Full wwPDB EM Validation Report (i)

Sep 16, 2026 – 07:56 PM EDT

PDB ID	:	8EIU / pdb_00008eiu
EMDB ID	:	EMD-28165
Title	:	E. coli 70S ribosome with A-loop mutations U2554C and U2555C
Authors	:	Nissley, A.J.; Penev, P.I.; Watson, Z.L.; Banfield, J.F.; Cate, J.H.D.
Deposited on	:	2022-09-15
Resolution	:	2.24 Å(reported)
Based on initial model	:	7K00

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

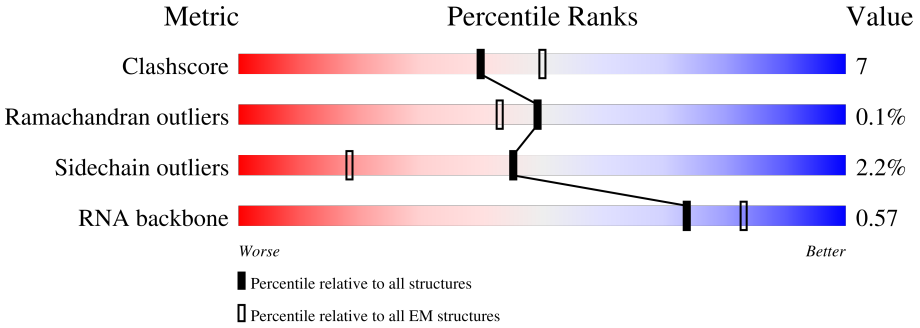
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

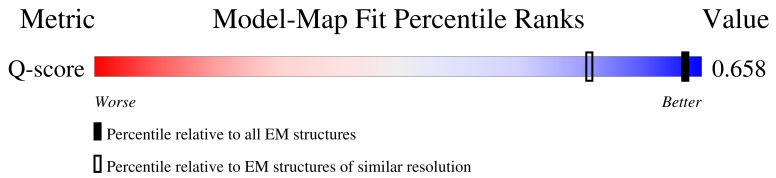
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.24 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	3381 (1.75 - 2.74)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	16% 69% 24% 7%
2	1	46	• 89% 11%
3	2	65	• 91% 8% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	13% 79% 21%
5	4	70	74% 40% 40% 6% 14%
6	A	1542	10% 58% 36% 5% •
7	B	241	80% 62% 30% • 7%
8	C	233	20% 75% 13% 12%
9	D	206	16% 82% 17%
10	E	167	6% 77% 17% 7%
11	F	135	24% 49% 27% • 24%
12	G	179	36% 61% 23% • 15%
13	H	130	5% 84% 15% •
14	I	130	31% 74% 23% • •
15	J	103	55% 63% 30% • 5%
16	K	129	16% 72% 19% 9%
17	L	124	6% 92% 7% •
18	M	118	19% 79% 17% • •
19	N	101	13% 84% 15% •
20	O	89	13% 87% 11% • •
21	P	82	12% 79% 18% • •
22	Q	84	14% 76% 18% 6%
23	R	75	21% 68% 20% 12%
24	S	92	22% 66% 25% 9%
25	T	87	15% 82% 17% •
26	U	71	61% 77% 21% •
27	X	27	11% 33% 7% • 56%
28	Y	75	64% 33% 47% 19% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	Z	75	15% 53% 39% 7%
29	a	2904	8% 63% 29% 5%
30	b	120	8% 62% 33%
31	c	273	85% 14%
32	d	209	6% 91% 9%
33	e	201	25% 82% 17%
34	f	179	48% 60% 39%
35	g	177	72% 69% 27%
36	h	149	23% 19% 8% 72%
37	i	142	7% 84% 16%
38	j	123	89% 11%
39	k	144	12% 86% 12%
40	l	136	84% 16%
41	m	127	83% 10% 7%
42	n	117	20% 79% 19%
43	o	115	10% 83% 16%
44	p	118	84% 14%
45	q	103	22% 85% 15%
46	r	110	5% 80% 19%
47	s	100	15% 78% 15% 7%
48	t	104	30% 74% 24%
49	u	94	27% 87% 12%
50	v	85	9% 88% 11%
51	w	78	12% 78% 21%
52	x	63	43% 87% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	y	59	8% 86% 12%
54	z	57	7% 74% 25%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 148825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	51	417	269	76	72	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	46	377	228	90	57	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	302	185	65	48	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	60	480	299	90	85	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	1519	32612	14552	5986	10555	1519	0	0

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	224	1753	1109	315	321	8	0	0

- Molecule 8 is a protein called 30S ribosomal protein S3.

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

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

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

- Molecule 11 is a protein called 30S ribosomal protein S6.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	153	1203	750	231	218	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

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

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	R	66	544	345	102	96	1	0	0

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	84	668	427	127	112	2	0	0

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

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

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	X	12	260	117	51	80	12	0	0

- Molecule 28 is a RNA chain called tRNA-fMET.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	Y	74	1581	704	287	516	74	0	0
28	Z	74	1581	704	287	516	74	0	0

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	a	2753	59130	26384	10899	19094	2753	0	0

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	b	119	2549	1135	466	829	119	0	0

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

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

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	41	303	194	54	54	1	0	0

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A0A7U9B8R8

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	v	84	628	388	126	113	1	0	0

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

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

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

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

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

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

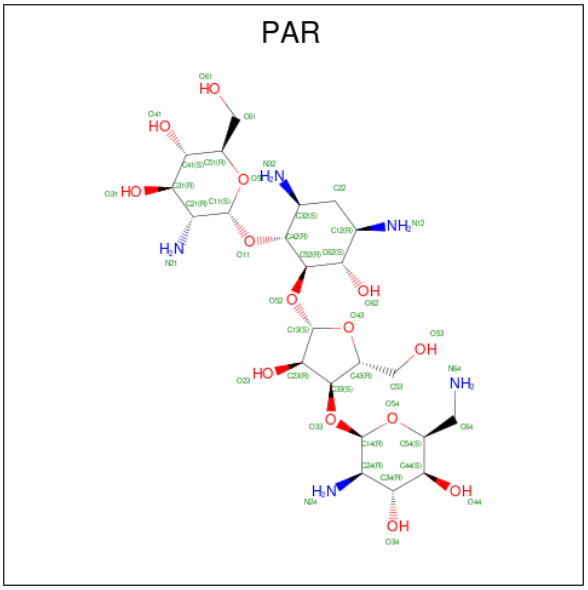
- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	3	1	1	1	0
			Total	Zn	
55	4	1	1	1	0

- Molecule 56 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
56	A	1	42	23	5	14	0

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

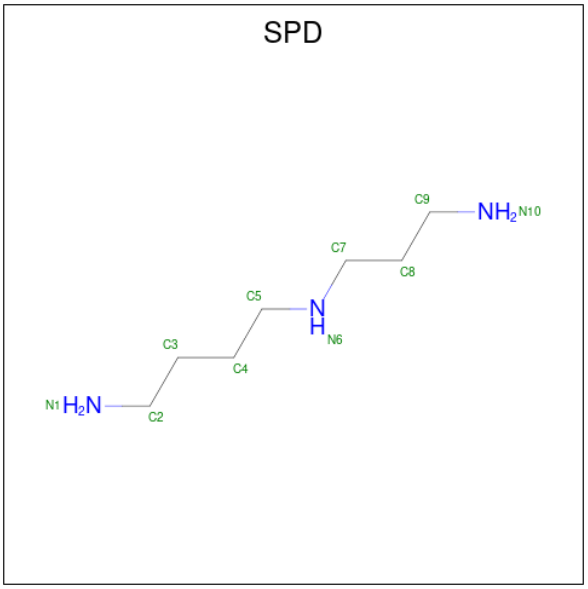
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	A	67	67	67	0
			Total	Mg	
57	N	1	1	1	0
			Total	Mg	
57	X	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	a	190	190	190	0
			Total	Mg	
57	b	5	5	5	0
			Total	Mg	
57	c	1	1	1	0
			Total	Mg	
57	d	1	1	1	0
			Total	Mg	
57	p	1	1	1	0
			Total	Mg	
57	z	1	1	1	0

- Molecule 58 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



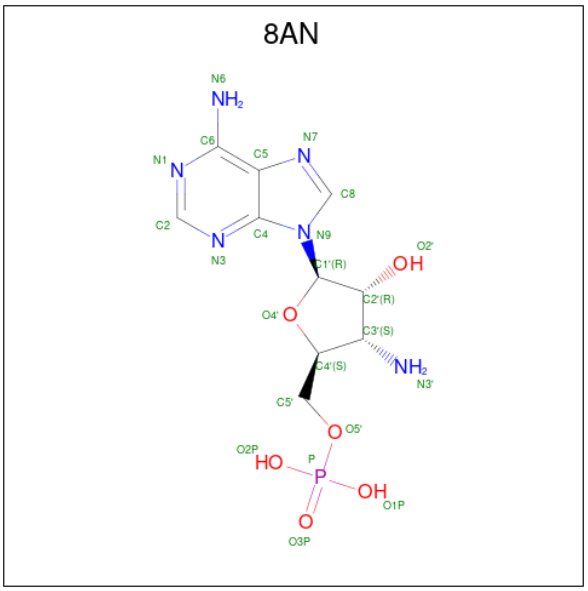
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
58	A	1	10	7	3	0
			Total	C	N	
58	A	1	10	7	3	0
			Total	C	N	
58	a	1	10	7	3	0
			Total	C	N	
58	a	1	10	7	3	0
			Total	C	N	
58	a	1	10	7	3	0

Continued on next page...

Continued from previous page...

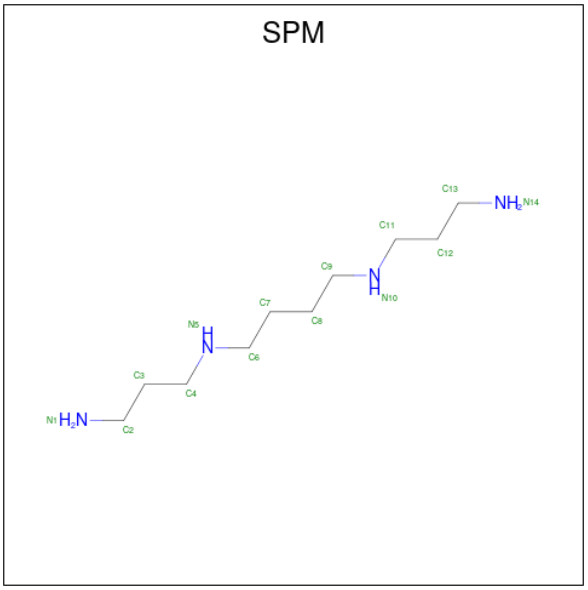
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0
58	a	1	10	7	3	0

- Molecule 59 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (CCD ID: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



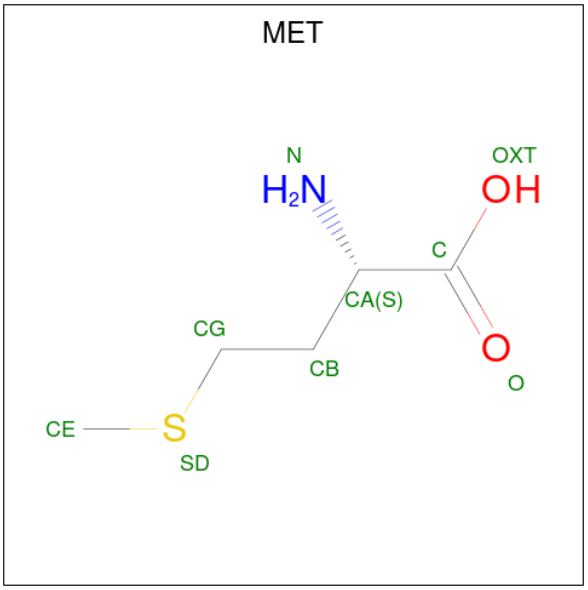
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	Y	1	22	10	6	5	1	0
			Total	C	N	O	P	
59	Z	1	22	10	6	5	1	0

- Molecule 60 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
60	a	1	14	10	4	0

- Molecule 61 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
61	a	1	8	5	1	1	1	0
			Total	C	N	O	S	
61	a	1	8	5	1	1	1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	0	11	11	11	0
			Total	O	
62	1	27	27	27	0
			Total	O	
62	2	27	27	27	0
			Total	O	
62	3	3	3	3	0
			Total	O	
62	4	3	3	3	0
			Total	O	
62	A	1860	1860	1860	0
			Total	O	
62	B	1	1	1	0
			Total	O	
62	C	42	42	42	0
			Total	O	
62	D	14	14	14	0
			Total	O	
62	E	15	15	15	0
			Total	O	
62	G	4	4	4	0
			Total	O	
62	H	23	23	23	0
			Total	O	
62	I	22	22	22	0
			Total	O	
62	J	18	18	18	0
			Total	O	
62	K	12	12	12	0
			Total	O	
62	L	25	25	25	0
			Total	O	
62	M	16	16	16	0
			Total	O	
62	N	38	38	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
62	O	12	Total O 12 12	0
62	P	11	Total O 11 11	0
62	Q	3	Total O 3 3	0
62	R	1	Total O 1 1	0
62	S	25	Total O 25 25	0
62	T	1	Total O 1 1	0
62	U	3	Total O 3 3	0
62	X	12	Total O 12 12	0
62	Y	6	Total O 6 6	0
62	Z	8	Total O 8 8	0
62	a	3758	Total O 3758 3758	0
62	b	167	Total O 167 167	0
62	c	95	Total O 95 95	0
62	d	40	Total O 40 40	0
62	e	52	Total O 52 52	0
62	f	34	Total O 34 34	0
62	h	5	Total O 5 5	0
62	i	14	Total O 14 14	0
62	j	13	Total O 13 13	0
62	k	51	Total O 51 51	0
62	l	28	Total O 28 28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	m	34	34	34	0
			Total	O	
62	n	39	39	39	0
			Total	O	
62	o	10	10	10	0
			Total	O	
62	p	32	32	32	0
			Total	O	
62	q	22	22	22	0
			Total	O	
62	r	26	26	26	0
			Total	O	
62	s	9	9	9	0
			Total	O	
62	t	3	3	3	0
			Total	O	
62	u	5	5	5	0
			Total	O	
62	v	20	20	20	0
			Total	O	
62	w	22	22	22	0
			Total	O	
62	x	2	2	2	0
			Total	O	
62	y	7	7	7	0
			Total	O	
62	z	25	25	25	0

3 Residue-property plots (i)

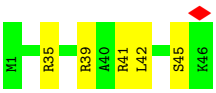
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 50S ribosomal protein L33

Chain 0:

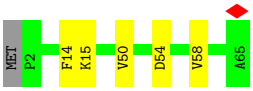
- Molecule 2: 50S ribosomal protein L34

Chain 1:



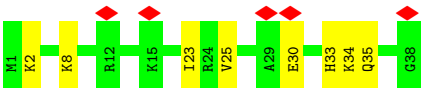
- Molecule 3: 50S ribosomal protein L35

Chain 2:



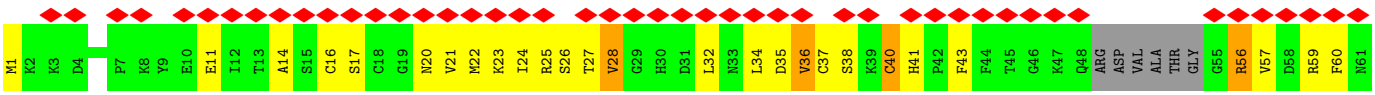
- Molecule 4: 50S ribosomal protein L36

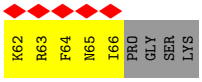
Chain 3:



- Molecule 5: 50S ribosomal protein L31

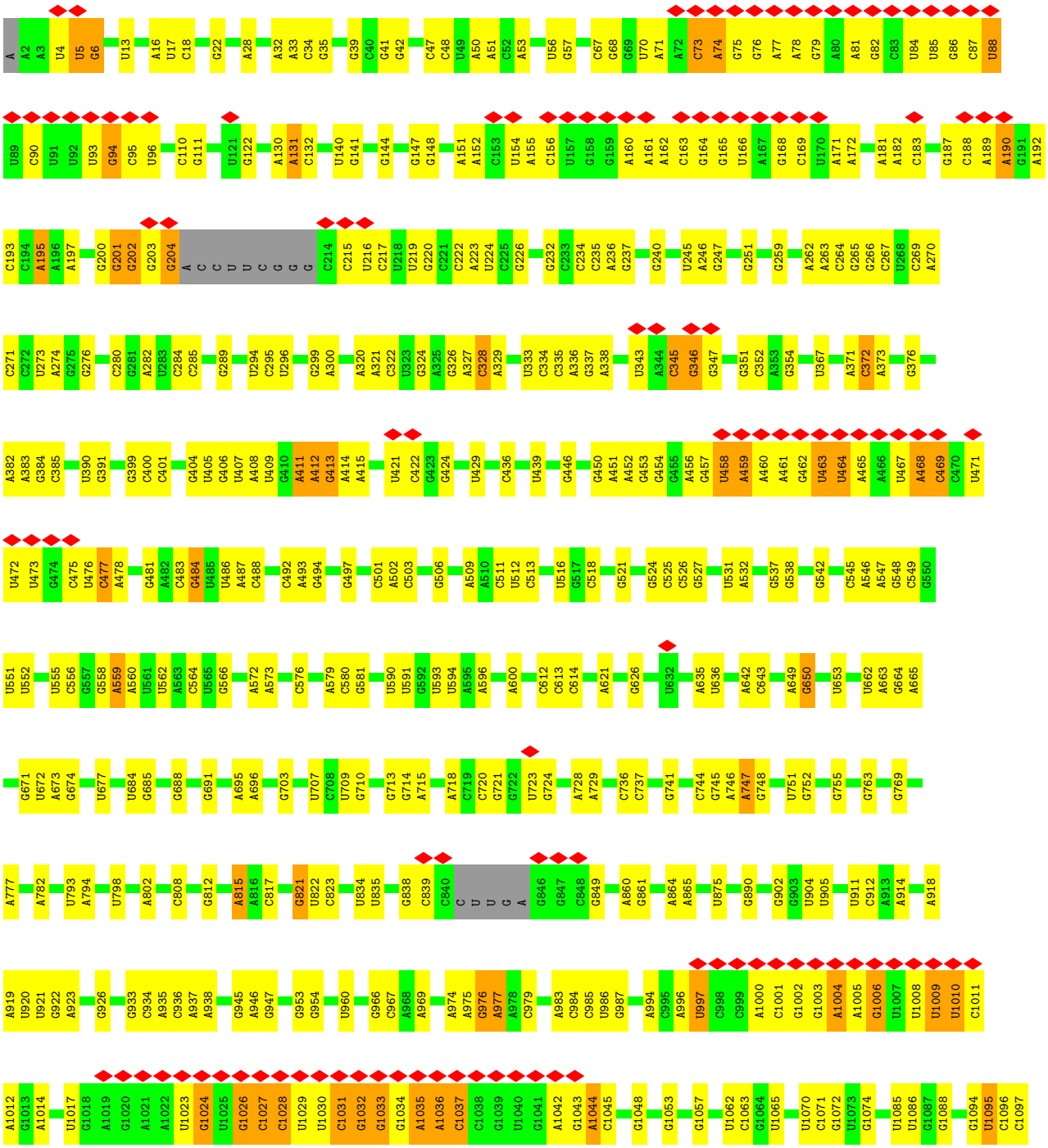
Chain 4:

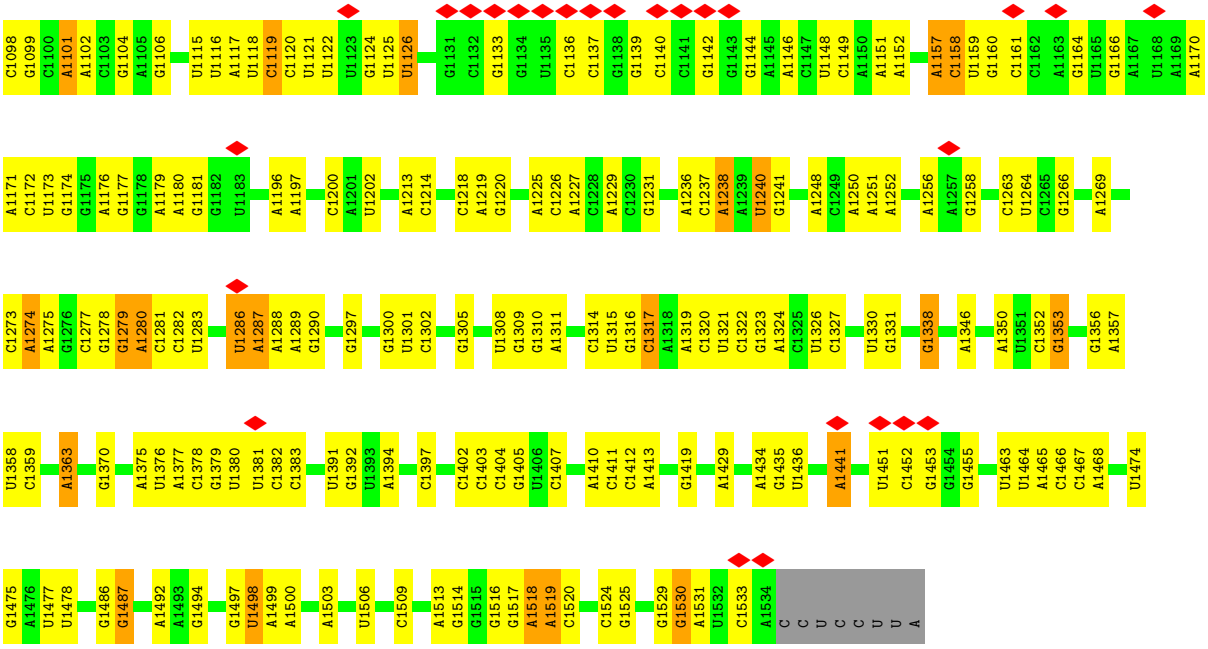




• Molecule 6: 16S rRNA

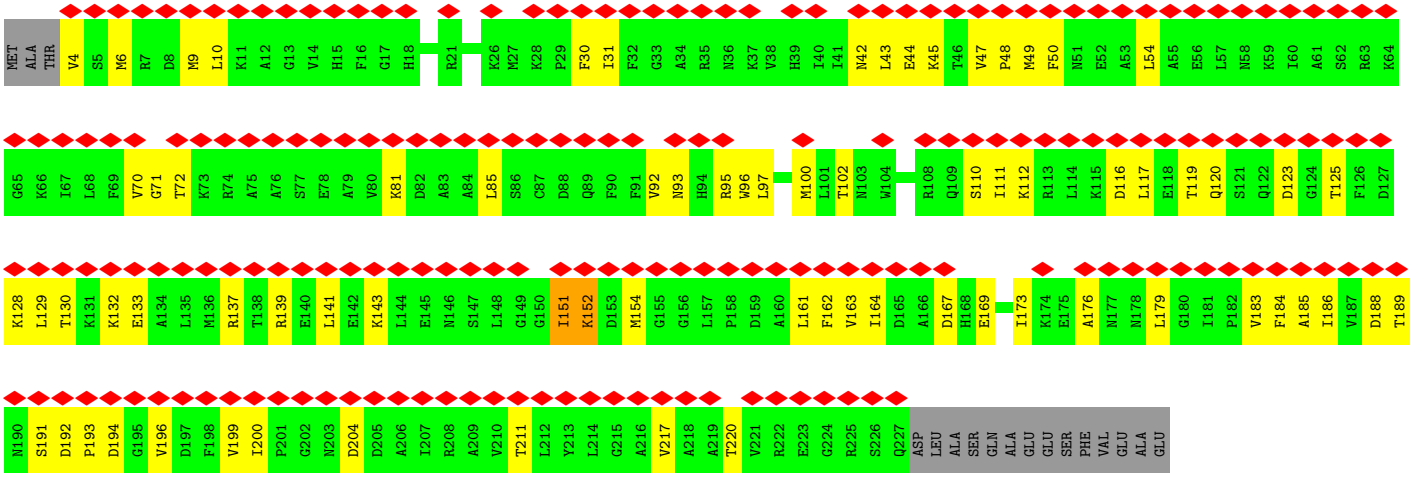
Chain A:





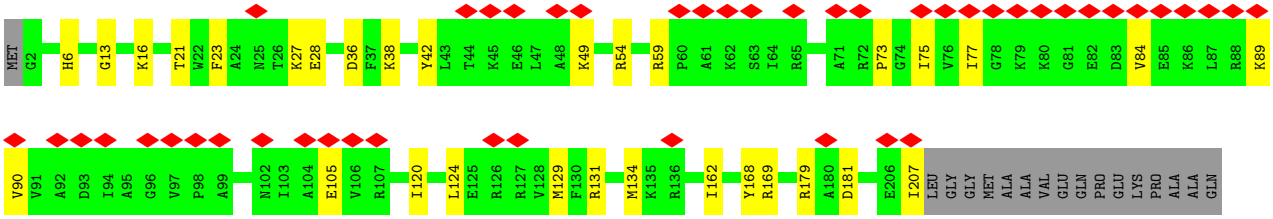
- Molecule 7: 30S ribosomal protein S2

Chain B:



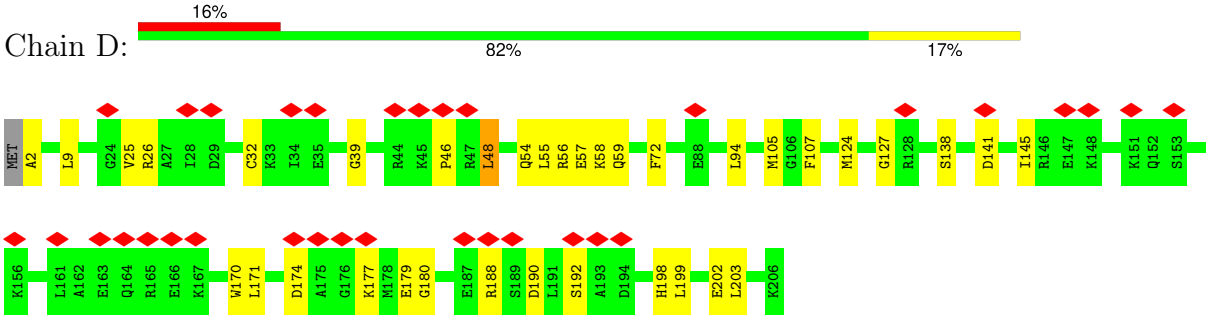
- Molecule 8: 30S ribosomal protein S3

Chain C:



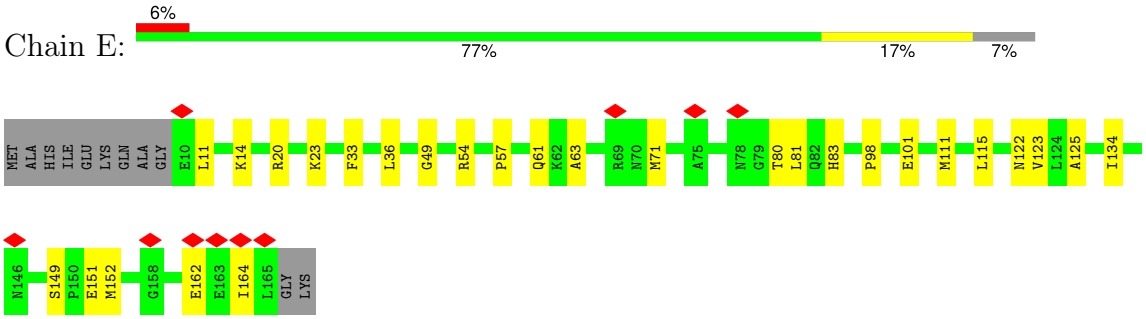
- Molecule 9: 30S ribosomal protein S4

Chain D:



