2:2:522:C:OP2	44:p:66:TYR:OH	2.20	0.46
2:2:552:U:H2'	2:2:553:A:H8	1.80	0.46
2:2:1226:C:OP2	45:q:102:THR:HG21	2.15	0.46
11:l:56:VAL:HB	11:l:124:VAL:HG12	1.98	0.46
35:g:87:LEU:O	35:g:91:VAL:HG23	2.16	0.46
1:1:2188:U:O4	1:1:2189:U:C5	2.68	0.46
2:2:1377:A:C6	39:k:7:ILE:HD13	2.50	0.46
37:i:153:VAL:HG23	37:i:164:ILE:HD13	1.97	0.46
54:z:79:C:H2'	54:z:80:U:O4'	2.16	0.46
55:B:5:MET:HA	55:B:8:ILE:HD12	1.98	0.46
1:1:247:G:O6	32:d:12:LYS:NZ	2.32	0.46
1:1:276:U:H1'	1:1:277:G:C8	2.50	0.46
1:1:403:U:O5'	1:1:403:U:H6	1.99	0.46
1:1:895:U:C2'	1:1:896:A:O4'	2.64	0.46
1:1:2012:G:OP1	20:R:11:ARG:NH2	2.47	0.46
1:1:2184:A:C8	1:1:2185:U:C5	3.03	0.46
1:1:2450:A:N6	1:1:2501:C:O2	2.49	0.46
2:2:1026:G:C6	2:2:1027:C:C5	3.04	0.46
2:2:1060:U:H4'	42:n:53:ILE:HG13	1.97	0.46
2:2:1498:UR3:O5'	2:2:1498:UR3:H6	2.16	0.46
42:n:57:VAL:O	42:n:57:VAL:HG13	2.16	0.46
43:o:65:VAL:O	43:o:69:ARG:HG3	2.16	0.46
45:q:106:ALA:HB3	45:q:110:LYS:HD3	1.98	0.46
54:z:69:G:H2'	54:z:70:U:H5'	1.97	0.46
1:1:2141:G:H2'	1:1:2142:A:C8	2.51	0.45
2:2:80:A:C2	2:2:90:C:N3	2.84	0.45
2:2:1035:A:C6	2:2:1036:A:C5	3.04	0.45
3:3:43:C:O2	8:F:92:ARG:NH2	2.48	0.45
5:C:170:ALA:O	5:C:186:ALA:N	2.41	0.45
42:n:12:ALA:HB3	42:n:18:ILE:HD12	1.98	0.45
1:1:335:C:O2	22:T:68:SER:OG	2.35	0.45
1:1:1069:A:O2'	1:1:1074:G:C2	2.69	0.45
1:1:1731:G:C2	1:1:1733:G:C4	3.03	0.45
1:1:2189:U:C2	1:1:2190:G:N7	2.84	0.45
2:2:406:G:N7	2:2:495:A:O2'	2.47	0.45
2:2:1323:G:H2'	2:2:1324:A:C8	2.51	0.45
2:2:1391:U:H2'	2:2:1392:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:52:PRO:O	19:Q:53:PHE:CD2	2.70	0.45
34:f:72:THR:HG22	34:f:93:ASN:C	2.42	0.45
35:g:7:PRO:O	35:g:11:ARG:HD3	2.16	0.45
2:2:309:A:O2'	2:2:607:A:N1	2.49	0.45
2:2:687:A:C2	2:2:704:A:C5	3.05	0.45
2:2:951:G:O2'	2:2:970:C:O2'	2.27	0.45
2:2:1020:G:N1	2:2:1021:A:C5	2.84	0.45
3:3:43:C:H5''	28:Z:1:MET:HG2	1.98	0.45
19:Q:34:GLU:HG2	19:Q:60:LYS:HG2	1.98	0.45
29:a:55:ILE:HG12	29:a:56:ALA:O	2.17	0.45
38:j:2:ARG:HB3	38:j:91:ARG:NH1	2.31	0.45
39:k:113:ASP:O	39:k:119:ARG:HD2	2.16	0.45
54:z:67:U:O2'	54:z:69:G:O6	2.35	0.45
1:1:322:A:P	7:E:162:ARG:HH11	2.38	0.45
1:1:570:G:H2'	1:1:2030:6MZ:N7	2.31	0.45
1:1:895:U:HO2'	1:1:896:A:C1'	2.29	0.45
1:1:1587:G:C2	1:1:1588:G:C8	3.05	0.45
1:1:1795:C:O2	5:C:253:LYS:HE2	2.16	0.45
1:1:2562:U:OP1	12:J:40:LYS:NZ	2.49	0.45
2:2:82:G:H1	2:2:86:G:H22	1.63	0.45
2:2:677:U:H3	2:2:713:G:H22	1.63	0.45
5:C:69:ARG:NH1	5:C:129:THR:OG1	2.49	0.45
29:a:40:ARG:HG3	29:a:41:HIS:ND1	2.31	0.45
34:f:129:LEU:CD2	34:f:134:ALA:HB2	2.43	0.45
34:f:173:ILE:HG22	34:f:177:ASN:OD1	2.17	0.45
35:g:47:LEU:N	35:g:47:LEU:CD1	2.80	0.45
39:k:9:GLN:NE2	39:k:10:ARG:HG2	2.32	0.45
45:q:81:MET:HE2	45:q:91:HIS:HB3	1.99	0.45
49:u:17:MET:HE3	49:u:20:SER:HB3	1.98	0.45
1:1:247:G:N7	1:1:249:C:C2	2.85	0.45
1:1:2602:A:C2'	1:1:2602:A:N3	2.79	0.45
2:2:1077:G:N2	2:2:1080:A:OP2	2.39	0.45
2:2:1152:A:P	42:n:72:ARG:HH22	2.39	0.45
2:2:1312:G:OP2	28:Z:63:ARG:NH2	2.49	0.45
5:C:130:LEU:O	5:C:135:ILE:HD11	2.16	0.45
5:C:174:LEU:O	5:C:181:MET:HA	2.16	0.45
11:I:89:PHE:O	11:I:93:ILE:HG12	2.15	0.45
42:n:54:SER:O	46:r:81:ARG:NH1	2.37	0.45
47:s:3:LEU:HB2	47:s:35:GLN:OE1	2.16	0.45
54:z:9:G:H22	54:z:13:G:H1	1.63	0.45
1:1:882:G:O6	1:1:894:U:C2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1107:G:C6	1:1:1108:U:C4	3.05	0.45
2:2:1368:A:OP1	42:n:64:GLN:NE2	2.44	0.45
7:E:152:GLU:CD	7:E:153:LEU:N	2.74	0.45
8:F:136:ILE:HD12	8:F:136:ILE:H	1.81	0.45
33:e:3:VAL:HA	33:e:36:ARG:O	2.17	0.45
37:i:111:MET:HG2	37:i:115:LEU:HD12	1.99	0.45
46:r:50:THR:HG22	51:w:13:LEU:CD1	2.47	0.45
51:w:40:ILE:HA	51:w:44:MET:SD	2.56	0.45
1:1:1452:G:O2'	1:1:2702:G:O6	2.35	0.45
1:1:2102:G:N1	1:1:2188:U:C2	2.85	0.45
10:H:135:HIS:HB3	10:H:138:VAL:H	1.82	0.45
12:J:90:ASN:O	12:J:92:GLU:OE1	2.34	0.45
12:J:109:SER:O	12:J:113:MET:HG3	2.16	0.45
13:K:74:THR:HG22	13:K:107:PHE:HB2	1.98	0.45
17:O:32:VAL:HG12	17:O:34:GLU:OE1	2.17	0.45
23:U:64:VAL:HG22	23:U:69:GLU:HG3	1.98	0.45
24:V:18:ALA:O	24:V:20:ARG:HD2	2.17	0.45
35:g:131:ARG:O	35:g:135:LYS:HG3	2.16	0.45
44:p:114:ARG:HB3	44:p:119:VAL:HB	1.99	0.45
45:q:11:ASP:HA	45:q:45:ILE:HB	1.98	0.45
1:1:549:G:H2'	1:1:550:C:C6	2.51	0.45
1:1:711:G:C6	1:1:721:A:C6	3.05	0.45
1:1:2220:U:C5'	10:H:112:LYS:HE3	2.47	0.45
1:1:2291:U:H2'	1:1:2292:U:C6	2.52	0.45
1:1:2602:A:N3	1:1:2602:A:O2'	2.45	0.45
2:2:1057:G:H2'	2:2:1058:G:O4'	2.16	0.45
2:2:1294:G:C6	2:2:1295:U:C4	3.05	0.45
2:2:1414:U:H2'	2:2:1415:G:H8	1.81	0.45
14:L:42:THR:HG22	14:L:93:VAL:HG12	1.98	0.45
37:i:18:VAL:HG12	37:i:19:ASN:N	2.32	0.45
42:n:22:THR:O	42:n:26:VAL:HG23	2.16	0.45
53:y:4:ILE:HD12	53:y:19:PHE:CD1	2.46	0.45
54:z:17:OMG:HN21	54:z:67:U:H6	1.65	0.45
55:B:1:FME:HB2	55:B:4:LYS:CB	2.44	0.45
1:1:848:C:H2'	1:1:849:A:C8	2.52	0.45
1:1:888:C:C6	45:q:92:ARG:HD2	2.52	0.45
1:1:1076:C:H2'	1:1:1077:A:H8	1.82	0.45
1:1:1170:C:C4	1:1:1171:G:N7	2.85	0.45
2:2:452:A:H62	2:2:480:U:H3	1.64	0.45
2:2:1157:A:C2	2:2:1181:G:C4	3.04	0.45
19:Q:91:GLN:OE1	19:Q:91:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:23:THR:HG23	27:Y:47:MET:HG2	1.99	0.45
37:i:111:MET:HA	37:i:114:VAL:HG12	1.98	0.45
42:n:90:LEU:HD23	42:n:90:LEU:C	2.42	0.45
45:q:22:ILE:HB	45:q:25:VAL:HG22	1.99	0.45
54:z:76:C:C2'	54:z:77:C:H5'	2.47	0.45
1:1:494:G:H4'	20:R:6:LYS:HB2	1.99	0.45
1:1:1089:A:N3	1:1:1090:A:N6	2.64	0.45
2:2:83:C:O2'	2:2:86:G:O6	2.33	0.45
2:2:552:U:H2'	2:2:553:A:C8	2.51	0.45
10:H:4:ILE:HA	10:H:17:ASP:O	2.17	0.45
21:S:61:LEU:HD11	21:S:82:LYS:HD3	1.99	0.45
49:u:19:LYS:HA	49:u:48:ASP:O	2.17	0.45
1:1:357:C:H2'	1:1:358:U:H6	1.80	0.44
1:1:1090:A:C6	1:1:1102:C:C2	3.05	0.44
1:1:1103:A:H3'	1:1:1104:C:C6	2.52	0.44
2:2:1270:G:HO2'	2:2:1313:U:HO2'	1.65	0.44
22:T:49:VAL:HG22	22:T:54:GLN:HB2	1.99	0.44
22:T:52:LEU:O	22:T:52:LEU:HD23	2.16	0.44
22:T:98:SER:O	22:T:99:ASN:OD1	2.34	0.44
34:f:221:VAL:HG23	34:f:222:ARG:N	2.32	0.44
44:p:102:LEU:N	44:p:102:LEU:HD12	2.31	0.44
54:z:19:C:H4'	54:z:20:U:O5'	2.18	0.44
54:z:60:C:N3	54:z:71:A:H1'	2.32	0.44
1:1:601:C:O5'	1:1:601:C:H6	1.99	0.44
1:1:720:U:H2'	1:1:721:A:H8	1.81	0.44
1:1:2579:C:O2'	6:D:136:ASN:OD1	2.33	0.44
2:2:750:C:H1'	47:s:21:ASP:O	2.18	0.44
2:2:1062:U:H2'	2:2:1063:C:C6	2.52	0.44
2:2:1316:G:N1	2:2:1319:A:OP2	2.50	0.44
6:D:45:TYR:OH	6:D:81:GLU:OE2	2.35	0.44
7:E:108:ILE:HB	13:K:1:MET:HE1	1.98	0.44
8:F:10:ASP:OD1	8:F:11:GLU:N	2.49	0.44
10:H:103:VAL:HG11	10:H:110:VAL:HG11	1.99	0.44
12:J:113:MET:HA	12:J:116:ILE:HG12	1.99	0.44
32:d:40:ARG:O	32:d:44:LEU:HG	2.18	0.44
39:k:47:LEU:HB3	39:k:58:GLU:HB3	1.98	0.44
49:u:11:ARG:HD2	49:u:58:VAL:HG22	1.99	0.44
51:w:19:VAL:O	51:w:23:VAL:HG23	2.17	0.44
2:2:1422:G:H4'	12:J:48:PRO:HB3	1.99	0.44
3:3:24:G:N7	3:3:56:G:H2'	2.31	0.44
3:3:40:U:N3	3:3:44:G:OP2	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:50:ARG:NH1	44:p:89:0TD:OD2	2.45	0.44
1:1:797:G:OP1	7:E:55:SER:OG	2.30	0.44
1:1:1175:A:H4'	1:1:1176:U:OP1	2.17	0.44
1:1:1535:A:OP2	1:1:1536:C:N4	2.51	0.44
1:1:1870:C:O2'	1:1:1871:A:H5'	2.16	0.44
1:1:2635:A:O2'	6:D:81:GLU:OE1	2.33	0.44
2:2:1218:C:H2'	2:2:1219:A:H8	1.83	0.44
3:3:74:U:O2	23:U:29:ILE:HD13	2.17	0.44
9:G:95:ARG:HG2	9:G:106:SER:HB2	1.99	0.44
10:H:131:SER:HA	10:H:140:ALA:O	2.18	0.44
15:M:114:GLU:OE1	15:M:118:ARG:NH1	2.48	0.44
28:Z:13:THR:HB	28:Z:31:ASP:OD1	2.18	0.44
34:f:68:LEU:HD11	34:f:92:VAL:HG23	2.00	0.44
45:q:65:VAL:HB	45:q:66:GLU:OE1	2.17	0.44
46:r:80:SER:O	46:r:84:VAL:HG23	2.16	0.44
1:1:2575:C:H5'	6:D:149:ASN:HB2	1.98	0.44
1:1:2788:C:H2'	1:1:2789:C:C6	2.53	0.44
13:K:127:VAL:HG12	13:K:128:THR:O	2.17	0.44
15:M:80:PHE:N	15:M:80:PHE:CD1	2.85	0.44
37:i:64:MET:O	37:i:68:ARG:HG3	2.17	0.44
55:B:5:MET:O	55:B:9:VAL:HG12	2.18	0.44
1:1:1680:U:H2'	1:1:1681:G:O4'	2.17	0.44
1:1:2102:G:C6	1:1:2188:U:N3	2.85	0.44
1:1:2313:C:H2'	1:1:2314:A:H8	1.82	0.44
2:2:1029:U:O2	2:2:1031:C:H1'	2.17	0.44
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.99	0.44
9:G:54:PRO:HG2	9:G:62:TRP:CE2	2.53	0.44
23:U:76:ASP:OD1	23:U:77:VAL:N	2.51	0.44
38:j:2:ARG:NE	38:j:91:ARG:HH12	2.10	0.44
41:m:15:SER:OG	41:m:78:ALA:HB2	2.17	0.44
1:1:1172:C:H2'	1:1:1173:U:N1	2.33	0.44
1:1:1417:C:O2'	1:1:1587:G:O2'	2.23	0.44
1:1:1452:G:H2'	1:1:1457:U:O4	2.17	0.44
2:2:355:C:C4	2:2:356:A:N7	2.86	0.44
23:U:9:ARG:HG2	23:U:41:GLU:HG2	1.99	0.44
23:U:61:LEU:HD12	23:U:61:LEU:N	2.33	0.44
24:V:9:SER:O	24:V:10:THR:HG23	2.18	0.44
54:z:1:G:H2'	54:z:2:G:H8	1.82	0.44
54:z:74:C:C2	54:z:75:C:C6	3.05	0.44
1:1:270:A:H5'	1:1:271:G:H5''	1.99	0.44
1:1:881:G:C6	1:1:882:G:N7	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1913:A:N1	2:2:1492:A:H2'	2.33	0.44
9:G:42:GLU:HA	9:G:55:ARG:NH2	2.33	0.44
10:H:14:SER:N	10:H:17:ASP:OD2	2.51	0.44
10:H:62:LEU:HD23	10:H:62:LEU:HA	1.79	0.44
20:R:10:ALA:HB3	20:R:101:SER:HB2	2.00	0.44
22:T:98:SER:C	22:T:100:SER:H	2.24	0.44
42:n:99:GLN:HA	42:n:99:GLN:NE2	2.33	0.44
54:z:53:A:H3'	54:z:54:A:H5'	1.99	0.44
55:B:19:GLY:O	55:B:21:ILE:HD11	2.18	0.44
1:1:1799:G:H8	5:C:180:GLU:OE1	2.01	0.44
1:1:2376:A:N3	16:N:111:ARG:NH1	2.66	0.44
1:1:2591:C:H2'	1:1:2592:G:C8	2.52	0.44
1:1:2728:U:O2'	1:1:2729:G:H8	2.00	0.44
2:2:1029:U:OP2	2:2:1029:U:C6	2.71	0.44
7:E:189:THR:HG22	7:E:191:ASP:H	1.83	0.44
8:F:37:ASN:HB3	8:F:153:ASP:OD1	2.17	0.44
14:L:53:MET:HG3	14:L:63:ILE:HD13	2.00	0.44
20:R:11:ARG:HH21	20:R:98:LYS:HE3	1.83	0.44
20:R:84:ARG:HG3	20:R:98:LYS:HD2	1.99	0.44
25:W:27:ARG:NH1	25:W:29:PHE:CZ	2.86	0.44
34:f:70:VAL:CG2	34:f:161:LEU:HD11	2.48	0.44
35:g:71:ALA:HA	35:g:106:VAL:HB	1.99	0.44
37:i:60:ILE:HG13	37:i:61:GLN:N	2.32	0.44
37:i:134:ILE:O	37:i:137:VAL:HG12	2.18	0.44
42:n:90:LEU:HD23	42:n:91:ASP:N	2.32	0.44
45:q:49:SER:HB3	45:q:52:GLN:HG3	1.98	0.44
1:1:1585:C:H2'	1:1:1586:A:O4'	2.17	0.43
1:1:2145:C:O2	1:1:2145:C:O2'	2.31	0.43
2:2:1458:G:OP1	52:x:30:THR:OG1	2.36	0.43
10:H:73:ASN:OD1	10:H:108:VAL:CG2	2.66	0.43
17:O:34:GLU:OE2	17:O:39:ARG:HG2	2.18	0.43
24:V:56:ASP:CG	24:V:58:THR:HG1	2.21	0.43
25:W:17:ASN:CG	25:W:27:ARG:HD2	2.43	0.43
33:e:23:ILE:HB	33:e:37:GLN:OE1	2.17	0.43
41:m:7:TYR:OH	41:m:9:THR:OG1	2.21	0.43
1:1:2190:G:H2'	1:1:2191:A:H8	1.83	0.43
2:2:235:C:H2'	2:2:236:A:C8	2.53	0.43
2:2:632:U:H5''	2:2:633:G:C8	2.52	0.43
2:2:891:U:H2'	2:2:892:A:H8	1.82	0.43
2:2:1010:U:H2'	2:2:1011:C:C5	2.52	0.43
8:F:144:ASP:C	8:F:146:VAL:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:32:ILE:O	32:d:32:ILE:HG22	2.19	0.43
35:g:47:LEU:HB3	35:g:50:ALA:HB3	2.00	0.43
38:j:18:VAL:HB	38:j:19:PRO:HD3	2.01	0.43
42:n:45:ARG:HB3	42:n:69:THR:HB	2.00	0.43
43:o:13:ARG:CZ	43:o:77:TYR:HE1	2.31	0.43
43:o:109:ASN:OD1	53:y:5:LYS:HG2	2.18	0.43
1:1:12:U:H2'	1:1:12:U:O2	2.17	0.43
1:1:901:C:C4	1:1:902:C:C4	3.06	0.43
1:1:1043:C:H2'	1:1:1044:C:O4'	2.18	0.43
1:1:1485:U:H2'	1:1:1486:U:C6	2.53	0.43
1:1:2101:A:N6	1:1:2189:U:N3	2.67	0.43
1:1:2184:A:H2'	1:1:2185:U:C6	2.52	0.43
1:1:2313:C:H2'	1:1:2314:A:C8	2.53	0.43
1:1:2800:A:C2	1:1:2895:G:H1'	2.54	0.43
2:2:120:A:O2'	2:2:122:G:N7	2.37	0.43
2:2:390:U:H2'	2:2:391:G:C8	2.53	0.43
2:2:518:C:H4'	2:2:519:C:H5''	2.00	0.43
2:2:1000:A:C6	2:2:1041:G:C6	3.05	0.43
3:3:119:A:H2'	3:3:120:U:O4'	2.19	0.43
6:D:86:GLU:OE1	6:D:86:GLU:N	2.47	0.43
12:J:110:GLU:H	12:J:110:GLU:CD	2.25	0.43
17:O:4:ILE:O	17:O:8:LEU:HD13	2.18	0.43
21:S:14:PRO:HD3	26:X:30:MET:SD	2.58	0.43
30:b:8:LYS:HD2	32:d:34:THR:HG21	2.00	0.43
35:g:130:PHE:O	35:g:134:MET:HG3	2.19	0.43
39:k:80:VAL:O	39:k:80:VAL:HG12	2.18	0.43
42:n:22:THR:HG23	42:n:23:ALA:N	2.32	0.43
42:n:36:VAL:O	42:n:36:VAL:HG23	2.16	0.43
1:1:880:G:H2'	1:1:880:G:N3	2.33	0.43
1:1:1293:C:C4	1:1:1294:U:C5	3.05	0.43
1:1:1494:A:H2'	1:1:1495:A:C8	2.53	0.43
1:1:2026:U:H2'	1:1:2027:G:O4'	2.18	0.43
1:1:2148:G:H2'	1:1:2149:U:H6	1.83	0.43
1:1:2820:A:OP2	15:M:2:ARG:NH2	2.51	0.43
2:2:212:G:C4	2:2:213:G:C8	3.06	0.43
2:2:1010:U:C2	2:2:1020:G:C2	3.06	0.43
2:2:1314:C:N4	51:w:2:PRO:O	2.51	0.43
7:E:153:LEU:HG	7:E:153:LEU:O	2.18	0.43
10:H:89:LYS:O	10:H:91:PHE:N	2.41	0.43
46:r:15:ALA:HA	46:r:18:ASP:OD2	2.19	0.43
50:v:18:VAL:HG22	50:v:20:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:y:40:LYS:O	53:y:44:GLU:HG3	2.18	0.43
1:1:1171:G:C5	1:1:1172:C:C5	3.07	0.43
1:1:1357:C:H2'	1:1:1358:G:O4'	2.18	0.43
1:1:1796:U:H2'	1:1:1797:G:H8	1.83	0.43
1:1:2123:G:H2'	1:1:2124:G:H8	1.81	0.43
1:1:2405:G:O2'	1:1:2411:A:N6	2.51	0.43
2:2:214:C:H2'	2:2:215:C:C6	2.52	0.43
2:2:1071:C:H2'	2:2:1072:G:H8	1.84	0.43
2:2:1497:G:O2'	2:2:1518:MA6:H103	2.19	0.43
7:E:150:THR:HG22	7:E:152:GLU:H	1.84	0.43
9:G:46:ALA:C	9:G:48:ASN:H	2.26	0.43
16:N:14:ALA:O	16:N:18:LEU:HD13	2.17	0.43
38:j:25:TYR:O	38:j:29:ILE:HG12	2.18	0.43
1:1:2140:G:C8	1:1:2140:G:C3'	3.02	0.43
1:1:2328:A:H2'	1:1:2329:U:C6	2.53	0.43
2:2:999:C:H2'	2:2:1000:A:H8	1.83	0.43
2:2:1032:G:H3'	2:2:1032:G:N3	2.34	0.43
5:C:225:MET:SD	5:C:230:HIS:HB2	2.59	0.43
8:F:119:ALA:HB1	8:F:167:ARG:HE	1.84	0.43
9:G:105:LEU:HD13	9:G:107:LEU:HD11	2.00	0.43
28:Z:42:PRO:O	28:Z:47:LYS:HG2	2.18	0.43
41:m:130:ARG:HH12	54:z:34:U:P	2.42	0.43
45:q:4:ILE:HG12	45:q:9:ILE:HD12	2.01	0.43
53:y:31:GLU:OE2	53:y:35:ARG:NE	2.51	0.43
1:1:1174:U:O2	1:1:1177:G:C6	2.72	0.43
1:1:1413:A:C5	1:1:1414:C:C5	3.07	0.43
1:1:2115:G:O3'	1:1:2165:C:O2	2.36	0.43
1:1:2298:A:OP1	8:F:71:ARG:NH2	2.51	0.43