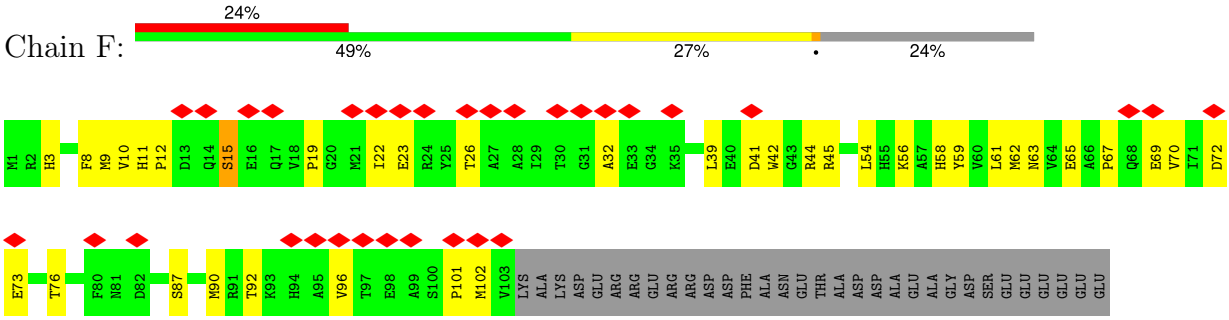
- Molecule 10: 30S ribosomal protein S5

Chain E:



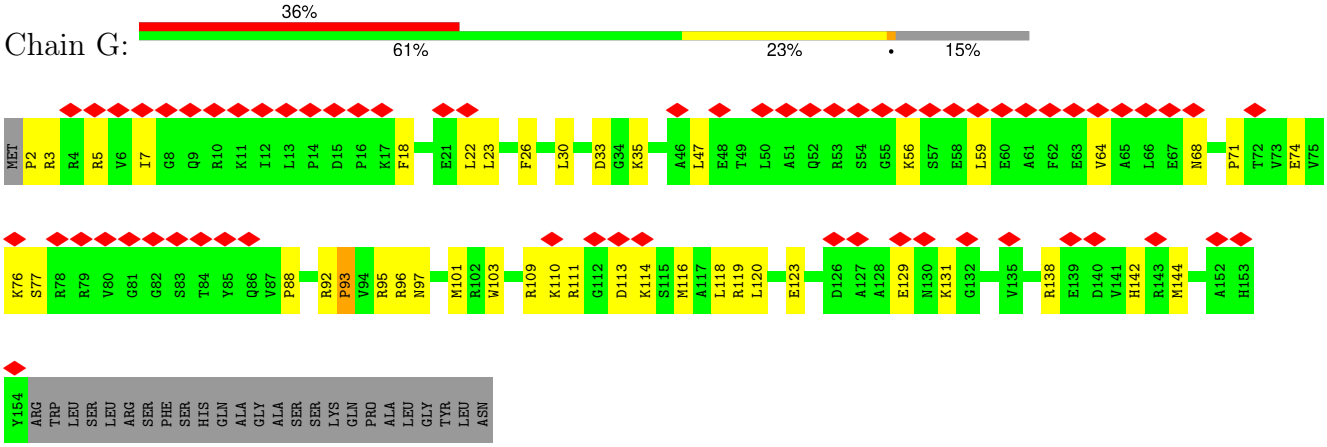
- Molecule 11: 30S ribosomal protein S6

Chain F:



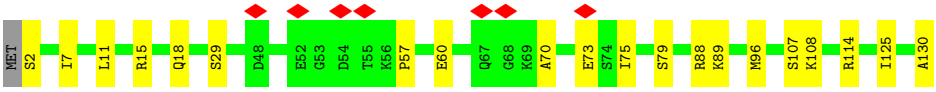
- Molecule 12: 30S ribosomal protein S7

Chain G:



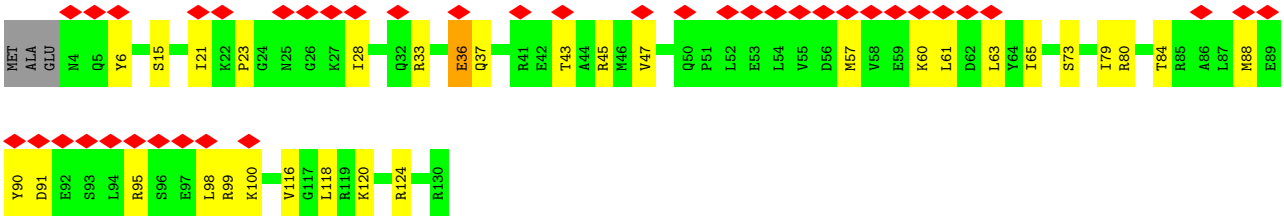
- Molecule 13: 30S ribosomal protein S8

Chain H:



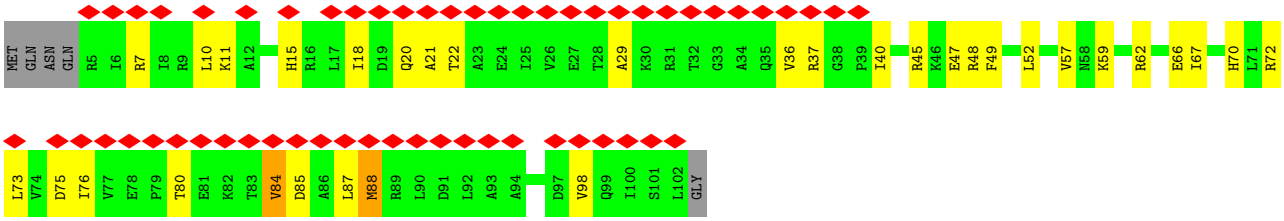
- Molecule 14: 30S ribosomal protein S9

Chain I:



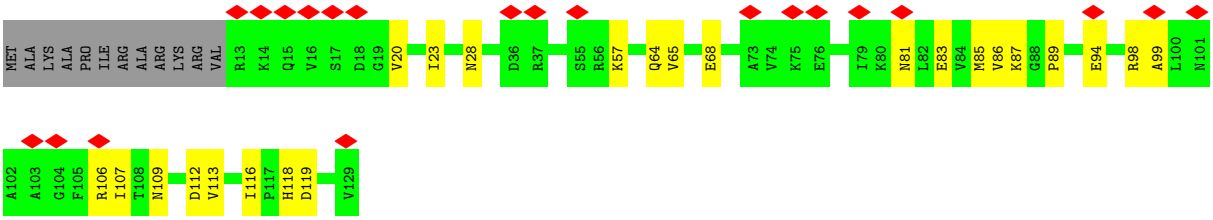
- Molecule 15: 30S ribosomal protein S10

Chain J:



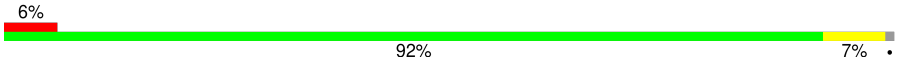
- Molecule 16: 30S ribosomal protein S11

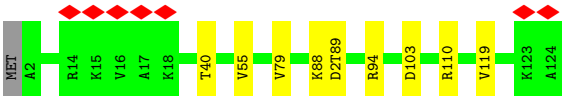
Chain K:



- Molecule 17: 30S ribosomal protein S12

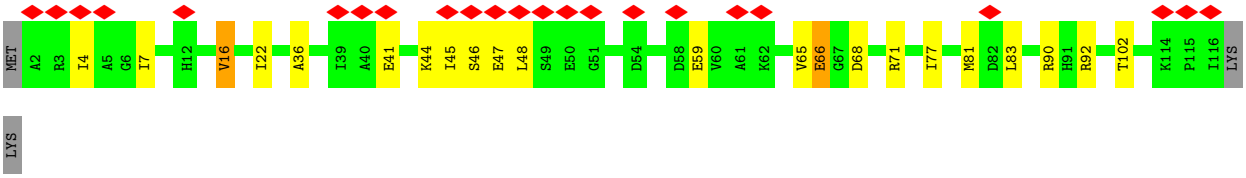
Chain L:





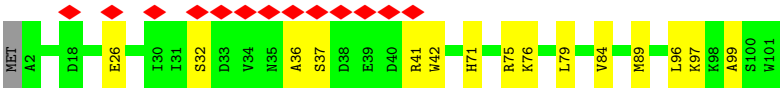
- Molecule 18: 30S ribosomal protein S13

Chain M:



- Molecule 19: 30S ribosomal protein S14

Chain N:

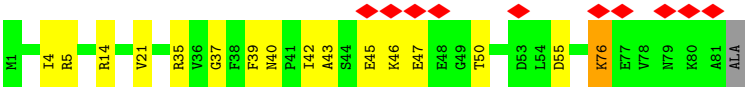


- Molecule 20: 30S ribosomal protein S15

Chain O:

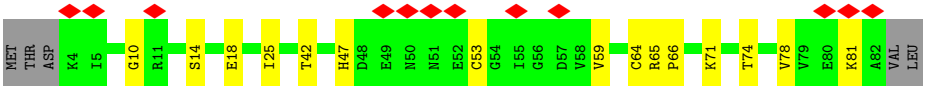
- Molecule 21: 30S ribosomal protein S16

Chain P:



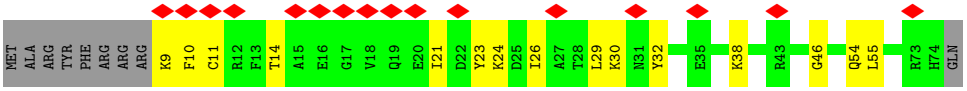
- Molecule 22: 30S ribosomal protein S17

Chain Q:



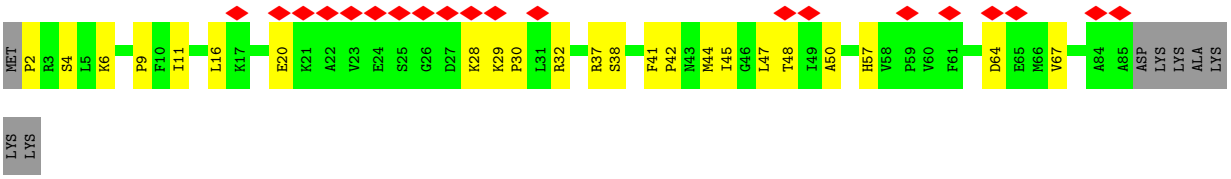
- Molecule 23: 30S ribosomal protein S18

Chain R:



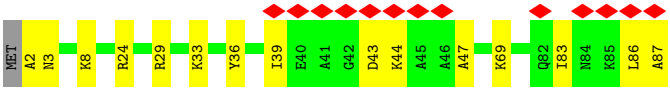
- Molecule 24: 30S ribosomal protein S19

Chain S:



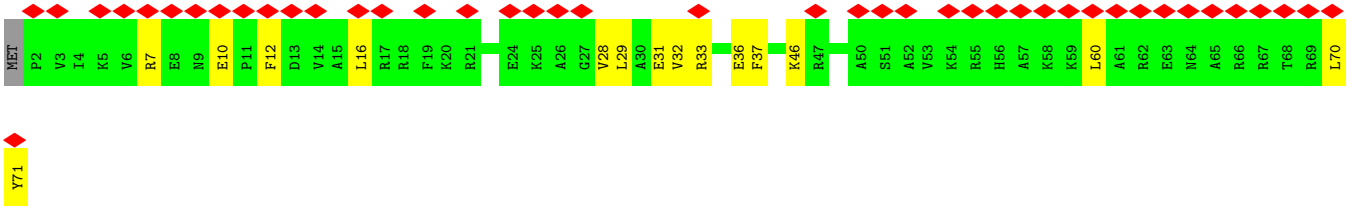
• Molecule 25: 30S ribosomal protein S20

Chain T:



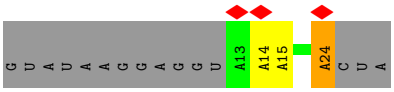
• Molecule 26: 30S ribosomal protein S21

Chain U:



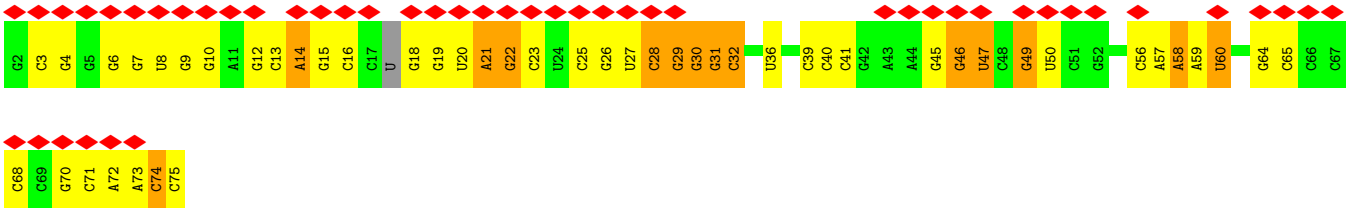
• Molecule 27: mRNA

Chain X:



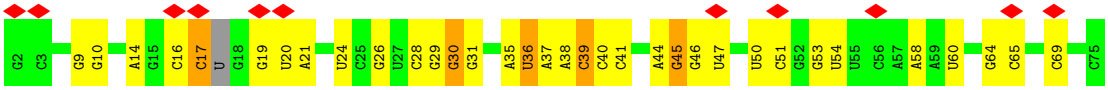
• Molecule 28: tRNA-fMET

Chain Y:



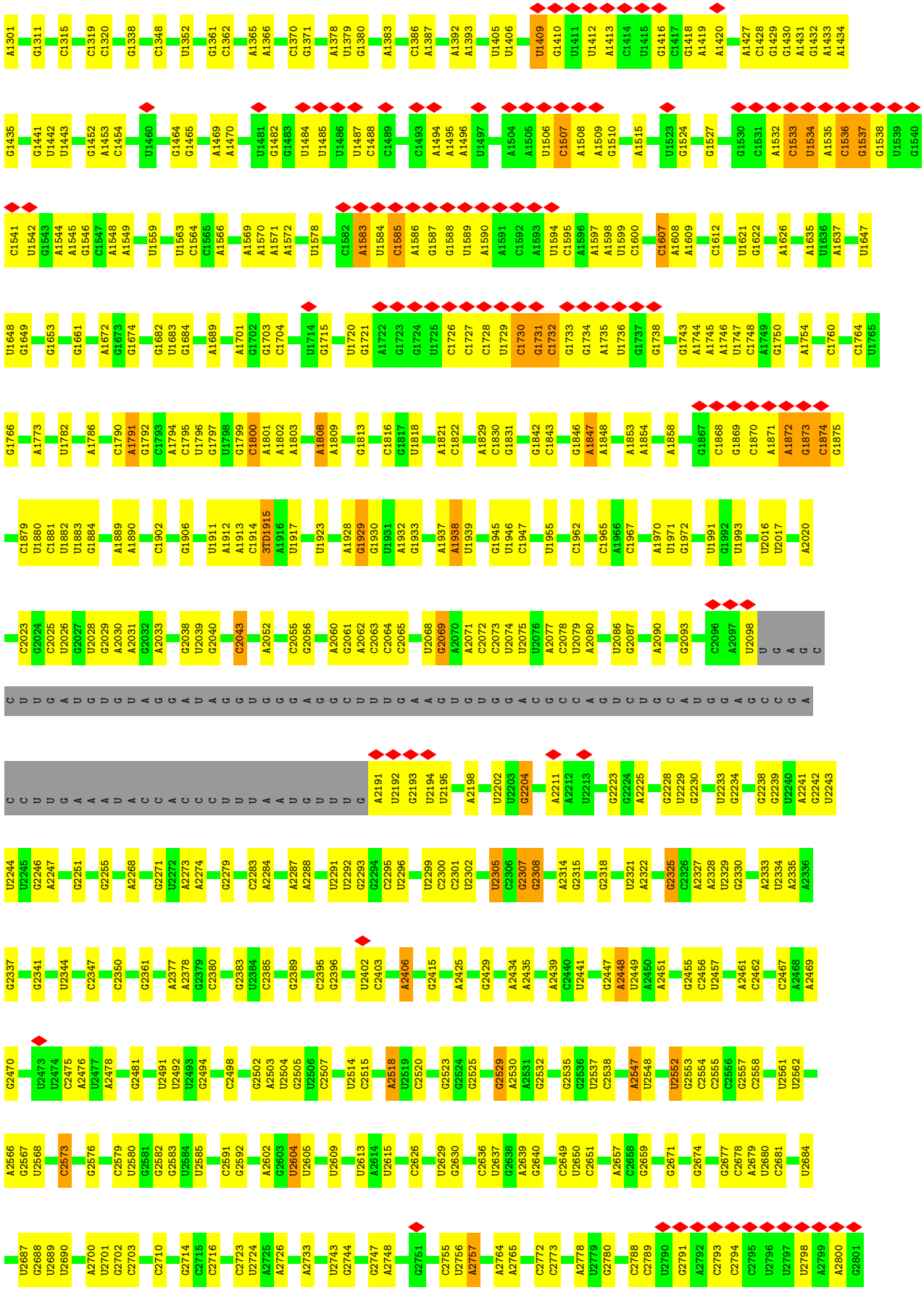
• Molecule 28: tRNA-fMET

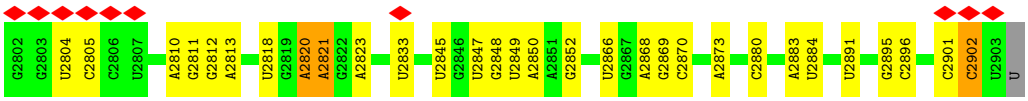
Chain Z:



- Molecule 29: 23S rRNA

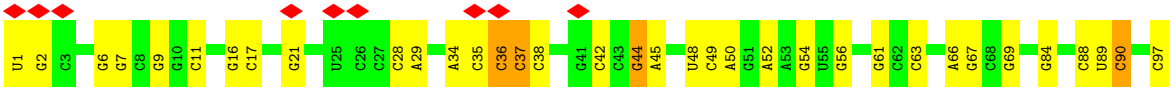
Chain a:

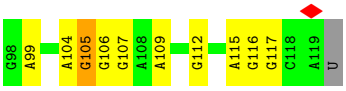

A1301 G1311 C1315 C1319 C1320 G1338 C1348 U1352 G1361 C1362 A1365 A1366 C1370 G1371 A1378 U1379 G1380 A1383 C1386 A1387 A1392 A1393 U1405 U1406 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434
G1435 G1441 U1442 U1443 G1452 A1453 C1454 U1460 G1464 G1465 A1469 A1470 U1481 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 C1493 A1494 A1495 A1496 U1497 A1504 A1505 U1506 C1507 A1508 A1509 G1510 A1515 U1523 G1524 G1527 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540
C1541 U1542 G1543 A1544 A1545 G1546 C1547 A1548 A1549 U1559 U1563 C1564 C1565 A1566 A1569 A1570 A1571 A1572 U1578 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1598 U1599 C1600 C1607 A1608 A1609 C1612 U1621 G1622 A1626 A1635 U1636 A1637 U1647
U1648 G1649 G1653 G1661 A1672 G1673 G1674 G1682 U1683 G1684 A1689 A1701 G1702 G1703 C1704 U1714 G1715 U1720 G1721 A1722 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 G1743 A1744 A1745 A1746 U1747 C1748 A1749 G1750 A1754 C1760 C1764 U1765
G1766 A1773 U1782 A1786 C1790 A1791 G1792 C1793 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 A1808 A1809 G1813 C1816 G1817 U1818 A1821 C1822 A1829 C1830 G1831 G1842 C1843 G1846 A1847 A1848 A1853 A1854 A1858 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875
C1879 U1880 C1881 U1882 U1883 G1884 A1889 A1890 C1902 G1906 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 U1923 A1928 G1929 G1930 U1931 A1932 G1933 A1937 A1938 U1939 G1945 U1946 C1947 U1955 C1962 C1965 A1966 C1967 A1970 U1971 G1972 U1991 G1992 U1993 U2016 U2017 A2020
C2023 G2024 C2025 U2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 G2038 U2039 G2040 C2043 A2052 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2076 A2077 C2078 U2079 A2080 U2086 G2087 A2090 G2093 C2096 A2097 U2098 U G A G C
C C U U U G A U G U G U A G G G A U A G G U G G G G A G G C U U U G A A G U G U G U U G C U U G G A C G G C C A G U C U U G C A U G G A G C C G A
C C U U U G A A A U A C C C A C C C C U U U U A A A U G U U U G A C A G U G U G U G A C G G C C A G U C U U G C A U G G A G C C G A
A2191 U2192 G2193 U2194 U2195 A2198 U2202 U2203 G2204 A2211 A2212 U2213 G2223 G2224 A2225 G2228 U2229 G2230 U2233 G2234 G2238 G2239 U2240 A2241 G2242 U2243
U2244 U2245 G2246 A2247 G2251 G2255 A2268 G2271 U2272 A2273 A2274 G2279 C2283 A2284 A2287 A2288 U2291 U2292 G2293 G2294 C2295 U2296 U2299 C2300 C2301 U2302 U2305 C2306 G2307 G2308 A2314 G2315 G2318 U2321 A2322 G2325 C2326 A2327 A2328 U2329 G2330 A2333 U2334 A2335 A2336
G2337 G2341 U2344 C2347 C2350 G2361 A2377 A2378 G2379 C2380 C2383 U2384 C2385 G2389 C2395 G2396 U2402 C2403 A2406 G2415 A2425 G2429 A2434 A2435 A2439 C2440 U2441 G2447 A2448 U2449 A2450 A2451 G2455 C2456 U2457 A2461 C2462 C2467 A2468 A2469
G2470 U2473 U2474 C2475 A2476 U2477 A2478 G2481 U2491 U2492 U2493 G2494 C2498 G2502 A2503 U2504 G2505 U2506 C2507 U2514 C2515 A2518 U2519 C2520 G2523 G2524 G2525 G2529 A2530 A2531 G2532 G2535 G2536 U2537 C2538 A2547 U2548 U2552 G2553 C2554 C2555 C2556 G2557 C2558 U2561 U2562
A2566 G2567 U2568 C2573 G2576 C2579 U2580 G2581 G2582 G2583 U2584 U2585 C2591 G2592 A2602 G2603 U2604 U2605 U2609 U2613 A2614 U2615 C2626 U2629 G2630 C2636 U2637 G2638 A2639 G2640 C2649 U2650 C2651 A2657 C2658 G2659 G2671 G2674 G2677 C2678 A2679 U2680 C2681 U2684
U2687 G2688 U2689 U2690 A2700 U2701 G2702 C2703 C2710 G2714 C2715 C2716 C2723 U2724 A2725 A2726 A2733 U2743 G2744 G2747 A2748 G2751 C2755 U2756 A2757 A2764 A2765 C2772 C2773 A2778 U2779 G2780 C2788 C2789 U2790 G2791 A2792 C2793 C2794 C2795 U2796 U2797 U2798 A2799 A2800 G2801



- Molecule 30: 5S rRNA

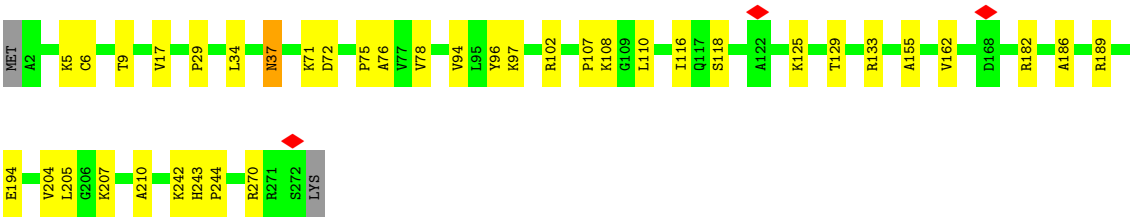
Chain b:





- Molecule 31: 50S ribosomal protein L2

Chain c:

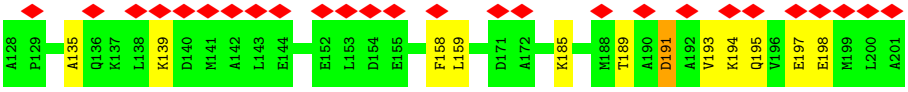


- Molecule 32: 50S ribosomal protein L3

Chain d:

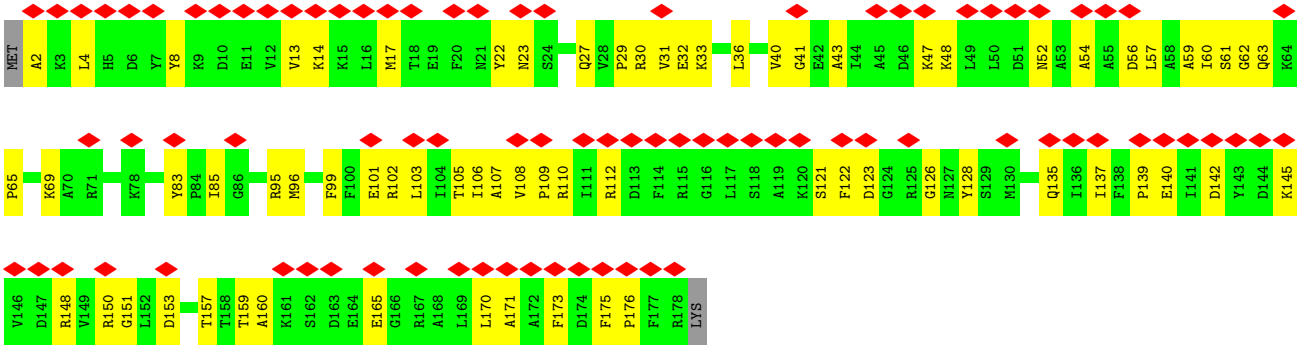
- Molecule 33: 50S ribosomal protein L4

Chain e:



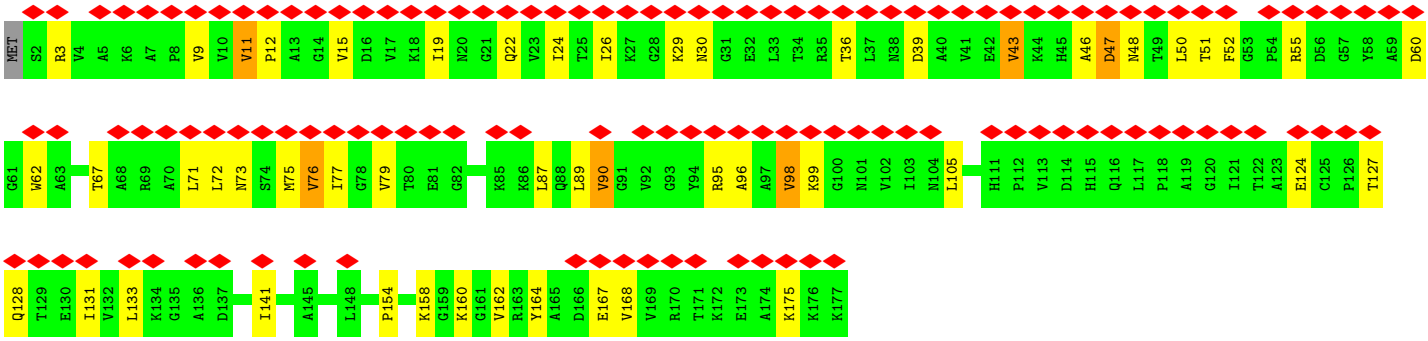
- Molecule 34: 50S ribosomal protein L5

Chain f:



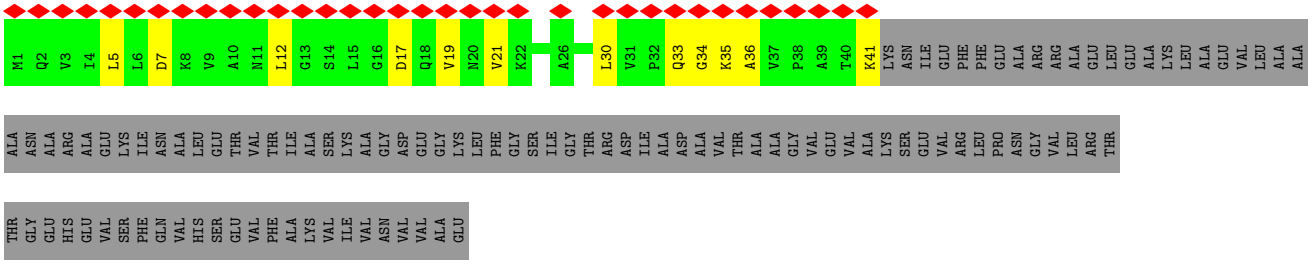
• Molecule 35: 50S ribosomal protein L6

Chain g:



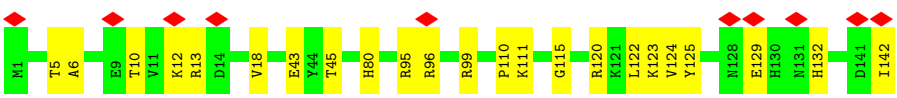
• Molecule 36: 50S ribosomal protein L9

Chain h:



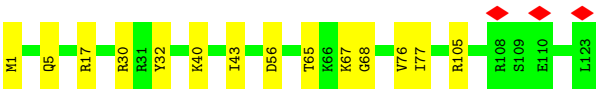
• Molecule 37: 50S ribosomal protein L13

Chain i:



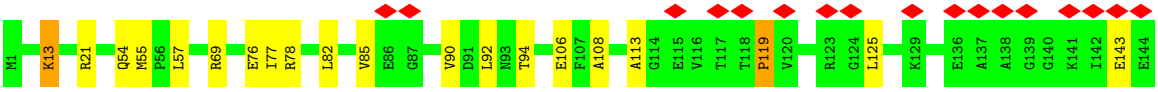
• Molecule 38: 50S ribosomal protein L14

Chain j:



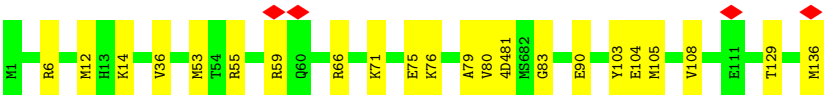
• Molecule 39: 50S ribosomal protein L15

Chain k:



• Molecule 40: 50S ribosomal protein L16

Chain l:

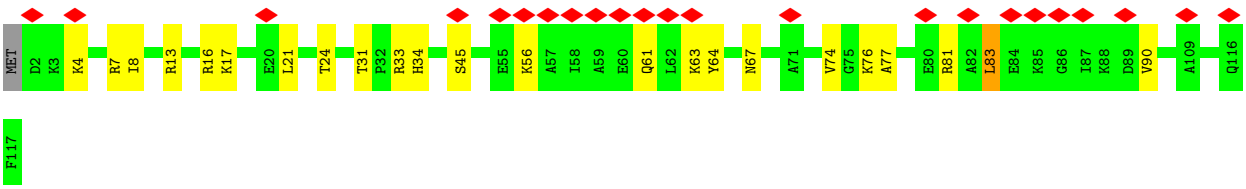


• Molecule 41: 50S ribosomal protein L17

Chain m:

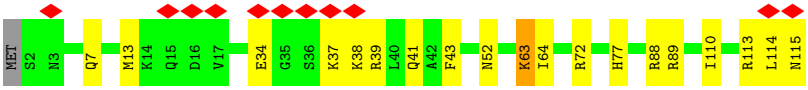
• Molecule 42: 50S ribosomal protein L18

Chain n:



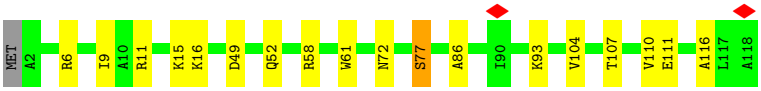
• Molecule 43: 50S ribosomal protein L19

Chain o:



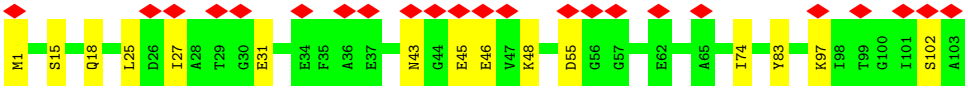
• Molecule 44: 50S ribosomal protein L20

Chain p:



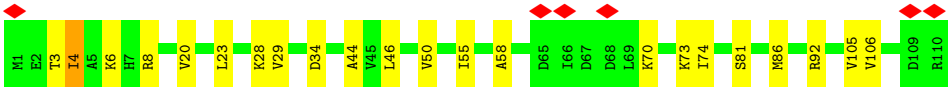
- Molecule 45: Ribosomal protein L21

Chain q:



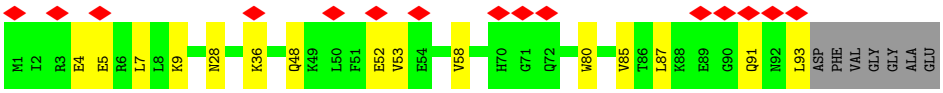
- Molecule 46: 50S ribosomal protein L22

Chain r:



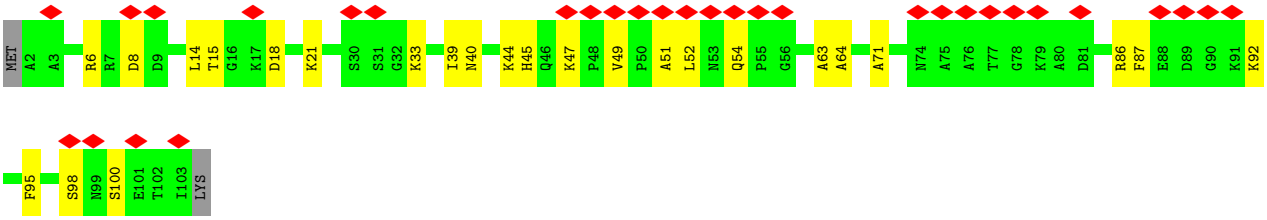
- Molecule 47: 50S ribosomal protein L23

Chain s:



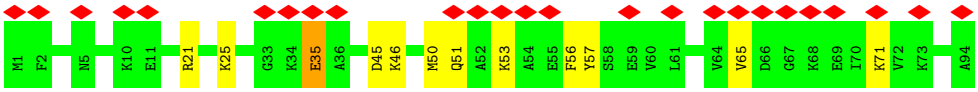
- Molecule 48: 50S ribosomal protein L24

Chain t:



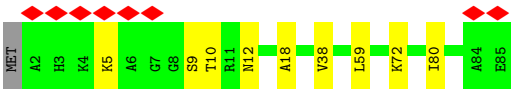
- Molecule 49: 50S ribosomal protein L25

Chain u:



- Molecule 50: 50S ribosomal protein L27

Chain v:

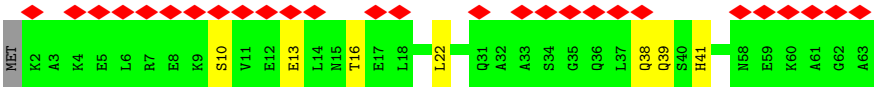


- Molecule 51: 50S ribosomal protein L28

Chain w:

- Molecule 52: 50S ribosomal protein L29

Chain x:

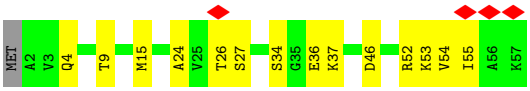


- Molecule 53: 50S ribosomal protein L30

Chain y:

- Molecule 54: 50S ribosomal protein L32

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114493	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.321	Depositor
Minimum map value	-0.132	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0329	Depositor
Map size (Å)	364.276, 364.276, 364.276	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8279, 0.8279, 0.8279	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, 3TD, OMU, 4D4, PAR, OMG, ZN, 2MG, H2U, MEQ, UR3, 5MU, D2T, MG, MS6, SPM, 8AN, IAS, G7M, OMC, PSU, MA6, 4OC, 6MZ, 2MA, 1MG, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	0	0.19	0/424	0.43	0/565
2	1	0.21	0/380	0.43	0/498
3	2	0.22	0/513	0.42	0/676
4	3	0.24	0/303	0.40	0/397
5	4	0.22	0/488	0.53	0/649
6	A	0.18	0/36236	0.35	0/56520
7	B	0.18	0/1784	0.45	0/2403
8	C	0.18	0/1651	0.40	0/2225
9	D	0.17	0/1665	0.41	0/2227
10	E	0.18	0/1165	0.44	0/1568
11	F	0.89	4/858 (0.5%)	1.01	4/1160 (0.3%)
12	G	0.78	3/1219 (0.2%)	1.03	4/1635 (0.2%)
13	H	0.16	0/989	0.39	0/1326
14	I	0.41	1/1034 (0.1%)	0.70	3/1375 (0.2%)
15	J	0.23	0/796	0.56	1/1077 (0.1%)
16	K	0.17	0/884	0.44	0/1191
17	L	0.15	0/960	0.41	0/1286
18	M	0.17	0/900	0.46	1/1204 (0.1%)
19	N	0.17	0/817	0.36	0/1088
20	O	0.17	0/722	0.38	0/964
21	P	0.16	0/653	0.44	0/877
22	Q	0.16	0/650	0.49	0/871
23	R	0.17	0/553	0.44	0/742
24	S	0.23	0/685	0.53	0/922
25	T	0.21	0/676	0.45	0/895
26	U	0.18	0/597	0.45	0/792
27	X	0.17	0/292	0.26	0/453
28	Y	0.19	0/1765	0.39	0/2748
28	Z	0.20	0/1765	0.41	0/2748
29	a	0.26	0/65651	0.39	1/102413 (0.0%)
30	b	0.21	0/2850	0.35	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.23	0/2121	0.42	0/2852
32	d	0.22	0/1576	0.41	0/2119
33	e	0.21	0/1571	0.40	0/2113
34	f	0.22	0/1434	0.48	0/1926
35	g	0.22	0/1343	0.49	0/1816
36	h	0.17	0/306	0.53	0/413
37	i	0.21	0/1152	0.39	0/1551
38	j	0.23	0/955	0.42	0/1279
39	k	0.24	0/1062	0.49	0/1413
40	l	0.22	0/1073	0.39	0/1433
41	m	0.24	0/958	0.45	0/1281
42	n	0.20	0/902	0.43	0/1209
43	o	0.22	0/929	0.40	0/1242
44	p	0.23	0/960	0.39	0/1278
45	q	0.21	0/829	0.38	0/1107
46	r	0.22	0/864	0.38	0/1156
47	s	0.21	0/744	0.47	0/994
48	t	0.22	0/787	0.51	0/1051
49	u	0.20	0/766	0.42	0/1025
50	v	0.20	0/636	0.44	0/841
51	w	0.19	0/635	0.40	0/848
52	x	0.21	0/502	0.38	0/667
53	y	0.20	0/453	0.39	0/605
54	z	0.22	0/450	0.38	0/599
All	All	0.24	8/152933 (0.0%)	0.41	14/228757 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	N	0	1
35	g	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	93	PRO	CG-CD	-23.00	0.72	1.50
11	F	101	PRO	CG-CD	-22.48	0.74	1.50
14	I	23	PRO	CG-CD	-9.88	1.17	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	93	PRO	N-CD	8.73	1.59	1.47
11	F	101	PRO	CB-CG	8.13	1.90	1.49
12	G	93	PRO	CB-CG	6.66	1.82	1.49
11	F	67	PRO	CG-CD	-5.86	1.30	1.50
11	F	101	PRO	N-CD	5.53	1.55	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	93	PRO	N-CD-CG	-32.90	53.85	103.20
11	F	101	PRO	N-CD-CG	-23.49	67.96	103.20
12	G	93	PRO	CA-CB-CG	-14.65	76.66	104.50
11	F	101	PRO	CA-CB-CG	-14.02	77.87	104.50
14	I	23	PRO	CA-N-CD	-12.56	94.42	112.00
14	I	23	PRO	N-CD-CG	-11.65	85.72	103.20
14	I	23	PRO	CA-CB-CG	-8.74	87.89	104.50
11	F	67	PRO	N-CD-CG	-8.31	90.73	103.20
11	F	67	PRO	CA-CB-CG	-6.45	92.24	104.50
18	M	66	GLU	CB-CA-C	-6.30	109.30	116.54
29	a	512	G	O4'-C1'-N9	5.99	117.18	108.20
12	G	93	PRO	N-CA-CB	-5.29	97.57	103.23
12	G	93	PRO	CA-N-CD	-5.19	104.74	112.00
15	J	88	MET	N-CA-CB	5.06	117.54	110.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	N	32	SER	Peptide
35	g	46	ALA	Peptide
35	g	47	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	377	0	418	5	0
3	2	504	0	572	4	0
4	3	302	0	340	6	0
5	4	480	0	477	65	0
6	A	32612	0	16432	396	0
7	B	1753	0	1780	50	0
8	C	1624	0	1696	21	0
9	D	1643	0	1707	25	0
10	E	1152	0	1196	18	0
11	F	839	0	833	25	0
12	G	1203	0	1254	40	0
13	H	979	0	1031	15	0
14	I	1022	0	1070	21	0
15	J	786	0	828	27	0
16	K	877	0	884	20	0
17	L	957	0	1017	3	0
18	M	891	0	952	14	0
19	N	805	0	844	12	0
20	O	714	0	734	8	0
21	P	643	0	661	11	0
22	Q	641	0	682	17	0
23	R	544	0	565	13	0
24	S	668	0	693	61	0
25	T	670	0	719	10	0
26	U	589	0	629	13	0
27	X	260	0	130	1	0
28	Y	1581	0	804	39	0
28	Z	1581	0	804	15	0
29	a	59130	0	29769	515	0
30	b	2549	0	1291	28	0
31	c	2082	0	2154	27	0
32	d	1566	0	1618	12	0
33	e	1552	0	1619	23	0
34	f	1410	0	1444	50	0
35	g	1323	0	1371	35	0
36	h	303	0	327	8	0
37	i	1129	0	1162	15	0
38	j	946	0	1023	10	0
39	k	1053	0	1129	16	0
40	l	1075	0	1146	12	0
41	m	945	0	989	8	0
42	n	892	0	923	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	o	917	0	962	19	0
44	p	947	0	1019	15	0
45	q	816	0	839	9	0
46	r	857	0	922	15	0
47	s	738	0	807	9	0
48	t	779	0	831	16	0
49	u	753	0	780	7	0
50	v	628	0	642	7	0
51	w	625	0	652	6	0
52	x	501	0	531	5	0
53	y	449	0	488	5	0
54	z	444	0	458	9	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
56	A	42	0	45	1	0
57	A	67	0	0	0	0
57	N	1	0	0	0	0
57	X	1	0	0	0	0
57	a	190	0	0	0	0
57	b	5	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	p	1	0	0	0	0
57	z	1	0	0	0	0
58	A	20	0	38	2	0
58	a	140	0	266	13	0
59	Y	22	0	11	2	0
59	Z	22	0	11	2	0
60	a	14	0	26	2	0
61	a	16	0	16	4	0
62	0	11	0	0	0	0
62	1	27	0	0	0	0
62	2	27	0	0	0	0
62	3	3	0	0	0	0
62	4	3	0	0	1	0
62	A	1860	0	0	37	0
62	B	1	0	0	0	0
62	C	42	0	0	0	0
62	D	14	0	0	0	0
62	E	15	0	0	0	0
62	G	4	0	0	0	0
62	H	23	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	I	22	0	0	0	0
62	J	18	0	0	1	0
62	K	12	0	0	0	0
62	L	25	0	0	0	0
62	M	16	0	0	1	0
62	N	38	0	0	1	0
62	O	12	0	0	0	0
62	P	11	0	0	0	0
62	Q	3	0	0	0	0
62	R	1	0	0	0	0
62	S	25	0	0	1	0
62	T	1	0	0	0	0
62	U	3	0	0	0	0
62	X	12	0	0	0	0
62	Y	6	0	0	0	0
62	Z	8	0	0	1	0
62	a	3758	0	0	55	0
62	b	167	0	0	12	0
62	c	95	0	0	1	0
62	d	40	0	0	0	0
62	e	52	0	0	2	0
62	f	34	0	0	7	0
62	h	5	0	0	0	0
62	i	14	0	0	1	0
62	j	13	0	0	1	0
62	k	51	0	0	3	0
62	l	28	0	0	1	0
62	m	34	0	0	0	0
62	n	39	0	0	3	0
62	o	10	0	0	0	0
62	p	32	0	0	1	0
62	q	22	0	0	0	0
62	r	26	0	0	0	0
62	s	9	0	0	1	0
62	t	3	0	0	0	0
62	u	5	0	0	0	0
62	v	20	0	0	0	0
62	w	22	0	0	0	0
62	x	2	0	0	0	0
62	y	7	0	0	0	0
62	z	25	0	0	0	0
All	All	148825	0	95512	1663	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 7.