1:1:2728:U:HO2'	1:1:2729:G:H8	1.66	0.43
2:2:485:U:H5'	2:2:485:U:O2	2.18	0.43
2:2:556:C:H2'	2:2:557:G:O4'	2.17	0.43
2:2:672:U:H2'	2:2:673:A:C8	2.54	0.43
2:2:767:A:H2'	2:2:768:A:O4'	2.19	0.43
2:2:1054:C:C5	2:2:1196:A:C8	3.07	0.43
5:C:144:VAL:HB	5:C:154:LEU:HB2	2.00	0.43
10:H:86:ASP:O	10:H:87:GLU:HB2	2.18	0.43
15:M:80:PHE:N	15:M:80:PHE:HD1	2.16	0.43
34:f:114:LEU:HD12	34:f:144:LEU:HB3	2.01	0.43
42:n:87:LEU:HD12	42:n:87:LEU:C	2.42	0.43
43:o:29:ASN:OD1	43:o:30:THR:N	2.50	0.43
49:u:14:SER:HA	49:u:55:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:A:H2'	1:1:143:C:C6	2.54	0.43
1:1:414:C:O2	1:1:1864:U:O2'	2.33	0.43
1:1:1276:A:O2'	15:M:16:HIS:NE2	2.44	0.43
1:1:1581:G:C6	1:1:1582:C:C4	3.06	0.43
1:1:1827:U:H2'	1:1:1828:G:O4'	2.19	0.43
1:1:2300:C:O2'	1:1:2301:C:H5'	2.18	0.43
1:1:2496:C:H2'	1:1:2497:A:O4'	2.18	0.43
2:2:1039:G:H2'	2:2:1040:U:H6	1.83	0.43
12:J:1:MET:SD	12:J:67:LYS:NZ	2.81	0.43
34:f:167:ASP:OD1	34:f:168:HIS:N	2.52	0.43
35:g:191:THR:HG21	35:g:196:ILE:HD12	2.01	0.43
40:l:20:ALA:HB3	40:l:22:LYS:HG2	2.01	0.43
44:p:44:LYS:HB3	44:p:45:PRO:HD3	2.01	0.43
44:p:89:0TD:C	44:p:89:0TD:OD1	2.66	0.43
46:r:54:ASP:HA	46:r:59:ARG:HD3	1.99	0.43
54:z:78:C:H2'	54:z:79:C:H5'	2.00	0.43
1:1:1:G:H2'	1:1:2:G:H8	1.84	0.43
1:1:278:A:C6	1:1:362:A:C8	3.07	0.43
1:1:833:A:H2'	1:1:834:G:C8	2.54	0.43
1:1:996:A:OP1	19:Q:10:LYS:HD2	2.19	0.43
1:1:1540:G:C6	1:1:1541:C:C4	3.06	0.43
2:2:109:A:C6	2:2:326:G:C6	3.06	0.43
2:2:463:U:H3'	2:2:464:U:C6	2.53	0.43
2:2:579:A:H2'	2:2:580:C:C6	2.54	0.43
2:2:977:A:O2'	2:2:979:C:OP2	2.35	0.43
2:2:1006:G:C6	2:2:1024:G:C2	3.06	0.43
3:3:2:G:H2'	3:3:3:C:H6	1.84	0.43
7:E:97:ASN:HB2	7:E:100:MET:SD	2.58	0.43
9:G:103:ILE:O	9:G:114:ASP:HA	2.19	0.43
16:N:34:HIS:CG	16:N:53:THR:HG1	2.35	0.43
36:h:118:VAL:HG12	36:h:131:ASN:O	2.18	0.43
37:i:142:ASP:HA	37:i:145:GLU:HG2	2.01	0.43
1:1:1584:U:H4'	1:1:1585:C:H5''	1.99	0.43
1:1:2117:A:N6	1:1:2170:A:H61	2.17	0.43
1:1:2189:U:O2'	1:1:2190:G:H5''	2.18	0.43
1:1:2425:A:H5''	1:1:2427:C:O4'	2.19	0.43
1:1:2545:G:H2'	1:1:2546:U:O4'	2.19	0.43
2:2:203:G:H2'	2:2:204:G:C8	2.54	0.43
2:2:420:U:O2'	2:2:421:U:O2	2.30	0.43
2:2:1145:A:O2'	2:2:1146:A:H5''	2.19	0.43
8:F:175:PHE:HA	8:F:176:PRO:HD3	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:130:VAL:O	10:H:130:VAL:HG23	2.19	0.43
13:K:29:LYS:HG3	13:K:30:THR:HG23	2.00	0.43
34:f:120:GLN:O	34:f:126:PHE:HB2	2.19	0.43
43:o:15:GLN:NE2	43:o:78:GLY:O	2.52	0.43
46:r:46:LEU:O	46:r:50:THR:HG23	2.19	0.43
54:z:86:C:C2'	54:z:87:C:O5'	2.67	0.43
1:1:796:C:OP1	7:E:57:LYS:NZ	2.40	0.42
1:1:1045:C:O2	1:1:1047:G:N1	2.51	0.42
1:1:1047:G:O2'	1:1:1110:G:N1	2.31	0.42
1:1:1565:C:O2'	1:1:1567:G:N7	2.50	0.42
1:1:1817:G:O5'	5:C:156:ARG:NH2	2.52	0.42
1:1:2133:G:N3	1:1:2158:A:N6	2.66	0.42
1:1:2178:C:H2'	1:1:2179:C:H5	1.84	0.42
1:1:2902:C:H2'	1:1:2903:U:H5''	2.01	0.42
2:2:247:G:C6	2:2:278:G:C2	3.07	0.42
2:2:780:A:C2	2:2:801:U:C5	3.06	0.42
2:2:857:C:H2'	2:2:858:G:O4'	2.18	0.42
34:f:122:GLN:CD	34:f:123:ASP:N	2.77	0.42
39:k:60:GLU:O	39:k:64:VAL:HG23	2.18	0.42
54:z:28:C:H2'	54:z:29:A:H8	1.84	0.42
55:B:19:GLY:O	55:B:21:ILE:CD1	2.67	0.42
1:1:886:A:C2'	1:1:887:A:O5'	2.67	0.42
1:1:971:G:H2'	1:1:972:A:O4'	2.19	0.42
1:1:1215:G:H1	1:1:1234:U:H3	1.67	0.42
1:1:2183:A:H2'	1:1:2184:A:C8	2.54	0.42
1:1:2249:U:O2'	1:1:2252:G:OP2	2.24	0.42
1:1:2350:C:H2'	1:1:2351:G:O4'	2.19	0.42
22:T:36:VAL:HG11	22:T:39:ILE:HD12	1.99	0.42
24:V:59:LEU:HD13	24:V:80:ILE:HD12	2.01	0.42
28:Z:56:ARG:O	28:Z:59:ARG:HG2	2.18	0.42
37:i:15:LEU:C	37:i:15:LEU:HD12	2.45	0.42
49:u:75:LEU:C	49:u:75:LEU:HD12	2.43	0.42
54:z:5:A:H2'	54:z:6:G:O4'	2.19	0.42
1:1:553:G:C6	1:1:554:U:C4	3.08	0.42
1:1:1042:G:C4	1:1:1043:C:C5	3.08	0.42
1:1:2134:A:H4'	1:1:2159:G:H21	1.83	0.42
1:1:2450:A:N6	1:1:2501:C:C2	2.86	0.42
2:2:519:C:H2'	2:2:520:A:O4'	2.19	0.42
2:2:539:A:H2'	2:2:540:G:C8	2.55	0.42
2:2:1012:A:C2	2:2:1018:G:C2	3.07	0.42
8:F:61:SER:O	8:F:63:GLN:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:111:GLU:HG2	14:L:112:LEU:N	2.35	0.42
17:O:29:LYS:HB2	17:O:83:SER:OG	2.19	0.42
34:f:27:MET:HE1	34:f:187:VAL:HG11	2.01	0.42
34:f:104:TRP:HE1	34:f:108:ARG:HH21	1.67	0.42
41:m:83:ILE:O	41:m:87:LEU:HD13	2.19	0.42
43:o:86:VAL:HG11	43:o:93:ARG:HE	1.84	0.42
55:B:4:LYS:O	55:B:8:ILE:HG13	2.19	0.42
1:1:475:C:N3	1:1:479:A:N7	2.67	0.42
1:1:887:A:O2'	1:1:889:C:OP2	2.38	0.42
1:1:1153:C:H2'	1:1:1154:G:O4'	2.20	0.42
1:1:1298:C:H2'	1:1:1299:G:O4'	2.19	0.42
1:1:1584:U:C5'	1:1:1585:C:C6	3.03	0.42
2:2:844:G:N3	2:2:844:G:H5''	2.34	0.42
2:2:1463:U:OP1	17:O:109:ARG:NE	2.49	0.42
2:2:1530:G:H2'	2:2:1531:A:C8	2.54	0.42
11:I:114:LEU:O	11:I:118:MET:HG3	2.19	0.42
18:P:80:ILE:O	18:P:84:LYS:HG2	2.19	0.42
34:f:74:ARG:O	34:f:74:ARG:HD3	2.19	0.42
36:h:159:LEU:O	36:h:163:GLU:HG2	2.19	0.42
39:k:5:ARG:NH1	39:k:7:ILE:HA	2.35	0.42
40:l:113:ASP:OD1	40:l:113:ASP:N	2.52	0.42
50:v:14:THR:CG2	50:v:48:ARG:HG3	2.49	0.42
54:z:63:G:C2'	54:z:64:G:O5'	2.67	0.42
1:1:837:C:N3	1:1:941:A:N6	2.66	0.42
1:1:894:U:HO2'	1:1:895:U:P	2.40	0.42
1:1:1883:U:H2'	1:1:1884:G:O4'	2.19	0.42
1:1:1922:G:C2'	1:1:1923:U:H5'	2.50	0.42
2:2:212:G:C2	2:2:213:G:C8	3.08	0.42
2:2:413:G:H22	2:2:429:U:P	2.42	0.42
3:3:48:U:OP1	16:N:30:ARG:NH2	2.47	0.42
13:K:20:GLY:HA2	13:K:28:GLY:O	2.19	0.42
15:M:118:ARG:O	15:M:118:ARG:HG2	2.20	0.42
25:W:72:ARG:NH1	25:W:78:TYR:OH	2.44	0.42
26:X:3:ALA:O	26:X:7:ARG:HG3	2.20	0.42
54:z:9:G:HO2'	54:z:10:U:P	2.41	0.42
1:1:279:A:C6	1:1:362:A:H5'	2.54	0.42
1:1:571:U:C4	1:1:2030:6MZ:H9	2.54	0.42
1:1:964:C:O2	1:1:2273:A:H2	2.01	0.42
1:1:1629:U:C4	1:1:1630:A:N7	2.87	0.42
1:1:2081:U:H2'	1:1:2082:A:H8	1.85	0.42
1:1:2311:A:O2'	1:1:2312:U:O4'	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:269:C:H2'	2:2:270:A:C8	2.54	0.42
2:2:844:G:N1	2:2:846:G:H1'	2.35	0.42
2:2:999:C:H2'	2:2:1000:A:C8	2.54	0.42
8:F:37:ASN:OD1	8:F:38:MET:N	2.53	0.42
13:K:92:LEU:O	13:K:96:LYS:HG3	2.20	0.42
34:f:130:THR:CG2	34:f:133:GLU:HB3	2.49	0.42
35:g:11:ARG:NH2	35:g:177:THR:O	2.49	0.42
36:h:129:VAL:HB	36:h:146:ARG:NH2	2.34	0.42
39:k:66:LEU:O	39:k:70:ARG:HG3	2.20	0.42
49:u:25:ILE:HD11	49:u:61:ILE:HD11	2.00	0.42
1:1:125:A:C5	31:c:10:LEU:HD13	2.54	0.42
1:1:653:U:H3'	1:1:654:A:C8	2.54	0.42
1:1:894:U:O2'	1:1:895:U:H6	2.02	0.42
1:1:930:G:H1'	27:Y:25:LEU:HD21	2.02	0.42
1:1:1506:U:H2'	1:1:1507:C:C6	2.54	0.42
1:1:2236:U:H2'	1:1:2237:G:O4'	2.19	0.42
1:1:2751:G:H5'	1:1:2752:C:C5	2.54	0.42
2:2:1006:G:N1	2:2:1023:U:C2	2.87	0.42
2:2:1158:C:N3	2:2:1160:G:C8	2.88	0.42
2:2:1315:U:H2'	2:2:1316:G:O4'	2.20	0.42
8:F:123:ASP:OD2	8:F:127:ASN:HB2	2.19	0.42
8:F:136:ILE:O	8:F:136:ILE:HG22	2.20	0.42
10:H:47:PHE:HA	10:H:51:ARG:HB2	2.01	0.42
10:H:78:VAL:O	10:H:78:VAL:HG13	2.19	0.42
24:V:18:ALA:O	24:V:20:ARG:NH1	2.42	0.42
27:Y:40:ASP:OD1	27:Y:45:ARG:NE	2.45	0.42
34:f:69:PHE:HB3	34:f:80:VAL:CG2	2.49	0.42
34:f:119:THR:O	34:f:124:GLY:CA	2.67	0.42
38:j:33:GLU:O	38:j:33:GLU:CD	2.63	0.42
38:j:72:ASP:OD1	38:j:72:ASP:C	2.63	0.42
43:o:89:PRO:HB3	53:y:29:LEU:HD23	2.01	0.42
49:u:58:VAL:CG1	49:u:79:VAL:HG23	2.49	0.42
53:y:28:VAL:CG2	53:y:29:LEU:N	2.83	0.42
1:1:373:U:H2'	1:1:374:A:H8	1.84	0.42
1:1:1062:G:C6	1:1:1077:A:N6	2.88	0.42
1:1:1856:U:H2'	1:1:1857:G:O4'	2.20	0.42
1:1:2698:U:H2'	1:1:2699:C:C6	2.55	0.42
2:2:978:A:C4	2:2:1319:A:C2	3.07	0.42
2:2:1004:A:C6	2:2:1026:G:C8	3.07	0.42
2:2:1060:U:OP1	46:r:85:ARG:NH1	2.50	0.42
5:C:80:ARG:NH1	5:C:82:GLU:OE2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:170:ARG:HB2	9:G:170:ARG:NH2	2.35	0.42
14:L:47:GLU:OE1	14:L:51:ARG:CZ	2.67	0.42
22:T:48:PRO:HG3	22:T:55:PRO:O	2.20	0.42
24:V:20:ARG:O	24:V:39:ARG:NH1	2.53	0.42
43:o:19:GLY:O	43:o:82:LEU:HD12	2.20	0.42
49:u:57:ASP:OD1	49:u:80:GLU:O	2.38	0.42
54:z:42:G:C2'	54:z:43:U:H5'	2.49	0.42
54:z:66:5MU:H2'	54:z:67:U:O4'	2.19	0.42
1:1:322:A:H2	1:1:339:U:O4	2.02	0.42
1:1:781:A:P	5:C:217:ARG:HH22	2.43	0.42
1:1:877:A:O2'	1:1:900:A:N6	2.52	0.42
1:1:1062:G:N1	1:1:1063:G:C6	2.88	0.42
1:1:1084:A:N3	1:1:1105:U:O2'	2.50	0.42
1:1:2250:G:H5'	1:1:2250:G:N3	2.34	0.42
2:2:701:U:O2	2:2:703:G:N1	2.53	0.42
2:2:999:C:C2	2:2:1042:A:N1	2.87	0.42
5:C:91:ILE:HD12	5:C:103:TYR:CD1	2.55	0.42
6:D:32:ASN:HD22	6:D:52:THR:HB	1.85	0.42
7:E:78:TRP:N	7:E:78:TRP:CD1	2.86	0.42
11:I:139:VAL:HG12	11:I:140:LEU:N	2.34	0.42
15:M:114:GLU:OE1	15:M:118:ARG:NE	2.52	0.42
18:P:35:ALA:O	18:P:39:VAL:HG23	2.20	0.42
34:f:123:ASP:O	34:f:125:THR:HG23	2.20	0.42
37:i:90:THR:O	37:i:90:THR:HG22	2.20	0.42
41:m:35:LEU:HD21	41:m:48:VAL:CG2	2.50	0.42
45:q:52:GLN:O	45:q:56:LEU:HG	2.20	0.42
54:z:66:5MU:O4	54:z:70:U:H5	2.03	0.42
55:B:1:FME:CG	55:B:4:LYS:HG3	2.50	0.42
1:1:161:A:OP2	1:1:162:U:O2'	2.32	0.42
1:1:560:C:H2'	1:1:561:G:O4'	2.20	0.42
1:1:1009:A:N3	1:1:1153:C:O2'	2.51	0.42
1:1:2144:G:H1'	1:1:2147:A:N6	2.35	0.42
1:1:2394:C:H5''	13:K:63:LYS:HE2	2.01	0.42
2:2:714:G:H2'	2:2:715:A:C8	2.55	0.42
2:2:1005:A:OP2	2:2:1024:G:N2	2.52	0.42
2:2:1029:U:O2	2:2:1033:G:C6	2.73	0.42
8:F:36:LEU:HD12	8:F:36:LEU:N	2.35	0.42
10:H:88:GLY:C	10:H:90:LEU:H	2.28	0.42
15:M:59:SER:O	15:M:63:ARG:HG2	2.19	0.42
21:S:61:LEU:C	21:S:61:LEU:HD12	2.45	0.42
36:h:47:ARG:HG2	36:h:47:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:o:53:ARG:HD2	43:o:53:ARG:HA	1.91	0.42
51:w:3:ARG:NH1	51:w:10:PHE:HB2	2.35	0.42
1:1:1186:G:H2'	1:1:1187:G:O4'	2.20	0.41
1:1:1682:G:OP2	1:1:1699:G:N2	2.51	0.41
1:1:2164:C:OP2	1:1:2170:A:N7	2.53	0.41
1:1:2322:A:H2'	1:1:2323:G:O4'	2.20	0.41
1:1:2556:C:H2'	1:1:2557:G:O4'	2.20	0.41
1:1:2756:U:OP2	33:e:19:ARG:NE	2.46	0.41
2:2:90:C:H2'	2:2:91:U:C6	2.54	0.41
2:2:335:C:O2	2:2:1433:A:H2	2.03	0.41
2:2:1308:U:H2'	2:2:1309:G:H8	1.85	0.41
2:2:1417:G:C6	2:2:1482:G:C6	3.08	0.41
10:H:53:GLU:O	10:H:57:LYS:HD3	2.19	0.41
21:S:31:VAL:HG22	21:S:84:TYR:CD1	2.55	0.41
34:f:97:LEU:H	34:f:100:MET:HE3	1.85	0.41
39:k:140:ASP:OD1	39:k:143:ARG:NH1	2.53	0.41
42:n:39:PRO:HA	42:n:74:VAL:HG22	2.02	0.41
53:y:36:GLU:HG3	53:y:37:PHE:CD2	2.55	0.41
2:2:381:C:H2'	2:2:382:A:O4'	2.21	0.41
2:2:465:A:H2'	2:2:466:A:C8	2.55	0.41
2:2:620:C:H2'	2:2:621:A:O4'	2.20	0.41
6:D:64:GLU:HG2	6:D:68:PHE:CE2	2.56	0.41
6:D:64:GLU:HG2	6:D:68:PHE:HE2	1.84	0.41
8:F:5:HIS:NE2	8:F:9:LYS:HD2	2.35	0.41
10:H:3:VAL:HG23	10:H:37:VAL:O	2.20	0.41
17:O:33:VAL:HG22	17:O:38:LYS:HG2	2.02	0.41
21:S:4:GLU:O	21:S:8:LEU:HG	2.21	0.41
35:g:8:ASN:O	35:g:12:LEU:HG	2.20	0.41
35:g:140:ASN:OD1	35:g:143:ARG:NH2	2.50	0.41
43:o:47:ALA:HB1	43:o:62:ALA:HB1	2.01	0.41
44:p:108:LYS:O	44:p:109:ASP:CG	2.63	0.41
54:z:62:G:C2'	54:z:63:G:H5'	2.51	0.41
55:B:20:PHE:HD2	55:B:22:THR:H	1.68	0.41
1:1:2:G:H2'	1:1:3:U:C6	2.55	0.41
1:1:306:U:H2'	1:1:307:G:O4'	2.20	0.41
1:1:362:A:C6	1:1:363:G:C5	3.08	0.41
1:1:1955:U:C5	1:1:2552:OMU:H1'	2.55	0.41
1:1:1963:U:O5'	1:1:1963:U:H6	2.03	0.41
1:1:1996:C:H5	12:J:32:TYR:OH	2.02	0.41
2:2:1522:U:H5''	43:o:128:ARG:NH2	2.36	0.41
3:3:66:A:O5'	3:3:108:A:N6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:90:ASN:O	12:J:92:GLU:CD	2.63	0.41
15:M:63:ARG:HD3	15:M:80:PHE:CD2	2.55	0.41
20:R:46:LEU:O	20:R:50:VAL:HG23	2.20	0.41
37:i:142:ASP:O	37:i:145:GLU:HG2	2.20	0.41
43:o:13:ARG:NH1	43:o:77:TYR:HE1	2.18	0.41
45:q:29:ARG:O	45:q:33:ILE:HG12	2.20	0.41
54:z:14:A:H3'	54:z:15:G:C5'	2.47	0.41
1:1:481:G:O2'	1:1:507:A:N1	2.53	0.41
1:1:1376:C:H2'	1:1:1377:G:O4'	2.20	0.41
1:1:1445:G:C6	1:1:1446:C:C4	3.09	0.41
1:1:1870:C:O2'	1:1:1871:A:C1'	2.68	0.41
1:1:2148:G:H2'	1:1:2149:U:C5	2.55	0.41
1:1:2508:G:O6	1:1:2580:PSU:O2	2.37	0.41
1:1:2902:C:H2'	1:1:2903:U:C4'	2.51	0.41
2:2:41:G:H2'	2:2:42:G:H8	1.86	0.41
2:2:181:A:N6	2:2:195:A:C8	2.88	0.41
2:2:213:G:N7	2:2:214:C:C5	2.88	0.41
2:2:477:C:H2'	2:2:478:A:C8	2.56	0.41
2:2:1174:G:O2'	2:2:1175:G:H5'	2.21	0.41
8:F:108:VAL:HB	8:F:109:PRO:HD3	2.01	0.41
12:J:109:SER:O	12:J:113:MET:CG	2.69	0.41
14:L:53:MET:O	14:L:57:VAL:HG22	2.20	0.41
38:j:40:GLU:OE2	38:j:99:ALA:HA	2.20	0.41
41:m:52:LEU:HD22	41:m:57:MET:HB2	2.02	0.41
43:o:35:THR:OG1	43:o:40:ASN:N	2.53	0.41
51:w:47:LEU:O	51:w:62:VAL:HG23	2.20	0.41
1:1:1197:G:H2'	1:1:1198:U:H6	1.85	0.41
1:1:2100:G:C2	1:1:2101:A:N7	2.88	0.41
2:2:1120:C:H2'	2:2:1121:U:C6	2.56	0.41
7:E:171:ASP:OD1	7:E:172:ALA:N	2.51	0.41
8:F:7:TYR:O	8:F:10:ASP:OD1	2.38	0.41
9:G:73:ASN:O	9:G:77:ILE:HG12	2.21	0.41
19:Q:37:GLU:OE1	19:Q:37:GLU:O	2.37	0.41
34:f:129:LEU:HD23	34:f:129:LEU:H	1.86	0.41
35:g:132:ARG:HD3	35:g:136:ARG:HH21	1.85	0.41
36:h:150:LYS:HG3	36:h:178:MET:SD	2.60	0.41
37:i:11:LEU:CD2	37:i:71:MET:HE1	2.49	0.41
1:1:356:G:C5	1:1:357:C:C4	3.09	0.41
1:1:558:U:H2'	1:1:559:G:C8	2.56	0.41
1:1:645:C:H2'	1:1:647:G:N7	2.35	0.41
1:1:807:U:OP2	13:K:41:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:889:C:H2'	1:1:890:C:O4'	2.21	0.41
1:1:1174:U:P	1:1:1175:A:N1	2.94	0.41
1:1:1538:G:H2'	1:1:1539:U:C6	2.55	0.41
1:1:2102:G:C6	1:1:2188:U:C4	3.08	0.41
2:2:1217:C:P	46:r:9:ARG:HH21	2.43	0.41
2:2:1305:G:HO2'	2:2:1306:A:H8	1.62	0.41
5:C:143:ASN:OD1	5:C:152:GLY:HA3	2.20	0.41
10:H:110:VAL:HG22	10:H:111:ALA:N	2.35	0.41
10:H:117:LEU:HD23	10:H:122:LEU:HD21	2.01	0.41
15:M:87:PHE:HD1	15:M:90:ARG:HD3	1.85	0.41
20:R:81:SER:HB3	20:R:97:LEU:HD12	2.01	0.41
23:U:56:PHE:CE1	23:U:61:LEU:HD21	2.56	0.41
29:a:3:VAL:HG22	29:a:4:GLN:N	2.36	0.41