All (1663) 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)
5:4:56:ARG:HD3	24:S:64:ASP:CG	1.43	1.42
5:4:56:ARG:HD3	24:S:64:ASP:OD1	1.17	1.30
5:4:60:PHE:CD2	24:S:42:PRO:HD3	1.83	1.13
5:4:64:PHE:CE2	24:S:9:PRO:HB3	1.85	1.12
5:4:56:ARG:CD	24:S:64:ASP:OD1	1.99	1.10
5:4:56:ARG:HD2	24:S:64:ASP:O	1.50	1.06
5:4:56:ARG:CZ	24:S:64:ASP:HA	1.84	1.05
5:4:56:ARG:NH1	24:S:64:ASP:HA	1.72	1.05
5:4:37:CYS:SG	5:4:40:CYS:HB3	2.02	0.99
5:4:60:PHE:CE2	24:S:42:PRO:HD2	1.97	0.99
5:4:64:PHE:CG	24:S:9:PRO:HG3	1.98	0.98
5:4:56:ARG:HD2	24:S:64:ASP:C	1.89	0.98
5:4:60:PHE:CD2	24:S:42:PRO:CD	2.46	0.97
24:S:29:LYS:HG2	24:S:30:PRO:HD2	1.47	0.96
5:4:56:ARG:CD	24:S:64:ASP:CG	2.38	0.96
5:4:56:ARG:NH1	24:S:64:ASP:OD1	1.99	0.94
5:4:64:PHE:CD2	24:S:9:PRO:HB3	2.08	0.88
5:4:59:ARG:NH1	6:A:1311:A:OP1	2.06	0.88
5:4:56:ARG:CD	24:S:64:ASP:O	2.23	0.87
5:4:60:PHE:CE2	24:S:42:PRO:CD	2.58	0.87
11:F:44:ARG:HG2	11:F:56:LYS:HG2	1.57	0.86
28:Y:10:G:O6	28:Y:45:G:N2	2.09	0.86
6:A:346:G:OP1	43:o:41:GLN:NE2	2.08	0.85
6:A:1028:C:N4	6:A:1033:G:O6	2.11	0.83
6:A:673:A:H2'	6:A:674:G:C8	2.14	0.82
29:a:544:C:O2	29:a:549:G:N2	2.12	0.82
6:A:664:G:H22	6:A:741:G:H1	1.27	0.82
5:4:64:PHE:CD2	24:S:9:PRO:HG3	2.16	0.81
36:h:30:LEU:HA	36:h:35:LYS:HZ1	1.43	0.81
39:k:143:GLU:OE1	62:k:201:HOH:O	2.00	0.80
15:J:85:ASP:HA	15:J:88:MET:SD	2.22	0.80
59:Z:101:8AN:HO2'	61:a:6206:MET:N	1.79	0.79
7:B:111:ILE:HD12	7:B:152:LYS:HA	1.64	0.79
40:l:105:MET:HE3	40:l:108:VAL:HG21	1.63	0.79
29:a:1434:A:H2'	29:a:1435:G:H8	1.50	0.77
5:4:56:ARG:CD	24:S:64:ASP:C	2.57	0.77
34:f:4:LEU:HD13	34:f:101:GLU:HG3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:37:ASN:O	31:c:37:ASN:ND2	2.18	0.77
12:G:26:PHE:HB2	12:G:101:MET:HE2	1.66	0.76
29:a:544:C:N3	29:a:549:G:N1	2.29	0.76
10:E:151:GLU:N	10:E:151:GLU:OE1	2.18	0.76
6:A:81:A:N6	6:A:88:U:O4	2.17	0.76
7:B:112:LYS:NZ	7:B:116:ASP:OD1	2.18	0.75
7:B:70:VAL:HB	7:B:163:VAL:HG12	1.69	0.75
34:f:23:ASN:OD1	62:f:201:HOH:O	2.05	0.75
6:A:946:A:H2'	6:A:947:G:C8	2.21	0.75
24:S:44:MET:HA	24:S:47:LEU:HD12	1.69	0.75
25:T:2:ALA:HB3	25:T:8:LYS:HG3	1.68	0.75
37:i:129:GLU:N	37:i:129:GLU:OE1	2.20	0.75
29:a:626:A:N7	62:a:6319:HOH:O	2.20	0.74
29:a:2529:G:H4'	35:g:175:LYS:HD3	1.67	0.74
5:4:64:PHE:CB	24:S:9:PRO:HG3	2.17	0.74
29:a:258:G:N7	62:a:6328:HOH:O	2.21	0.74
6:A:203:G:N2	6:A:204:G:O6	2.21	0.74
34:f:56:ASP:O	34:f:60:ILE:HG12	1.88	0.74
45:q:46:GLU:OE2	45:q:48:LYS:NZ	2.21	0.74
5:4:56:ARG:HD3	24:S:64:ASP:CB	2.18	0.73
29:a:2415:G:N7	62:a:6330:HOH:O	2.21	0.73
40:l:12:MET:HE2	40:l:71:LYS:HG3	1.69	0.73
5:4:60:PHE:HE2	24:S:42:PRO:HD2	1.49	0.73
6:A:1088:G:H4'	26:U:70:LEU:HD21	1.71	0.73
7:B:6:MET:HE2	7:B:43:LEU:HD12	1.68	0.73
30:b:6:G:OP1	62:b:301:HOH:O	2.07	0.73
6:A:1441:A:N1	43:o:114:LEU:HD11	2.04	0.73
29:a:1434:A:H2'	29:a:1435:G:C8	2.23	0.72
5:4:1:MET:N	62:4:201:HOH:O	2.21	0.72
5:4:56:ARG:CD	24:S:64:ASP:CA	2.66	0.72
29:a:568:U:H1'	29:a:2030:6MZ:H9C1	1.70	0.72
29:a:549:G:H2'	29:a:550:C:C6	2.25	0.72
29:a:2674:G:H4'	38:j:30:ARG:HD2	1.70	0.72
29:a:1621:U:OP1	62:a:6301:HOH:O	2.08	0.72
6:A:1086:U:H3	6:A:1099:G:H22	1.38	0.71
5:4:64:PHE:HB3	24:S:9:PRO:HG3	1.72	0.71
29:a:327:G:N7	58:a:6198:SPD:N10	2.39	0.71
31:c:270:ARG:NH1	62:c:401:HOH:O	2.24	0.71
29:a:1534:U:O2'	29:a:1537:G:O6	2.07	0.71
29:a:2582:G:OP1	62:a:6302:HOH:O	2.09	0.70
29:a:549:G:H2'	29:a:550:C:H6	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1031:C:O2'	6:A:1032:G:N2	2.24	0.70
6:A:1356:G:H2'	6:A:1357:A:C8	2.26	0.70
8:C:129:MET:HE3	8:C:131:ARG:HB2	1.72	0.70
4:3:23:ILE:HD13	29:a:1032:A:H1'	1.74	0.70
5:4:56:ARG:HH11	24:S:64:ASP:CG	1.99	0.70
29:a:593:U:H2'	29:a:594:U:C6	2.27	0.69
5:4:56:ARG:NE	24:S:64:ASP:HA	2.08	0.69
48:t:49:VAL:HG12	48:t:51:ALA:H	1.58	0.69
15:J:18:ILE:O	15:J:22:THR:HG23	1.93	0.68
25:T:29:ARG:O	25:T:33:LYS:HG3	1.93	0.68
29:a:460:A:OP2	62:a:6303:HOH:O	2.10	0.68
6:A:662:U:H2'	6:A:663:A:C8	2.28	0.68
28:Y:3:C:H2'	28:Y:4:G:H8	1.58	0.68
47:s:53:VAL:HB	47:s:91:GLN:HB3	1.76	0.68
9:D:57:GLU:HG3	9:D:199:LEU:HD12	1.76	0.68
16:K:23:ILE:HD12	16:K:86:VAL:HG22	1.75	0.68
29:a:1766:G:N7	62:a:6383:HOH:O	2.27	0.68
5:4:64:PHE:CG	24:S:9:PRO:CG	2.76	0.67
6:A:1104:G:N7	62:A:1752:HOH:O	2.27	0.67
29:a:331:C:OP2	62:a:6304:HOH:O	2.11	0.67
34:f:8:TYR:HB2	34:f:173:PHE:HZ	1.60	0.67
51:w:72:ARG:NH1	51:w:78:TYR:OH	2.28	0.67
5:4:64:PHE:CD2	24:S:9:PRO:CB	2.78	0.67
31:c:29:PRO:HG2	31:c:34:LEU:HD11	1.76	0.67
42:n:7:ARG:NH1	62:n:203:HOH:O	2.27	0.67
6:A:714:G:H2'	6:A:715:A:C8	2.29	0.67
33:e:92:HIS:O	62:e:301:HOH:O	2.12	0.67
41:m:56:LYS:NZ	41:m:94:TYR:OH	2.27	0.67
6:A:269:C:H2'	6:A:270:A:C8	2.29	0.66
29:a:2328:A:H2'	29:a:2329:U:C6	2.31	0.66
29:a:1431:A:H4'	58:a:6199:SPD:H32	1.77	0.66
30:b:36:C:OP2	62:b:303:HOH:O	2.13	0.66
39:k:85:VAL:HB	39:k:94:THR:HG22	1.77	0.66
5:4:56:ARG:HG3	5:4:57:VAL:N	2.11	0.66
5:4:66:ILE:HD12	19:N:42:TRP:CD2	2.31	0.66
7:B:97:LEU:H	7:B:100:MET:HE3	1.60	0.66
29:a:2255:G:H21	50:v:9:SER:HB3	1.59	0.66
6:A:94:G:H5"	6:A:95:C:H5	1.60	0.66
34:f:61:SER:O	62:f:203:HOH:O	2.14	0.66
5:4:56:ARG:NH1	24:S:64:ASP:CA	2.55	0.66
29:a:374:A:OP2	62:a:6306:HOH:O	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:585:G:N7	44:p:6:ARG:NH2	2.40	0.66
29:a:1124:G:N7	62:a:6395:HOH:O	2.29	0.66
28:Y:28:C:O2'	28:Y:29:G:O5'	2.14	0.66
34:f:52:ASN:HB2	34:f:150:ARG:HH22	1.59	0.66
6:A:555:U:H2'	6:A:556:C:C6	2.31	0.65
6:A:581:G:O6	62:A:1701:HOH:O	2.13	0.65
31:c:107:PRO:HD2	31:c:110:LEU:HD22	1.78	0.65
5:4:28:VAL:HG13	34:f:140:GLU:HA	1.77	0.65
6:A:451:A:O2'	58:A:1669:SPD:N1	2.28	0.65
41:m:86:ARG:NH2	41:m:117:ASP:OD1	2.25	0.65
44:p:11:ARG:NH1	62:p:301:HOH:O	2.07	0.65
7:B:139:ARG:HG2	7:B:143:LYS:NZ	2.11	0.65
6:A:187:G:N2	6:A:190:A:OP2	2.28	0.65
16:K:116:ILE:HG12	26:U:31:GLU:HG2	1.77	0.65
18:M:68:ASP:HA	18:M:71:ARG:NH1	2.12	0.65
26:U:36:GLU:HG2	26:U:37:PHE:CE2	2.31	0.65
6:A:1391:U:H2'	6:A:1392:G:C8	2.31	0.65
6:A:216:U:H2'	6:A:217:C:C6	2.31	0.65
47:s:36:LYS:HD3	47:s:80:TRP:HA	1.78	0.65
6:A:823:C:HO2'	13:H:2:SER:N	1.95	0.65
6:A:1048:G:N7	62:A:1767:HOH:O	2.28	0.65
18:M:44:LYS:HB2	18:M:47:GLU:HG3	1.78	0.65
29:a:1244:A:OP2	62:a:6305:HOH:O	2.14	0.65
29:a:2068:U:OP2	62:a:6307:HOH:O	2.15	0.65
58:a:6201:SPD:H31	46:r:86:MET:SD	2.37	0.64
46:r:28:LYS:HG3	46:r:70:LYS:HE3	1.78	0.64
6:A:79:G:H1	6:A:90:C:H42	1.45	0.64
28:Y:29:G:H2'	28:Y:30:G:C8	2.31	0.64
29:a:684:G:N7	62:a:6408:HOH:O	2.30	0.64
29:a:2591:C:H2'	29:a:2592:G:C8	2.32	0.64
6:A:53:A:OP2	62:A:1704:HOH:O	2.15	0.64
6:A:1202:U:OP1	62:A:1702:HOH:O	2.15	0.64
29:a:747:5MU:H1'	46:r:92:ARG:HH21	1.62	0.64
29:a:2341:G:N7	62:a:6393:HOH:O	2.29	0.64
29:a:2823:A:OP2	62:a:6308:HOH:O	2.15	0.64
42:n:63:LYS:NZ	62:n:205:HOH:O	2.30	0.64
48:t:18:ASP:HB3	48:t:21:LYS:HD3	1.77	0.64
6:A:1152:A:OP1	15:J:70:HIS:ND1	2.31	0.64
35:g:90:VAL:HG22	35:g:160:LYS:HA	1.79	0.64
3:2:54:ASP:HB3	39:k:57:LEU:HD22	1.79	0.64
6:A:728:A:H2'	6:A:729:A:C8	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:946:A:H2'	6:A:947:G:H8	1.62	0.64
34:f:47:LYS:HD2	34:f:47:LYS:N	2.13	0.64
29:a:1607:C:N4	29:a:1622:G:OP2	2.26	0.64
29:a:2243:U:H2'	29:a:2244:U:C6	2.32	0.64
35:g:19:ILE:HG12	35:g:24:ILE:HG13	1.80	0.64
9:D:198:HIS:O	9:D:202:GLU:HG3	1.97	0.64
34:f:69:LYS:O	62:f:204:HOH:O	2.15	0.64
47:s:5:GLU:HG2	52:x:22:LEU:HD13	1.80	0.63
5:4:60:PHE:HD2	24:S:42:PRO:CD	2.11	0.63
6:A:1098:C:O2'	26:U:71:TYR:O	2.13	0.63
28:Y:3:C:H2'	28:Y:4:G:C8	2.33	0.63
29:a:1386:C:H2'	29:a:1387:A:C8	2.33	0.63
25:T:44:LYS:HD3	25:T:87:ALA:HA	1.81	0.63
6:A:919:A:OP1	62:A:1703:HOH:O	2.15	0.63
6:A:17:U:H2'	6:A:18:C:C6	2.34	0.63
9:D:46:PRO:HB2	9:D:48:LEU:HD13	1.80	0.63
5:4:56:ARG:CD	24:S:64:ASP:HA	2.28	0.63
6:A:1000:A:H2'	6:A:1001:C:C6	2.34	0.63
7:B:167:ASP:OD2	7:B:191:SER:HA	1.98	0.63
29:a:1235:G:OP1	62:a:6311:HOH:O	2.16	0.63
29:a:2852:G:O6	58:a:6192:SPD:N10	2.29	0.63
4:3:25:VAL:HB	4:3:35:GLN:HG2	1.80	0.63
34:f:63:GLN:OE1	62:f:205:HOH:O	2.16	0.63
8:C:129:MET:HE3	8:C:131:ARG:H	1.63	0.62
14:I:100:LYS:HE3	14:I:100:LYS:HA	1.80	0.62
29:a:2820:A:OP1	62:a:6309:HOH:O	2.15	0.62
29:a:84:A:N1	29:a:98:G:O2'	2.31	0.62
34:f:135:GLN:NE2	34:f:148:ARG:O	2.22	0.62
15:J:40:ILE:HB	15:J:73:LEU:HB3	1.80	0.62
46:r:29:VAL:HB	46:r:55:ILE:HD11	1.81	0.62
6:A:337:G:H2'	6:A:338:A:C8	2.34	0.62
23:R:9:LYS:HA	23:R:46:GLY:HA3	1.79	0.62
5:4:64:PHE:CD2	24:S:9:PRO:CG	2.83	0.62
35:g:26:ILE:HD13	35:g:76:VAL:HG23	1.81	0.62
53:y:45:ARG:HH22	53:y:59:GLU:HG2	1.64	0.62
6:A:677:U:H3	6:A:713:G:H22	1.46	0.62
45:q:1:MET:SD	45:q:43:ASN:ND2	2.73	0.62
48:t:54:GLN:H	48:t:54:GLN:NE2	1.97	0.62
6:A:147:G:H2'	6:A:148:G:C8	2.34	0.62
10:E:36:LEU:HD22	10:E:134:ILE:HD13	1.81	0.62
29:a:2052:A:H4'	32:d:148:GLN:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:133:LEU:HB3	35:g:141:ILE:HD11	1.81	0.62
6:A:1441:A:C2	43:o:114:LEU:HD11	2.35	0.62
9:D:72:PHE:HE1	9:D:94:LEU:HD11	1.65	0.62
11:F:12:PRO:O	11:F:44:ARG:NH2	2.33	0.62
29:a:856:G:H2'	29:a:857:G:C8	2.34	0.62
7:B:161:LEU:HD22	7:B:176:ALA:HB2	1.80	0.62
12:G:26:PHE:HD1	12:G:101:MET:HG2	1.64	0.62
38:j:105:ARG:NH2	43:o:34:GLU:OE2	2.33	0.62
40:l:66:ARG:NH1	40:l:104:GLU:OE2	2.32	0.62
29:a:1469:A:H2'	29:a:1470:A:C8	2.35	0.61
29:a:1720:U:H2'	29:a:1721:G:O4'	2.00	0.61
6:A:75:G:H2'	6:A:76:G:H8	1.65	0.61
6:A:405:U:O4	9:D:2:ALA:N	2.33	0.61
6:A:1074:G:O2'	6:A:1101:A:N1	2.31	0.61
20:O:26:GLU:OE2	20:O:77:ARG:NH2	2.34	0.61
32:d:157:LYS:HG2	37:i:80:HIS:CE1	2.35	0.61
8:C:134:MET:HE2	8:C:168:TYR:CD2	2.36	0.61
29:a:5:A:H2'	29:a:6:A:C8	2.36	0.61
29:a:2547:A:H2'	29:a:2548:U:C6	2.36	0.61
29:a:505:A:OP2	62:a:6311:HOH:O	2.16	0.61
2:1:45:SER:OG	29:a:126:A:OP1	2.16	0.61
30:b:115:A:H2'	30:b:116:G:C8	2.35	0.61
29:a:2291:U:H2'	29:a:2292:U:C6	2.35	0.61
31:c:133:ARG:HB3	31:c:186:ALA:HB1	1.82	0.61
43:o:88:ARG:NH2	43:o:110:ILE:O	2.33	0.61
5:4:56:ARG:HD3	24:S:64:ASP:CA	2.30	0.61
12:G:116:MET:HA	12:G:119:ARG:HE	1.65	0.61
29:a:881:G:O6	29:a:895:U:O2	2.18	0.61
6:A:1412:C:H2'	6:A:1413:A:C8	2.35	0.61
15:J:36:VAL:HG12	15:J:76:ILE:HD13	1.81	0.61
29:a:230:G:N7	62:a:6419:HOH:O	2.31	0.60
29:a:2301:C:H2'	29:a:2302:U:C6	2.36	0.60
6:A:1004:A:H2'	6:A:1005:A:O4'	2.02	0.60
11:F:69:GLU:O	11:F:73:GLU:HG2	2.01	0.60
29:a:2788:C:H2'	29:a:2789:C:C6	2.36	0.60
30:b:84:G:N7	62:b:311:HOH:O	2.31	0.60
5:4:56:ARG:HH21	24:S:67:VAL:HG21	1.66	0.60
15:J:37:ARG:HB2	15:J:75:ASP:HB2	1.84	0.60
19:N:36:ALA:HB3	19:N:41:ARG:HH12	1.66	0.60
39:k:106:GLU:OE1	62:k:202:HOH:O	2.16	0.60
5:4:16:CYS:SG	5:4:17:SER:N	2.75	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:177:LYS:HD2	9:D:179:GLU:HG3	1.83	0.60
29:a:851:C:H2'	29:a:852:U:C6	2.36	0.60
44:p:104:VAL:HG11	45:q:45:GLU:HG2	1.82	0.60
21:P:39:PHE:HD1	21:P:50:THR:HG22	1.65	0.60
48:t:49:VAL:HB	48:t:52:LEU:O	2.01	0.60
6:A:1356:G:H2'	6:A:1357:A:H8	1.67	0.60
29:a:2327:A:H2'	29:a:2328:A:C8	2.37	0.60
34:f:122:PHE:CE1	34:f:128:TYR:HB2	2.37	0.60
6:A:974:A:OP1	62:A:1705:HOH:O	2.16	0.60
29:a:2537:U:H2'	29:a:2538:C:C6	2.37	0.60
62:b:302:HOH:O	42:n:56:LYS:NZ	2.28	0.60
6:A:161:A:H2'	6:A:162:A:C8	2.36	0.60
29:a:639:U:H2'	29:a:640:C:C6	2.36	0.60
35:g:22:GLN:HE21	35:g:39:ASP:HA	1.67	0.60
8:C:73:PRO:HG3	8:C:105:GLU:HG2	1.84	0.59
31:c:75:PRO:HG2	31:c:97:LYS:HG3	1.84	0.59
45:q:27:ILE:HD11	45:q:31:GLU:HB2	1.83	0.59
6:A:475:C:H2'	6:A:476:U:C6	2.37	0.59
5:4:56:ARG:HG3	5:4:57:VAL:H	1.67	0.59
22:Q:25:ILE:HB	22:Q:42:THR:HG23	1.84	0.59
29:a:742:A:H2'	29:a:743:A:C8	2.37	0.59
29:a:645:C:H2'	29:a:647:G:C8	2.36	0.59
6:A:77:A:H2'	6:A:78:A:C8	2.38	0.59
29:a:226:A:OP1	58:a:6196:SPD:N1	2.36	0.59
6:A:1266:G:N2	6:A:1269:A:OP2	2.30	0.59
29:a:414:C:H2'	29:a:415:A:C8	2.37	0.59
29:a:813:U:H2'	29:a:814:C:C6	2.37	0.59
11:F:32:ALA:HB2	11:F:70:VAL:HG21	1.85	0.59
29:a:1527:G:N1	29:a:1544:A:OP2	2.31	0.59
6:A:933:G:O6	12:G:3:ARG:NH2	2.34	0.59
6:A:1071:C:H2'	6:A:1072:G:H8	1.67	0.59
6:A:1218:C:H2'	6:A:1219:A:C8	2.36	0.59
10:E:80:THR:OG1	10:E:122:ASN:O	2.20	0.59
29:a:2071:A:H2'	29:a:2072:C:C6	2.38	0.59
35:g:67:THR:O	35:g:71:LEU:HD12	2.02	0.59
6:A:235:C:H2'	6:A:236:A:C8	2.38	0.59
6:A:1286:U:H2'	6:A:1287:A:H5'	1.83	0.59
7:B:54:LEU:HD22	7:B:220:THR:HG21	1.83	0.59
18:M:77:ILE:HG22	18:M:81:MET:HE2	1.85	0.59
23:R:21:ILE:HG13	23:R:54:GLN:HB3	1.84	0.59
29:a:2561:U:O3'	38:j:40:LYS:HE2	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:201:G:HO2'	6:A:469:C:HO2'	1.51	0.59
28:Z:38:A:N7	62:Z:202:HOH:O	2.32	0.59
51:w:53:ALA:HA	51:w:56:MET:HG3	1.85	0.59
22:Q:10:GLY:HA3	22:Q:25:ILE:HD13	1.85	0.58
22:Q:47:HIS:HB3	22:Q:74:THR:HG22	1.84	0.58
28:Y:14:A:N1	28:Y:21:A:O2'	2.35	0.58
6:A:707:U:OP1	62:A:1706:HOH:O	2.17	0.58
29:a:1179:G:H2'	29:a:1180:U:C6	2.38	0.58
29:a:851:C:H2'	29:a:852:U:H6	1.68	0.58
11:F:15:SER:OG	11:F:58:HIS:ND1	2.34	0.58
29:a:2568:U:O2	62:a:6310:HOH:O	2.16	0.58
43:o:89:ARG:HH21	43:o:113:ARG:HH21	1.49	0.58
5:4:28:VAL:HG11	5:4:32:LEU:HD21	1.84	0.58
5:4:56:ARG:HH21	24:S:67:VAL:CG2	2.16	0.58
28:Y:27:U:H2'	28:Y:28:C:H5'	1.85	0.58
6:A:471:U:H2'	6:A:472:U:C6	2.39	0.58
7:B:188:ASP:HB2	7:B:204:ASP:OD2	2.04	0.58
52:x:13:GLU:HA	52:x:16:THR:HG22	1.85	0.58
6:A:75:G:H2'	6:A:76:G:C8	2.38	0.58
6:A:1124:G:OP1	15:J:37:ARG:NH1	2.37	0.58
6:A:1441:A:C2	43:o:114:LEU:CD1	2.86	0.58
29:a:624:C:O2'	29:a:657:U:OP1	2.22	0.58
30:b:61:G:N2	62:b:312:HOH:O	2.31	0.58
6:A:1117:A:N3	62:A:1802:HOH:O	2.32	0.57
6:A:1477:U:H2'	6:A:1478:U:C6	2.39	0.57
29:a:2026:U:OP2	62:a:6312:HOH:O	2.17	0.57
7:B:72:THR:OG1	7:B:169:GLU:OE1	2.18	0.57
9:D:107:PHE:HB3	9:D:145:ILE:HD11	1.85	0.57
6:A:1530:G:O2'	62:A:1709:HOH:O	2.17	0.57
34:f:59:ALA:O	62:f:207:HOH:O	2.18	0.57
30:b:1:U:H2'	30:b:2:G:H8	1.69	0.57
22:Q:18:GLU:N	22:Q:18:GLU:OE2	2.36	0.57
6:A:215:C:O2'	6:A:465:A:N7	2.34	0.57
6:A:131:A:H2'	6:A:132:C:C6	2.39	0.57
6:A:151:A:OP2	6:A:169:C:N4	2.36	0.57
6:A:691:G:N7	62:A:1806:HOH:O	2.33	0.57
6:A:1287:A:H2'	6:A:1288:A:C8	2.39	0.57
6:A:1305:G:N2	6:A:1331:G:H1'	2.18	0.57
24:S:44:MET:HA	24:S:47:LEU:CD1	2.34	0.57
29:a:1802:A:H2'	29:a:1803:A:C8	2.39	0.57
6:A:1171:A:H2'	6:A:1172:C:H6	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:102:THR:HA	7:B:179:LEU:HD11	1.86	0.56
8:C:42:TYR:CZ	8:C:90:VAL:HG11	2.40	0.56
24:S:11:ILE:HG13	24:S:38:SER:HB3	1.87	0.56
29:a:2246:G:H2'	29:a:2247:A:C8	2.39	0.56
32:d:85:ALA:HB3	32:d:88:GLU:HG3	1.86	0.56
39:k:108:ALA:HB3	39:k:125:LEU:HD22	1.86	0.56
6:A:216:U:H2'	6:A:217:C:H6	1.69	0.56
29:a:1583:A:O2'	29:a:1585:C:N4	2.37	0.56
6:A:190:A:O5'	6:A:190:A:H8	1.87	0.56
6:A:526:C:OP2	17:L:88:LYS:HE3	2.06	0.56
6:A:1035:A:O2'	6:A:1036:A:O5'	2.17	0.56
6:A:1314:C:OP2	24:S:4:SER:OG	2.18	0.56
7:B:117:LEU:HG	7:B:141:LEU:HB2	1.87	0.56
12:G:5:ARG:NH2	12:G:7:ILE:O	2.37	0.56
29:a:92:U:H2'	29:a:93:G:O4'	2.06	0.56
36:h:12:LEU:HD13	36:h:19:VAL:HG11	1.87	0.56
54:z:52:ARG:CZ	54:z:54:VAL:HG12	2.35	0.56
2:1:39:ARG:NH2	29:a:468:G:N7	2.45	0.56
6:A:1126:U:OP1	15:J:7:ARG:NH2	2.37	0.56
6:A:996:A:H2'	6:A:997:U:C6	2.40	0.56
15:J:10:LEU:HD22	15:J:98:VAL:HG22	1.88	0.56
29:a:2514:U:H2'	29:a:2515:C:C6	2.40	0.56
49:u:51:GLN:OE1	49:u:57:TYR:OH	2.21	0.56
29:a:306:U:H2'	29:a:307:G:O4'	2.04	0.56
29:a:1311:G:OP2	29:a:1311:G:N2	2.30	0.56
35:g:73:ASN:O	35:g:77:ILE:HG13	2.06	0.56
11:F:72:ASP:O	11:F:76:THR:HG23	2.06	0.56
29:a:5:A:H2'	29:a:6:A:H8	1.71	0.56
29:a:2494:G:O2'	40:l:79:ALA:HA	2.04	0.56
5:4:56:ARG:NE	24:S:64:ASP:O	2.38	0.56
6:A:202:G:O2'	6:A:468:A:N3	2.32	0.56
6:A:695:A:H2'	6:A:696:A:C8	2.41	0.56
12:G:110:LYS:O	12:G:110:LYS:HG3	2.05	0.56
12:G:111:ARG:NH1	12:G:123:GLU:OE1	2.36	0.56
28:Y:7:G:O2'	28:Y:49:G:H5'	2.05	0.56
29:a:1939:5MU:OP1	29:a:2604:PSU:O2'	2.21	0.56
30:b:115:A:H2'	30:b:116:G:H8	1.70	0.56
34:f:62:GLY:O	34:f:95:ARG:NH1	2.38	0.56
6:A:1014:A:C2	6:A:1219:A:H1'	2.41	0.56
29:a:1047:G:O2'	29:a:1109:C:N4	2.39	0.56
29:a:1250:G:H5"	44:p:6:ARG:HD3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:24:ILE:HD12	5:4:24:ILE:O	2.05	0.56
6:A:235:C:H2'	6:A:236:A:H8	1.70	0.56
6:A:1071:C:H2'	6:A:1072:G:C8	2.40	0.56
7:B:45:LYS:O	7:B:49:MET:HG3	2.06	0.56
6:A:1125:U:O2	6:A:1126:U:O2'	2.19	0.55
11:F:102:MET:HE1	23:R:24:LYS:O	2.06	0.55
6:A:382:A:H2'	6:A:383:A:C8	2.41	0.55
24:S:44:MET:CA	24:S:47:LEU:HD12	2.35	0.55
42:n:33:ARG:HG2	42:n:34:HIS:CD2	2.41	0.55
6:A:713:G:H2'	6:A:714:G:C8	2.41	0.55
6:A:1119:C:H2'	6:A:1120:C:H6	1.71	0.55
6:A:1317:C:O2	24:S:37:ARG:NH2	2.39	0.55
29:a:2334:U:C4	42:n:16:ARG:HG3	2.41	0.55
29:a:2562:U:OP2	62:a:6313:HOH:O	2.18	0.55
35:g:71:LEU:O	35:g:75:MET:HB2	2.06	0.55
37:i:120:ARG:NH2	62:i:201:HOH:O	2.36	0.55
5:4:36:VAL:HG12	5:4:37:CYS:H	1.72	0.55
6:A:1520:C:OP1	62:A:1710:HOH:O	2.18	0.55
29:a:351:C:H2'	29:a:352:A:C8	2.42	0.55
31:c:37:ASN:HD22	31:c:37:ASN:C	2.14	0.55
32:d:35:THR:HG22	32:d:73:VAL:HG21	1.89	0.55
33:e:191:ASP:O	33:e:195:GLN:HG3	2.06	0.55
34:f:17:MET:HE3	34:f:22:TYR:HB2	1.87	0.55
5:4:14:ALA:HB1	5:4:34:LEU:HD21	1.88	0.55
15:J:48:ARG:NH1	62:J:201:HOH:O	2.33	0.55
29:a:1495:A:H2'	29:a:1496:A:C8	2.42	0.55
35:g:9:VAL:HG21	35:g:73:ASN:HA	1.88	0.55
6:A:376:G:H5"	21:P:5:ARG:HB2	1.88	0.55
6:A:1518:MA6:H103	6:A:1519:MA6:H102	1.89	0.55
18:M:92:ARG:NH2	29:a:887:U:H5"	2.21	0.55
42:n:77:ALA:O	42:n:81:ARG:HG3	2.06	0.55
46:r:73:LYS:HB2	46:r:106:VAL:HB	1.87	0.55
4:3:34:LYS:NZ	29:a:2743:U:OP1	2.32	0.55
6:A:481:G:O2'	6:A:483:C:N4	2.39	0.55
6:A:1323:G:H2'	6:A:1324:A:C8	2.42	0.55
29:a:849:A:H2'	29:a:850:U:C6	2.42	0.55
29:a:1570:A:H2'	29:a:1571:A:C8	2.41	0.55
23:R:11:CYS:SG	23:R:14:THR:HG23	2.47	0.54
29:a:909:A:H2'	29:a:912:C:C5	2.42	0.54
5:4:60:PHE:HD2	24:S:42:PRO:HD3	1.60	0.54
6:A:613:C:H2'	6:A:614:C:C6	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:49:G:H2'	28:Y:50:U:C6	2.42	0.54
33:e:135:ALA:O	33:e:139:LYS:HE2	2.07	0.54
34:f:60:ILE:HG22	34:f:99:PHE:HE2	1.72	0.54
6:A:812:G:N7	62:A:1810:HOH:O	2.33	0.54
11:F:19:PRO:O	11:F:23:GLU:HG2	2.07	0.54
20:O:26:GLU:OE1	20:O:77:ARG:HB3	2.08	0.54
28:Y:18:G:H21	28:Y:58:A:H5'	1.73	0.54
35:g:95:ARG:HB2	35:g:128:GLN:HB2	1.89	0.54
5:4:63:ARG:HG3	5:4:64:PHE:CG	2.43	0.54
16:K:64:GLN:O	16:K:68:GLU:HG3	2.08	0.54
29:a:78:U:H2'	29:a:79:C:C6	2.41	0.54
29:a:1889:A:H2'	29:a:1890:A:C8	2.42	0.54
34:f:106:ILE:O	34:f:110:ARG:HG3	2.07	0.54
6:A:1516:2MG:N2	6:A:1519:MA6:OP2	2.39	0.54
29:a:64:A:H2'	29:a:65:U:C6	2.43	0.54
29:a:2901:C:H2'	29:a:2902:C:C6	2.43	0.54
48:t:98:SER:OG	48:t:98:SER:O	2.24	0.54
29:a:1405:U:H2'	29:a:1406:U:C6	2.42	0.54
6:A:56:U:H2'	6:A:57:G:C8	2.42	0.54
29:a:132:G:H2'	29:a:133:U:C6	2.43	0.54
29:a:386:G:O2'	58:a:6197:SPD:H82	2.08	0.54
29:a:608:A:H2'	29:a:609:A:C8	2.43	0.54
29:a:2074:U:H2'	29:a:2075:U:C6	2.42	0.54
20:O:26:GLU:HG3	20:O:81:LEU:HD22	1.88	0.54
6:A:458:U:H2'	6:A:459:A:C8	2.43	0.54
7:B:217:VAL:HA	7:B:220:THR:HG22	1.90	0.54
10:E:20:ARG:HG3	10:E:33:PHE:CE2	2.42	0.54
23:R:32:TYR:HB3	23:R:55:LEU:HD21	1.90	0.54
6:A:94:G:H5"	6:A:95:C:C5	2.42	0.54
6:A:345:C:H4'	6:A:346:G:O5'	2.07	0.54
7:B:42:ASN:HD21	7:B:44:GLU:HB2	1.72	0.54
9:D:177:LYS:HD2	9:D:179:GLU:CG	2.38	0.54
14:I:88:MET:CE	14:I:95:ARG:HG3	2.37	0.54
29:a:1225:G:OP1	62:a:6315:HOH:O	2.18	0.54
35:g:98:VAL:HG11	35:g:124:GLU:HA	1.90	0.54
6:A:215:C:H2'	6:A:216:U:C6	2.43	0.53
11:F:41:ASP:OD1	11:F:58:HIS:NE2	2.32	0.53
6:A:1005:A:H3'	6:A:1006:G:H8	1.73	0.53
7:B:129:LEU:HB3	7:B:133:GLU:HG2	1.91	0.53
29:a:365:U:H2'	29:a:366:C:C6	2.43	0.53
34:f:170:LEU:O	34:f:175:PHE:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:55:ASP:N	45:q:55:ASP:OD1	2.38	0.53
6:A:938:A:N3	6:A:1376:U:O2'	2.38	0.53
6:A:1171:A:H2'	6:A:1172:C:C6	2.42	0.53
35:g:29:LYS:CD	35:g:29:LYS:H	2.21	0.53
41:m:24:MET:HG2	41:m:44:LEU:HD22	1.91	0.53
6:A:1102:A:O3'	7:B:95:ARG:NH2	2.42	0.53
29:a:1361:G:H2'	29:a:1362:C:C6	2.43	0.53
6:A:384:G:H2'	6:A:385:C:C6	2.43	0.53
28:Y:28:C:O2'	28:Y:29:G:H8	1.92	0.53
29:a:54:G:N7	62:a:6346:HOH:O	2.34	0.53
29:a:1197:G:H2'	29:a:1198:U:H6	1.74	0.53
6:A:945:G:C2	6:A:946:A:C8	2.96	0.53
15:J:66:GLU:HB3	19:N:99:ALA:HB2	1.91	0.53
28:Z:64:G:H2'	28:Z:65:C:C6	2.42	0.53
29:a:2337:G:OP2	62:a:6314:HOH:O	2.18	0.53
6:A:28:A:O2'	6:A:296:U:OP1	2.21	0.53
6:A:1062:U:H2'	6:A:1063:C:C6	2.44	0.53
20:O:75:VAL:O	20:O:79:THR:HG23	2.09	0.53
30:b:1:U:H2'	30:b:2:G:C8	2.43	0.53
39:k:82:LEU:HD22	39:k:90:VAL:HG21	1.91	0.53
29:a:617:G:OP1	33:e:102:ARG:NH1	2.42	0.53
34:f:32:GLU:O	62:f:206:HOH:O	2.17	0.53
3:2:14:PHE:O	3:2:15:LYS:HD3	2.08	0.53
7:B:30:PHE:CZ	7:B:49:MET:HE1	2.44	0.53
14:I:57:MET:HG2	14:I:60:LYS:HB2	1.91	0.53
28:Y:31:G:O2'	28:Y:32:C:O2	2.26	0.53
29:a:191:A:H2'	29:a:192:C:C6	2.44	0.53
29:a:1412:U:H2'	29:a:1413:A:C8	2.44	0.53
34:f:126:GLY:HA3	34:f:160:ALA:HB3	1.90	0.53
25:T:39:ILE:HD11	25:T:83:ILE:HG13	1.92	0.52
29:a:910:A:H2'	29:a:911:A:C8	2.45	0.52
6:A:147:G:H2'	6:A:148:G:H8	1.74	0.52
6:A:920:U:H2'	6:A:921:U:C6	2.44	0.52
25:T:39:ILE:HG23	25:T:86:LEU:HD22	1.90	0.52
29:a:634:C:H2'	29:a:635:C:C6	2.45	0.52
29:a:1661:G:OP2	62:a:6316:HOH:O	2.19	0.52
46:r:23:LEU:HD22	54:z:24:ALA:HB2	1.90	0.52
6:A:1359:C:OP1	62:A:1712:HOH:O	2.18	0.52
62:A:3539:HOH:O	24:S:2:PRO:HG2	2.10	0.52
16:K:20:VAL:HG22	16:K:83:GLU:HB2	1.91	0.52
29:a:2064:C:H2'	29:a:2065:C:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2233:U:H2'	29:a:2234:G:C8	2.45	0.52
6:A:459:A:H2'	6:A:460:A:C8	2.44	0.52
6:A:1513:A:H2'	6:A:1514:G:C8	2.44	0.52
8:C:77:ILE:HA	8:C:84:VAL:HG13	1.92	0.52
18:M:22:ILE:HG23	18:M:66:GLU:OE2	2.09	0.52
24:S:16:LEU:O	24:S:20:GLU:HG2	2.09	0.52
29:a:1873:G:H2'	29:a:1874:C:C6	2.44	0.52
47:s:87:LEU:HB3	47:s:91:GLN:HB2	1.92	0.52
7:B:164:ILE:HD13	7:B:186:ILE:HG13	1.91	0.52
11:F:45:ARG:O	11:F:56:LYS:HG3	2.10	0.52
29:a:367:G:H2'	29:a:368:A:C8	2.44	0.52
6:A:1176:A:H2'	6:A:1177:G:C8	2.45	0.52
6:A:1290:G:OP1	12:G:35:LYS:NZ	2.43	0.52
6:A:1310:G:O6	62:A:1707:HOH:O	2.17	0.52
6:A:1465:A:H2'	6:A:1466:C:C6	2.44	0.52
7:B:4:VAL:HG22	7:B:9:MET:HE2	1.92	0.52
29:a:419:U:H2'	29:a:420:C:C6	2.44	0.52
30:b:7:G:O6	62:b:304:HOH:O	2.19	0.52
6:A:1273:C:H2'	6:A:1274:A:O4'	2.10	0.52
12:G:71:PRO:HG3	12:G:103:TRP:CZ3	2.45	0.52
29:a:1589:U:H2'	29:a:1590:A:C8	2.44	0.52
6:A:171:A:H2'	6:A:172:A:C8	2.45	0.52
6:A:236:A:H2'	6:A:237:G:C8	2.44	0.52
6:A:512:U:H2'	6:A:513:C:C6	2.44	0.52
29:a:2847:U:H2'	29:a:2848:G:O4'	2.10	0.52
30:b:106:G:H2'	30:b:107:G:O4'	2.10	0.52
33:e:127:GLU:H	33:e:127:GLU:CD	2.18	0.52
37:i:96:ARG:NH2	37:i:99:ARG:HD2	2.24	0.52
54:z:53:LYS:NZ	54:z:55:ILE:O	2.42	0.52
6:A:404:G:N7	9:D:2:ALA:HB3	2.24	0.52
18:M:36:ALA:HB3	18:M:59:GLU:OE1	2.10	0.52
28:Y:64:G:H2'	28:Y:65:C:C6	2.44	0.52
40:l:75:GLU:HB2	40:l:90:GLU:HG3	1.92	0.52
54:z:36:GLU:OE1	54:z:46:ASP:HB2	2.10	0.52
6:A:459:A:H2'	6:A:460:A:H8	1.74	0.52
6:A:911:U:H2'	6:A:912:C:C6	2.45	0.52
6:A:1032:G:H2'	6:A:1033:G:H4'	1.90	0.52
23:R:26:ILE:HG22	23:R:30:LYS:HD2	1.91	0.52
29:a:355:U:H2'	29:a:356:G:H8	1.73	0.52
34:f:2:ALA:N	62:f:210:HOH:O	2.43	0.52
43:o:13:MET:HE3	43:o:77:HIS:NE2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:u:46:LYS:O	49:u:50:MET:HG2	2.09	0.52
28:Y:29:G:O2'	28:Y:30:G:H5'	2.11	0.51
29:a:78:U:H2'	29:a:79:C:H6	1.74	0.51
29:a:987:C:O2'	29:a:1000:A:N3	2.39	0.51
6:A:412:A:O2'	6:A:413:G:H4'	2.11	0.51
6:A:460:A:H2'	6:A:461:A:H8	1.75	0.51
6:A:1121:U:H2'	6:A:1122:U:C6	2.45	0.51
6:A:1326:U:H2'	6:A:1327:C:C6	2.45	0.51
10:E:81:LEU:HB2	10:E:98:PRO:HG3	1.93	0.51
29:a:580:U:H2'	29:a:581:C:C6	2.45	0.51
38:j:65:THR:HG22	38:j:68:GLY:H	1.74	0.51
7:B:139:ARG:HG2	7:B:143:LYS:HZ1	1.74	0.51
9:D:25:VAL:HG13	9:D:26:ARG:HG2	1.92	0.51
21:P:39:PHE:CD1	21:P:50:THR:HG22	2.45	0.51
29:a:1113:U:OP1	35:g:3:ARG:NH1	2.43	0.51
29:a:1532:A:H2'	29:a:1533:C:C6	2.46	0.51
35:g:87:LEU:HB2	35:g:131:ILE:HB	1.93	0.51
29:a:279:A:N6	29:a:361:G:H1'	2.26	0.51
29:a:581:C:H2'	29:a:582:A:C8	2.45	0.51
29:a:2780:G:OP1	62:a:6317:HOH:O	2.19	0.51
29:a:2895:G:H2'	29:a:2896:C:C6	2.46	0.51
34:f:47:LYS:HB2	34:f:48:LYS:NZ	2.25	0.51
52:x:39:GLN:HB3	52:x:41:HIS:CE1	2.46	0.51
6:A:746:A:H2'	6:A:747:A:C8	2.46	0.51
7:B:92:VAL:HG21	7:B:96:TRP:HE3	1.76	0.51
29:a:348:A:H2'	29:a:349:U:O4'	2.10	0.51
29:a:355:U:H2'	29:a:356:G:C8	2.45	0.51
29:a:661:A:H4'	39:k:13:LYS:HE3	1.91	0.51
29:a:1487:U:H2'	29:a:1488:C:H6	1.76	0.51
29:a:2591:C:H2'	29:a:2592:G:H8	1.74	0.51
34:f:106:ILE:O	34:f:109:PRO:HD2	2.10	0.51
35:g:11:VAL:CG1	35:g:48:ASN:HB3	2.41	0.51
43:o:13:MET:HE3	43:o:77:HIS:CE1	2.45	0.51
6:A:769:G:H4'	6:A:1513:A:H4'	1.93	0.51
15:J:47:GLU:OE1	19:N:76:LYS:HD3	2.10	0.51
29:a:1028:A:N6	29:a:1125:G:H2'	2.26	0.51
38:j:43:ILE:HD12	38:j:56:ASP:HB2	1.91	0.51
42:n:64:TYR:HB3	42:n:67:ASN:HD22	1.75	0.51
11:F:42:TRP:CZ2	23:R:24:LYS:HD2	2.45	0.51
29:a:367:G:H2'	29:a:368:A:H8	1.75	0.51
29:a:2552:OMU:H6	29:a:2552:OMU:O5'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2747:G:O6	29:a:2755:C:H5”	2.11	0.51
6:A:450:G:N7	62:A:1819:HOH:O	2.34	0.51
6:A:453:G:H2’	6:A:454:G:H8	1.75	0.51
7:B:185:ALA:HB3	7:B:196:VAL:HG11	1.91	0.51
29:a:414:C:H2’	29:a:415:A:H8	1.74	0.51
29:a:1796:U:H2’	29:a:1797:G:H8	1.76	0.51
6:A:1435:G:H2’	6:A:1436:U:C6	2.46	0.51
14:I:116:VAL:HG11	15:J:62:ARG:HG3	1.93	0.51
28:Y:39:C:H2’	28:Y:40:C:C6	2.46	0.51
29:a:151:C:H2’	29:a:152:A:H8	1.76	0.51
29:a:2329:U:H2’	29:a:2330:G:C8	2.46	0.51
38:j:77:ILE:HG12	43:o:72:ARG:HG2	1.93	0.51
6:A:471:U:H2’	6:A:472:U:H6	1.75	0.51
6:A:475:C:H2’	6:A:476:U:H6	1.75	0.51
29:a:144:A:H2’	29:a:145:C:C6	2.46	0.51