34:f:15:HIS:HB3	34:f:43:LEU:HD11	2.03	0.41
36:h:113:GLU:OE2	36:h:154:ARG:HD2	2.21	0.41
39:k:113:ASP:C	39:k:119:ARG:HD2	2.46	0.41
47:s:53:ARG:O	47:s:57:LEU:HG	2.20	0.41
1:1:545:U:HO2'	1:1:547:A:P	2.43	0.41
1:1:711:G:H2'	1:1:712:G:O4'	2.21	0.41
1:1:883:G:N2	1:1:884:U:C4	2.89	0.41
1:1:891:G:C6	1:1:892:A:N7	2.88	0.41
1:1:995:C:O2	11:I:3:THR:OG1	2.27	0.41
1:1:1130:U:O4	6:D:151:THR:O	2.39	0.41
1:1:1841:U:C4	1:1:1842:G:N7	2.89	0.41
1:1:2766:A:N3	1:1:2766:A:H2'	2.36	0.41
1:1:2880:C:O3'	15:M:90:ARG:NH2	2.54	0.41
2:2:61:G:N7	52:x:6:SER:OG	2.45	0.41
2:2:1010:U:C2	2:2:1020:G:N3	2.88	0.41
2:2:1027:C:C5	2:2:1034:G:N1	2.89	0.41
2:2:1028:C:O2	2:2:1034:G:C2	2.74	0.41
5:C:145:GLU:HB2	5:C:188:CYS:HB3	2.02	0.41
16:N:100:HIS:CD2	16:N:101:GLY:N	2.88	0.41
19:Q:6:GLN:HB2	19:Q:37:GLU:OE2	2.19	0.41
34:f:113:ARG:HA	34:f:116:ASP:OD2	2.20	0.41
41:m:92:GLU:HG3	41:m:92:GLU:O	2.21	0.41
54:z:44:G:H2'	54:z:45:U:O4'	2.21	0.41
54:z:50:G:C6	54:z:56:G:C6	3.09	0.41
54:z:65:G:O2'	54:z:66:5MU:H5''	2.20	0.41
1:1:1064:C:O2'	1:1:1065:U:O5'	2.36	0.41
1:1:1067:A:C3'	1:1:1068:G:H5''	2.51	0.41
1:1:1407:G:H3'	1:1:1408:G:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:204:G:C5	2:2:465:A:C6	3.08	0.41
2:2:205:A:H2'	2:2:206:C:C6	2.56	0.41
2:2:1305:G:O2'	2:2:1306:A:H8	2.03	0.41
8:F:110:ARG:O	45:q:3:ARG:NH2	2.53	0.41
8:F:122:PHE:HB2	8:F:163:ASP:OD2	2.21	0.41
8:F:144:ASP:OD1	8:F:145:LYS:HG2	2.21	0.41
8:F:167:ARG:HG3	8:F:177:PHE:CE2	2.55	0.41
10:H:88:GLY:O	10:H:90:LEU:N	2.53	0.41
19:Q:58:VAL:CG1	19:Q:102:SER:HB3	2.50	0.41
34:f:27:MET:HE1	34:f:193:PRO:HB3	2.03	0.41
34:f:27:MET:HE2	34:f:193:PRO:HD3	2.01	0.41
34:f:28:LYS:N	34:f:29:PRO:CD	2.84	0.41
34:f:79:ALA:O	34:f:82:ASP:OD1	2.38	0.41
34:f:113:ARG:CZ	34:f:117:LEU:HD21	2.51	0.41
54:z:47:U:H2'	54:z:48:A:C8	2.56	0.41
55:B:20:PHE:O	55:B:21:ILE:HD13	2.20	0.41
1:1:11:C:H6	1:1:11:C:O5'	2.04	0.41
1:1:510:C:H2'	1:1:511:U:H5'	2.02	0.41
1:1:878:A:C8	1:1:879:G:C8	3.09	0.41
1:1:885:C:H2'	1:1:886:A:H8	1.84	0.41
1:1:1064:C:HO2'	1:1:1065:U:P	2.43	0.41
1:1:1248:G:OP1	7:E:44:ARG:NH2	2.35	0.41
1:1:1432:G:H2'	1:1:1433:A:C8	2.56	0.41
1:1:1534:U:H3'	1:1:1536:C:N4	2.35	0.41
1:1:1870:C:O2'	1:1:1871:A:C8	2.74	0.41
1:1:2031:A:C6	1:1:2498:OMC:HI'	2.55	0.41
1:1:2133:G:N3	1:1:2158:A:C6	2.89	0.41
1:1:2140:G:C5'	1:1:2140:G:H8	2.34	0.41
1:1:2225:A:H4'	1:1:2226:C:C6	2.55	0.41
1:1:2286:G:H4'	1:1:2287:A:O4'	2.21	0.41
1:1:2314:A:O4'	8:F:155:THR:HG21	2.21	0.41
1:1:2639:A:H2'	1:1:2640:G:O4'	2.21	0.41
1:1:2798:U:H4'	1:1:2799:A:H5'	2.01	0.41
2:2:451:A:H61	2:2:481:G:H5'	1.85	0.41
2:2:458:U:H3	2:2:474:G:H1	1.68	0.41
2:2:768:A:N3	2:2:1512:U:O2'	2.50	0.41
2:2:1244:G:C6	2:2:1294:G:C6	3.09	0.41
2:2:1309:G:P	45:q:87:ARG:HH11	2.40	0.41
2:2:1425:U:H2'	2:2:1426:G:H8	1.85	0.41
5:C:240:PHE:CD2	5:C:240:PHE:O	2.74	0.41
10:H:50:ARG:HE	10:H:51:ARG:NH2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:90:LEU:HD11	10:H:123:ARG:HA	2.03	0.41
18:P:26:GLY:O	18:P:30:ARG:NH1	2.47	0.41
19:Q:52:PRO:CD	19:Q:53:PHE:N	2.80	0.41
25:W:43:GLU:OE1	25:W:45:ARG:NE	2.54	0.41
32:d:55:LEU:O	32:d:58:VAL:HG22	2.21	0.41
34:f:128:LYS:HE3	34:f:128:LYS:HB3	1.88	0.41
34:f:207:ILE:HA	34:f:210:VAL:HG22	2.03	0.41
37:i:82:GLN:OE1	37:i:149:SER:HA	2.21	0.41
38:j:3:HIS:ND1	38:j:94:HIS:C	2.79	0.41
42:n:73:LEU:C	42:n:73:LEU:HD23	2.46	0.41
49:u:29:VAL:HG22	49:u:30:LYS:N	2.36	0.41
52:x:78:ASN:O	52:x:82:GLN:HG2	2.21	0.41
54:z:40:G:H2'	54:z:41:U:H5'	2.03	0.41
55:B:14:ALA:C	55:B:16:LYS:N	2.75	0.41
1:1:243:U:OP2	32:d:8:ARG:NH1	2.54	0.41
1:1:635:C:O2'	1:1:639:U:OP1	2.38	0.41
1:1:2025:C:H2'	1:1:2026:U:C6	2.56	0.41
1:1:2811:G:H2'	1:1:2812:G:O4'	2.21	0.41
2:2:275:G:H5'	49:u:16:LYS:HD2	2.01	0.41
2:2:439:U:O2	2:2:439:U:O4'	2.39	0.41
2:2:933:G:OP2	39:k:3:ARG:HB2	2.21	0.41
2:2:1010:U:H2'	2:2:1011:C:C6	2.56	0.41
2:2:1064:G:O2'	2:2:1190:G:N2	2.54	0.41
7:E:108:ILE:HG21	7:E:108:ILE:HD13	1.78	0.41
10:H:12:LEU:HD23	10:H:12:LEU:N	2.36	0.41
24:V:41:ARG:NE	24:V:41:ARG:HA	2.36	0.41
35:g:122:SER:O	35:g:126:ARG:HG2	2.21	0.41
36:h:47:ARG:HA	36:h:47:ARG:CZ	2.51	0.41
36:h:106:GLY:HA3	36:h:162:ALA:HB2	2.03	0.41
41:m:88:MET:CE	41:m:104:VAL:HG12	2.51	0.41
55:B:5:MET:O	55:B:8:ILE:HB	2.21	0.41
1:1:1417:C:H2'	1:1:1418:G:O4'	2.20	0.40
2:2:41:G:H2'	2:2:42:G:C8	2.56	0.40
2:2:246:A:C2	2:2:282:A:C5	3.09	0.40
2:2:390:U:H2'	2:2:391:G:H8	1.86	0.40
2:2:1008:U:O2	2:2:1009:U:C2	2.74	0.40
2:2:1021:A:N1	2:2:1022:A:C5	2.89	0.40
2:2:1120:C:H2'	2:2:1121:U:H6	1.86	0.40
11:I:19:ASP:OD1	11:I:58:ASN:ND2	2.37	0.40
12:J:7:MET:SD	12:J:20:MET:HB2	2.61	0.40
18:P:36:PHE:O	18:P:40:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:146:ARG:HG2	36:h:147:GLU:N	2.35	0.40
40:l:35:ALA:O	40:l:39:VAL:HG23	2.22	0.40
1:1:143:C:O2	1:1:143:C:H2'	2.21	0.40
1:1:898:C:H2'	1:1:899:A:O4'	2.21	0.40
1:1:955:PSU:HN3	1:1:962:G:H1	1.68	0.40
1:1:1021:A:N3	1:1:1021:A:H3'	2.37	0.40
1:1:1835:2MG:O6	1:1:1969:A:H5''	2.21	0.40
1:1:2127:G:H21	1:1:2173:A:H1'	1.86	0.40
1:1:2271:G:H5''	24:V:18:ALA:CB	2.51	0.40
2:2:456:A:C6	2:2:457:G:C5	3.09	0.40
2:2:640:A:O2'	40:l:108:LYS:HE3	2.21	0.40
9:G:10:VAL:CA	9:G:49:THR:HG22	2.50	0.40
17:O:63:LYS:HE2	17:O:65:SER:OG	2.21	0.40
29:a:33:THR:OG1	29:a:51:GLY:HA2	2.20	0.40
31:c:8:SER:OG	31:c:11:LYS:HB3	2.21	0.40
34:f:218:ALA:HA	34:f:221:VAL:CG2	2.51	0.40
41:m:21:ILE:HD13	41:m:63:LEU:HG	2.02	0.40
42:n:59:LYS:HE2	42:n:62:ARG:NH2	2.37	0.40
49:u:7:THR:C	49:u:8:LEU:HD12	2.46	0.40
1:1:136:G:C6	1:1:137:U:C4	3.09	0.40
1:1:308:G:H2'	1:1:309:A:C8	2.57	0.40
1:1:1069:A:H4'	1:1:1070:A:H5''	2.04	0.40
1:1:2116:G:H3'	1:1:2117:A:C4	2.56	0.40
1:1:2140:G:C8	1:1:2140:G:H3'	2.56	0.40
1:1:2190:G:H2'	1:1:2191:A:C8	2.56	0.40
1:1:2314:A:H1'	8:F:155:THR:HG21	2.03	0.40
1:1:2902:C:C2'	1:1:2903:U:H5''	2.51	0.40
2:2:439:U:O2	36:h:120:HIS:CD2	2.74	0.40
2:2:444:G:C6	2:2:491:G:C6	3.10	0.40
2:2:1180:A:P	41:m:99:ARG:HH12	2.44	0.40
9:G:127:THR:HG22	9:G:128:GLN:N	2.37	0.40
11:I:92:MET:HE2	11:I:92:MET:HB3	2.00	0.40
11:I:118:MET:HA	11:I:121:LYS:HE2	2.02	0.40
33:e:4:ARG:O	33:e:37:GLN:HA	2.21	0.40
34:f:129:LEU:HD21	34:f:134:ALA:CB	2.48	0.40
35:g:21:THR:O	35:g:58:GLU:HG3	2.22	0.40
36:h:156:LYS:O	36:h:160:GLU:HG2	2.20	0.40
42:n:10:LEU:HG	42:n:98:VAL:HG12	2.02	0.40
1:1:104:A:C5	1:1:105:C:C5	3.10	0.40
1:1:591:U:O2	32:d:2:PRO:N	2.54	0.40
1:1:634:C:O5'	1:1:634:C:H6	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1416:G:C6	1:1:1583:A:N1	2.89	0.40
1:1:1607:C:H4'	1:1:1608:A:H5'	2.04	0.40
1:1:1671:U:O2'	1:1:1673:G:N7	2.48	0.40
1:1:1720:U:H2'	1:1:1721:G:O4'	2.21	0.40
1:1:2107:G:C8	1:1:2107:G:C4'	3.05	0.40
1:1:2570:G:H2'	1:1:2571:U:O4'	2.21	0.40
2:2:1004:A:C6	2:2:1005:A:C2	3.09	0.40
2:2:1004:A:N1	2:2:1026:G:C4	2.90	0.40
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.97	0.40
7:E:28:VAL:O	7:E:32:VAL:HG23	2.21	0.40
8:F:7:TYR:CE1	8:F:11:GLU:OE1	2.75	0.40
10:H:103:VAL:CG1	10:H:110:VAL:HG12	2.51	0.40
13:K:86:GLU:OE1	13:K:86:GLU:N	2.55	0.40
28:Z:60:PHE:CD2	51:w:67:VAL:HG12	2.57	0.40
37:i:46:VAL:HG22	37:i:118:ALA:HA	2.03	0.40
1:1:45:G:H5''	1:1:46:G:H5'	2.03	0.40
1:1:1256:G:H21	7:E:77:ILE:CG2	2.34	0.40
1:1:1365:A:OP1	25:W:3:ARG:NH2	2.42	0.40
1:1:1445:G:C5	1:1:1446:C:C5	3.09	0.40
1:1:2585:U:C5	55:B:25:ASP:O	2.75	0.40
2:2:721:G:H4'	2:2:722:G:O4'	2.21	0.40
2:2:1175:G:O2'	2:2:1176:A:H8	2.05	0.40
3:3:75:G:H2'	3:3:76:G:O4'	2.22	0.40
5:C:51:THR:HG23	5:C:54:ILE:HD12	2.03	0.40
8:F:49:LEU:O	8:F:150:ARG:NH2	2.54	0.40
8:F:78:LYS:HD2	8:F:78:LYS:C	2.46	0.40
9:G:102:VAL:HG12	9:G:103:ILE:N	2.35	0.40
10:H:127:GLU:HA	10:H:145:ASN:HA	2.03	0.40
14:L:126:ILE:HD13	14:L:126:ILE:HG21	1.79	0.40
34:f:70:VAL:HG21	34:f:161:LEU:HD11	2.04	0.40
34:f:124:GLY:O	34:f:125:THR:OG1	2.35	0.40
39:k:17:LYS:HG2	39:k:18:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	269/271 (99%)	256 (95%)	13 (5%)	0	100	100
6	D	207/209 (99%)	200 (97%)	4 (2%)	3 (1%)	9	36
7	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
8	F	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	21	56
9	G	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
10	H	147/149 (99%)	137 (93%)	8 (5%)	2 (1%)	9	36
11	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
12	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
13	K	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	L	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
15	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
16	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
17	O	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
18	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
19	Q	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	6	28
20	R	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
21	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	T	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
23	U	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
24	V	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
25	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
26	X	60/62 (97%)	60 (100%)	0	0	100	100
27	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
28	Z	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
29	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	b	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
31	c	44/46 (96%)	44 (100%)	0	0	100	100
32	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
33	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	f	223/225 (99%)	209 (94%)	14 (6%)	0	100	100
35	g	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
36	h	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
37	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
38	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	k	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
40	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
41	m	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
42	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
43	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
44	p	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
45	q	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
46	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
47	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
48	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
49	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
50	v	64/66 (97%)	64 (100%)	0	0	100	100
51	w	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
52	x	84/86 (98%)	84 (100%)	0	0	100	100
53	y	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	B	25/27 (93%)	19 (76%)	5 (20%)	1 (4%)	2	14
All	All	5637/5738 (98%)	5420 (96%)	208 (4%)	9 (0%)	44	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	152	PRO
6	D	153	GLY
6	D	154	LYS
10	H	90	LEU
19	Q	52	PRO
19	Q	53	PHE
10	H	89	LYS
8	F	124	GLY
55	B	23	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	216/216 (100%)	216 (100%)	0	100	100
6	D	164/164 (100%)	163 (99%)	1 (1%)	78	88
7	E	165/165 (100%)	165 (100%)	0	100	100
8	F	148/148 (100%)	148 (100%)	0	100	100
9	G	136/136 (100%)	136 (100%)	0	100	100
10	H	114/114 (100%)	113 (99%)	1 (1%)	70	85
11	I	116/116 (100%)	116 (100%)	0	100	100
12	J	104/104 (100%)	104 (100%)	0	100	100
13	K	103/103 (100%)	103 (100%)	0	100	100
14	L	109/109 (100%)	109 (100%)	0	100	100
15	M	99/99 (100%)	99 (100%)	0	100	100
16	N	86/86 (100%)	86 (100%)	0	100	100
17	O	99/99 (100%)	99 (100%)	0	100	100
18	P	89/89 (100%)	89 (100%)	0	100	100
19	Q	84/84 (100%)	84 (100%)	0	100	100
20	R	93/93 (100%)	93 (100%)	0	100	100
21	S	81/81 (100%)	80 (99%)	1 (1%)	63	82
22	T	84/84 (100%)	84 (100%)	0	100	100
23	U	78/78 (100%)	78 (100%)	0	100	100
24	V	59/59 (100%)	58 (98%)	1 (2%)	53	78
25	W	67/67 (100%)	67 (100%)	0	100	100
26	X	54/54 (100%)	54 (100%)	0	100	100
27	Y	48/48 (100%)	48 (100%)	0	100	100
28	Z	59/59 (100%)	59 (100%)	0	100	100
29	a	47/47 (100%)	47 (100%)	0	100	100
30	b	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	c	38/38 (100%)	38 (100%)	0	100	100
32	d	51/51 (100%)	50 (98%)	1 (2%)	48	76
33	e	34/34 (100%)	34 (100%)	0	100	100
34	f	187/187 (100%)	187 (100%)	0	100	100
35	g	171/171 (100%)	171 (100%)	0	100	100
36	h	172/172 (100%)	172 (100%)	0	100	100
37	i	119/119 (100%)	119 (100%)	0	100	100
38	j	91/91 (100%)	90 (99%)	1 (1%)	65	83
39	k	124/124 (100%)	124 (100%)	0	100	100
40	l	104/104 (100%)	104 (100%)	0	100	100
41	m	105/105 (100%)	105 (100%)	0	100	100
42	n	86/86 (100%)	85 (99%)	1 (1%)	63	82
43	o	90/90 (100%)	90 (100%)	0	100	100
44	p	102/102 (100%)	102 (100%)	0	100	100
45	q	94/94 (100%)	94 (100%)	0	100	100
46	r	83/83 (100%)	83 (100%)	0	100	100
47	s	76/76 (100%)	76 (100%)	0	100	100
48	t	65/65 (100%)	65 (100%)	0	100	100
49	u	74/74 (100%)	74 (100%)	0	100	100
50	v	57/57 (100%)	57 (100%)	0	100	100
51	w	72/72 (100%)	72 (100%)	0	100	100
52	x	65/65 (100%)	64 (98%)	1 (2%)	57	80
53	y	60/60 (100%)	60 (100%)	0	100	100
55	B	20/20 (100%)	18 (90%)	2 (10%)	7	29
All	All	4689/4689 (100%)	4679 (100%)	10 (0%)	85	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	151	THR
10	H	122	LEU
21	S	72	GLN
24	V	10	THR
32	d	31	HIS

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Mol	Chain	Res	Type
38	j	72	ASP
42	n	87	LEU
52	x	57	ILE
55	B	9	VAL
55	B	12	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	70	ASN
5	C	226	ASN
7	E	90	GLN
7	E	136	GLN
9	G	48	ASN
10	H	33	GLN
13	K	54	GLN
14	L	60	GLN
15	M	9	GLN
15	M	18	GLN
16	N	98	GLN
16	N	116	GLN
18	P	71	GLN
19	Q	12	HIS
21	S	70	HIS
21	S	72	GLN
22	T	54	GLN
25	W	36	HIS
26	X	45	GLN
32	d	31	HIS
37	i	12	GLN
37	i	121	HIS
38	j	94	HIS
41	m	75	GLN
42	n	58	ASN
43	o	81	ASN
46	r	71	HIS
47	s	40	GLN
52	x	20	HIS
52	x	61	GLN
52	x	82	GLN
53	y	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	500 (17%)	14 (0%)
2	2	1532/1534 (99%)	250 (16%)	4 (0%)
3	3	119/120 (99%)	15 (12%)	0
4	4	5/6 (83%)	0	0
54	z	87/88 (98%)	31 (35%)	0
All	All	4645/4651 (99%)	796 (17%)	18 (0%)

All (796) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A

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Mol	Chain	Res	Type
1	1	248	G
1	1	249	C
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	399	U
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C

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Mol	Chain	Res	Type
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	609	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	702	U
1	1	717	C
1	1	726	G
1	1	730	A
1	1	747	5MU
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A

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Mol	Chain	Res	Type
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	898	C
1	1	907	G
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G

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Mol	Chain	Res	Type
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U

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Mol	Chain	Res	Type
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1411	U
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U

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Mol	Chain	Res	Type
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1618	6MZ
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G

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Mol	Chain	Res	Type
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1862	G
1	1	1865	U
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U

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Mol	Chain	Res	Type
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2104	C
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2143	C

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Mol	Chain	Res	Type
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2168	G
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U

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Mol	Chain	Res	Type
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G

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Mol	Chain	Res	Type
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A

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Mol	Chain	Res	Type
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
1	1	2903	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A

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Mol	Chain	Res	Type
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U

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Mol	Chain	Res	Type
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G

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Mol	Chain	Res	Type
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	884	U
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U

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Mol	Chain	Res	Type
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1009	U
2	2	1019	A
2	2	1020	G
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1104	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1175	G

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Mol	Chain	Res	Type
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1335	U
2	2	1336	C
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1446	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U

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Mol	Chain	Res	Type
2	2	1517	G
2	2	1519	MA6
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	24	G
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
54	z	2	G
54	z	8	U
54	z	10	U
54	z	13	G
54	z	14	A
54	z	15	G
54	z	17	OMG
54	z	18	G
54	z	19	C
54	z	20	U
54	z	21	G
54	z	22	A
54	z	23	A
54	z	24	G
54	z	40	G
54	z	45	U
54	z	46	A
54	z	51	G
54	z	52	C
54	z	53	A
54	z	54	A
54	z	55	C

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Mol	Chain	Res	Type
54	z	56	G
54	z	60	C
54	z	61	G
54	z	67	U
54	z	76	C
54	z	79	C
54	z	85	G
54	z	86	C
54	z	88	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	887	A
1	1	891	G
1	1	894	U
1	1	1175	A
1	1	1379	U
1	1	2116	G
1	1	2118	U
1	1	2127	G
1	1	2146	C
1	1	2189	U
1	1	2756	U
2	2	516	PSU
2	2	966	2MG
2	2	1109	C
2	2	1145	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

37 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
2	PSU	2	516	2,56	18,21,22	1.04	1 (5%)	22,30,33	1.90	4 (18%)
2	MA6	2	1519	2	23,26,27	1.70	6 (26%)	34,38,41	3.16	11 (32%)
1	PSU	1	2457	1	18,21,22	1.20	2 (11%)	22,30,33	2.12	5 (22%)
1	PSU	1	955	1,56	18,21,22	1.11	1 (5%)	22,30,33	2.08	4 (18%)
54	5MU	z	66	54	19,22,23	4.51	7 (36%)	28,32,35	3.82	11 (39%)
1	6MZ	1	2030	1	22,25,26	2.58	6 (27%)	30,36,39	3.29	12 (40%)
2	UR3	2	1498	2,56	19,22,23	2.39	6 (31%)	26,32,35	0.99	2 (7%)
2	MA6	2	1518	2	23,26,27	1.70	6 (26%)	34,38,41	3.36	11 (32%)
2	G7M	2	527	2	23,26,27	2.81	9 (39%)	35,39,42	2.24	11 (31%)
1	PSU	1	2605	1	18,21,22	1.08	1 (5%)	22,30,33	2.00	4 (18%)
2	2MG	2	1516	2	23,26,27	2.55	8 (34%)	32,38,41	2.10	10 (31%)
1	OMC	1	2498	1,56	19,22,23	2.46	6 (31%)	26,31,34	1.00	2 (7%)
1	3TD	1	1915	1	18,22,23	3.87	6 (33%)	22,32,35	1.41	2 (9%)
1	2MG	1	2445	1	23,26,27	2.50	7 (30%)	32,38,41	1.91	9 (28%)
44	0TD	p	89	44	7,9,10	1.38	0	6,11,13	1.93	2 (33%)
2	2MG	2	966	2	23,26,27	2.65	8 (34%)	32,38,41	2.01	7 (21%)
1	PSU	1	1917	1	18,21,22	1.03	1 (5%)	22,30,33	2.03	5 (22%)
1	PSU	1	746	1,56	18,21,22	1.03	1 (5%)	22,30,33	1.76	3 (13%)
1	5MC	1	1962	1	18,22,23	3.07	7 (38%)	26,32,35	1.10	3 (11%)
2	5MC	2	1407	2	18,22,23	3.03	7 (38%)	26,32,35	0.91	1 (3%)
1	PSU	1	2580	1,56	18,21,22	1.14	2 (11%)	22,30,33	1.82	5 (22%)
1	5MU	1	1939	1,56	19,22,23	4.17	7 (36%)	28,32,35	3.76	9 (32%)
1	PSU	1	1911	1	18,21,22	1.01	1 (5%)	22,30,33	1.95	5 (22%)
1	6MZ	1	1618	1	22,25,26	2.47	7 (31%)	30,36,39	3.31	11 (36%)
1	OMU	1	2552	1	19,22,23	2.64	6 (31%)	26,31,34	1.78	6 (23%)
2	5MC	2	967	2	18,22,23	3.23	7 (38%)	26,32,35	1.01	2 (7%)
55	FME	B	1	55	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
2	2MG	2	1207	2	23,26,27	2.58	8 (34%)	32,38,41	1.94	10 (31%)
1	OMG	1	2251	1,54	23,26,27	2.13	6 (26%)	33,38,41	1.66	8 (24%)
54	OMG	z	17	54	27,27,27	3.41	9 (33%)	40,41,41	6.54	15 (37%)
1	G7M	1	2069	1	23,26,27	2.73	8 (34%)	35,39,42	2.19	12 (34%)
2	4OC	2	1402	2	20,23,24	2.68	8 (40%)	26,32,35	1.09	1 (3%)
1	5MU	1	747	1	19,22,23	4.42	7 (36%)	28,32,35	3.78	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1	2503	1,56	22,25,26	3.47	10 (45%)	33,37,40	2.23	9 (27%)
1	PSU	1	2504	1	18,21,22	1.08	1 (5%)	22,30,33	1.93	5 (22%)
1	2MG	1	1835	1	23,26,27	2.52	9 (39%)	32,38,41	1.99	8 (25%)
1	1MG	1	745	1	22,26,27	2.77	7 (31%)	33,39,42	2.15	7 (21%)