6:A:265:G:OP1	22:Q:65:ARG:NH2	2.44	0.50
6:A:453:G:H2’	6:A:454:G:C8	2.46	0.50
6:A:904:U:H2’	6:A:905:U:C6	2.46	0.50
6:A:1251:A:H2’	6:A:1252:A:C8	2.45	0.50
17:L:110:ARG:HB3	17:L:119:VAL:HG21	1.94	0.50
29:a:277:G:H5’	29:a:278:A:OP1	2.11	0.50
29:a:1338:G:O2’	29:a:1393:A:N1	2.43	0.50
29:a:2314:A:H2’	29:a:2315:G:C8	2.45	0.50
44:p:49:ASP:HA	44:p:52:GLN:HB2	1.91	0.50
6:A:834:U:H2’	6:A:835:U:C6	2.46	0.50
10:E:162:GLU:OE2	10:E:162:GLU:N	2.44	0.50
12:G:26:PHE:CD1	12:G:101:MET:HG2	2.44	0.50
28:Y:18:G:N2	28:Y:58:A:H5’	2.26	0.50
29:a:103:A:H2’	29:a:104:A:O4’	2.12	0.50
29:a:811:U:H2’	39:k:21:ARG:HA	1.92	0.50
29:a:1141:U:H4’	29:a:1142:A:O4’	2.11	0.50
44:p:107:THR:O	44:p:111:GLU:HG2	2.11	0.50
8:C:16:LYS:NZ	8:C:181:ASP:OD1	2.44	0.50
10:E:57:PRO:O	10:E:61:GLN:HG3	2.11	0.50
10:E:164:ILE:O	13:H:114:ARG:NH2	2.44	0.50
29:a:2273:A:H2’	29:a:2274:A:C8	2.46	0.50
29:a:2291:U:OP1	29:a:2380:C:O2’	2.26	0.50
7:B:31:ILE:HD11	7:B:189:THR:HB	1.93	0.50
12:G:22:LEU:O	12:G:101:MET:HE1	2.10	0.50
34:f:41:GLY:HA2	34:f:85:ILE:HB	1.92	0.50
50:v:59:LEU:HD12	50:v:80:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:57:MET:HE1	14:I:90:TYR:CZ	2.46	0.50
18:M:7:ILE:HG22	34:f:112:ARG:NH2	2.26	0.50
18:M:45:ILE:O	18:M:48:LEU:HB2	2.12	0.50
29:a:1348:C:OP1	62:a:6320:HOH:O	2.20	0.50
6:A:333:U:H2'	6:A:334:C:H6	1.77	0.50
6:A:346:G:OP1	43:o:39:ARG:NH2	2.30	0.50
9:D:138:SER:HG	9:D:141:ASP:CG	2.20	0.50
11:F:92:THR:HG21	11:F:96:VAL:HG21	1.92	0.50
29:a:833:A:H2'	29:a:834:G:C8	2.46	0.50
29:a:1599:U:H2'	29:a:1600:C:C6	2.47	0.50
37:i:5:THR:HG23	37:i:45:THR:HG21	1.93	0.50
38:j:65:THR:HG22	38:j:67:LYS:N	2.27	0.50
42:n:4:LYS:O	42:n:8:ILE:HG12	2.12	0.50
33:e:94:GLN:OE1	62:e:302:HOH:O	2.19	0.50
6:A:76:G:O6	6:A:93:U:O4	2.29	0.50
29:a:150:U:H2'	29:a:151:C:C6	2.46	0.50
29:a:747:5MU:H1'	46:r:92:ARG:NH2	2.26	0.50
29:a:1746:A:H2'	29:a:1747:U:C6	2.47	0.50
29:a:2246:G:H2'	29:a:2247:A:H8	1.77	0.50
6:A:937:A:O2'	12:G:76:LYS:NZ	2.45	0.50
29:a:909:A:H2'	29:a:912:C:H5	1.75	0.50
30:b:117:G:OP1	42:n:56:LYS:HE2	2.11	0.50
6:A:33:A:H2'	6:A:34:C:C6	2.46	0.49
11:F:10:VAL:CG2	11:F:58:HIS:HB3	2.42	0.49
29:a:646:U:H5"	29:a:647:G:H5"	1.93	0.49
29:a:1183:U:H2'	29:a:1184:U:C6	2.47	0.49
29:a:1794:A:H2'	29:a:1795:C:C6	2.47	0.49
29:a:2659:G:OP2	35:g:158:LYS:NZ	2.45	0.49
34:f:31:VAL:O	34:f:96:MET:HE1	2.12	0.49
5:4:41:HIS:NE2	5:4:43:PHE:HB3	2.27	0.49
6:A:5:U:H4'	6:A:6:G:O5'	2.11	0.49
6:A:922:G:H2'	6:A:923:A:C8	2.46	0.49
6:A:923:A:N7	62:A:1831:HOH:O	2.35	0.49
6:A:1352:C:H2'	6:A:1353:G:C8	2.47	0.49
10:E:101:GLU:HA	10:E:122:ASN:ND2	2.26	0.49
12:G:138:ARG:HD3	12:G:142:HIS:CE1	2.47	0.49
25:T:47:ALA:HB1	25:T:83:ILE:HG12	1.94	0.49
29:a:1009:A:N3	29:a:1153:C:O2'	2.43	0.49
29:a:1612:C:OP2	62:a:6318:HOH:O	2.19	0.49
29:a:2455:G:H2'	29:a:2456:C:C6	2.46	0.49
62:a:9694:HOH:O	37:i:111:LYS:HG2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:460:A:H2'	6:A:461:A:C8	2.47	0.49
6:A:1263:C:H2'	6:A:1264:U:C6	2.47	0.49
21:P:4:ILE:HG12	21:P:21:VAL:HG22	1.94	0.49
29:a:594:U:H2'	29:a:595:C:C6	2.46	0.49
29:a:1418:G:N7	62:a:6467:HOH:O	2.34	0.49
42:n:24:THR:HG22	42:n:90:VAL:HG12	1.95	0.49
47:s:58:VAL:HG22	47:s:85:VAL:HG22	1.94	0.49
6:A:501:C:H2'	6:A:502:A:H8	1.77	0.49
14:I:6:TYR:HB2	14:I:21:ILE:CG1	2.43	0.49
28:Y:19:G:H4'	28:Y:20:U:OP2	2.11	0.49
29:a:548:G:H2'	29:a:549:G:H1'	1.94	0.49
29:a:1932:A:H2'	29:a:1933:G:O4'	2.13	0.49
5:4:26:SER:OG	5:4:27:THR:N	2.45	0.49
6:A:1057:G:OP1	62:A:1716:HOH:O	2.20	0.49
6:A:1530:G:H2'	6:A:1531:A:C8	2.47	0.49
8:C:134:MET:HE2	8:C:168:TYR:HD2	1.76	0.49
29:a:1028:A:H2'	29:a:1029:A:C8	2.48	0.49
39:k:119:PRO:HG2	39:k:119:PRO:O	2.13	0.49
44:p:11:ARG:O	44:p:15:LYS:HG3	2.12	0.49
6:A:41:G:H2'	6:A:42:G:C8	2.48	0.49
6:A:407:U:H2'	6:A:408:A:H8	1.77	0.49
6:A:492:C:H2'	6:A:493:A:C8	2.47	0.49
6:A:736:C:H2'	6:A:737:C:C6	2.47	0.49
7:B:97:LEU:H	7:B:100:MET:CE	2.26	0.49
7:B:133:GLU:O	7:B:137:ARG:HG3	2.11	0.49
29:a:948:C:H2'	29:a:949:G:H8	1.78	0.49
29:a:1800:C:OP2	31:c:182:ARG:NH1	2.42	0.49
6:A:232:G:H1'	6:A:262:A:N1	2.28	0.49
6:A:1225:A:H2'	6:A:1226:C:C5	2.48	0.49
6:A:1229:A:H4'	28:Z:30:G:P	2.53	0.49
6:A:1314:C:OP1	24:S:6:LYS:NZ	2.36	0.49
14:I:47:VAL:HG13	14:I:80:ARG:HD3	1.94	0.49
29:a:518:G:H2'	29:a:519:U:C6	2.48	0.49
29:a:581:C:H2'	29:a:582:A:H8	1.77	0.49
29:a:2301:C:H2'	29:a:2302:U:H6	1.77	0.49
29:a:2576:G:O2'	29:a:2579:C:OP2	2.27	0.49
53:y:4:THR:HA	53:y:38:ARG:O	2.13	0.49
7:B:6:MET:SD	7:B:10:LEU:HD23	2.53	0.49
29:a:2334:U:H1'	42:n:13:ARG:HG3	1.95	0.49
40:l:36:VAL:HG21	40:l:129:THR:HG23	1.95	0.49
6:A:333:U:H2'	6:A:334:C:C6	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:407:U:H2'	6:A:408:A:C8	2.47	0.49
6:A:439:U:OP2	62:A:1715:HOH:O	2.20	0.49
6:A:1475:G:H4'	29:a:1689:A:H4'	1.95	0.49
11:F:10:VAL:HG22	11:F:58:HIS:HB3	1.94	0.49
29:a:1199:U:H2'	29:a:1200:C:C6	2.48	0.49
29:a:1790:C:H2'	29:a:1791:A:C5	2.47	0.49
29:a:2243:U:H2'	29:a:2244:U:H6	1.74	0.49
31:c:5:LYS:HD3	31:c:17:VAL:HG22	1.95	0.49
12:G:129:GLU:HG3	12:G:131:LYS:HE2	1.94	0.49
29:a:1532:A:H2'	29:a:1533:C:H6	1.77	0.49
51:w:74:ARG:NH2	51:w:76:GLU:OE2	2.46	0.49
5:4:64:PHE:CZ	24:S:9:PRO:HB3	2.44	0.48
7:B:42:ASN:ND2	7:B:44:GLU:HB2	2.28	0.48
11:F:96:VAL:HG12	11:F:96:VAL:O	2.12	0.48
12:G:26:PHE:HE2	12:G:120:LEU:HD21	1.77	0.48
31:c:37:ASN:ND2	31:c:37:ASN:C	2.69	0.48
5:4:56:ARG:CZ	24:S:64:ASP:OD1	2.58	0.48
6:A:524:G:H2'	6:A:525:C:C6	2.48	0.48
6:A:1119:C:H2'	6:A:1120:C:C6	2.47	0.48
6:A:1236:A:H2'	6:A:1237:C:C6	2.48	0.48
29:a:1597:A:H5"	29:a:1598:A:H5'	1.94	0.48
35:g:52:PHE:CZ	35:g:72:LEU:HD12	2.48	0.48
1:0:9:ILE:HD12	1:0:51:GLU:HG3	1.94	0.48
6:A:461:A:H2'	6:A:462:G:H8	1.77	0.48
6:A:1314:C:H2'	6:A:1315:U:C6	2.48	0.48
16:K:85:MET:HE2	16:K:113:VAL:HG11	1.96	0.48
29:a:1242:U:H2'	29:a:1243:C:C6	2.49	0.48
29:a:1599:U:H2'	29:a:1600:C:H6	1.78	0.48
29:a:1881:C:H2'	29:a:1882:U:O4'	2.14	0.48
30:b:66:A:N6	30:b:107:G:H2'	2.28	0.48
4:3:8:LYS:NZ	29:a:2467:C:OP1	2.31	0.48
6:A:41:G:H2'	6:A:42:G:H8	1.78	0.48
6:A:337:G:H2'	6:A:338:A:H8	1.76	0.48
31:c:155:ALA:HB2	31:c:162:VAL:HG23	1.94	0.48
6:A:270:A:H2'	6:A:271:C:C6	2.49	0.48
11:F:90:MET:HE1	23:R:23:TYR:OH	2.14	0.48
14:I:88:MET:HE2	14:I:95:ARG:HG3	1.94	0.48
29:a:1796:U:H2'	29:a:1797:G:C8	2.49	0.48
29:a:2461:A:H2'	29:a:2462:C:C6	2.48	0.48
6:A:76:G:H1	6:A:93:U:H3	1.62	0.48
6:A:546:A:H4'	6:A:548:G:O3'	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:124:MET:HE2	9:D:127:GLY:C	2.39	0.48
29:a:285:G:C2	29:a:286:U:H1'	2.48	0.48
29:a:1874:C:H2'	29:a:1875:G:O4'	2.13	0.48
38:j:5:GLN:NE2	62:j:201:HOH:O	2.26	0.48
6:A:860:A:H2'	6:A:861:G:O4'	2.14	0.48
13:H:7:ILE:O	13:H:11:LEU:HG	2.13	0.48
28:Y:74:C:H2'	28:Y:75:C:O4'	2.13	0.48
29:a:1378:A:O2'	29:a:1380:G:N7	2.46	0.48
29:a:1487:U:H2'	29:a:1488:C:C6	2.49	0.48
44:p:61:TRP:CZ2	44:p:93:LYS:HG3	2.48	0.48
6:A:399:G:H2'	6:A:400:C:C6	2.49	0.48
12:G:2:PRO:HG2	12:G:5:ARG:H	1.78	0.48
29:a:480:A:OP2	48:t:44:LYS:HE2	2.14	0.48
29:a:642:U:O2'	29:a:644:A:N7	2.33	0.48
29:a:945:A:H1'	58:a:6191:SPD:H82	1.96	0.48
6:A:130:A:H1'	6:A:263:A:O2'	2.14	0.48
6:A:751:U:H2'	6:A:752:G:O4'	2.13	0.48
15:J:88:MET:SD	15:J:88:MET:N	2.83	0.48
29:a:172:A:H2'	29:a:173:A:C8	2.47	0.48
29:a:494:G:OP1	46:r:8:ARG:HD3	2.14	0.48
29:a:2389:G:O6	62:a:6326:HOH:O	2.20	0.48
35:g:29:LYS:HD3	35:g:79:VAL:O	2.13	0.48
45:q:25:LEU:HB3	45:q:27:ILE:HG22	1.96	0.48
46:r:74:ILE:HD12	46:r:105:VAL:HG22	1.96	0.48
6:A:335:C:H2'	6:A:336:A:H8	1.78	0.48
6:A:626:G:OP1	21:P:35:ARG:NH2	2.46	0.48
13:H:96:MET:HE3	13:H:130:ALA:HB1	1.96	0.48
29:a:12:U:O2	29:a:2626:C:H4'	2.14	0.48
29:a:280:U:H2'	29:a:281:C:C6	2.49	0.48
29:a:1114:C:H2'	29:a:1115:G:C8	2.48	0.48
44:p:58:ARG:HA	44:p:61:TRP:CE3	2.48	0.48
48:t:14:LEU:HD11	48:t:71:ALA:HB2	1.96	0.48
6:A:1375:A:H2'	6:A:1376:U:O4'	2.13	0.47
29:a:272:A:H2'	29:a:273:G:H8	1.79	0.47
29:a:548:G:H2'	29:a:549:G:C1'	2.44	0.47
37:i:18:VAL:HG21	37:i:142:ILE:HD12	1.95	0.47
6:A:612:C:H2'	6:A:613:C:C6	2.49	0.47
6:A:1357:A:OP1	62:A:1717:HOH:O	2.20	0.47
14:I:28:ILE:HG12	14:I:63:LEU:HD12	1.96	0.47
16:K:89:PRO:HG3	26:U:32:VAL:HG11	1.95	0.47
24:S:41:PHE:H	24:S:44:MET:HE3	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:756:A:H2'	29:a:757:G:O4'	2.13	0.47
29:a:1672:A:C2	29:a:2582:G:H5'	2.49	0.47
43:o:37:LYS:HD2	43:o:38:LYS:H	1.78	0.47
29:a:172:A:H2'	29:a:173:A:H8	1.79	0.47
29:a:720:U:H2'	29:a:721:A:C8	2.49	0.47
29:a:967:U:H2'	29:a:968:C:C6	2.48	0.47
29:a:1563:U:H2'	29:a:1564:C:C6	2.50	0.47
33:e:121:VAL:HG23	33:e:189:THR:HG22	1.95	0.47
48:t:86:ARG:NH1	48:t:100:SER:OG	2.44	0.47
53:y:10:THR:CG2	53:y:56:LYS:HG2	2.44	0.47
6:A:234:C:H4'	22:Q:66:PRO:HG3	1.96	0.47
6:A:1475:G:H4'	29:a:1689:A:C4'	2.44	0.47
16:K:87:LYS:HB2	16:K:87:LYS:HE2	1.70	0.47
29:a:813:U:H2'	29:a:814:C:H6	1.78	0.47
29:a:1011:G:OP1	44:p:77:SER:OG	2.30	0.47
29:a:1315:C:O2'	29:a:1392:A:N3	2.45	0.47
35:g:89:LEU:HD22	35:g:162:VAL:HG22	1.95	0.47
5:4:11:GLU:HA	5:4:25:ARG:HA	1.97	0.47
6:A:1151:A:HO2'	6:A:1152:A:H8	1.61	0.47
6:A:1231:G:O2'	62:A:1708:HOH:O	2.17	0.47
29:a:2016:U:H2'	29:a:2017:U:C6	2.49	0.47
29:a:2194:U:H2'	29:a:2195:U:C6	2.49	0.47
29:a:2532:G:O2'	29:a:2657:A:N1	2.44	0.47
38:j:1:MET:HE3	38:j:32:TYR:CZ	2.50	0.47
5:4:20:ASN:HD22	5:4:21:VAL:N	2.12	0.47
6:A:411:A:H4'	6:A:412:A:O5'	2.14	0.47
6:A:1326:U:H2'	6:A:1327:C:H6	1.80	0.47
7:B:92:VAL:HG21	7:B:96:TRP:CE3	2.50	0.47
29:a:1370:C:H2'	29:a:1371:G:O4'	2.13	0.47
30:b:90:C:OP2	62:b:305:HOH:O	2.21	0.47
33:e:189:THR:O	33:e:193:VAL:HG23	2.14	0.47
33:e:194:LYS:O	33:e:198:GLU:HG2	2.14	0.47
6:A:56:U:H2'	6:A:57:G:H8	1.78	0.47
6:A:73:C:O2'	6:A:74:A:H8	1.98	0.47
6:A:983:A:H2	6:A:984:C:C6	2.33	0.47
6:A:986:U:H2'	6:A:987:G:O4'	2.15	0.47
6:A:1023:U:H2'	6:A:1024:G:C8	2.49	0.47
6:A:1115:U:H2'	6:A:1116:U:C6	2.49	0.47
6:A:1240:U:OP1	12:G:119:ARG:NH2	2.48	0.47
6:A:1338:G:N3	28:Z:41:C:O2'	2.47	0.47
7:B:81:LYS:O	7:B:85:LEU:HG	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:120:GLN:HB3	7:B:125:THR:HB	1.96	0.47
14:I:6:TYR:HB2	14:I:21:ILE:HD11	1.97	0.47
14:I:21:ILE:O	14:I:21:ILE:HG13	2.14	0.47
24:S:50:ALA:HB1	24:S:57:HIS:HB3	1.96	0.47
29:a:223:A:OP2	62:a:6327:HOH:O	2.21	0.47
29:a:2679:A:OP1	62:a:6325:HOH:O	2.20	0.47
31:c:71:LYS:HG3	31:c:102:ARG:HH12	1.80	0.47
34:f:103:LEU:HD12	34:f:107:ALA:HB3	1.96	0.47
44:p:72:ASN:HB3	44:p:110:VAL:HG11	1.96	0.47
6:A:493:A:H2'	6:A:494:G:C8	2.49	0.47
6:A:918:A:H2'	6:A:919:A:C8	2.50	0.47
6:A:1095:U:H2'	6:A:1096:C:C6	2.50	0.47
10:E:115:LEU:HD13	10:E:123:VAL:HG11	1.96	0.47
11:F:22:ILE:HD13	11:F:39:LEU:HD11	1.97	0.47
12:G:109:ARG:HA	12:G:116:MET:HE1	1.97	0.47
15:J:45:ARG:NH2	15:J:47:GLU:OE2	2.48	0.47
29:a:982:C:N3	62:a:6482:HOH:O	2.35	0.47
6:A:67:C:H2'	6:A:68:G:C8	2.50	0.47
6:A:463:U:H2'	6:A:464:U:C6	2.49	0.47
6:A:1277:C:O2'	6:A:1279:G:N3	2.41	0.47
8:C:13:GLY:HA3	19:N:97:LYS:NZ	2.30	0.47
9:D:170:TRP:CZ3	9:D:190:ASP:HB3	2.50	0.47
12:G:5:ARG:NH1	12:G:7:ILE:HB	2.30	0.47
28:Z:50:U:H2'	28:Z:51:C:C6	2.50	0.47
29:a:1683:U:H2'	29:a:1684:G:C8	2.50	0.47
29:a:2292:U:H2'	29:a:2293:G:C8	2.50	0.47
29:a:2850:A:OP2	58:a:6192:SPD:H91	2.14	0.47
35:g:52:PHE:CE2	35:g:72:LEU:HD12	2.49	0.47
42:n:17:LYS:HE2	42:n:21:LEU:HD11	1.97	0.47
4:3:30:GLU:HG2	4:3:33:HIS:CD2	2.50	0.47
6:A:299:G:H2'	6:A:300:A:C8	2.50	0.47
6:A:1157:A:C2	6:A:1181:G:C4	3.03	0.47
6:A:1350:A:O2'	12:G:33:ASP:OD1	2.32	0.47
29:a:417:C:H2'	29:a:418:C:C6	2.50	0.47
33:e:49:ARG:O	33:e:74:LYS:HD2	2.15	0.47
6:A:371:A:H2'	6:A:372:C:O4'	2.15	0.46
6:A:501:C:H2'	6:A:502:A:C8	2.49	0.46
6:A:707:U:OP1	16:K:87:LYS:HE3	2.15	0.46
6:A:709:U:H2'	6:A:710:G:C8	2.51	0.46
6:A:1179:A:OP2	14:I:99:ARG:NH2	2.49	0.46
18:M:90:ARG:NH1	62:M:203:HOH:O	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:17:ASP:N	36:h:17:ASP:OD1	2.48	0.46
46:r:34:ASP:OD2	54:z:37:LYS:HE3	2.15	0.46
6:A:472:U:H2'	6:A:473:U:H6	1.80	0.46
16:K:81:ASN:HB3	16:K:106:ARG:CZ	2.46	0.46
29:a:151:C:H2'	29:a:152:A:C8	2.50	0.46
29:a:361:G:O2'	29:a:362:A:O5'	2.33	0.46
29:a:709:U:H2'	29:a:710:U:C6	2.50	0.46
29:a:2271:G:OP1	50:v:18:ALA:HB1	2.15	0.46
29:a:2557:G:H2'	29:a:2558:C:C6	2.50	0.46
29:a:2636:C:H2'	29:a:2637:U:C6	2.50	0.46
46:r:20:VAL:HG11	46:r:44:ALA:HA	1.98	0.46
6:A:160:A:H2'	6:A:161:A:C8	2.49	0.46
6:A:246:A:C2	6:A:282:A:C5	3.03	0.46
9:D:48:LEU:HD21	9:D:56:ARG:HG3	1.97	0.46
12:G:74:GLU:O	12:G:88:PRO:HA	2.15	0.46
16:K:81:ASN:HB3	16:K:106:ARG:NH2	2.30	0.46
29:a:182:A:H2'	29:a:183:C:C6	2.51	0.46
29:a:381:G:N7	62:a:6486:HOH:O	2.36	0.46
29:a:542:C:H2'	29:a:543:G:H8	1.80	0.46
29:a:586:A:N1	29:a:809:G:O2'	2.41	0.46
29:a:2469:A:N6	29:a:2481:G:O2'	2.48	0.46
6:A:461:A:H2'	6:A:462:G:C8	2.50	0.46
29:a:1682:G:H2'	29:a:1683:U:C6	2.49	0.46
29:a:2025:C:H2'	29:a:2026:U:C6	2.50	0.46
29:a:2800:A:C2	29:a:2895:G:H1'	2.50	0.46
6:A:642:A:C8	13:H:107:SER:HA	2.51	0.46
6:A:1248:A:N6	62:A:1836:HOH:O	2.36	0.46
6:A:1315:U:H2'	6:A:1316:G:O4'	2.16	0.46
30:b:44:G:H3'	62:b:308:HOH:O	2.16	0.46
39:k:78:ARG:HG2	39:k:113:ALA:HB3	1.98	0.46
52:x:13:GLU:HA	52:x:16:THR:CG2	2.46	0.46
54:z:37:LYS:HB2	54:z:37:LYS:NZ	2.30	0.46
6:A:736:C:H2'	6:A:737:C:H6	1.80	0.46
6:A:1179:A:H2'	6:A:1180:A:O4'	2.15	0.46
6:A:1394:A:N1	6:A:1500:A:O2'	2.48	0.46
11:F:9:MET:HE3	11:F:59:TYR:CZ	2.51	0.46
16:K:116:ILE:HD11	26:U:28:VAL:HG13	1.98	0.46
24:S:42:PRO:O	24:S:45:ILE:HG13	2.15	0.46
29:a:721:A:H8	29:a:721:A:OP2	1.99	0.46
29:a:737:C:OP1	62:a:6301:HOH:O	2.20	0.46
29:a:1853:A:H2'	29:a:1854:A:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:12:LEU:HD13	36:h:19:VAL:HG21	1.96	0.46
6:A:718:A:N7	62:A:1842:HOH:O	2.36	0.46
6:A:1463:U:H2'	6:A:1464:U:C6	2.50	0.46
19:N:79:LEU:HB2	19:N:84:VAL:HG23	1.97	0.46
29:a:1187:G:H5"	45:q:83:TYR:CE1	2.50	0.46
29:a:1730:C:H1'	29:a:1731:G:C2	2.50	0.46
29:a:1946:U:H2'	29:a:1947:C:C6	2.50	0.46
31:c:5:LYS:HD2	31:c:6:CYS:N	2.31	0.46
48:t:86:ARG:HG3	48:t:95:PHE:CE2	2.51	0.46
6:A:219:U:H2'	6:A:220:G:H8	1.81	0.46
6:A:1070:U:OP2	62:A:1718:HOH:O	2.21	0.46
25:T:43:ASP:OD1	25:T:44:LYS:N	2.49	0.46
28:Y:26:G:C5	28:Y:27:U:C5	3.03	0.46
28:Z:10:G:N2	28:Z:26:G:H1'	2.31	0.46
33:e:14:VAL:HG12	33:e:197:GLU:HG3	1.98	0.46
35:g:50:LEU:HD23	35:g:50:LEU:HA	1.79	0.46
36:h:7:ASP:HB2	36:h:35:LYS:HA	1.98	0.46
40:l:76:LYS:O	62:l:201:HOH:O	2.21	0.46
42:n:64:TYR:HB3	42:n:67:ASN:ND2	2.31	0.46
6:A:264:C:O2'	22:Q:66:PRO:O	2.29	0.46
6:A:390:U:H2'	6:A:391:G:C8	2.50	0.46
6:A:1280:A:O2'	6:A:1281:C:H5'	2.16	0.46
11:F:42:TRP:CH2	23:R:24:LYS:HD2	2.50	0.46
15:J:67:ILE:HG13	19:N:96:LEU:HD13	1.97	0.46
16:K:28:ASN:O	16:K:57:LYS:HG2	2.15	0.46
29:a:1585:C:H2'	29:a:1586:A:O4'	2.16	0.46
29:a:2530:A:H5'	35:g:175:LYS:HE3	1.96	0.46
35:g:30:ASN:HB3	35:g:79:VAL:HA	1.97	0.46
6:A:985:C:H2'	6:A:986:U:C6	2.51	0.46
9:D:138:SER:OG	9:D:141:ASP:OD1	2.31	0.46
10:E:149:SER:OG	10:E:152:MET:HG2	2.16	0.46
12:G:26:PHE:HZ	12:G:120:LEU:HD11	1.80	0.46
22:Q:25:ILE:HB	22:Q:42:THR:CG2	2.46	0.46
29:a:1026:G:H8	29:a:1026:G:OP2	1.99	0.46
29:a:1115:G:N3	29:a:1116:G:C8	2.84	0.46
29:a:2202:U:O2'	29:a:2204:G:OP1	2.31	0.46
29:a:2295:C:O2'	29:a:2296:U:H5'	2.16	0.46
40:l:53:MET:HE1	40:l:103:TYR:CD2	2.50	0.46
47:s:9:LYS:HA	47:s:9:LYS:HD3	1.70	0.46
49:u:71:LYS:HA	49:u:71:LYS:HD3	1.74	0.46
51:w:51:VAL:HG22	51:w:52:SER:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:977:A:O2'	6:A:979:C:OP2	2.32	0.45
11:F:63:ASN:HD22	11:F:96:VAL:HB	1.81	0.45
28:Y:40:C:H2'	28:Y:41:C:O4'	2.17	0.45
29:a:1484:U:H2'	29:a:1485:U:C6	2.51	0.45
29:a:2514:U:H2'	29:a:2515:C:H6	1.80	0.45
37:i:95:ARG:HH21	37:i:96:ARG:NH1	2.13	0.45
43:o:43:PHE:CZ	43:o:63:LYS:HG2	2.51	0.45
51:w:3:ARG:O	51:w:12:PRO:HD3	2.16	0.45
1:0:5:ILE:HG22	29:a:2284:A:OP1	2.15	0.45
6:A:487:A:H2'	6:A:488:C:O4'	2.16	0.45
7:B:183:VAL:HG12	7:B:196:VAL:HG13	1.99	0.45
20:O:35:GLN:HA	20:O:35:GLN:OE1	2.17	0.45
28:Y:30:G:O2'	28:Y:31:G:H2'	2.17	0.45
29:a:886:A:O2'	29:a:890:C:N4	2.48	0.45
29:a:947:A:H2'	29:a:948:C:C6	2.52	0.45
29:a:1735:A:H2'	29:a:1736:U:C6	2.52	0.45
15:J:80:THR:O	15:J:84:VAL:HG23	2.15	0.45
28:Y:14:A:H2'	28:Y:15:G:O4'	2.17	0.45
29:a:146:A:H2'	29:a:147:C:C6	2.51	0.45
29:a:1198:U:H2'	29:a:1199:U:C6	2.51	0.45
29:a:1506:U:H2'	29:a:1507:C:C6	2.50	0.45
29:a:2518:A:OP2	58:a:6194:SPD:H52	2.17	0.45
29:a:2793:C:H2'	29:a:2794:C:C6	2.51	0.45
29:a:2812:G:H2'	29:a:2813:A:C8	2.52	0.45
34:f:40:VAL:HG12	34:f:43:ALA:HB2	1.98	0.45
42:n:76:LYS:HE2	62:n:224:HOH:O	2.17	0.45
49:u:21:ARG:HA	49:u:25:LYS:O	2.15	0.45
4:3:2:LYS:NZ	29:a:2478:A:OP2	2.35	0.45
5:4:37:CYS:SG	5:4:40:CYS:CB	2.92	0.45
6:A:265:G:P	22:Q:65:ARG:HH21	2.39	0.45
6:A:1011:C:H2'	6:A:1012:A:H8	1.80	0.45
6:A:1014:A:H2	6:A:1219:A:H1'	1.79	0.45
6:A:1321:U:H2'	6:A:1322:C:C5	2.51	0.45
9:D:9:LEU:HD13	9:D:32:CYS:HB3	1.99	0.45
12:G:26:PHE:CB	12:G:101:MET:HE2	2.42	0.45
15:J:20:GLN:HG3	15:J:21:ALA:N	2.30	0.45
29:a:1366:A:H1'	62:a:8072:HOH:O	2.16	0.45
29:a:2649:C:H2'	29:a:2650:U:H6	1.82	0.45
30:b:11:C:N3	62:b:317:HOH:O	2.36	0.45
32:d:184:ARG:HH12	43:o:7:GLN:HG2	1.80	0.45
6:A:335:C:H2'	6:A:336:A:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:98:ARG:NH1	26:U:16:LEU:HD23	2.32	0.45
18:M:65:VAL:HG23	18:M:66:GLU:HG2	1.97	0.45
29:a:500:G:N1	29:a:503:A:OP2	2.45	0.45
29:a:877:A:H1'	29:a:900:A:H61	1.81	0.45
29:a:1442:U:H2'	29:a:1443:U:C6	2.51	0.45
29:a:2241:A:H2'	29:a:2242:G:C8	2.52	0.45
29:a:2299:U:H2'	29:a:2300:C:H6	1.80	0.45
34:f:47:LYS:HE3	34:f:83:TYR:OH	2.17	0.45
35:g:60:ASP:O	35:g:62:TRP:N	2.49	0.45
47:s:4:GLU:O	47:s:4:GLU:HG2	2.16	0.45
6:A:1279:G:OP2	15:J:11:LYS:NZ	2.40	0.45
28:Y:49:G:H2'	28:Y:50:U:H6	1.81	0.45
29:a:1149:G:H2'	29:a:1150:C:C6	2.51	0.45
29:a:2901:C:H2'	29:a:2902:C:H6	1.80	0.45
6:A:815:A:N7	6:A:1509:C:O2'	2.44	0.45
29:a:139:U:H5'	29:a:140:C:H5	1.82	0.45
29:a:589:U:H2'	29:a:590:A:C8	2.52	0.45
29:a:889:C:H5"	29:a:890:C:OP2	2.16	0.45
29:a:1545:A:H2'	29:a:1546:G:O4'	2.17	0.45
29:a:2228:G:H2'	29:a:2229:U:C6	2.52	0.45
39:k:13:LYS:HD2	39:k:13:LYS:HA	1.66	0.45
2:1:35:ARG:HG2	2:1:42:LEU:HD21	1.99	0.45
6:A:502:A:H2'	6:A:503:C:O4'	2.17	0.45
6:A:542:G:H5'	9:D:39:GLY:HA3	1.98	0.45
7:B:162:PHE:HA	7:B:184:PHE:O	2.15	0.45
11:F:11:HIS:NE2	11:F:54:LEU:HD21	2.32	0.45
12:G:116:MET:HE2	12:G:119:ARG:HE	1.81	0.45
14:I:33:ARG:NH1	14:I:37:GLN:O	2.49	0.45
3:2:14:PHE:C	3:2:15:LYS:HD3	2.42	0.45
6:A:320:A:H2'	6:A:321:A:O4'	2.17	0.45
6:A:1278:G:O5'	6:A:1279:G:H5'	2.17	0.45
20:O:7:ALA:O	20:O:11:ILE:HD12	2.17	0.45
28:Y:10:G:P	28:Y:46:G:H5"	2.57	0.45
28:Y:25:C:C2	28:Y:26:G:C8	3.05	0.45
28:Z:17:C:OP1	28:Z:60:U:O2'	2.29	0.45
29:a:320:A:H4'	29:a:322:A:N7	2.32	0.45
29:a:832:U:H2'	29:a:833:A:C8	2.52	0.45
29:a:1182:G:H2'	29:a:1183:U:O4'	2.16	0.45
29:a:1842:G:H2'	29:a:1843:C:H6	1.82	0.45
29:a:1869:G:O2'	29:a:1872:A:N6	2.49	0.45
29:a:2325:G:OP2	62:a:6323:HOH:O	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2756:U:H1'	29:a:2757:A:H5"	1.97	0.45
34:f:108:VAL:HG11	34:f:176:PRO:HG3	1.98	0.45
1:0:7:GLU:OE1	1:0:28:ARG:NH2	2.50	0.45
6:A:273:U:O2'	22:Q:18:GLU:OE1	2.19	0.45
6:A:821:G:H2'	6:A:822:U:C6	2.52	0.45
6:A:1308:U:H2'	6:A:1309:G:H8	1.82	0.45
12:G:74:GLU:OE2	12:G:95:ARG:NH2	2.48	0.45
21:P:40:ASN:HB3	21:P:43:ALA:HB2	1.99	0.45
29:a:1494:A:H2'	29:a:1495:A:C8	2.52	0.45
29:a:1733:G:H2'	29:a:1734:G:C8	2.51	0.45
29:a:2469:A:H4'	40:l:55:ARG:HD2	1.98	0.45
37:i:12:LYS:HE3	37:i:13:ARG:C	2.41	0.45
6:A:34:C:H2'	6:A:35:G:H8	1.81	0.44
6:A:345:C:H3'	43:o:39:ARG:NH2	2.32	0.44
6:A:875:U:O2'	13:H:15:ARG:HD2	2.17	0.44
6:A:1008:U:H3'	6:A:1009:U:H5"	1.99	0.44
6:A:1288:A:H2'	6:A:1289:A:O4'	2.17	0.44
7:B:163:VAL:HG21	7:B:173:ILE:HD11	1.98	0.44
29:a:949:G:N7	62:a:6487:HOH:O	2.36	0.44
29:a:1537:G:H2'	29:a:1538:G:O4'	2.16	0.44
29:a:2395:C:H2'	29:a:2396:G:O4'	2.17	0.44
29:a:2507:C:H5'	29:a:2573:C:N4	2.31	0.44
34:f:32:GLU:OE1	34:f:157:THR:HG22	2.17	0.44
38:j:17:ARG:HA	38:j:17:ARG:HD3	1.77	0.44
49:u:51:GLN:HB2	49:u:57:TYR:OH	2.17	0.44
5:4:24:ILE:HB	34:f:102:ARG:HD2	1.99	0.44
6:A:165:G:H2'	6:A:166:U:C6	2.53	0.44
6:A:476:U:H2'	6:A:477:C:C6	2.52	0.44
6:A:642:A:H2'	6:A:643:C:H6	1.81	0.44
6:A:983:A:H5'	6:A:984:C:OP2	2.17	0.44
6:A:1121:U:H2'	6:A:1122:U:H6	1.81	0.44
28:Y:22:G:H2'	28:Y:23:C:H6	1.82	0.44
28:Z:53:G:H2'	28:Z:54:U:C6	2.52	0.44
29:a:64:A:H2'	29:a:65:U:H6	1.82	0.44
29:a:742:A:H2'	29:a:743:A:H8	1.81	0.44
29:a:766:U:O4	60:a:6205:SPM:H81	2.17	0.44
29:a:1248:G:OP1	33:e:44:ARG:NH1	2.41	0.44
29:a:1853:A:N1	29:a:2087:G:H1'	2.32	0.44
29:a:2072:C:H2'	29:a:2073:C:H6	1.82	0.44
29:a:2377:A:H2'	29:a:2378:A:C8	2.51	0.44
29:a:2849:U:H4'	29:a:2868:A:C2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:37:C:H2'	30:b:38:C:O4'	2.17	0.44
6:A:77:A:H2'	6:A:78:A:H8	1.82	0.44
6:A:1410:A:H2'	6:A:1411:C:C6	2.53	0.44
7:B:139:ARG:HG2	7:B:143:LYS:HZ3	1.78	0.44
13:H:73:GLU:HB3	13:H:130:ALA:OXT	2.17	0.44
29:a:132:G:H2'	29:a:133:U:H6	1.81	0.44
29:a:630:G:N2	29:a:633:A:OP2	2.41	0.44
29:a:2020:A:H5'	54:z:9:THR:CG2	2.47	0.44
29:a:2582:G:OP2	62:a:6322:HOH:O	2.21	0.44
33:e:119:ILE:HD11	33:e:185:LYS:HD2	1.97	0.44
6:A:649:A:H2'	6:A:650:G:O4'	2.17	0.44
6:A:1160:G:C2	6:A:1161:C:C6	3.05	0.44
7:B:50:PHE:CD1	7:B:200:ILE:HD13	2.53	0.44
8:C:36:ASP:OD1	8:C:59:ARG:NH2	2.40	0.44
8:C:162:ILE:HD13	27:X:24:A:O3'	2.17	0.44
29:a:247:G:H4'	29:a:386:G:C5	2.52	0.44
29:a:265:A:N1	29:a:427:U:O2'	2.47	0.44
29:a:580:U:H2'	29:a:581:C:H6	1.83	0.44
29:a:657:U:H2'	29:a:658:U:C6	2.53	0.44
29:a:1821:A:H2'	29:a:1822:C:C6	2.53	0.44
36:h:34:GLY:O	36:h:36:ALA:N	2.50	0.44
50:v:10:THR:CG2	50:v:12:ASN:H	2.30	0.44
2:1:41:ARG:HG3	2:1:41:ARG:HH11	1.82	0.44
6:A:82:G:N3	6:A:82:G:H2'	2.32	0.44
6:A:472:U:H2'	6:A:473:U:C6	2.52	0.44
6:A:688:G:OP1	62:A:1720:HOH:O	2.21	0.44
6:A:1023:U:H2'	6:A:1024:G:H8	1.82	0.44
15:J:47:GLU:HG2	15:J:49:PHE:CZ	2.53	0.44
15:J:59:LYS:HE2	15:J:62:ARG:NH2	2.33	0.44
28:Z:24:U:O2'	29:a:1923:U:OP1	2.36	0.44
29:a:347:A:H2'	29:a:348:A:C8	2.53	0.44
29:a:391:A:H1'	29:a:411:G:O4'	2.17	0.44
29:a:483:A:C8	48:t:45:HIS:HD2	2.35	0.44
29:a:1197:G:H2'	29:a:1198:U:C6	2.52	0.44
29:a:2615:U:C2	54:z:4:GLN:HA	2.53	0.44
29:a:2895:G:H2'	29:a:2896:C:H6	1.81	0.44
34:f:14:LYS:HE3	34:f:14:LYS:HB3	1.90	0.44
6:A:294:U:H2'	6:A:295:C:C6	2.52	0.44
6:A:555:U:H2'	6:A:556:C:H6	1.80	0.44
6:A:1524:C:H2'	6:A:1525:G:C8	2.53	0.44
8:C:49:LYS:HD2	8:C:49:LYS:HA	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:23:LEU:HD12	12:G:23:LEU:HA	1.86	0.44
18:M:16:VAL:CG2	18:M:41:GLU:HB3	2.48	0.44
23:R:23:TYR:HA	23:R:29:LEU:HD11	2.00	0.44
28:Z:36:U:H2'	28:Z:37:A:H8	1.83	0.44
29:a:347:A:H2'	29:a:348:A:H8	1.83	0.44
29:a:1014:A:H2'	29:a:1015:U:C6	2.52	0.44
29:a:1731:G:H2'	29:a:1732:C:H5"	2.00	0.44
31:c:72:ASP:HA	31:c:118:SER:O	2.18	0.44
34:f:29:PRO:HG2	34:f:165:GLU:HB3	1.98	0.44
6:A:1474:U:H4'	29:a:1701:A:N3	2.33	0.44
22:Q:81:LYS:HD2	22:Q:81:LYS:N	2.32	0.44
29:a:866:A:C8	29:a:914:G:C5	3.05	0.44
29:a:1020:A:OP1	62:a:6331:HOH:O	2.21	0.44
29:a:1818:U:OP2	62:a:6333:HOH:O	2.21	0.44
29:a:1842:G:H2'	29:a:1843:C:C6	2.53	0.44
29:a:2328:A:H2'	29:a:2329:U:H6	1.79	0.44
35:g:99:LYS:HD2	35:g:99:LYS:O	2.17	0.44
39:k:55:MET:HB3	62:k:225:HOH:O	2.17	0.44
2:1:41:ARG:HG3	2:1:41:ARG:NH1	2.33	0.44
3:2:50:VAL:HG11	3:2:58:VAL:HG21	1.99	0.44
6:A:259:G:OP1	25:T:36:TYR:OH	2.25	0.44
6:A:1151:A:O2'	6:A:1152:A:H8	2.00	0.44
6:A:1330:U:OP1	62:A:1722:HOH:O	2.21	0.44
6:A:1530:G:O6	26:U:46:LYS:NZ	2.36	0.44
7:B:128:LYS:H	7:B:128:LYS:HD2	1.83	0.44
14:I:84:THR:HG23	14:I:98:LEU:HD13	1.98	0.44
29:a:881:G:C2	29:a:882:G:C8	3.06	0.44
6:A:590:U:H2'	6:A:591:U:C6	2.53	0.44
6:A:600:A:OP2	13:H:88:ARG:HD2	2.17	0.44
6:A:798:U:OP1	62:A:1719:HOH:O	2.21	0.44
6:A:1305:G:H22	6:A:1331:G:H1'	1.83	0.44
15:J:52:LEU:HD12	15:J:62:ARG:HD3	1.98	0.44
29:a:1:G:H2'	29:a:2:G:C8	2.53	0.44
29:a:1001:A:H2'	29:a:1002:G:O4'	2.17	0.44
29:a:1754:A:N1	29:a:2716:C:O2'	2.44	0.44
35:g:96:ALA:HB2	35:g:105:LEU:HD23	1.98	0.44
5:4:11:GLU:HG2	5:4:23:LYS:NZ	2.33	0.43
6:A:671:G:H2'	6:A:672:U:O4'	2.18	0.43
12:G:5:ARG:O	12:G:5:ARG:HG3	2.18	0.43
13:H:18:GLN:CD	13:H:70:ALA:HB1	2.43	0.43
14:I:65:ILE:HG21	14:I:79:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:182:A:H2'	29:a:183:C:H6	1.82	0.43
29:a:1409:U:H2'	29:a:1410:G:H8	1.83	0.43
31:c:108:LYS:HE3	31:c:194:GLU:OE1	2.18	0.43
31:c:205:LEU:HB3	31:c:210:ALA:HB3	1.99	0.43
34:f:106:ILE:HG21	34:f:139:PRO:HG2	1.99	0.43
6:A:188:C:H2'	6:A:189:A:O4'	2.19	0.43
6:A:593:U:H2'	6:A:594:U:C6	2.52	0.43
6:A:635:A:H2'	6:A:636:U:C6	2.53	0.43
8:C:6:HIS:CG	19:N:89:MET:HB3	2.52	0.43
11:F:62:MET:HE2	11:F:62:MET:HB2	1.86	0.43
26:U:29:LEU:O	26:U:33:ARG:HG3	2.17	0.43
29:a:2090:A:OP2	62:a:6336:HOH:O	2.21	0.43
30:b:50:A:OP1	42:n:67:ASN:HB2	2.18	0.43
32:d:7:LYS:HE3	32:d:7:LYS:HB2	1.67	0.43
37:i:43:GLU:N	37:i:43:GLU:CD	2.76	0.43
6:A:545:C:OP1	9:D:58:LYS:NZ	2.51	0.43
6:A:612:C:H2'	6:A:613:C:H6	1.82	0.43
6:A:1363:A:OP1	62:A:1724:HOH:O	2.21	0.43
22:Q:59:VAL:HG12	22:Q:78:VAL:HG22	2.00	0.43
28:Z:44:A:H2'	28:Z:45:G:C8	2.53	0.43
29:a:158:U:H2'	29:a:159:G:C8	2.53	0.43
29:a:760:G:H2'	29:a:761:A:O4'	2.18	0.43
31:c:76:ALA:HB2	31:c:96:TYR:CD1	2.52	0.43
6:A:154:U:H2'	6:A:155:A:H8	1.82	0.43
6:A:451:A:H4'	6:A:452:A:O4'	2.18	0.43
6:A:1101:A:H4'	6:A:1102:A:O5'	2.19	0.43
8:C:23:PHE:CZ	15:J:11:LYS:HB3	2.53	0.43
10:E:83:HIS:CG	13:H:96:MET:HG2	2.54	0.43
10:E:111:MET:HE2	10:E:125:ALA:HB1	2.00	0.43
15:J:29:ALA:HB2	15:J:87:LEU:HD21	2.00	0.43
17:L:79:VAL:O	17:L:103:ASP:HB2	2.18	0.43
24:S:29:LYS:HG2	24:S:30:PRO:CD	2.33	0.43
24:S:30:PRO:HG3	24:S:48:THR:CG2	2.48	0.43
24:S:32:ARG:O	62:S:102:HOH:O	2.21	0.43
28:Z:50:U:H3	28:Z:64:G:H1	1.66	0.43
29:a:82:U:H2'	29:a:83:A:C8	2.54	0.43
29:a:157:C:H2'	29:a:158:U:O4'	2.18	0.43
29:a:208:C:H2'	29:a:209:C:C6	2.53	0.43
29:a:871:U:H2'	29:a:872:U:C6	2.54	0.43
29:a:1155:A:OP2	62:a:6324:HOH:O	2.20	0.43
29:a:1292:G:H2'	29:a:1293:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1319:C:O2'	29:a:1320:C:H5'	2.18	0.43
32:d:62:LYS:HE2	32:d:62:LYS:HB3	1.61	0.43
39:k:69:ARG:NH1	39:k:69:ARG:HG2	2.33	0.43
6:A:580:C:H2'	6:A:581:G:O4'	2.19	0.43
6:A:821:G:H2'	6:A:822:U:H6	1.83	0.43
6:A:1263:C:H2'	6:A:1264:U:H6	1.83	0.43
6:A:1391:U:H2'	6:A:1392:G:H8	1.80	0.43
13:H:29:SER:HB3	13:H:57:PRO:HB2	2.00	0.43
24:S:44:MET:C	24:S:47:LEU:HD12	2.43	0.43
28:Y:29:G:H2'	28:Y:30:G:H8	1.77	0.43
29:a:588:U:H2'	29:a:589:U:C6	2.54	0.43
29:a:609:A:H2'	29:a:610:C:O4'	2.19	0.43
29:a:1808:A:H3'	29:a:1809:A:C8	2.53	0.43
29:a:2299:U:H2'	29:a:2300:C:C6	2.53	0.43
29:a:2329:U:H2'	29:a:2330:G:H8	1.83	0.43
29:a:2469:A:H2'	29:a:2470:G:O4'	2.19	0.43
32:d:121:THR:HB	32:d:127:PHE:CD2	2.54	0.43
41:m:69:ARG:C	41:m:71:ARG:H	2.27	0.43
6:A:223:A:H2'	6:A:224:U:C6	2.53	0.43
6:A:1148:U:H2'	6:A:1149:C:O4'	2.17	0.43
12:G:68:ASN:O	12:G:138:ARG:NH2	2.50	0.43
21:P:76:LYS:HE2	21:P:76:LYS:HB2	1.82	0.43
29:a:133:U:O2'	29:a:134:G:H5'	2.19	0.43
29:a:2229:U:H2'	29:a:2230:G:H8	1.83	0.43
30:b:16:G:N2	30:b:69:G:H1'	2.33	0.43
34:f:36:LEU:HA	34:f:153:ASP:O	2.19	0.43
43:o:89:ARG:CZ	43:o:115:ASN:O	2.67	0.43
48:t:40:ASN:HB3	48:t:63:ALA:O	2.19	0.43
49:u:35:GLU:H	49:u:35:GLU:HG3	1.52	0.43
5:4:35:ASP:CG	5:4:36:VAL:HG23	2.44	0.43
6:A:501:C:H1'	6:A:549:C:H1'	2.01	0.43
6:A:1238:A:H2	6:A:1241:G:N3	2.16	0.43
9:D:72:PHE:CE1	9:D:94:LEU:HD11	2.48	0.43
28:Y:71:C:H2'	28:Y:72:A:C8	2.53	0.43
29:a:244:A:H2'	29:a:245:G:O4'	2.19	0.43
29:a:601:C:OP2	62:a:6329:HOH:O	2.21	0.43
29:a:784:G:H5'	29:a:785:G:OP1	2.19	0.43
29:a:934:U:H2'	29:a:935:C:C6	2.54	0.43
29:a:1534:U:H2'	29:a:1536:C:C6	2.53	0.43
29:a:1541:C:H2'	29:a:1542:U:C6	2.53	0.43
29:a:1928:A:H2'	29:a:1929:G:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2191:A:H2'	29:a:2192:U:C6	2.54	0.43
29:a:2639:A:H2'	29:a:2640:G:O4'	2.18	0.43
29:a:2680:U:O2'	29:a:2681:C:H5'	2.19	0.43
34:f:29:PRO:HA	34:f:159:THR:OG1	2.18	0.43
41:m:38:LEU:HB3	41:m:39:PRO:HD3	1.99	0.43
5:4:60:PHE:HZ	24:S:41:PHE:CE1	2.37	0.43
6:A:154:U:H2'	6:A:155:A:C8	2.54	0.43
6:A:1229:A:H4'	28:Z:29:G:O3'	2.19	0.43
6:A:1498:UR3:O4'	6:A:1519:MA6:H2	2.19	0.43
11:F:61:LEU:HD22	23:R:24:LYS:HE3	2.00	0.43
12:G:113:ASP:HB3	12:G:118:LEU:HD23	2.01	0.43
29:a:713:G:H21	29:a:718:A:H62	1.66	0.43
29:a:918:A:H5"	30:b:97:C:O2'	2.18	0.43
29:a:2078:C:H2'	29:a:2079:U:C6	2.53	0.43
29:a:2845:U:H5"	43:o:52:ASN:O	2.18	0.43
29:a:2901:C:C2	29:a:2902:C:C5	3.06	0.43
32:d:148:GLN:HB2	32:d:152:PRO:HD2	2.00	0.43
33:e:158:PHE:CD1	33:e:159:LEU:HD23	2.53	0.43
1:0:30:LYS:HB3	1:0:32:GLU:OE2	2.19	0.43
6:A:181:A:N6	6:A:195:A:C8	2.87	0.43
6:A:192:A:H2'	6:A:193:C:O4'	2.19	0.43
6:A:219:U:H2'	6:A:220:G:C8	2.54	0.43
6:A:684:U:H2'	6:A:685:G:O4'	2.19	0.43
6:A:744:C:H2'	6:A:745:G:H8	1.84	0.43
6:A:1277:C:H1'	6:A:1282:C:O2	2.19	0.43
10:E:23:LYS:HE2	10:E:23:LYS:HB2	1.69	0.43
18:M:7:ILE:HG22	34:f:112:ARG:HH21	1.83	0.43
24:S:28:LYS:HD3	24:S:29:LYS:N	2.33	0.43
28:Y:58:A:O2'	28:Y:60:U:OP2	2.20	0.43
29:a:155:A:H2'	29:a:156:A:C8	2.54	0.43
29:a:409:G:OP1	62:a:6335:HOH:O	2.21	0.43
29:a:749:A:H4'	29:a:1271:G:N3	2.34	0.43
29:a:956:G:O6	40:l:14:LYS:HE3	2.19	0.43
29:a:1469:A:H2'	29:a:1470:A:H8	1.81	0.43
29:a:1653:G:H3'	41:m:2:ARG:HG2	2.00	0.43
29:a:1794:A:H2'	29:a:1795:C:H6	1.83	0.43
29:a:2038:G:H2'	29:a:2039:U:O4'	2.18	0.43
29:a:2251:OMG:HM23	29:a:2251:OMG:H1'	1.73	0.43
29:a:2451:A:N7	62:a:6500:HOH:O	2.36	0.43
35:g:164:TYR:HB2	35:g:167:GLU:HB2	2.01	0.43
6:A:537:G:H2'	6:A:538:G:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:782:A:H4'	6:A:1514:G:O2'	2.19	0.43
6:A:1250:A:H2'	6:A:1251:A:C8	2.54	0.43
6:A:1402:4OC:H2'	6:A:1403:C:O4'	2.19	0.43
28:Y:19:G:O6	29:a:897:C:O2'	2.37	0.43
29:a:327:G:O6	58:a:6198:SPD:H82	2.18	0.43
29:a:542:C:H2'	29:a:543:G:C8	2.53	0.43
29:a:639:U:H2'	29:a:640:C:H6	1.81	0.43
35:g:127:THR:HG22	35:g:128:GLN:H	1.83	0.43
45:q:15:SER:O	45:q:18:GLN:HB2	2.19	0.43
50:v:5:LYS:HE3	50:v:5:LYS:HB3	1.86	0.43
6:A:273:U:O4	6:A:274:A:N6	2.52	0.42
6:A:506:G:O6	62:A:1723:HOH:O	2.21	0.42
6:A:1001:C:C2	6:A:1002:G:C8	3.07	0.42
6:A:1404:C:H2'	6:A:1405:G:C8	2.54	0.42
13:H:79:SER:HB3	13:H:125:ILE:O	2.19	0.42
16:K:64:GLN:HG3	16:K:99:ALA:HB2	2.00	0.42
26:U:7:ARG:O	26:U:10:GLU:HB3	2.19	0.42
29:a:323:C:H6	29:a:1205:A:C2	2.36	0.42
29:a:1048:A:N7	29:a:1111:A:C6	2.87	0.42
29:a:1813:G:N7	62:a:6498:HOH:O	2.36	0.42
29:a:2439:A:H62	61:a:6207:MET:CE	2.32	0.42
30:b:52:A:N7	42:n:64:TYR:OH	2.40	0.42
34:f:13:VAL:O	34:f:17:MET:HG3	2.18	0.42
37:i:96:ARG:HB3	37:i:99:ARG:HG3	2.01	0.42
43:o:63:LYS:HB2	43:o:63:LYS:HE2	1.45	0.42
5:4:38:SER:HB2	34:f:105:THR:HA	2.02	0.42
6:A:1513:A:H2'	6:A:1514:G:H8	1.83	0.42
6:A:1525:G:OP2	62:A:1725:HOH:O	2.22	0.42
10:E:14:LYS:HZ2	10:E:14:LYS:HG3	1.54	0.42
28:Z:39:C:H2'	28:Z:40:C:H6	1.85	0.42
29:a:694:U:O4	60:a:6205:SPM:H112	2.20	0.42
29:a:987:C:H2'	29:a:988:A:O4'	2.19	0.42
29:a:1571:A:H2'	29:a:1572:A:C8	2.54	0.42
29:a:1846:G:O2'	29:a:1847:A:H5'	2.19	0.42
29:a:1883:U:H2'	29:a:1884:G:O4'	2.19	0.42
29:a:2650:U:H2'	29:a:2651:C:H6	1.84	0.42
34:f:57:LEU:O	34:f:61:SER:OG	2.35	0.42
6:A:5:U:H5'	6:A:6:G:OP1	2.19	0.42
6:A:151:A:H2'	6:A:152:A:O4'	2.19	0.42
6:A:718:A:C2	23:R:38:LYS:HG2	2.54	0.42
12:G:47:LEU:HD12	12:G:47:LEU:HA	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:56:LYS:HB3	12:G:56:LYS:HE2	1.64	0.42
29:a:248:G:H5'	29:a:250:G:N7	2.34	0.42
29:a:652:U:H3'	29:a:653:U:C5	2.54	0.42
29:a:1269:A:H2'	29:a:1270:C:C6	2.54	0.42
30:b:34:A:N6	62:b:322:HOH:O	2.41	0.42
30:b:104:A:H2'	30:b:105:G:O4'	2.19	0.42
34:f:107:ALA:HB1	34:f:137:ILE:HD12	2.00	0.42
36:h:33:GLN:HG3	36:h:35:LYS:HE2	1.99	0.42
39:k:69:ARG:HG2	39:k:69:ARG:HH11	1.84	0.42
1:0:11:LEU:HD21	1:0:34:LEU:HD23	2.00	0.42
6:A:326:G:O6	58:A:1670:SPD:N10	2.51	0.42
6:A:458:U:H2'	6:A:459:A:H8	1.83	0.42
12:G:2:PRO:HG3	12:G:7:ILE:HD11	2.01	0.42
25:T:69:LYS:HB2	25:T:69:LYS:HE3	1.83	0.42
59:Y:101:8AN:H2	29:a:2583:G:N3	2.34	0.42
30:b:54:G:N2	62:b:332:HOH:O	2.51	0.42
42:n:83:LEU:HD12	42:n:83:LEU:HA	1.80	0.42
51:w:64:ILE:O	51:w:68:LEU:HG	2.20	0.42
6:A:408:A:H2'	6:A:409:U:O4'	2.19	0.42
6:A:1382:C:H2'	6:A:1383:C:H6	1.84	0.42
9:D:54:GLN:HB3	9:D:203:LEU:HB2	2.02	0.42
29:a:52:A:H2'	29:a:53:A:C8	2.55	0.42
29:a:576:U:H2'	29:a:577:G:C8	2.55	0.42
29:a:1744:A:H3'	29:a:1745:A:H8	1.85	0.42
33:e:1:MET:HE3	33:e:1:MET:HB3	1.87	0.42
33:e:5:LEU:HD11	33:e:12:LEU:HB2	2.01	0.42
33:e:98:LYS:O	33:e:102:ARG:HG3	2.20	0.42
45:q:97:LYS:HE3	45:q:97:LYS:HB2	1.67	0.42
6:A:16:A:N1	6:A:919:A:H2	2.16	0.42
6:A:270:A:H2'	6:A:271:C:H6	1.84	0.42
6:A:284:C:H2'	6:A:285:C:H6	1.85	0.42
6:A:1070:U:H2'	6:A:1071:C:C6	2.55	0.42
7:B:119:THR:O	7:B:123:ASP:HB2	2.20	0.42
11:F:8:PHE:HA	11:F:87:SER:HA	2.02	0.42
12:G:71:PRO:O	12:G:96:ARG:HG2	2.19	0.42
16:K:81:ASN:OD1	16:K:106:ARG:NH2	2.51	0.42
29:a:156:A:H2'	29:a:157:C:C6	2.55	0.42
29:a:224:U:O4	29:a:420:C:H5'	2.19	0.42
29:a:898:C:H2'	29:a:899:A:O4'	2.19	0.42
29:a:1405:U:H2'	29:a:1406:U:H6	1.84	0.42
29:a:1432:G:H2'	29:a:1433:A:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2810:A:H2'	29:a:2811:G:O4'	2.20	0.42
47:s:7:LEU:O	62:s:201:HOH:O	2.22	0.42
6:A:328:C:H4'	6:A:329:A:H5'	2.01	0.42
6:A:1032:G:C6	6:A:1033:G:H1'	2.53	0.42
6:A:1043:G:O2'	6:A:1044:A:O5'	2.34	0.42
6:A:1133:G:C6	6:A:1142:G:C6	3.07	0.42
6:A:1274:A:N1	62:A:1849:HOH:O	2.37	0.42
6:A:1358:U:P	19:N:75:ARG:HD2	2.59	0.42
14:I:118:LEU:HD22	14:I:124:ARG:HG2	2.01	0.42
25:T:24:ARG:HA	25:T:24:ARG:HD3	1.75	0.42
29:a:1429:G:H2'	29:a:1430:G:H8	1.85	0.42
50:v:38:VAL:HG12	50:v:59:LEU:HB2	2.00	0.42
1:0:37:LYS:CD	1:0:48:ILE:HD12	2.49	0.42
6:A:73:C:O2'	6:A:74:A:O5'	2.33	0.42
6:A:200:G:O2'	6:A:201:G:H5'	2.19	0.42
6:A:346:G:H3'	6:A:346:G:N3	2.35	0.42
6:A:864:A:H2'	6:A:865:A:C8	2.54	0.42
6:A:1158:C:C4	6:A:1160:G:C8	3.08	0.42
6:A:1170:A:O5'	6:A:1170:A:H8	2.03	0.42
7:B:152:LYS:HE2	7:B:152:LYS:HB3	1.74	0.42
8:C:129:MET:HE3	8:C:131:ARG:CB	2.47	0.42
28:Y:56:C:OP2	40:l:59:ARG:NH1	2.52	0.42
28:Z:36:U:H2'	28:Z:37:A:C8	2.54	0.42
29:a:30:G:H2'	29:a:31:C:C6	2.55	0.42
29:a:1013:C:H2'	29:a:1014:A:H8	1.84	0.42
29:a:1830:C:H2'	29:a:1831:G:H8	1.85	0.42
29:a:2649:C:H2'	29:a:2650:U:C6	2.55	0.42
29:a:2820:A:O2'	29:a:2821:A:OP1	2.35	0.42
31:c:78:VAL:HG22	31:c:94:VAL:HG12	2.01	0.42
48:t:87:PHE:CE1	48:t:92:LYS:HB2	2.55	0.42
49:u:51:GLN:HA	49:u:56:PHE:CG	2.54	0.42
5:4:66:ILE:CD1	19:N:42:TRP:CD2	3.02	0.42
6:A:487:A:H3'	6:A:488:C:H6	1.85	0.42
6:A:1173:U:H2'	6:A:1174:G:O4'	2.19	0.42
7:B:81:LYS:HE3	7:B:81:LYS:HB2	1.93	0.42
9:D:105:MET:HE2	9:D:171:LEU:HD22	2.00	0.42
22:Q:47:HIS:HA	22:Q:71:LYS:HZ1	1.84	0.42
29:a:37:C:H4'	29:a:451:U:OP1	2.20	0.42
29:a:594:U:H2'	29:a:595:C:H6	1.85	0.42
29:a:1799:G:OP2	31:c:270:ARG:NH2	2.48	0.42
29:a:1902:C:H4'	31:c:242:LYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2191:A:H2'	29:a:2192:U:H6	1.85	0.42
29:a:2636:C:H2'	29:a:2637:U:H6	1.85	0.42
34:f:54:ALA:HB1	34:f:65:PRO:HG2	2.01	0.42
37:i:110:PRO:O	37:i:115:GLY:HA3	2.19	0.42
6:A:269:C:H2'	6:A:270:A:H8	1.78	0.42
12:G:18:PHE:HB3	12:G:59:LEU:HD11	2.02	0.42
26:U:16:LEU:HD12	26:U:16:LEU:HA	1.87	0.42
29:a:171:U:H2'	29:a:172:A:H8	1.85	0.42
29:a:285:G:H2'	29:a:286:U:O4'	2.19	0.42
29:a:1464:G:H2'	29:a:1465:G:C8	2.54	0.42
29:a:2028:U:H2'	29:a:2029:G:C8	2.55	0.42
29:a:2553:G:H2'	29:a:2554:C:O4'	2.20	0.42
29:a:2684:U:OP1	62:a:6334:HOH:O	2.21	0.42
29:a:2723:C:H2'	29:a:2724:U:O4'	2.19	0.42
29:a:2869:G:H2'	29:a:2870:C:O4'	2.19	0.42
50:v:72:LYS:HE3	50:v:72:LYS:HB2	1.72	0.42
28:Y:6:G:H2'	28:Y:7:G:C8	2.55	0.41
28:Y:26:G:C4	28:Y:27:U:C6	3.08	0.41
29:a:95:A:H4'	52:x:38:GLN:O	2.20	0.41
29:a:729:G:C6	31:c:207:LYS:HB2	2.55	0.41
29:a:927:A:H2'	29:a:928:A:C8	2.55	0.41
29:a:1635:A:OP2	62:a:6337:HOH:O	2.21	0.41
29:a:1726:C:H2'	29:a:1727:C:O4'	2.19	0.41
29:a:1945:G:H2'	29:a:1946:U:C6	2.55	0.41
29:a:2804:U:H2'	29:a:2805:C:C6	2.55	0.41
30:b:112:G:N2	42:n:45:SER:O	2.44	0.41
6:A:321:A:H2'	6:A:322:C:C6	2.55	0.41
6:A:718:A:C8	16:K:118:HIS:HB3	2.55	0.41
12:G:22:LEU:HD21	12:G:97:ASN:ND2	2.35	0.41
12:G:116:MET:HE2	12:G:119:ARG:NE	2.35	0.41
29:a:1271:G:O6	58:a:6201:SPD:H21	2.20	0.41
29:a:1409:U:H2'	29:a:1410:G:C8	2.55	0.41
29:a:1441:G:H2'	29:a:1442:U:C6	2.55	0.41
29:a:1594:U:H2'	29:a:1595:C:C6	2.56	0.41
29:a:1786:A:H1'	29:a:1938:A:N6	2.36	0.41
29:a:1803:A:OP2	62:a:6332:HOH:O	2.21	0.41
29:a:2077:A:OP2	62:a:6338:HOH:O	2.22	0.41
29:a:2307:G:H4'	29:a:2308:G:O4'	2.20	0.41
30:b:28:C:H2'	30:b:29:A:O4'	2.20	0.41
34:f:142:ASP:OD1	34:f:145:LYS:HB2	2.20	0.41
6:A:222:C:H2'	6:A:223:A:H8	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:720:C:H2'	6:A:721:G:N7	2.35	0.41
6:A:1283:U:O4	62:A:1721:HOH:O	2.21	0.41
6:A:1486:G:H2'	6:A:1487:G:O4'	2.20	0.41
7:B:70:VAL:O	7:B:163:VAL:HA	2.21	0.41
7:B:193:PRO:HB2	7:B:199:VAL:HG21	2.02	0.41
8:C:27:LYS:HB3	8:C:28:GLU:OE1	2.20	0.41
9:D:55:LEU:O	9:D:59:GLN:HG2	2.21	0.41
16:K:107:ILE:HG13	26:U:12:PHE:CE1	2.55	0.41
28:Y:9:G:O2'	28:Y:10:G:N7	2.49	0.41
29:a:2305:U:C2	34:f:151:GLY:HA3	2.55	0.41
29:a:2406:A:H1'	58:a:6196:SPD:H51	2.02	0.41
31:c:243:HIS:HA	31:c:244:PRO:HD3	1.96	0.41
41:m:69:ARG:O	41:m:71:ARG:N	2.51	0.41
6:A:1434:A:H2'	6:A:1435:G:O4'	2.20	0.41
6:A:1494:G:O2'	29:a:1912:A:O2'	2.22	0.41
10:E:11:LEU:HD13	10:E:71:MET:HE1	2.02	0.41
13:H:89:LYS:HE3	13:H:89:LYS:HB3	1.86	0.41
18:M:83:LEU:HD23	18:M:83:LEU:HA	1.75	0.41
28:Y:15:G:H5"	28:Y:16:C:OP2	2.20	0.41
29:a:340:A:H2'	29:a:341:C:O4'	2.20	0.41
29:a:589:U:H2'	29:a:590:A:H8	1.86	0.41
29:a:948:C:H2'	29:a:949:G:C8	2.55	0.41
29:a:2687:U:H2'	29:a:2688:G:O4'	2.21	0.41
31:c:116:ILE:HA	31:c:125:LYS:NZ	2.35	0.41
33:e:83:VAL:HB	33:e:86:ALA:HB2	2.01	0.41
35:g:24:ILE:HD11	35:g:43:VAL:HG21	2.02	0.41
37:i:5:THR:HG22	37:i:6:ALA:O	2.20	0.41
48:t:47:LYS:HA	48:t:47:LYS:HD3	1.83	0.41
6:A:33:A:H2'	6:A:34:C:H6	1.85	0.41
6:A:537:G:H2'	6:A:538:G:H8	1.85	0.41
6:A:1118:U:H2'	6:A:1119:C:O4'	2.21	0.41
7:B:71:GLY:O	7:B:93:ASN:HA	2.20	0.41
8:C:42:TYR:CE1	8:C:90:VAL:HG11	2.55	0.41
9:D:188:ARG:HD2	9:D:188:ARG:HA	1.62	0.41
16:K:65:VAL:HA	16:K:68:GLU:HG3	2.02	0.41
21:P:43:ALA:HB1	21:P:47:GLU:HG2	2.02	0.41
29:a:285:G:O6	29:a:355:U:O2	2.39	0.41
29:a:352:A:H8	29:a:352:A:O5'	2.04	0.41
29:a:848:C:H2'	29:a:849:A:C8	2.55	0.41
29:a:1548:A:H2'	29:a:1549:A:C8	2.56	0.41
34:f:69:LYS:HA	34:f:83:TYR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:23:THR:OG1	1:0:24:THR:N	2.54	0.41
6:A:953:G:H2'	6:A:954:G:O4'	2.20	0.41
6:A:976:G:OP2	6:A:1358:U:O2'	2.35	0.41
14:I:57:MET:HE2	14:I:61:LEU:HD21	2.02	0.41
19:N:71:HIS:NE2	62:N:307:HOH:O	2.37	0.41
29:a:308:G:H2'	29:a:309:A:C8	2.54	0.41
29:a:819:A:C4	29:a:1189:A:C2	3.08	0.41
29:a:852:U:H2'	29:a:853:C:C6	2.56	0.41
29:a:1913:A:OP2	62:a:6340:HOH:O	2.22	0.41
29:a:2072:C:H2'	29:a:2073:C:C6	2.56	0.41
30:b:48:U:H2'	30:b:49:C:C6	2.56	0.41
33:e:2:GLU:OE2	33:e:2:GLU:N	2.51	0.41
37:i:125:TYR:OH	37:i:132:HIS:NE2	2.51	0.41
46:r:46:LEU:O	46:r:50:VAL:HG23	2.21	0.41
53:y:3:LYS:HB3	53:y:3:LYS:HE2	1.64	0.41
6:A:236:A:H2'	6:A:237:G:H8	1.86	0.41
6:A:1220:G:N7	62:A:1852:HOH:O	2.37	0.41
7:B:97:LEU:N	7:B:100:MET:HE3	2.32	0.41
13:H:108:LYS:HD2	13:H:108:LYS:HA	1.84	0.41
20:O:69:TYR:OH	20:O:73:LYS:HE2	2.20	0.41
24:S:32:ARG:HA	24:S:50:ALA:HB3	2.03	0.41
24:S:44:MET:O	24:S:47:LEU:HD12	2.20	0.41
29:a:413:C:H2'	29:a:414:C:C6	2.56	0.41
29:a:451:U:H4'	33:e:47:LYS:HE2	2.03	0.41
29:a:570:G:H2'	29:a:2030:6MZ:N7	2.36	0.41
29:a:933:A:H5'	29:a:934:U:OP2	2.20	0.41
29:a:1177:G:H8	29:a:1177:G:OP1	2.03	0.41
29:a:1274:A:N3	29:a:1297:C:H1'	2.36	0.41
29:a:1727:C:H2'	29:a:1728:C:C6	2.56	0.41
29:a:1792:G:H5'	31:c:204:VAL:HG13	2.02	0.41
32:d:149:ASN:OD1	32:d:150:MEQ:N	2.53	0.41
33:e:123:LYS:HD3	33:e:123:LYS:HA	1.96	0.41
48:t:33:LYS:HB3	48:t:64:ALA:HB1	2.03	0.41
53:y:10:THR:HG22	53:y:56:LYS:NZ	2.36	0.41
6:A:1010:U:H2'	6:A:1011:C:C6	2.56	0.41
6:A:1026:G:C5	6:A:1027:C:C5	3.08	0.41
6:A:1096:C:H2'	6:A:1097:C:C6	2.55	0.41
6:A:1120:C:H2'	6:A:1121:U:H6	1.86	0.41
6:A:1308:U:H2'	6:A:1309:G:C8	2.56	0.41
14:I:36:GLU:HG3	14:I:45:ARG:NH2	2.36	0.41
21:P:45:GLU:O	21:P:46:LYS:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1637:A:H5'	29:a:1760:C:O2'	2.21	0.41
29:a:2229:U:H2'	29:a:2230:G:C8	2.56	0.41
29:a:2523:G:O2'	29:a:2764:A:O2'	2.35	0.41
31:c:72:ASP:CG	31:c:189:ARG:HH22	2.29	0.41
35:g:11:VAL:HA	35:g:12:PRO:HD3	1.93	0.41
35:g:39:ASP:O	35:g:55:ARG:HD2	2.21	0.41
5:4:56:ARG:HH11	24:S:64:ASP:CB	2.33	0.41
6:A:110:C:H2'	6:A:111:G:O4'	2.21	0.41
6:A:390:U:H2'	6:A:391:G:H8	1.85	0.41
6:A:401:C:O2'	6:A:621:A:N3	2.53	0.41
6:A:590:U:H2'	6:A:591:U:H6	1.86	0.41
6:A:1036:A:H2'	6:A:1037:C:H5'	2.02	0.41
7:B:161:LEU:HD12	7:B:161:LEU:HA	1.81	0.41
8:C:120:ILE:O	8:C:124:LEU:HG	2.21	0.41
13:H:11:LEU:HD22	13:H:75:ILE:HD11	2.03	0.41
14:I:90:TYR:CD2	14:I:91:ASP:HB2	2.56	0.41
15:J:15:HIS:O	15:J:18:ILE:HG22	2.21	0.41
15:J:84:VAL:O	15:J:87:LEU:N	2.53	0.41
21:P:35:ARG:HD3	21:P:37:GLY:H	1.86	0.41
28:Y:28:C:C2	28:Y:29:G:C8	3.09	0.41
29:a:372:G:O2'	29:a:400:G:O6	2.35	0.41
29:a:493:G:H2'	29:a:494:G:O4'	2.21	0.41
29:a:593:U:H2'	29:a:594:U:H6	1.84	0.41
29:a:880:G:C6	29:a:881:G:C5	3.09	0.41
29:a:1223:G:C6	29:a:1227:G:C6	3.09	0.41
29:a:1226:A:OP1	44:p:16:LYS:NZ	2.42	0.41
29:a:1879:C:H2'	29:a:1880:U:O4'	2.21	0.41
29:a:1946:U:H2'	29:a:1947:C:H6	1.86	0.41
29:a:2192:U:H2'	29:a:2193:G:O4'	2.20	0.41
29:a:2554:C:N4	29:a:2555:C:H41	2.19	0.41
29:a:2615:U:OP1	62:a:6341:HOH:O	2.22	0.41
29:a:2650:U:H2'	29:a:2651:C:C6	2.55	0.41
29:a:2700:A:H2'	29:a:2701:U:C6	2.56	0.41
29:a:2804:U:H2'	29:a:2805:C:H6	1.85	0.41
30:b:63:C:N4	62:b:338:HOH:O	2.54	0.41
31:c:71:LYS:HG3	31:c:102:ARG:NH1	2.36	0.41
34:f:33:LYS:HA	34:f:96:MET:SD	2.60	0.41
40:l:136:MET:HE3	40:l:136:MET:HB3	1.72	0.41
43:o:89:ARG:HE	43:o:113:ARG:NH2	2.19	0.41
46:r:4:ILE:HG12	46:r:106:VAL:HG22	2.01	0.41
48:t:39:ILE:HD13	48:t:39:ILE:HA	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:195:A:H1'	6:A:222:C:O2'	2.21	0.41
6:A:324:G:N1	6:A:327:A:OP2	2.54	0.41
6:A:763:G:O6	62:A:1714:HOH:O	2.20	0.41
6:A:1118:U:H1'	6:A:1179:A:C5	2.56	0.41
6:A:1359:C:OP2	19:N:75:ARG:NE	2.48	0.41
11:F:3:HIS:CE1	11:F:65:GLU:HG3	2.56	0.41
12:G:56:LYS:NZ	12:G:64:VAL:HG21	2.35	0.41
22:Q:59:VAL:HG12	22:Q:78:VAL:HA	2.03	0.41
23:R:10:PHE:O	23:R:10:PHE:CG	2.73	0.41
29:a:170:U:H2'	29:a:171:U:C6	2.56	0.41
29:a:794:A:H2'	29:a:795:C:C6	2.55	0.41
29:a:1117:C:O2'	29:a:1118:C:H5'	2.21	0.41
29:a:1230:A:H2'	29:a:1231:U:C6	2.56	0.41
29:a:1743:G:H8	29:a:1743:G:O5'	2.04	0.41
29:a:2086:U:H2'	29:a:2087:G:C8	2.55	0.41
34:f:8:TYR:OH	34:f:30:ARG:HG2	2.20	0.41
34:f:22:TYR:CG	34:f:27:GLN:HB2	2.56	0.41
35:g:67:THR:HG22	35:g:71:LEU:CD1	2.51	0.41
6:A:70:U:H1'	6:A:71:A:N7	2.35	0.40
6:A:155:A:H2'	6:A:156:C:O4'	2.21	0.40
6:A:334:C:H2'	6:A:335:C:H6	1.86	0.40
6:A:838:G:C6	6:A:839:C:C4	3.09	0.40
6:A:1319:A:C8	6:A:1323:G:C6	3.08	0.40
6:A:1377:A:OP1	12:G:92:ARG:NH2	2.54	0.40
6:A:1494:G:N7	56:A:1601:PAR:N32	2.69	0.40
7:B:192:ASP:OD2	7:B:194:ASP:HB2	2.21	0.40
10:E:54:ARG:HG3	10:E:54:ARG:HH11	1.86	0.40
22:Q:64:CYS:SG	22:Q:74:THR:HG23	2.61	0.40
29:a:16:C:H4'	54:z:15:MET:HE3	2.03	0.40
29:a:84:A:OP1	48:t:6:ARG:NH2	2.54	0.40
29:a:263:G:H2'	29:a:264:C:O4'	2.21	0.40
29:a:282:A:H2'	29:a:283:G:C8	2.56	0.40
29:a:302:C:H2'	29:a:303:G:H8	1.86	0.40
29:a:492:A:H2'	29:a:493:G:O4'	2.21	0.40
29:a:1118:C:H2'	29:a:1119:U:O4'	2.21	0.40
29:a:2866:U:O4	58:a:6192:SPD:N10	2.50	0.40
34:f:171:ALA:C	34:f:173:PHE:H	2.28	0.40
44:p:61:TRP:CE2	44:p:93:LYS:HG3	2.56	0.40
47:s:48:GLN:O	47:s:52:GLU:HA	2.21	0.40
6:A:162:A:H8	6:A:162:A:O5'	2.04	0.40
6:A:1152:A:P	15:J:72:ARG:HH22	2.43	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1467:C:H2'	6:A:1468:A:C8	2.57	0.40
62:A:2908:HOH:O	14:I:120:LYS:HB3	2.22	0.40
8:C:89:LYS:HE2	8:C:89:LYS:HB2	1.83	0.40
9:D:9:LEU:HD13	9:D:32:CYS:SG	2.62	0.40
9:D:105:MET:SD	9:D:180:GLY:HA3	2.62	0.40
16:K:94:GLU:H	16:K:94:GLU:HG2	1.68	0.40
29:a:337:C:H2'	29:a:338:G:O4'	2.21	0.40
29:a:846:U:H4'	29:a:847:U:H5	1.85	0.40
29:a:1198:U:H5'	44:p:9:ILE:HD11	2.01	0.40
29:a:1747:U:H2'	29:a:1748:C:C6	2.56	0.40
29:a:2039:U:H2'	29:a:2040:G:C8	2.56	0.40
29:a:2585:U:H4'	61:a:6207:MET:HE2	2.03	0.40
29:a:2710:C:OP1	41:m:15:SER:OG	2.36	0.40
31:c:118:SER:HB2	31:c:129:THR:HB	2.03	0.40
35:g:11:VAL:HG11	35:g:48:ASN:HB3	2.03	0.40
35:g:154:PRO:HA	35:g:160:LYS:O	2.21	0.40
36:h:19:VAL:HG13	36:h:21:VAL:HG13	2.03	0.40
46:r:3:THR:HG21	46:r:58:ALA:N	2.36	0.40
6:A:168:G:C6	6:A:169:C:C5	3.09	0.40
6:A:483:C:H2'	6:A:484:G:C8	2.56	0.40
6:A:551:U:H2'	6:A:552:U:C6	2.56	0.40
6:A:558:G:OP2	6:A:559:A:O2'	2.36	0.40
6:A:560:A:H5'	6:A:566:G:N2	2.37	0.40
6:A:1053:G:N7	6:A:1200:C:H5"	2.35	0.40
6:A:1226:C:O2'	18:M:102:THR:O	2.39	0.40
7:B:47:VAL:HB	7:B:48:PRO:HD3	2.03	0.40
28:Y:21:A:N6	28:Y:47:U:O2'	2.54	0.40
29:a:494:G:H4'	46:r:6:LYS:HB2	2.03	0.40
29:a:526:A:O2'	29:a:2043:C:O2	2.38	0.40
29:a:1587:G:H2'	29:a:1588:G:H8	1.87	0.40
29:a:2677:G:H2'	29:a:2678:C:C6	2.56	0.40
33:e:18:THR:HA	33:e:106:LYS:HG2	2.03	0.40
33:e:52:VAL:O	33:e:74:LYS:HD3	2.21	0.40
37:i:122:LEU:HG	37:i:124:VAL:HG23	2.03	0.40
6:A:1297:G:H21	12:G:114:LYS:HB3	1.86	0.40
6:A:1465:A:H2'	6:A:1466:C:H6	1.85	0.40
7:B:151:ILE:HB	7:B:154:MET:HG3	2.02	0.40
10:E:49:GLY:HA3	10:E:63:ALA:O	2.22	0.40
12:G:92:ARG:HB2	12:G:93:PRO:HD3	2.03	0.40
16:K:112:ASP:OD2	26:U:28:VAL:HG11	2.21	0.40
28:Y:71:C:H2'	28:Y:72:A:H8	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Z:101:8AN:O2'	61:a:6206:MET:N	2.50	0.40
29:a:825:A:O2'	39:k:54:GLN:HB2	2.22	0.40
29:a:876:C:H2'	29:a:877:A:O4'	2.22	0.40
29:a:945:A:C4	29:a:2448:A:C2	3.09	0.40
29:a:1586:A:H3'	29:a:1587:G:H8	1.86	0.40
29:a:2194:U:H2'	29:a:2195:U:H6	1.86	0.40
44:p:86:ALA:HB2	44:p:116:ALA:HB2	2.02	0.40
5:4:56:ARG:HG3	5:4:57:VAL:HG23	2.03	0.40
6:A:130:A:O2'	62:A:1711:HOH:O	2.18	0.40
6:A:276:G:OP1	22:Q:14:SER:OG	2.27	0.40
6:A:808:C:OP1	20:O:48:LYS:HD3	2.22	0.40
6:A:1106:G:O2'	8:C:169:ARG:NH1	2.54	0.40
7:B:130:THR:O	7:B:132:LYS:N	2.54	0.40
8:C:179:ARG:HD2	8:C:207:ILE:HG12	2.03	0.40
14:I:63:LEU:HD13	14:I:65:ILE:HD11	2.03	0.40
21:P:14:ARG:HB3	21:P:42:ILE:HD11	2.03	0.40
22:Q:53:CYS:SG	22:Q:59:VAL:HG11	2.61	0.40
28:Y:75:C:H2'	59:Y:101:8AN:C8	2.52	0.40
29:a:272:A:H2'	29:a:273:G:C8	2.56	0.40
29:a:667:U:H2'	29:a:668:A:O4'	2.22	0.40
29:a:1703:G:H2'	29:a:1704:C:C6	2.57	0.40
29:a:2702:G:H2'	29:a:2703:C:H6	1.86	0.40
29:a:2772:C:H2'	29:a:2773:C:C6	2.57	0.40
30:b:28:C:H5"	42:n:31:THR:HG21	2.03	0.40
32:d:40:LEU:HD23	32:d:40:LEU:HA	1.94	0.40
32:d:152:PRO:HG3	32:d:156:PHE:CZ	2.56	0.40
39:k:76:GLU:C	39:k:77:ILE:HD13	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
7	B	222/241 (92%)	202 (91%)	20 (9%)	0	100	100
8	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
9	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
10	E	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
11	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
12	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
15	J	96/103 (93%)	90 (94%)	4 (4%)	2 (2%)	5	2
16	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
17	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
18	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
19	N	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
22	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
23	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
24	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
25	T	84/87 (97%)	84 (100%)	0	0	100	100
26	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
31	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
32	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
33	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
34	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
35	g	174/177 (98%)	164 (94%)	9 (5%)	1 (1%)	21	20
36	h	39/149 (26%)	33 (85%)	6 (15%)	0	100	100
37	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
39	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
40	l	132/136 (97%)	128 (97%)	3 (2%)	1 (1%)	16	13
41	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
42	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
43	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
46	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
48	t	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
49	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
50	v	82/85 (96%)	79 (96%)	3 (4%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
53	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
54	z	54/57 (95%)	54 (100%)	0	0	100	100
All	All	5487/5913 (93%)	5285 (96%)	198 (4%)	4 (0%)	49	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	J	57	VAL
35	g	47	ASP
40	l	83	GLY
15	J	84	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	48 (87%)	7 (13%)	4	2
7	B	186/199 (94%)	182 (98%)	4 (2%)	45	54
8	C	170/190 (90%)	166 (98%)	4 (2%)	43	51
9	D	172/173 (99%)	169 (98%)	3 (2%)	53	63
10	E	119/126 (94%)	119 (100%)	0	100	100
11	F	90/116 (78%)	88 (98%)	2 (2%)	45	54
12	G	126/147 (86%)	123 (98%)	3 (2%)	43	51
13	H	104/105 (99%)	103 (99%)	1 (1%)	68	76
14	I	105/107 (98%)	101 (96%)	4 (4%)	29	34
15	J	86/90 (96%)	86 (100%)	0	100	100
16	K	89/98 (91%)	88 (99%)	1 (1%)	65	74
17	L	102/103 (99%)	99 (97%)	3 (3%)	37	44
18	M	93/96 (97%)	90 (97%)	3 (3%)	34	40
19	N	83/84 (99%)	81 (98%)	2 (2%)	43	51
20	O	76/77 (99%)	75 (99%)	1 (1%)	61	71
21	P	65/65 (100%)	63 (97%)	2 (3%)	35	41
22	Q	73/78 (94%)	73 (100%)	0	100	100
23	R	57/65 (88%)	57 (100%)	0	100	100
24	S	72/79 (91%)	72 (100%)	0	100	100
25	T	65/66 (98%)	64 (98%)	1 (2%)	57	66
26	U	60/61 (98%)	59 (98%)	1 (2%)	53	63
31	c	216/218 (99%)	214 (99%)	2 (1%)	70	78
32	d	163/163 (100%)	160 (98%)	3 (2%)	51	61
33	e	165/165 (100%)	159 (96%)	6 (4%)	31	36
34	f	148/150 (99%)	146 (99%)	2 (1%)	59	69
35	g	137/138 (99%)	128 (93%)	9 (7%)	15	13
36	h	32/114 (28%)	30 (94%)	2 (6%)	16	14
37	i	116/116 (100%)	114 (98%)	2 (2%)	53	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	104/104 (100%)	103 (99%)	1 (1%)	68	76
39	k	103/103 (100%)	100 (97%)	3 (3%)	37	44
40	l	107/107 (100%)	105 (98%)	2 (2%)	50	59
41	m	98/103 (95%)	97 (99%)	1 (1%)	68	76
42	n	86/87 (99%)	83 (96%)	3 (4%)	32	37
43	o	99/100 (99%)	97 (98%)	2 (2%)	48	58
44	p	89/90 (99%)	88 (99%)	1 (1%)	65	74
45	q	84/84 (100%)	82 (98%)	2 (2%)	43	51
46	r	93/93 (100%)	91 (98%)	2 (2%)	45	54
47	s	80/84 (95%)	78 (98%)	2 (2%)	42	50
48	t	83/85 (98%)	81 (98%)	2 (2%)	43	51
49	u	78/78 (100%)	74 (95%)	4 (5%)	21	21
50	v	61/63 (97%)	61 (100%)	0	100	100
51	w	67/68 (98%)	63 (94%)	4 (6%)	17	16
52	x	54/55 (98%)	53 (98%)	1 (2%)	50	59
53	y	48/49 (98%)	48 (100%)	0	100	100
54	z	47/48 (98%)	44 (94%)	3 (6%)	16	14
All	All	4575/4825 (95%)	4474 (98%)	101 (2%)	45	54