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
2	PSU	2	516	2,56	-	2/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	2/11/29/30	0/3/3/3
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1,56	-	0/7/25/26	0/2/2/2
54	5MU	z	66	54	-	2/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	4/9/27/28	0/3/3/3
2	UR3	2	1498	2,56	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
2	G7M	2	527	2	-	3/7/25/26	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
1	OMC	1	2498	1,56	-	0/9/27/28	0/2/2/2
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
44	0TD	p	89	44	-	2/7/12/14	-
2	2MG	2	966	2	-	2/9/27/28	0/3/3/3
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1	746	1,56	-	1/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1,56	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1,56	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	4/9/27/28	0/3/3/3
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
55	FME	B	1	55	-	4/7/9/11	-
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1	2251	1,54	-	0/9/27/28	0/3/3/3
54	OMG	z	17	54	-	3/12/28/28	0/3/3/3
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	2MA	1	2503	1,56	-	2/7/25/26	0/3/3/3
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	11.21	1.48	1.35
54	z	66	5MU	C2-N1	10.77	1.55	1.38
1	1	2503	2MA	C4-N3	10.67	1.47	1.34
1	1	747	5MU	C2-N1	10.18	1.54	1.38
54	z	17	OMG	O6-C6	-10.11	1.04	1.23
54	z	66	5MU	C6-N1	9.75	1.54	1.38
1	1	747	5MU	C6-N1	9.21	1.53	1.38
1	1	1939	5MU	C2-N1	9.04	1.53	1.38
1	1	2030	6MZ	C6-N6	9.01	1.43	1.34
1	1	1618	6MZ	C6-N6	8.67	1.43	1.34
54	z	66	5MU	C4-C5	8.54	1.59	1.44
1	1	1915	3TD	C2-N1	8.52	1.48	1.37
1	1	1939	5MU	C6-N1	8.48	1.52	1.38
1	1	747	5MU	C4-C5	8.48	1.58	1.44
54	z	17	OMG	C4-N3	8.47	1.54	1.34
1	1	1939	5MU	C4-C5	8.33	1.58	1.44
1	1	2069	G7M	C5-N7	-8.04	1.29	1.39
54	z	17	OMG	C2-N3	8.02	1.52	1.33
1	1	747	5MU	C4-N3	-8.02	1.23	1.38
1	1	1939	5MU	C4-N3	-7.99	1.24	1.38
2	2	967	5MC	C6-C5	7.96	1.47	1.34
2	2	527	G7M	C5-N7	-7.95	1.29	1.39
2	2	1407	5MC	C6-C5	7.75	1.47	1.34
1	1	745	1MG	C2-N2	7.57	1.47	1.34
54	z	66	5MU	C4-N3	-7.51	1.24	1.38
1	1	1962	5MC	C6-C5	7.24	1.46	1.34
2	2	966	2MG	C2-N3	7.12	1.45	1.31
2	2	1207	2MG	C2-N3	6.87	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1835	2MG	C2-N3	6.69	1.44	1.31
2	2	1516	2MG	C2-N3	6.49	1.44	1.31
1	1	2445	2MG	C2-N3	6.32	1.44	1.31
1	1	1962	5MC	C4-N3	6.18	1.44	1.34
2	2	967	5MC	C4-N3	6.07	1.44	1.34
2	2	1402	4OC	C4-N3	6.03	1.43	1.32
1	1	2552	OMU	C2-N3	5.90	1.48	1.38
2	2	527	G7M	C4-N3	5.90	1.48	1.34
2	2	1498	UR3	C6-C5	5.88	1.48	1.35
2	2	966	2MG	C4-N3	5.84	1.48	1.34
1	1	2503	2MA	C2-N3	5.75	1.44	1.34
2	2	1207	2MG	C4-N3	5.74	1.47	1.34
2	2	967	5MC	C2-N3	5.61	1.47	1.36
1	1	2552	OMU	C2-N1	5.59	1.47	1.38
1	1	1962	5MC	C2-N3	5.54	1.47	1.36
1	1	1835	2MG	C4-N3	5.40	1.47	1.34
1	1	745	1MG	C4-N3	5.37	1.47	1.34
2	2	1402	4OC	C2-N3	5.37	1.47	1.36
2	2	1407	5MC	C4-N3	5.36	1.43	1.34
2	2	1516	2MG	C4-N3	5.34	1.46	1.34
1	1	1915	3TD	C6-N1	5.32	1.45	1.36
2	2	1402	4OC	C6-C5	5.19	1.47	1.35
1	1	2251	OMG	C4-N3	5.16	1.46	1.34
2	2	527	G7M	C2-N3	5.13	1.45	1.33
2	2	1407	5MC	C2-N3	5.10	1.46	1.36
1	1	2498	OMC	C2-N3	5.08	1.46	1.36
1	1	2498	OMC	C6-C5	5.07	1.46	1.35
1	1	2445	2MG	C4-N3	5.04	1.46	1.34
54	z	66	5MU	C6-C5	5.02	1.42	1.34
54	z	17	OMG	C2-N1	5.01	1.50	1.37
1	1	2069	G7M	C4-N3	4.96	1.46	1.34
1	1	2503	2MA	C6-N1	4.82	1.41	1.35
2	2	1498	UR3	C2-N1	4.81	1.45	1.38
1	1	747	5MU	C6-C5	4.79	1.42	1.34
1	1	2552	OMU	C6-C5	4.78	1.46	1.35
1	1	2503	2MA	C2-N1	4.55	1.42	1.34
1	1	2251	OMG	C2-N3	4.54	1.44	1.33
2	2	966	2MG	C2-N2	4.49	1.43	1.33
2	2	1207	2MG	C2-N2	4.48	1.43	1.33
1	1	745	1MG	C5-N7	-4.38	1.30	1.39
1	1	1915	3TD	C2-N3	4.32	1.48	1.38
2	2	527	G7M	C2-N2	4.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1939	5MU	C6-C5	4.27	1.41	1.34
1	1	745	1MG	C2-N3	4.27	1.42	1.34
2	2	1498	UR3	C2-N3	4.24	1.47	1.39
1	1	2503	2MA	C6-N6	-4.16	1.23	1.34
2	2	1519	MA6	C5-C4	-4.16	1.31	1.39
2	2	1516	2MG	C2-N2	4.08	1.42	1.33
1	1	2445	2MG	C2-N2	4.06	1.42	1.33
2	2	967	5MC	C4-N4	4.05	1.44	1.34
2	2	1518	MA6	C5-C4	-4.05	1.31	1.39
1	1	745	1MG	O6-C6	-4.05	1.14	1.23
1	1	2069	G7M	C2-N3	4.01	1.42	1.33
1	1	2445	2MG	C5-N7	-3.99	1.31	1.39
1	1	1835	2MG	C2-N2	3.97	1.42	1.33
1	1	2503	2MA	C5-C6	3.93	1.52	1.41
1	1	2030	6MZ	C5-N7	-3.92	1.31	1.39
1	1	2498	OMC	C4-N3	3.89	1.42	1.34
2	2	966	2MG	C2-N1	3.82	1.42	1.36
2	2	1516	2MG	C2-N1	3.80	1.42	1.36
1	1	2251	OMG	C5-N7	-3.80	1.31	1.39
1	1	1962	5MC	C4-N4	3.80	1.44	1.34
1	1	2030	6MZ	C5-C4	-3.74	1.32	1.39
1	1	1835	2MG	C5-N7	-3.73	1.31	1.39
1	1	1618	6MZ	C5-C4	-3.71	1.32	1.39
2	2	1407	5MC	C4-N4	3.70	1.43	1.34
1	1	2498	OMC	C4-N4	3.69	1.42	1.33
2	2	967	5MC	C2-N1	3.64	1.47	1.40
1	1	1618	6MZ	C5-N7	-3.54	1.32	1.39
1	1	2069	G7M	C2-N2	3.53	1.42	1.34
2	2	1407	5MC	C6-N1	3.52	1.44	1.38
2	2	1402	4OC	C4-N4	3.51	1.43	1.35
1	1	747	5MU	O4-C4	-3.51	1.16	1.23
1	1	2552	OMU	C4-N3	3.50	1.44	1.38
2	2	1516	2MG	C5-N7	-3.49	1.32	1.39
2	2	1207	2MG	C2-N1	3.45	1.42	1.36
1	1	2498	OMC	O2-C2	-3.41	1.17	1.23
2	2	967	5MC	C6-N1	3.41	1.43	1.38
2	2	966	2MG	C5-N7	-3.39	1.32	1.39
2	2	1207	2MG	C5-N7	-3.38	1.32	1.39
54	z	17	OMG	C2-N2	3.36	1.42	1.34
1	1	1962	5MC	C2-N1	3.36	1.47	1.40
2	2	1407	5MC	O2-C2	-3.32	1.17	1.23
2	2	1498	UR3	C3U-N3	-3.32	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	745	1MG	C4-N9	-3.31	1.29	1.38
1	1	1939	5MU	O4-C4	-3.29	1.17	1.23
54	z	17	OMG	C5-N7	-3.29	1.32	1.39
1	1	2503	2MA	C5-N7	-3.28	1.32	1.39
1	1	2503	2MA	C4-N9	-3.25	1.30	1.37
54	z	66	5MU	O4-C4	-3.25	1.17	1.23
2	2	1402	4OC	C2-N1	3.25	1.47	1.40
1	1	2030	6MZ	C8-N9	-3.23	1.31	1.37
1	1	1962	5MC	O2-C2	-3.19	1.17	1.23
1	1	2498	OMC	C2-N1	3.18	1.46	1.40
1	1	1962	5MC	C6-N1	3.15	1.43	1.38
1	1	2069	G7M	CN7-N7	-3.14	1.41	1.46
2	2	1402	4OC	O2-C2	-3.14	1.17	1.23
1	1	2251	OMG	O6-C6	-3.13	1.17	1.23
2	2	1518	MA6	C5-N7	-3.10	1.33	1.39
1	1	2069	G7M	C4-N9	-3.09	1.30	1.38
1	1	1835	2MG	C2-N1	3.09	1.41	1.36
1	1	2445	2MG	O6-C6	-3.06	1.17	1.23
1	1	2445	2MG	C4-N9	-3.05	1.30	1.38
1	1	2552	OMU	O4-C4	-3.04	1.18	1.24
1	1	2445	2MG	C2-N1	3.04	1.41	1.36
2	2	967	5MC	O2-C2	-3.04	1.18	1.23
1	1	2030	6MZ	C6-N1	-3.03	1.30	1.35
1	1	2069	G7M	O6-C6	-3.03	1.17	1.23
2	2	1516	2MG	C4-N9	-3.02	1.30	1.38
2	2	1518	MA6	C8-N9	-2.98	1.32	1.37
2	2	1519	MA6	C8-N9	-2.95	1.32	1.37
1	1	2251	OMG	C4-N9	-2.95	1.30	1.38
1	1	1835	2MG	O6-C6	-2.95	1.18	1.23
2	2	1519	MA6	C5-N7	-2.95	1.33	1.39
2	2	1407	5MC	C2-N1	2.93	1.46	1.40
1	1	2552	OMU	O2-C2	-2.92	1.17	1.23
2	2	527	G7M	C5-C6	2.91	1.51	1.43
1	1	1939	5MU	O2-C2	-2.87	1.17	1.23
1	1	1618	6MZ	C6-N1	-2.84	1.30	1.35
1	1	1618	6MZ	C8-N9	-2.81	1.32	1.37
54	z	17	OMG	C6-N1	2.73	1.43	1.38
2	2	527	G7M	O6-C6	-2.71	1.18	1.23
1	1	747	5MU	O2-C2	-2.70	1.18	1.23
2	2	1516	2MG	O6-C6	-2.70	1.18	1.23
2	2	1207	2MG	O6-C6	-2.69	1.18	1.23
1	1	2069	G7M	C5-C6	2.68	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1519	MA6	C4-N9	-2.67	1.31	1.37
2	2	1402	4OC	C5-C4	2.65	1.46	1.40
2	2	1519	MA6	C6-N6	2.61	1.44	1.36
1	1	1915	3TD	O2-C2	-2.61	1.18	1.23
1	1	2030	6MZ	C5-C6	-2.60	1.35	1.41
2	2	1207	2MG	C4-N9	-2.57	1.31	1.38
1	1	1835	2MG	C4-N9	-2.57	1.31	1.38
2	2	1518	MA6	C6-N6	2.54	1.44	1.36
2	2	1518	MA6	C4-N9	-2.52	1.32	1.37
1	1	1618	6MZ	C5-C6	-2.52	1.35	1.41
54	z	17	OMG	C5-C6	2.51	1.53	1.44
54	z	66	5MU	O2-C2	-2.48	1.18	1.23
1	1	2251	OMG	C2-N2	2.46	1.40	1.34
2	2	966	2MG	O6-C6	-2.45	1.18	1.23
2	2	966	2MG	C4-N9	-2.44	1.31	1.38
1	1	1915	3TD	O4-C4	-2.44	1.18	1.23
2	2	1498	UR3	O2-C2	-2.44	1.18	1.22
1	1	2504	PSU	C4-C5	-2.44	1.37	1.44
1	1	2605	PSU	C4-C5	-2.44	1.37	1.44
1	1	2503	2MA	C5-C4	-2.43	1.34	1.39
1	1	2457	PSU	C4-C5	-2.43	1.37	1.44
1	1	2503	2MA	C8-N9	-2.41	1.33	1.37
1	1	745	1MG	C5-C6	2.41	1.51	1.45
1	1	2580	PSU	C4-C5	-2.41	1.37	1.44
2	2	527	G7M	CN7-N7	-2.40	1.42	1.46
1	1	955	PSU	C4-C5	-2.36	1.37	1.44
2	2	1516	2MG	C5-C6	2.29	1.52	1.44
1	1	1911	PSU	C4-C5	-2.29	1.37	1.44
2	2	966	2MG	C5-C6	2.27	1.52	1.44
2	2	516	PSU	C4-C5	-2.27	1.37	1.44
2	2	1518	MA6	C5-C6	-2.22	1.35	1.41
1	1	1917	PSU	C4-C5	-2.20	1.37	1.44
54	z	17	OMG	C4-N9	-2.20	1.32	1.38
2	2	527	G7M	C4-N9	-2.17	1.32	1.38
2	2	1207	2MG	C5-C6	2.16	1.52	1.44
2	2	527	G7M	C2-N1	2.14	1.43	1.37
2	2	1402	4OC	C6-N1	2.14	1.43	1.38
1	1	746	PSU	C4-C5	-2.10	1.38	1.44
2	2	1498	UR3	C6-N1	2.08	1.43	1.38
1	1	1835	2MG	C8-N9	-2.06	1.33	1.37
2	2	1519	MA6	C5-C6	-2.06	1.36	1.41
1	1	2457	PSU	O4'-C1'	-2.06	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1835	2MG	C5-C6	2.05	1.52	1.44
1	1	2580	PSU	C6-N1	-2.03	1.32	1.36
1	1	1618	6MZ	C4-N9	-2.02	1.33	1.37

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	17	OMG	O6-C6-N1	-29.76	63.06	120.12
54	z	17	OMG	O6-C6-C5	-23.83	63.37	126.60
2	2	1518	MA6	N1-C6-N6	-14.31	101.43	117.08
2	2	1519	MA6	N1-C6-N6	-13.10	102.76	117.08
54	z	66	5MU	C5-C4-N3	12.53	126.01	115.31
1	1	747	5MU	C5-C4-N3	12.21	125.74	115.31
1	1	1939	5MU	C5-C4-N3	11.79	125.38	115.31
54	z	66	5MU	C5-C6-N1	-10.44	112.60	123.34
1	1	747	5MU	C5-C6-N1	-9.95	113.10	123.34
1	1	1939	5MU	C5-C6-N1	-9.73	113.33	123.34
1	1	2030	6MZ	C4-N9-C1'	-8.43	106.51	126.59
1	1	1618	6MZ	C4-N9-C1'	-8.33	106.75	126.59
1	1	2030	6MZ	C1'-N9-C8	8.24	145.73	127.14
1	1	1618	6MZ	C1'-N9-C8	8.20	145.66	127.14
54	z	66	5MU	O4-C4-C5	-7.06	116.72	124.90
1	1	745	1MG	C1'-N9-C4	-6.84	106.17	126.50
2	2	1518	MA6	C5-C6-N6	6.81	137.16	125.30
1	1	2030	6MZ	C5-C4-N3	-6.73	117.97	126.75
1	1	1618	6MZ	C5-C4-N3	-6.58	118.16	126.75
1	1	2503	2MA	C1'-N9-C8	-6.32	112.88	127.14
1	1	1939	5MU	C5M-C5-C4	6.30	125.70	118.77
1	1	745	1MG	C1'-N9-C8	6.11	144.10	126.70
54	z	17	OMG	OP3-P-OP1	-6.06	86.95	110.68
2	2	1519	MA6	C5-C6-N6	6.00	135.75	125.30
1	1	2030	6MZ	C4-C5-C6	5.97	121.44	116.81
1	1	747	5MU	O4-C4-C5	-5.93	118.03	124.90
54	z	17	OMG	OP3-P-O5'	-5.83	91.21	106.73
1	1	1939	5MU	C5M-C5-C6	-5.82	115.08	122.85
1	1	2457	PSU	C4-N3-C2	-5.73	118.08	126.34
54	z	17	OMG	C2-N1-C6	-5.58	114.92	125.10
54	z	66	5MU	C4-N3-C2	-5.46	120.28	127.35
1	1	2605	PSU	C4-N3-C2	-5.44	118.50	126.34
2	2	1518	MA6	N1-C2-N3	-5.41	120.14	128.60
2	2	1516	2MG	C2-N3-C4	5.39	118.72	112.04
1	1	1835	2MG	C2-N3-C4	5.38	118.71	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	516	PSU	C4-N3-C2	-5.36	118.61	126.34
1	1	747	5MU	C4-N3-C2	-5.34	120.44	127.35
1	1	1939	5MU	O4-C4-C5	-5.34	118.71	124.90
1	1	2457	PSU	N1-C2-N3	5.33	121.16	115.13
54	z	17	OMG	OP3-P-OP2	-5.29	87.43	107.64
1	1	955	PSU	C4-N3-C2	-5.27	118.75	126.34
1	1	2503	2MA	N9-C8-N7	-5.26	106.72	113.91
1	1	2552	OMU	C4-N3-C2	-5.25	119.66	126.58
2	2	966	2MG	C2-N3-C4	5.23	118.53	112.04
54	z	17	OMG	C5-C6-N1	5.21	126.43	113.19
1	1	1917	PSU	C4-N3-C2	-5.17	118.89	126.34
1	1	1835	2MG	C5-C4-N3	-5.15	120.11	128.46
1	1	1911	PSU	C4-N3-C2	-5.14	118.93	126.34
2	2	1519	MA6	N1-C2-N3	-5.12	120.59	128.60
2	2	1207	2MG	C2-N3-C4	5.10	118.36	112.04
1	1	746	PSU	C4-N3-C2	-5.05	119.06	126.34
2	2	966	2MG	C5-C4-N3	-5.02	120.32	128.46
1	1	2030	6MZ	N3-C4-N9	4.99	135.30	127.08
1	1	1917	PSU	N1-C2-N3	4.94	120.73	115.13
1	1	955	PSU	N1-C2-N3	4.88	120.66	115.13
1	1	2069	G7M	CN7-N7-C8	-4.88	117.31	124.84
2	2	1516	2MG	C2-N1-C6	-4.87	118.87	124.48
1	1	2504	PSU	C4-N3-C2	-4.87	119.33	126.34
1	1	2504	PSU	N1-C2-N3	4.80	120.57	115.13
2	2	1519	MA6	C5-C4-N3	-4.80	120.49	126.75
54	z	17	OMG	OP2-P-OP1	4.80	129.47	110.68
1	1	2580	PSU	C4-N3-C2	-4.79	119.43	126.34
1	1	2069	G7M	CN7-N7-C5	4.77	132.70	126.77
1	1	1618	6MZ	N3-C4-N9	4.75	134.91	127.08
1	1	1618	6MZ	N1-C2-N3	-4.74	121.18	128.60
1	1	1618	6MZ	C4-C5-C6	4.74	120.48	116.81
1	1	1911	PSU	N1-C2-N3	4.70	120.45	115.13
2	2	1207	2MG	C5-C4-N3	-4.68	120.86	128.46
1	1	1939	5MU	C4-N3-C2	-4.68	121.30	127.35
1	1	2445	2MG	C2-N3-C4	4.65	117.81	112.04
2	2	1518	MA6	C5-C4-N3	-4.63	120.71	126.75
1	1	747	5MU	C5M-C5-C6	-4.60	116.71	122.85
1	1	2605	PSU	N1-C2-N3	4.59	120.33	115.13
2	2	1516	2MG	C5-C4-N3	-4.59	121.01	128.46
1	1	2445	2MG	C5-C4-N3	-4.59	121.02	128.46
2	2	527	G7M	C5-C4-N3	-4.58	119.37	128.15
1	1	2251	OMG	C5-C4-N3	-4.56	121.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1835	2MG	C2-N1-C6	-4.55	119.24	124.48
2	2	527	G7M	C1'-N9-C4	4.53	139.97	126.50
2	2	527	G7M	C1'-N9-C8	-4.49	111.56	126.74
1	1	1618	6MZ	C9-N6-C6	-4.49	119.00	122.87
1	1	2503	2MA	C5-C4-N3	-4.43	122.20	127.19
1	1	2580	PSU	N1-C2-N3	4.43	120.15	115.13
1	1	2503	2MA	C4-N9-C1'	4.42	137.12	126.59
1	1	747	5MU	N3-C2-N1	4.30	120.60	114.89
2	2	966	2MG	C2-N1-C6	-4.30	119.53	124.48
1	1	746	PSU	N1-C2-N3	4.29	119.99	115.13
2	2	527	G7M	CN7-N7-C5	4.28	132.09	126.77
1	1	2030	6MZ	N1-C2-N3	-4.26	121.95	128.60
1	1	745	1MG	C5-C4-N3	-4.23	121.60	128.46
2	2	1518	MA6	N9-C8-N7	-4.22	108.14	113.91
2	2	1519	MA6	N9-C8-N7	-4.21	108.16	113.91
1	1	2445	2MG	C2-N1-C6	-4.17	119.68	124.48
1	1	747	5MU	C5M-C5-C4	4.13	123.31	118.77
2	2	1207	2MG	C2-N1-C6	-4.06	119.81	124.48
1	1	1915	3TD	N1-C2-N3	3.97	119.27	116.14
54	z	66	5MU	N3-C2-N1	3.95	120.14	114.89
2	2	516	PSU	N1-C2-N3	3.95	119.61	115.13
1	1	2503	2MA	C4-N9-C8	3.93	109.98	105.73
2	2	527	G7M	CN7-N7-C8	-3.91	118.80	124.84
1	1	1618	6MZ	C5-C6-N1	3.83	122.28	118.20
44	p	89	0TD	OD2-CG-CB	3.74	121.22	113.15
2	2	527	G7M	N9-C4-N3	3.73	133.43	125.94
1	1	1618	6MZ	C2-N3-C4	3.73	120.56	111.75
2	2	527	G7M	C2-N3-C4	3.71	118.91	112.30
1	1	2069	G7M	C5-C4-N3	-3.69	121.07	128.15
1	1	1915	3TD	C4-N3-C2	-3.69	120.60	124.61
1	1	2069	G7M	C2-N3-C4	3.65	118.81	112.30
1	1	2030	6MZ	N9-C8-N7	-3.64	108.94	113.91
1	1	2552	OMU	N3-C2-N1	3.62	119.70	114.89
1	1	1939	5MU	N3-C2-N1	3.54	119.58	114.89
1	1	2069	G7M	O6-C6-C5	-3.50	120.17	128.06
1	1	2030	6MZ	C2-N3-C4	3.49	120.00	111.75
1	1	2457	PSU	O2-C2-N1	-3.47	118.97	122.79
54	z	66	5MU	C5M-C5-C6	-3.41	118.29	122.85
1	1	955	PSU	C6-C5-C4	3.41	120.58	118.20
2	2	527	G7M	O6-C6-C5	-3.38	120.43	128.06
2	2	1402	4OC	CM4-N4-C4	-3.38	115.84	122.45
2	2	1519	MA6	C2-N3-C4	3.38	119.73	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2069	G7M	C1'-N9-C8	-3.37	115.36	126.74
1	1	2552	OMU	CM2-O2'-C2'	-3.35	105.74	114.52
1	1	1618	6MZ	N9-C8-N7	-3.31	109.38	113.91
1	1	2069	G7M	C5-C6-N1	3.31	118.70	111.79
54	z	17	OMG	O5'-P-OP1	3.31	115.75	106.47
1	1	2605	PSU	C6-C5-C4	3.30	120.50	118.20
2	2	527	G7M	C5-C6-N1	3.27	118.62	111.79
1	1	1917	PSU	C6-C5-C4	3.26	120.48	118.20
2	2	1516	2MG	CM2-N2-C2	-3.26	116.66	123.86
1	1	2251	OMG	C2-N1-C6	-3.26	119.16	125.10
2	2	1518	MA6	C2-N3-C4	3.25	119.44	111.75
54	z	17	OMG	C5-C4-N3	-3.22	123.23	128.46
1	1	1911	PSU	O2-C2-N1	-3.22	119.24	122.79
1	1	1835	2MG	CM2-N2-C2	-3.20	116.80	123.86
1	1	746	PSU	O2-C2-N1	-3.20	119.27	122.79
2	2	1518	MA6	N3-C4-N9	3.15	132.27	127.08
1	1	2251	OMG	C2-N3-C4	3.14	117.90	112.30
2	2	1518	MA6	C2-N1-C6	3.14	119.17	111.75
1	1	1917	PSU	O2-C2-N1	-3.13	119.35	122.79
1	1	2069	G7M	C2-N1-C6	-3.12	119.42	125.10
1	1	1835	2MG	N9-C4-N3	3.09	132.14	125.94
1	1	745	1MG	N9-C8-N7	-3.05	107.65	113.39
1	1	955	PSU	O2-C2-N1	-3.04	119.44	122.79
2	2	966	2MG	N9-C4-N3	3.01	131.97	125.94
1	1	2504	PSU	O2-C2-N1	-3.00	119.48	122.79
1	1	2030	6MZ	C6-C5-N7	-3.00	129.15	132.39
2	2	1519	MA6	C4-C5-C6	2.98	119.21	115.88
1	1	2069	G7M	C1'-N9-C4	2.97	135.33	126.50
1	1	2498	OMC	CM2-O2'-C2'	-2.97	106.73	114.52
54	z	17	OMG	OP2-P-O5'	2.94	114.54	106.73
2	2	527	G7M	C2-N1-C6	-2.93	119.75	125.10
2	2	1407	5MC	C5-C6-N1	-2.93	120.32	123.34
1	1	2552	OMU	O4-C4-C5	-2.91	120.05	125.16
2	2	1518	MA6	C4-C5-C6	2.90	119.13	115.88
1	1	2552	OMU	C5-C4-N3	2.89	119.17	114.84
2	2	1519	MA6	N3-C4-N9	2.88	131.83	127.08
1	1	2503	2MA	N3-C2-N1	-2.87	120.45	125.72
2	2	1519	MA6	C2-N1-C6	2.85	118.49	111.75
2	2	966	2MG	N9-C8-N7	-2.85	108.03	113.39
2	2	1518	MA6	C4-N9-C8	2.84	108.81	105.73
1	1	2503	2MA	C5-N7-C8	2.84	107.55	103.51
1	1	745	1MG	N9-C4-N3	2.84	131.64	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2580	PSU	O2-C2-N1	-2.84	119.66	122.79
1	1	2504	PSU	C6-C5-C4	2.82	120.17	118.20
1	1	2251	OMG	N9-C8-N7	-2.82	108.08	113.39
54	z	17	OMG	N9-C4-N3	2.81	131.58	125.94
2	2	1516	2MG	C1'-N9-C4	-2.81	118.17	126.50
1	1	2445	2MG	N9-C8-N7	-2.80	108.11	113.39
1	1	2251	OMG	CM2-O2'-C2'	-2.77	107.26	114.52
1	1	2030	6MZ	C5-C6-N1	2.76	121.14	118.20
2	2	967	5MC	CM5-C5-C6	-2.74	119.19	122.85
1	1	747	5MU	O2-C2-N1	-2.73	119.16	122.79
2	2	1516	2MG	N9-C8-N7	-2.73	108.26	113.39
1	1	745	1MG	C2-N3-C4	2.71	118.08	111.98
54	z	66	5MU	C6-C5-C4	2.71	120.30	118.03
2	2	1207	2MG	C1'-N9-C4	-2.70	118.49	126.50
1	1	2445	2MG	N9-C4-N3	2.69	131.34	125.94
2	2	1498	UR3	C4-N3-C2	-2.68	122.04	124.56
1	1	1939	5MU	O2-C2-N1	-2.66	119.25	122.79
54	z	66	5MU	O2-C2-N1	-2.64	119.27	122.79
1	1	2069	G7M	N2-C2-N1	2.62	122.29	116.71
1	1	2069	G7M	N9-C8-N7	-2.61	105.75	112.21
2	2	1519	MA6	C4-N9-C8	2.60	108.55	105.73
2	2	1207	2MG	N9-C8-N7	-2.60	108.49	113.39
1	1	1962	5MC	C5-C6-N1	-2.59	120.67	123.34
2	2	1207	2MG	N9-C4-N3	2.58	131.12	125.94
1	1	2030	6MZ	C5-N7-C8	2.57	107.16	103.51
1	1	1618	6MZ	C6-C5-N7	-2.50	129.69	132.39
1	1	2552	OMU	O2-C2-N1	-2.50	119.46	122.79
1	1	2445	2MG	CM2-N2-C2	-2.49	118.35	123.86
2	2	1516	2MG	C1'-N9-C8	2.48	133.77	126.70
2	2	1498	UR3	C1'-N1-C2	2.47	121.16	116.99
2	2	1516	2MG	C5-C6-N1	2.47	119.46	113.19
1	1	2503	2MA	N3-C4-N9	2.47	130.41	126.99
1	1	2445	2MG	O6-C6-C5	-2.47	120.06	126.60
2	2	967	5MC	C5-C6-N1	-2.46	120.81	123.34
54	z	17	OMG	C6-C5-N7	2.44	134.79	130.25
1	1	2251	OMG	N9-C4-N3	2.42	130.80	125.94
55	B	1	FME	O-C-CA	-2.42	118.44	124.78
2	2	1207	2MG	C1'-N9-C8	2.41	133.56	126.70
54	z	17	OMG	C1'-N9-C8	-2.40	119.86	126.70
1	1	1835	2MG	C5-C6-N1	2.40	119.28	113.19
54	z	66	5MU	C5M-C5-C4	2.40	121.41	118.77
1	1	1962	5MC	C5-C4-N4	-2.37	117.94	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	CM2-C2-N1	2.37	120.85	117.15
2	2	1516	2MG	O6-C6-C5	-2.36	120.35	126.60
2	2	1207	2MG	C5-C6-N1	2.35	119.17	113.19
1	1	2457	PSU	C6-N1-C2	-2.35	120.28	122.68
1	1	2251	OMG	O6-C6-C5	-2.34	120.40	126.60
1	1	747	5MU	C6-C5-C4	2.33	119.98	118.03
1	1	1835	2MG	N9-C8-N7	-2.33	109.00	113.39
54	z	66	5MU	C1'-N1-C2	2.32	121.77	117.57
1	1	745	1MG	CM1-N1-C2	-2.32	118.31	120.72
1	1	2445	2MG	C1'-N9-C4	-2.31	119.64	126.50
1	1	2605	PSU	O2-C2-N1	-2.31	120.25	122.79
44	p	89	0TD	OD1-CG-CB	-2.31	117.61	122.44
1	1	2504	PSU	C6-N1-C2	-2.29	120.34	122.68
1	1	2069	G7M	N9-C4-N3	2.28	130.52	125.94
2	2	1207	2MG	CM2-N2-C2	-2.28	118.83	123.86
1	1	1911	PSU	C6-C5-C4	2.27	119.78	118.20
2	2	966	2MG	C5-C6-N1	2.26	118.94	113.19
1	1	2251	OMG	C5-C6-N1	2.26	118.93	113.19
1	1	1962	5MC	CM5-C5-C6	-2.24	119.86	122.85
2	2	516	PSU	O2-C2-N1	-2.22	120.35	122.79
2	2	1516	2MG	N9-C4-N3	2.21	130.38	125.94
2	2	1207	2MG	O6-C6-C5	-2.20	120.77	126.60
1	1	1939	5MU	O4-C4-N3	-2.20	115.91	120.12
1	1	1835	2MG	O6-C6-C5	-2.19	120.79	126.60
1	1	1917	PSU	C6-N1-C2	-2.18	120.45	122.68
2	2	966	2MG	O6-C6-C5	-2.18	120.82	126.60
1	1	2445	2MG	C5-C6-N1	2.18	118.72	113.19
2	2	516	PSU	O4'-C1'-C2'	2.18	108.22	105.14
1	1	2580	PSU	O4'-C1'-C2'	2.18	108.22	105.14
1	1	1911	PSU	C6-N1-C2	-2.18	120.46	122.68
54	z	17	OMG	N9-C8-N7	-2.15	109.34	113.39
54	z	66	5MU	C1'-N1-C6	-2.15	117.55	121.12
1	1	2498	OMC	C2'-C1'-N1	-2.14	110.06	114.22
1	1	2030	6MZ	C9-N6-C6	-2.14	121.03	122.87
2	2	1519	MA6	C5-N7-C8	2.11	106.50	103.51
2	2	1518	MA6	C5-N7-C8	2.11	106.50	103.51
1	1	2580	PSU	C6-N1-C2	-2.10	120.53	122.68
1	1	2457	PSU	O4'-C1'-C2'	2.09	108.09	105.14
1	1	747	5MU	O4-C4-N3	-2.03	116.23	120.12
2	2	527	G7M	C6-C5-N7	-2.01	129.82	132.25

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2030	6MZ	N1-C6-N6-C9
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
54	z	17	OMG	C5'-O5'-P-OP3
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
55	B	1	FME	CA-CB-CG-SD
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
55	B	1	FME	N-CA-CB-CG
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
54	z	66	5MU	O4'-C4'-C5'-O5'
54	z	17	OMG	C5'-O5'-P-OP1
55	B	1	FME	O1-CN-N-CA
55	B	1	FME	CB-CG-SD-CE
54	z	66	5MU	C3'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
1	1	2030	6MZ	C5-C6-N6-C9
2	2	1402	4OC	C3'-C4'-C5'-O5'
44	p	89	0TD	CG-CB-SB-CSB
2	2	527	G7M	C4'-C5'-O5'-P
44	p	89	0TD	SB-CB-CG-OD1
1	1	2503	2MA	C3'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	17	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

18 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	516	PSU	2	0
2	2	1519	MA6	1	0
1	1	2457	PSU	1	0
1	1	955	PSU	1	0
54	z	66	5MU	5	0
1	1	2030	6MZ	3	0
2	2	1498	UR3	1	0
2	2	1518	MA6	1	0
2	2	1516	2MG	1	0
1	1	2498	OMC	1	0
1	1	1915	3TD	2	0
1	1	2445	2MG	1	0
44	p	89	0TD	2	0
1	1	2580	PSU	2	0
1	1	2552	OMU	1	0
55	B	1	FME	4	0
54	z	17	OMG	5	0
1	1	1835	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 418 ligands modelled in this entry, 418 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.

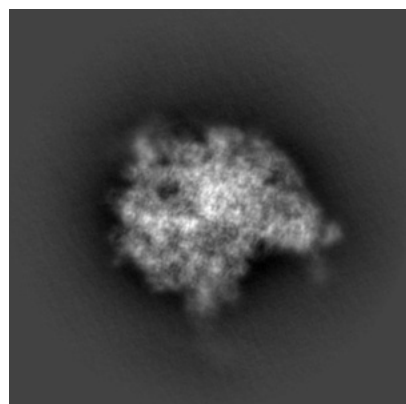
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12928. These allow visual inspection of the internal detail of the map and identification of artifacts.