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	22	MET
5	4	28	VAL
5	4	36	VAL
5	4	40	CYS
5	4	56	ARG
5	4	62	LYS
5	4	65	ASN
7	B	110	SER
7	B	151	ILE
7	B	152	LYS
7	B	211	THR
8	C	21	THR
8	C	38	LYS
8	C	54	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	C	75	ILE
9	D	48	LEU
9	D	174	ASP
9	D	192	SER
11	F	15	SER
11	F	26	THR
12	G	30	LEU
12	G	77	SER
12	G	144	MET
13	H	60	GLU
14	I	15	SER
14	I	36	GLU
14	I	43	THR
14	I	73	SER
16	K	109	ASN
17	L	40	THR
17	L	55	VAL
17	L	94	ARG
18	M	4	ILE
18	M	16	VAL
18	M	46	SER
19	N	26	GLU
19	N	37	SER
20	O	75	VAL
21	P	55	ASP
21	P	76	LYS
25	T	3	ASN
26	U	60	LEU
31	c	9	THR
31	c	37	ASN
32	d	52	THR
32	d	174	SER
32	d	181	ASP
33	e	2	GLU
33	e	13	THR
33	e	55	SER
33	e	107	SER
33	e	127	GLU
33	e	191	ASP
34	f	121	SER
34	f	123	ASP
35	g	11	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	g	15	VAL
35	g	36	THR
35	g	43	VAL
35	g	51	THR
35	g	76	VAL
35	g	90	VAL
35	g	98	VAL
35	g	168	VAL
36	h	5	LEU
36	h	41	LYS
37	i	10	THR
37	i	123	LYS
38	j	76	VAL
39	k	13	LYS
39	k	92	LEU
39	k	119	PRO
40	l	6	ARG
40	l	80	VAL
41	m	6	SER
42	n	61	GLN
42	n	74	VAL
42	n	83	LEU
43	o	63	LYS
43	o	64	ILE
44	p	77	SER
45	q	74	ILE
45	q	102	SER
46	r	4	ILE
46	r	81	SER
47	s	28	ASN
47	s	93	LEU
48	t	8	ASP
48	t	15	THR
49	u	35	GLU
49	u	45	ASP
49	u	53	LYS
49	u	65	VAL
51	w	2	SER
51	w	35	SER
51	w	40	VAL
51	w	66	THR
52	x	10	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	z	26	THR
54	z	27	SER
54	z	34	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	13	ASN
7	B	170	HIS
8	C	6	HIS
8	C	25	ASN
8	C	139	GLN
9	D	196	ASN
10	E	43	ASN
10	E	89	HIS
10	E	132	ASN
11	F	52	ASN
11	F	63	ASN
12	G	86	GLN
13	H	4	GLN
15	J	58	ASN
17	L	20	ASN
17	L	77	HIS
18	M	52	GLN
20	O	50	HIS
23	R	52	GLN
26	U	9	ASN
31	c	21	ASN
31	c	46	ASN
31	c	60	GLN
31	c	153	GLN
32	d	42	ASN
33	e	9	GLN
33	e	94	GLN
34	f	23	ASN
35	g	73	ASN
37	i	58	ASN
37	i	80	HIS
37	i	86	GLN
37	i	128	ASN
37	i	131	ASN
40	l	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	o	3	ASN
45	q	87	GLN
46	r	9	HIS
48	t	54	GLN
49	u	12	GLN
54	z	42	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	11/27 (40%)	3 (27%)	0
28	Y	72/75 (96%)	23 (31%)	0
28	Z	72/75 (96%)	18 (25%)	0
29	a	2749/2904 (94%)	319 (11%)	0
30	b	118/120 (98%)	17 (14%)	0
6	A	1516/1542 (98%)	212 (13%)	4 (0%)
All	All	4538/4743 (95%)	592 (13%)	4 (0%)