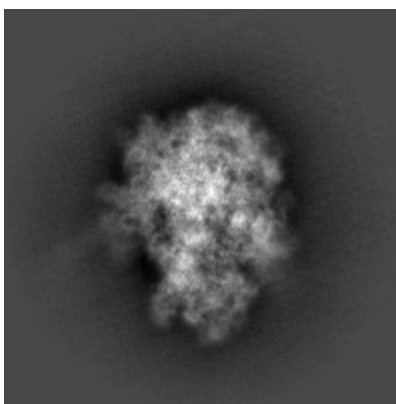
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

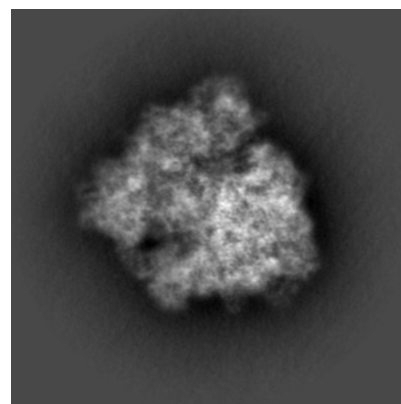
6.1.1 Primary map



X

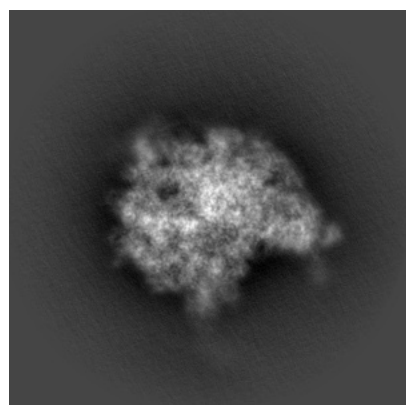


Y

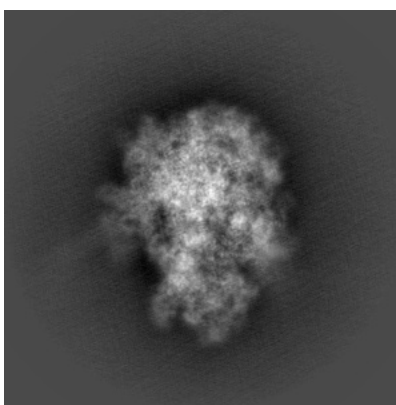


Z

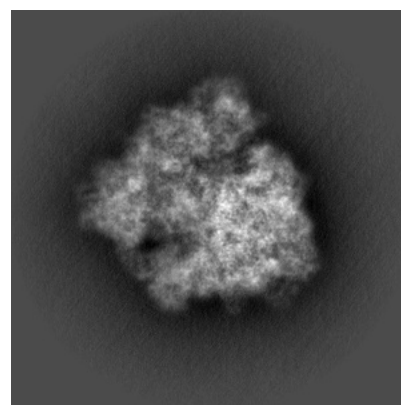
6.1.2 Raw map



X



Y

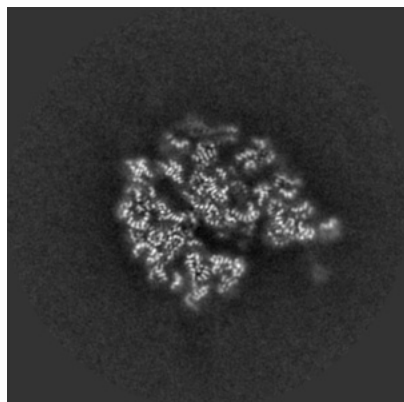


Z

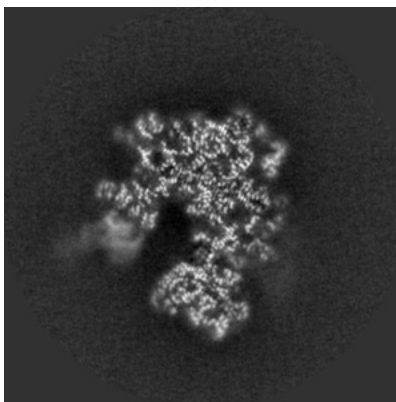
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

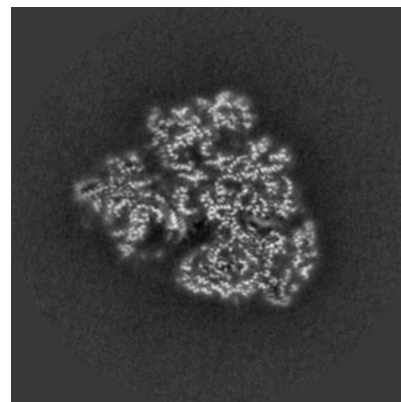
6.2.1 Primary map



X Index: 200

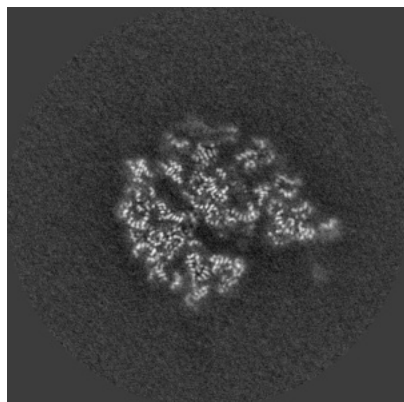


Y Index: 200

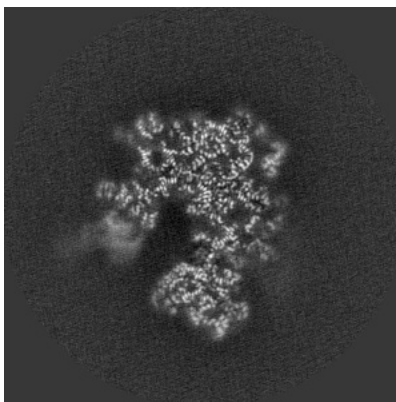


Z Index: 200

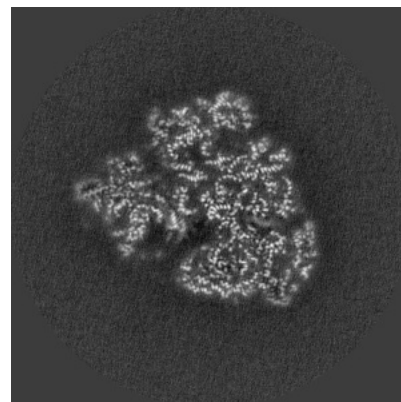
6.2.2 Raw map



X Index: 200



Y Index: 200

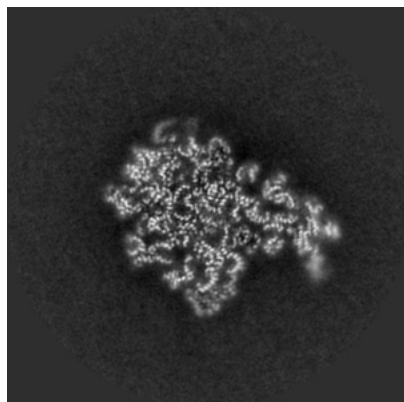


Z Index: 200

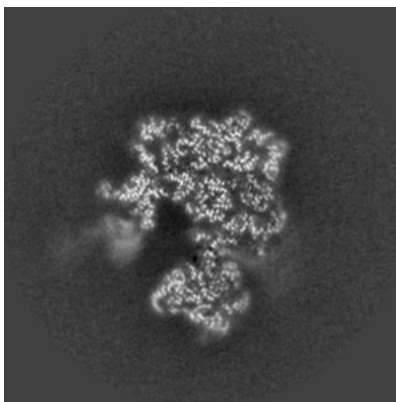
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

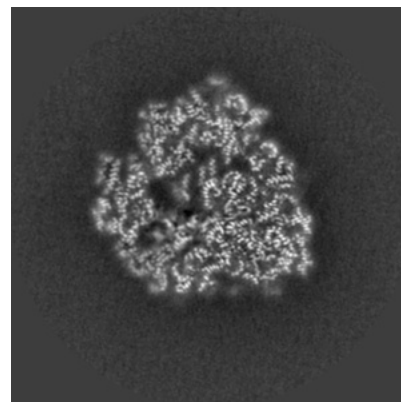
6.3.1 Primary map



X Index: 216

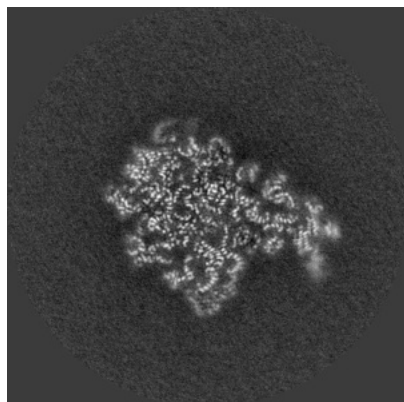


Y Index: 205

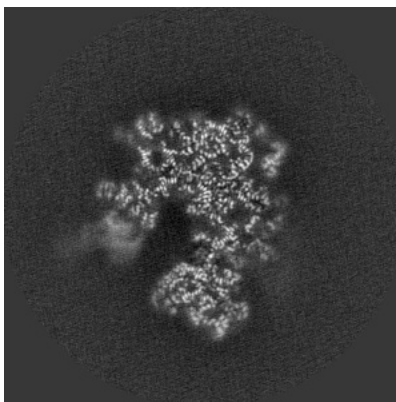


Z Index: 187

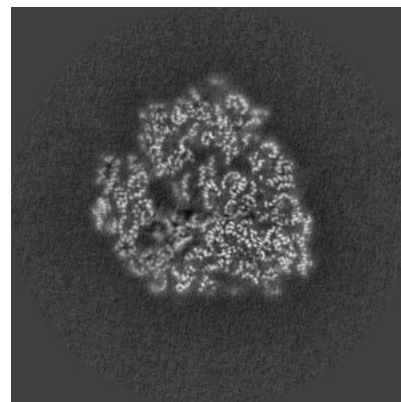
6.3.2 Raw map



X Index: 216



Y Index: 200

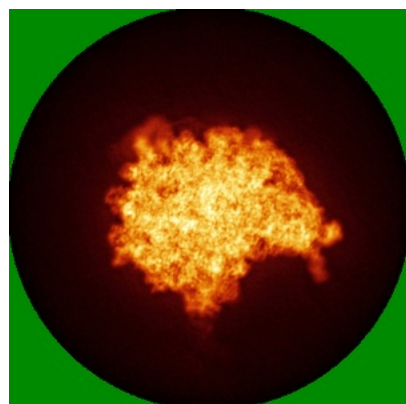


Z Index: 188

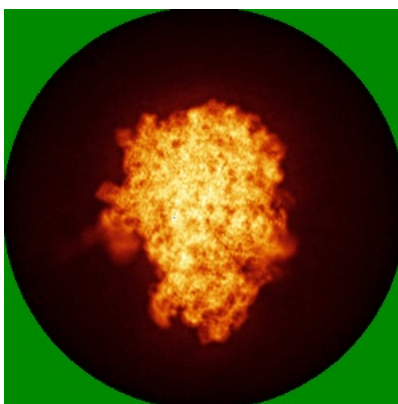
The images above show the largest variance slices of the map in three orthogonal directions.

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

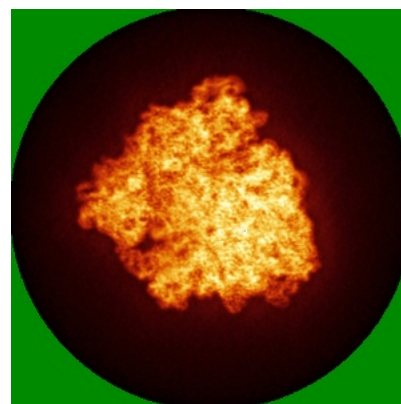
6.4.1 Primary map



X

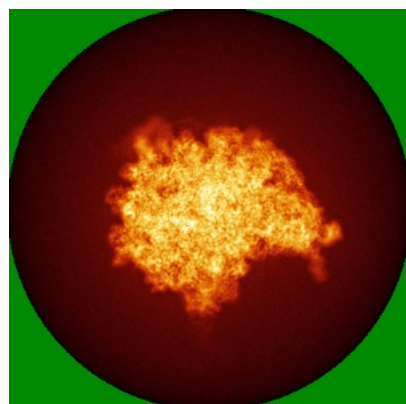


Y

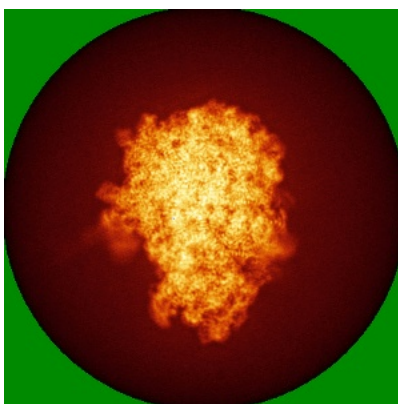


Z

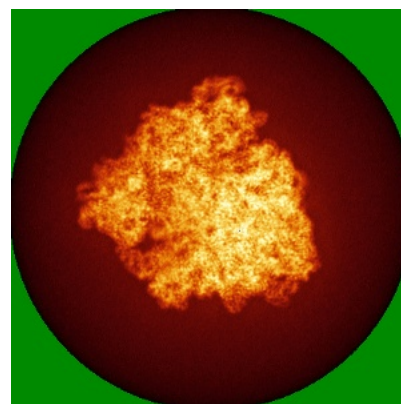
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

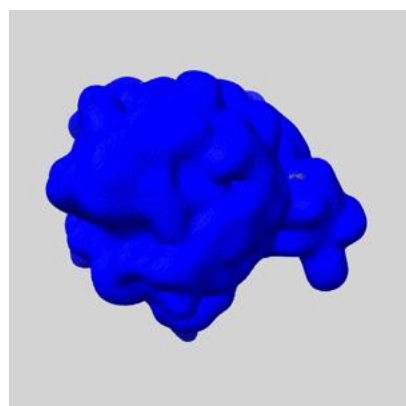
6.6 Mask visualisation [i](#)

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

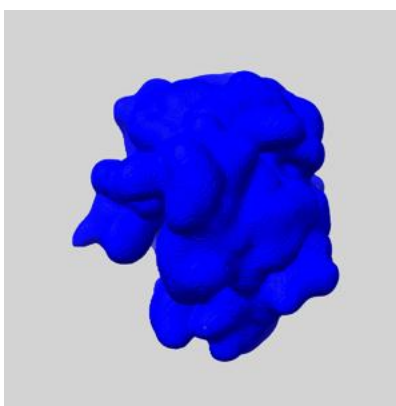
A mask typically either:

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

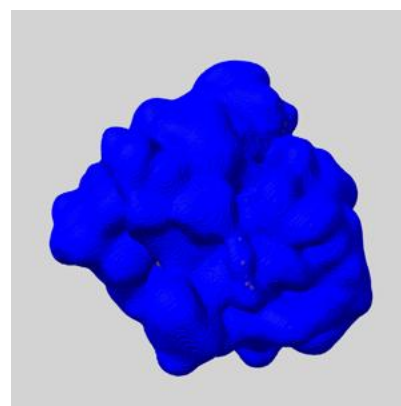
6.6.1 emd_12928_msk_1.map [i](#)



X



Y

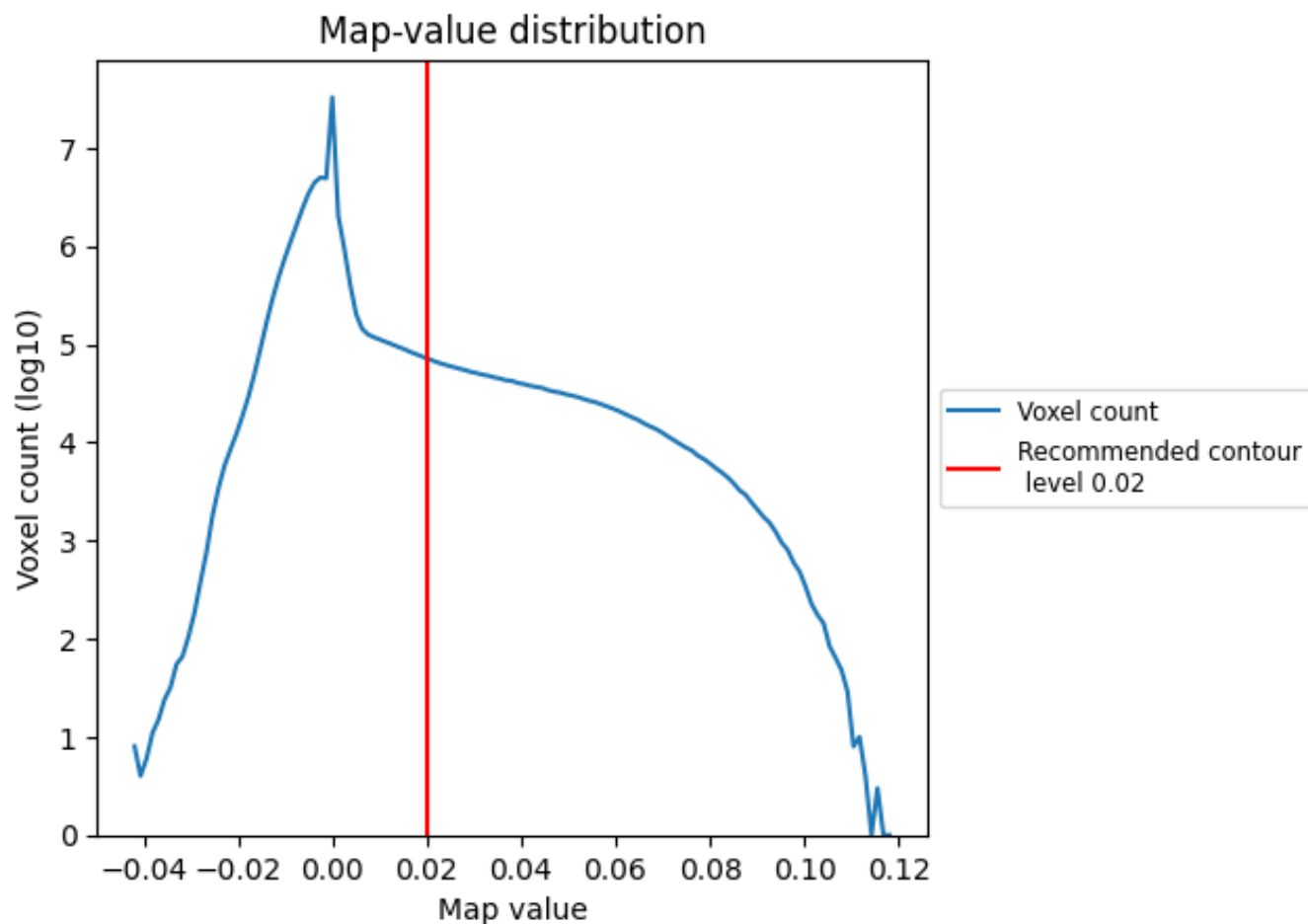


Z

7 Map analysis [i](#)

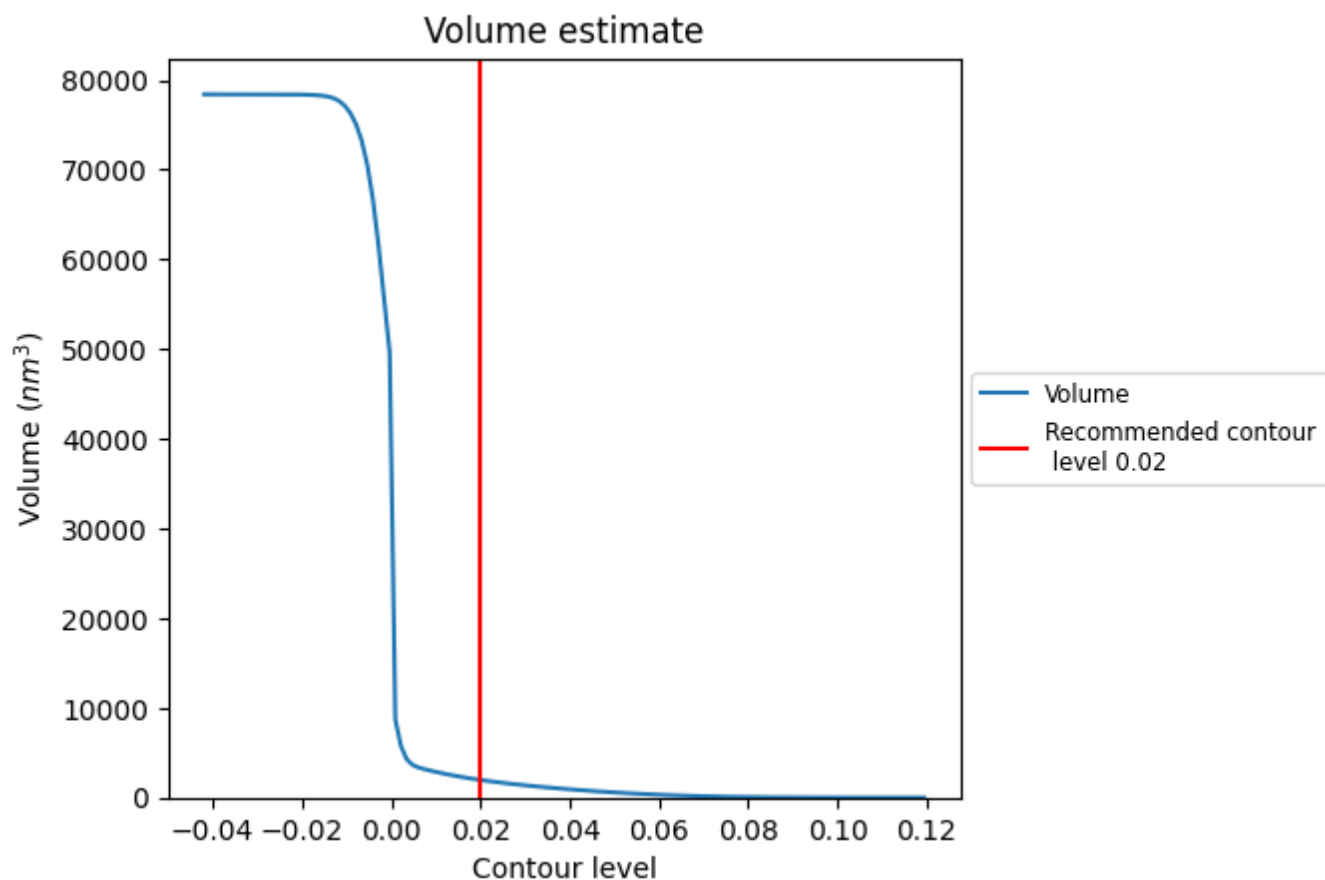
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

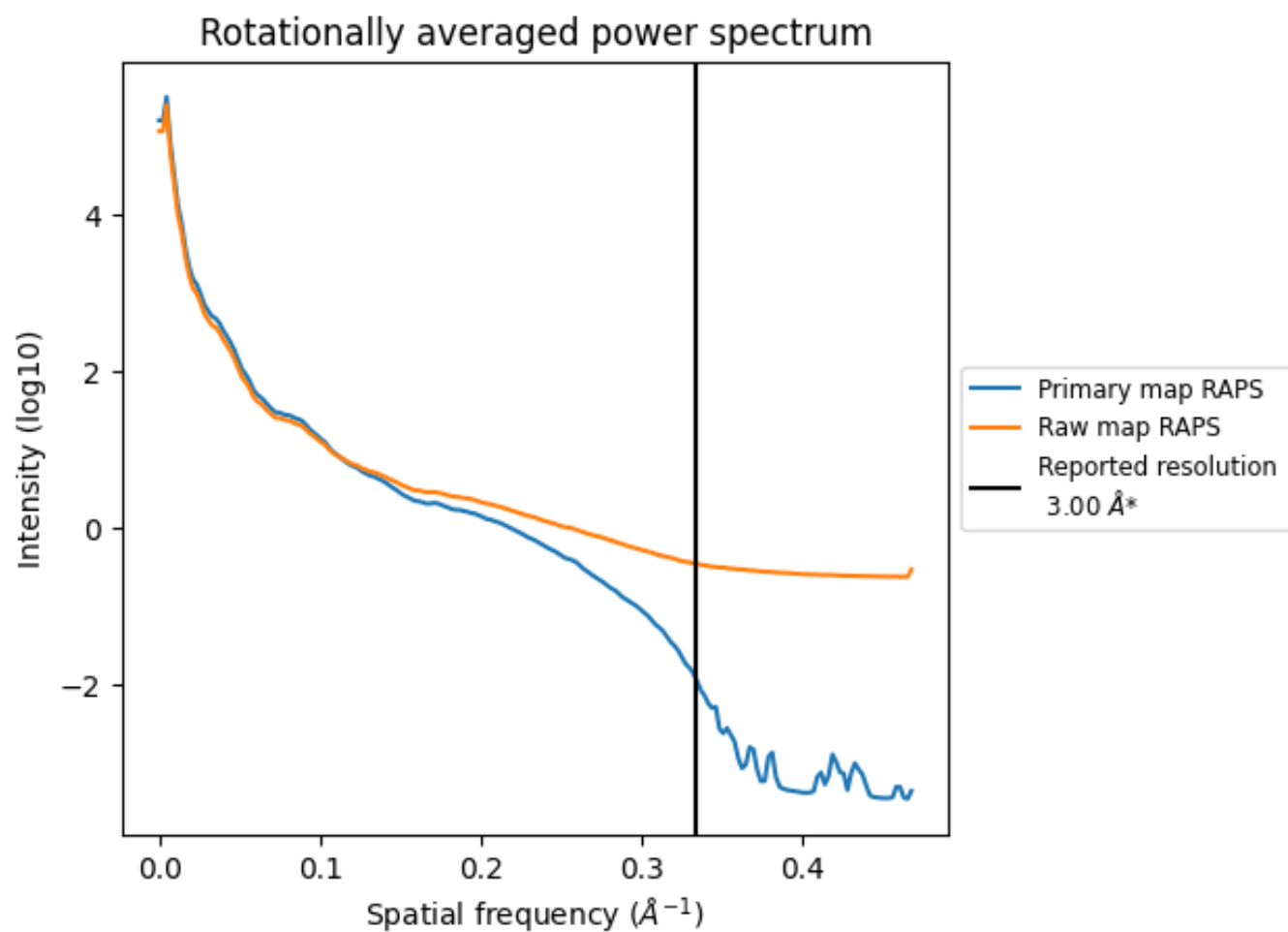
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1958 nm^3 ; this corresponds to an approximate mass of 1769 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

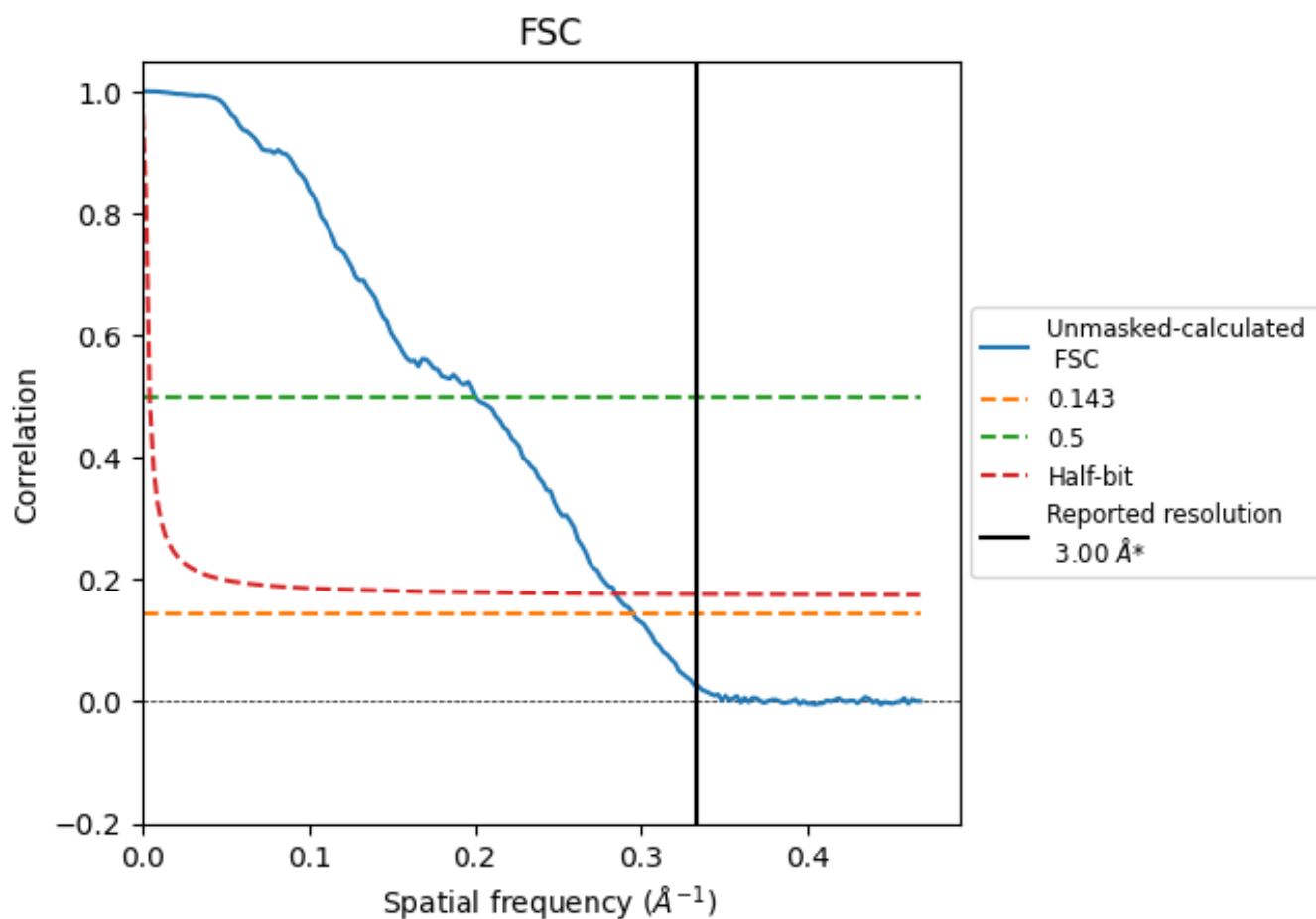


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

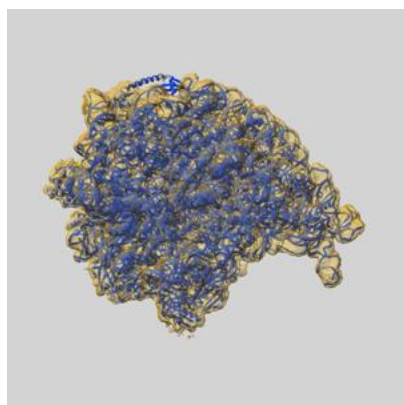
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	4.99	3.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 3.0 by more than 10 %

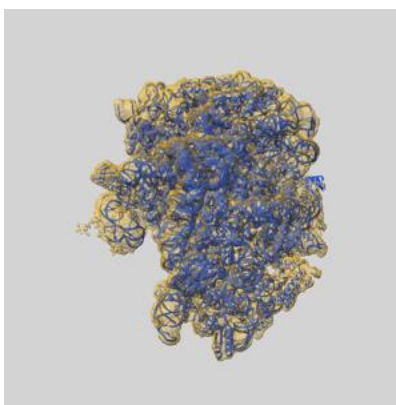
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12928 and PDB model 7OIF. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

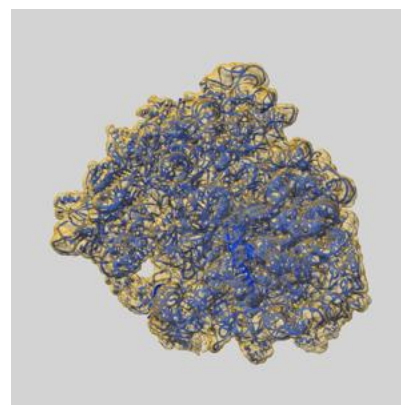
9.1 Map-model overlay [i](#)



X



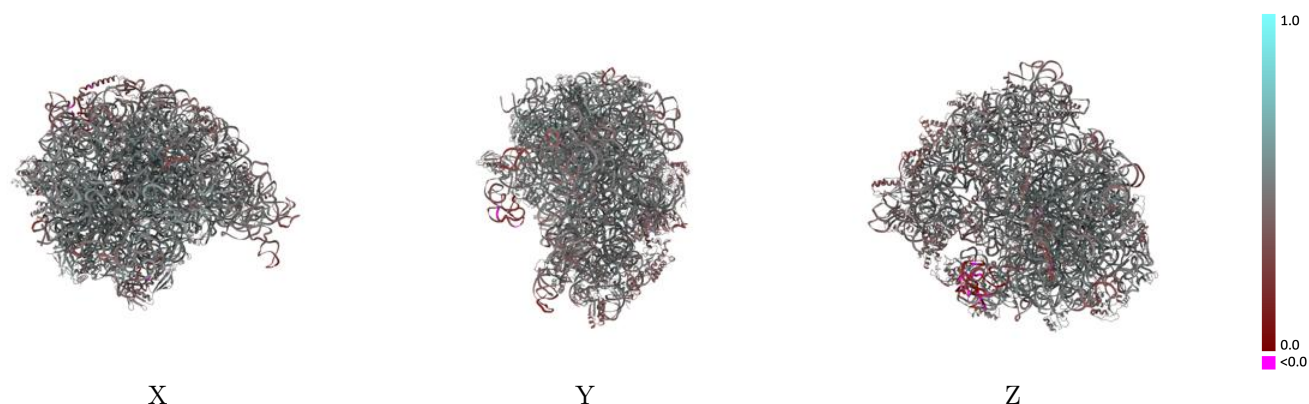
Y



Z

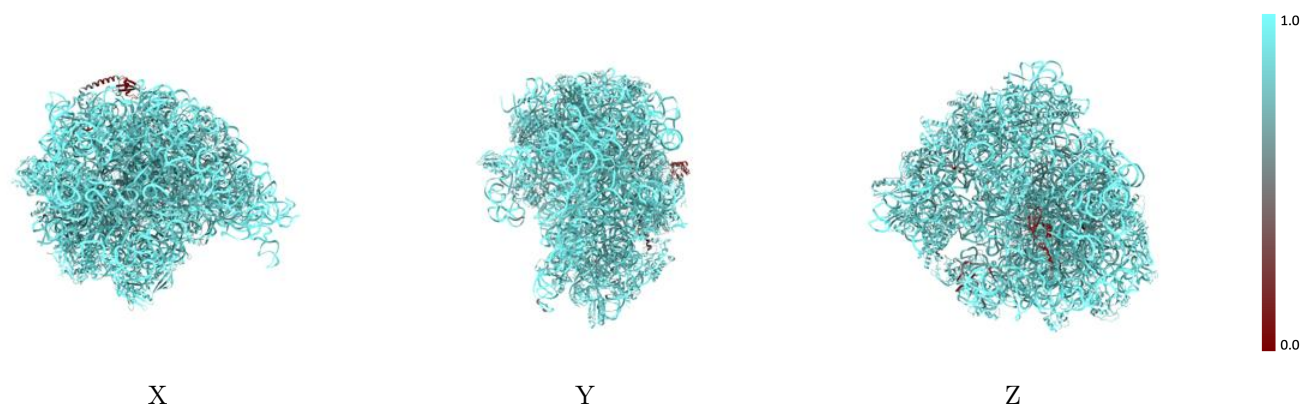
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



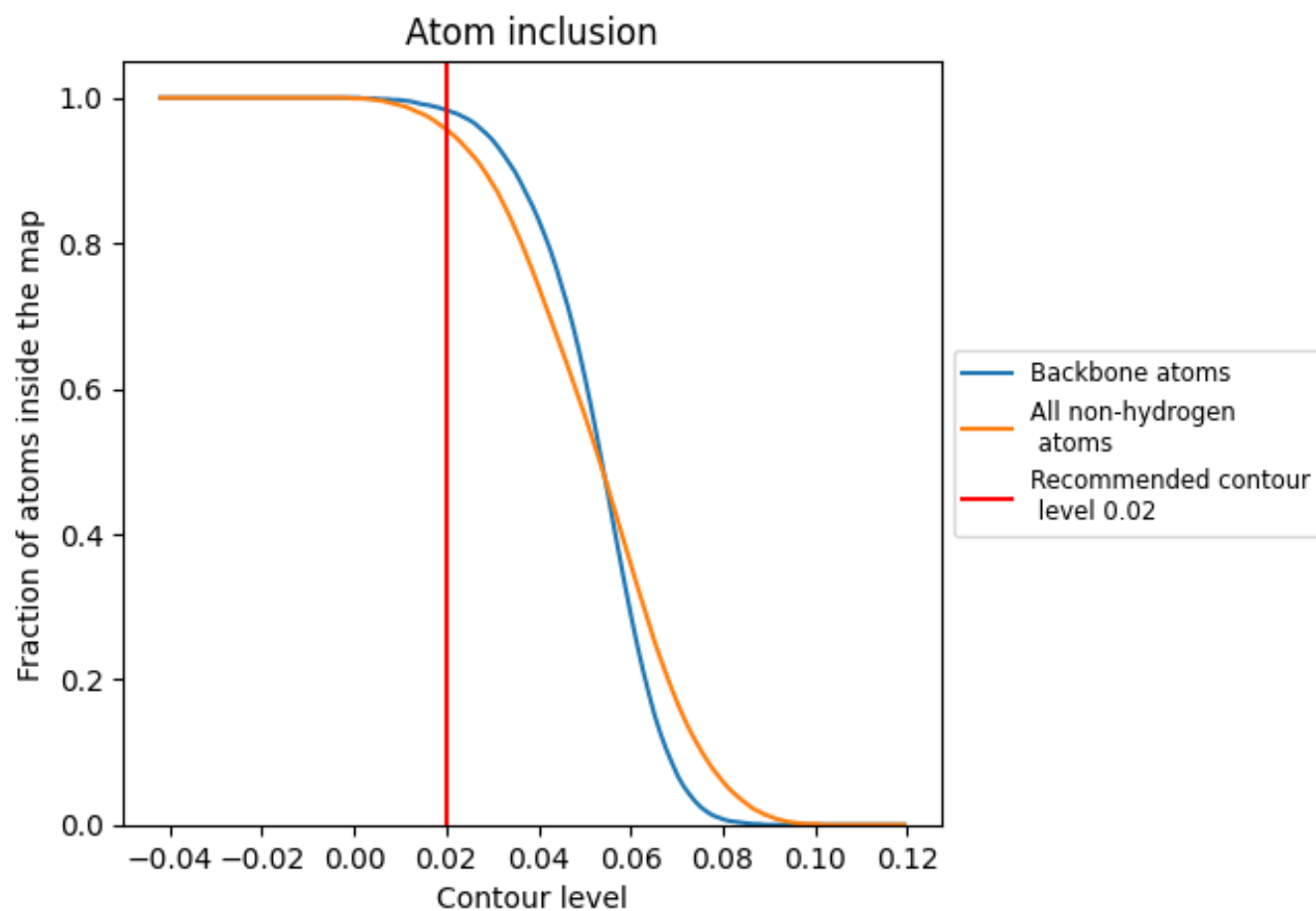
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.4680
1	 0.9860	 0.4780
2	 0.9950	 0.4720
3	 0.9970	 0.4700
4	 0.9610	 0.4570
B	 0.6130	 0.3050
C	 0.9030	 0.5150
D	 0.9140	 0.5060
E	 0.9070	 0.4720
F	 0.8940	 0.4250
G	 0.9250	 0.4350
H	 0.3850	 0.3300
I	 0.9120	 0.4930
J	 0.8570	 0.4940
K	 0.9190	 0.4880
L	 0.8940	 0.4910
M	 0.9400	 0.4950
N	 0.9370	 0.4470
O	 0.8740	 0.4830
P	 0.9350	 0.4840
Q	 0.9130	 0.4970
R	 0.8680	 0.4890
S	 0.8920	 0.4620
T	 0.9050	 0.4590
U	 0.8980	 0.4610
V	 0.8750	 0.5030
W	 0.9030	 0.4810
X	 0.8770	 0.4050
Y	 0.8940	 0.4750
Z	 0.8830	 0.3910
a	 0.8860	 0.4900
b	 0.8350	 0.4750
c	 0.9070	 0.5070
d	 0.9100	 0.5260
e	 0.9250	 0.5010



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Chain	Atom inclusion	Q-score
f	 0.8640	 0.3940
g	 0.8920	 0.4370
h	 0.8970	 0.4320
i	 0.9080	 0.4670
j	 0.8890	 0.4330
k	 0.8830	 0.4020
l	 0.8870	 0.4600
m	 0.9130	 0.4280
n	 0.8540	 0.4100
o	 0.9040	 0.4500
p	 0.8480	 0.4820
q	 0.9090	 0.4260
r	 0.9170	 0.4490
s	 0.9060	 0.4410
t	 0.9440	 0.4620
u	 0.8810	 0.4470
v	 0.9040	 0.4400
w	 0.9160	 0.4380
x	 0.9280	 0.4340
y	 0.7140	 0.3730
z	 0.9760	 0.4220