All (592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	6	G
6	A	13	U
6	A	22	G
6	A	32	A
6	A	39	G
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	73	C
6	A	74	A
6	A	84	U
6	A	85	U
6	A	86	G
6	A	87	C
6	A	88	U
6	A	94	G
6	A	96	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	122	G
6	A	131	A
6	A	140	U
6	A	141	G
6	A	144	G
6	A	163	C
6	A	164	G
6	A	182	A
6	A	183	C
6	A	190	A
6	A	195	A
6	A	197	A
6	A	201	G
6	A	202	G
6	A	204	G
6	A	226	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	280	C
6	A	289	G
6	A	328	C
6	A	343	U
6	A	345	C
6	A	346	G
6	A	347	G
6	A	351	G
6	A	352	C
6	A	354	G
6	A	367	U
6	A	372	C
6	A	373	A
6	A	406	G
6	A	411	A
6	A	412	A
6	A	413	G
6	A	414	A
6	A	415	A
6	A	421	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	422	C
6	A	424	G
6	A	429	U
6	A	436	C
6	A	446	G
6	A	456	A
6	A	457	G
6	A	458	U
6	A	459	A
6	A	463	U
6	A	464	U
6	A	467	U
6	A	468	A
6	A	469	C
6	A	477	C
6	A	478	A
6	A	484	G
6	A	486	U
6	A	497	G
6	A	509	A
6	A	511	C
6	A	518	C
6	A	521	G
6	A	531	U
6	A	532	A
6	A	547	A
6	A	559	A
6	A	562	U
6	A	564	C
6	A	572	A
6	A	573	A
6	A	576	C
6	A	579	A
6	A	596	A
6	A	650	G
6	A	653	U
6	A	665	A
6	A	703	G
6	A	723	U
6	A	724	G
6	A	747	A
6	A	748	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	802	A
6	A	815	A
6	A	817	C
6	A	821	G
6	A	849	G
6	A	890	G
6	A	902	G
6	A	914	A
6	A	926	G
6	A	934	C
6	A	935	A
6	A	936	C
6	A	960	U
6	A	966	2MG
6	A	969	A
6	A	975	A
6	A	976	G
6	A	977	A
6	A	994	A
6	A	997	U
6	A	1003	G
6	A	1004	A
6	A	1006	G
6	A	1009	U
6	A	1010	U
6	A	1017	U
6	A	1024	G
6	A	1027	C
6	A	1028	C
6	A	1029	U
6	A	1030	U
6	A	1031	C
6	A	1032	G
6	A	1033	G
6	A	1034	G
6	A	1036	A
6	A	1037	C
6	A	1042	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1044	A
6	A	1045	C
6	A	1065	U
6	A	1085	U
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1119	C
6	A	1126	U
6	A	1136	C
6	A	1137	C
6	A	1139	G
6	A	1140	C
6	A	1144	G
6	A	1146	A
6	A	1157	A
6	A	1158	C
6	A	1159	U
6	A	1164	G
6	A	1166	G
6	A	1196	A
6	A	1197	A
6	A	1213	A
6	A	1214	C
6	A	1227	A
6	A	1238	A
6	A	1256	A
6	A	1258	G
6	A	1274	A
6	A	1275	A
6	A	1279	G
6	A	1280	A
6	A	1286	U
6	A	1287	A
6	A	1300	G
6	A	1301	U
6	A	1302	C
6	A	1317	C
6	A	1320	C
6	A	1338	G
6	A	1346	A
6	A	1353	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1363	A
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1380	U
6	A	1381	U
6	A	1397	C
6	A	1419	G
6	A	1429	A
6	A	1441	A
6	A	1451	U
6	A	1452	C
6	A	1453	G
6	A	1455	G
6	A	1487	G
6	A	1492	A
6	A	1497	G
6	A	1499	A
6	A	1503	A
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
6	A	1533	C
27	X	14	A
27	X	15	A
27	X	24	A
28	Y	8	U
28	Y	12	G
28	Y	13	C
28	Y	14	A
28	Y	21	A
28	Y	22	G
28	Y	28	C
28	Y	29	G
28	Y	30	G
28	Y	31	G
28	Y	32	C
28	Y	36	U
28	Y	46	G
28	Y	47	U
28	Y	49	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	Y	57	A
28	Y	58	A
28	Y	59	A
28	Y	60	U
28	Y	68	C
28	Y	70	G
28	Y	73	A
28	Y	74	C
28	Z	9	G
28	Z	14	A
28	Z	16	C
28	Z	17	C
28	Z	19	G
28	Z	20	U
28	Z	21	A
28	Z	28	C
28	Z	30	G
28	Z	31	G
28	Z	35	A
28	Z	36	U
28	Z	39	C
28	Z	45	G
28	Z	46	G
28	Z	47	U
28	Z	58	A
28	Z	69	C
29	a	10	A
29	a	34	U
29	a	42	A
29	a	45	G
29	a	61	C
29	a	71	A
29	a	74	A
29	a	75	G
29	a	101	A
29	a	102	U
29	a	103	A
29	a	118	A
29	a	119	A
29	a	120	U
29	a	131	A
29	a	138	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	139	U
29	a	142	A
29	a	163	C
29	a	181	A
29	a	196	A
29	a	215	G
29	a	216	A
29	a	221	A
29	a	222	A
29	a	248	G
29	a	265	A
29	a	272	A
29	a	274	C
29	a	278	A
29	a	285	G
29	a	289	G
29	a	311	A
29	a	329	G
29	a	330	A
29	a	356	G
29	a	357	C
29	a	361	G
29	a	362	A
29	a	365	U
29	a	383	C
29	a	386	G
29	a	396	G
29	a	405	U
29	a	406	G
29	a	411	G
29	a	412	A
29	a	481	G
29	a	491	G
29	a	504	A
29	a	505	A
29	a	509	C
29	a	530	G
29	a	531	C
29	a	532	A
29	a	533	G
29	a	538	A
29	a	544	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	545	U
29	a	546	U
29	a	547	A
29	a	548	G
29	a	549	G
29	a	563	A
29	a	573	U
29	a	575	A
29	a	603	A
29	a	615	U
29	a	627	A
29	a	637	A
29	a	645	C
29	a	646	U
29	a	647	G
29	a	653	U
29	a	654	A
29	a	655	A
29	a	686	U
29	a	717	C
29	a	721	A
29	a	730	A
29	a	747	5MU
29	a	764	A
29	a	775	G
29	a	776	G
29	a	782	A
29	a	784	G
29	a	785	G
29	a	805	G
29	a	812	C
29	a	827	U
29	a	828	U
29	a	845	A
29	a	846	U
29	a	847	U
29	a	859	G
29	a	865	C
29	a	881	G
29	a	882	G
29	a	883	G
29	a	884	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	885	C
29	a	888	C
29	a	890	C
29	a	891	G
29	a	893	C
29	a	895	U
29	a	896	A
29	a	897	C
29	a	899	A
29	a	910	A
29	a	915	C
29	a	931	U
29	a	946	C
29	a	961	C
29	a	974	G
29	a	983	A
29	a	996	A
29	a	1005	C
29	a	1012	U
29	a	1013	C
29	a	1026	G
29	a	1033	U
29	a	1045	C
29	a	1046	A
29	a	1047	G
29	a	1110	G
29	a	1111	A
29	a	1112	G
29	a	1115	G
29	a	1116	G
29	a	1118	C
29	a	1132	U
29	a	1135	C
29	a	1142	A
29	a	1170	C
29	a	1171	G
29	a	1178	C
29	a	1205	A
29	a	1241	A
29	a	1253	A
29	a	1256	G
29	a	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	1272	A
29	a	1300	G
29	a	1301	A
29	a	1352	U
29	a	1365	A
29	a	1379	U
29	a	1383	A
29	a	1409	U
29	a	1416	G
29	a	1419	A
29	a	1420	A
29	a	1427	A
29	a	1428	C
29	a	1452	G
29	a	1453	A
29	a	1454	C
29	a	1482	G
29	a	1507	C
29	a	1508	A
29	a	1509	A
29	a	1510	G
29	a	1515	A
29	a	1524	G
29	a	1533	C
29	a	1534	U
29	a	1535	A
29	a	1536	C
29	a	1537	G
29	a	1559	U
29	a	1566	A
29	a	1569	A
29	a	1578	U
29	a	1583	A
29	a	1584	U
29	a	1585	C
29	a	1607	C
29	a	1608	A
29	a	1609	A
29	a	1626	A
29	a	1647	U
29	a	1648	U
29	a	1649	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	1674	G
29	a	1715	G
29	a	1729	U
29	a	1730	C
29	a	1731	G
29	a	1732	C
29	a	1738	G
29	a	1750	G
29	a	1764	C
29	a	1773	A
29	a	1782	U
29	a	1791	A
29	a	1800	C
29	a	1801	A
29	a	1808	A
29	a	1816	C
29	a	1829	A
29	a	1847	A
29	a	1848	A
29	a	1858	A
29	a	1868	C
29	a	1870	C
29	a	1871	A
29	a	1872	A
29	a	1873	G
29	a	1874	C
29	a	1906	G
29	a	1914	C
29	a	1915	3TD
29	a	1929	G
29	a	1930	G
29	a	1937	A
29	a	1938	A
29	a	1955	U
29	a	1965	C
29	a	1967	C
29	a	1970	A
29	a	1971	U
29	a	1972	G
29	a	1991	U
29	a	1993	U
29	a	2023	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	2031	A
29	a	2033	A
29	a	2043	C
29	a	2055	C
29	a	2056	G
29	a	2060	A
29	a	2061	G
29	a	2062	A
29	a	2063	C
29	a	2069	G7M
29	a	2080	A
29	a	2093	G
29	a	2098	U
29	a	2198	A
29	a	2204	G
29	a	2211	A
29	a	2223	G
29	a	2225	A
29	a	2238	G
29	a	2239	G
29	a	2268	A
29	a	2279	G
29	a	2283	C
29	a	2287	A
29	a	2288	A
29	a	2305	U
29	a	2307	G
29	a	2308	G
29	a	2318	G
29	a	2321	U
29	a	2322	A
29	a	2325	G
29	a	2333	A
29	a	2335	A
29	a	2344	U
29	a	2347	C
29	a	2350	C
29	a	2361	G
29	a	2383	G
29	a	2385	C
29	a	2402	U
29	a	2403	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	2406	A
29	a	2425	A
29	a	2429	G
29	a	2434	A
29	a	2435	A
29	a	2441	U
29	a	2447	G
29	a	2448	A
29	a	2475	C
29	a	2476	A
29	a	2491	U
29	a	2492	U
29	a	2502	G
29	a	2505	G
29	a	2518	A
29	a	2520	C
29	a	2525	G
29	a	2529	G
29	a	2535	G
29	a	2547	A
29	a	2566	A
29	a	2567	G
29	a	2573	C
29	a	2602	A
29	a	2609	U
29	a	2613	U
29	a	2629	U
29	a	2630	G
29	a	2671	G
29	a	2689	U
29	a	2690	U
29	a	2714	G
29	a	2726	A
29	a	2733	A
29	a	2744	G
29	a	2748	A
29	a	2757	A
29	a	2765	A
29	a	2778	A
29	a	2791	G
29	a	2798	U
29	a	2818	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	2820	A
29	a	2821	A
29	a	2833	U
29	a	2873	A
29	a	2880	C
29	a	2883	A
29	a	2884	U
29	a	2891	U
29	a	2902	C
30	b	9	G
30	b	17	C
30	b	21	G
30	b	35	C
30	b	36	C
30	b	37	C
30	b	42	C
30	b	44	G
30	b	45	A
30	b	56	G
30	b	67	G
30	b	88	C
30	b	89	U
30	b	90	C
30	b	99	A
30	b	105	G
30	b	109	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	5	U
6	A	1026	G
6	A	1035	A
6	A	1240	U

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

40 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	$\#\|Z\| > 2$
16	IAS	K	119	16	6,7,8	1.41	1 (16%)	3,8,10	1.11	0
6	5MC	A	967	6	19,22,23	0.73	1 (5%)	26,32,35	0.50	0
29	6MZ	a	1618	29	22,25,26	0.31	0	29,36,39	0.61	0
6	2MG	A	1207	6	23,26,27	0.38	0	33,38,41	0.44	0
6	5MC	A	1407	6	19,22,23	0.72	1 (5%)	26,32,35	0.58	0
29	OMG	a	2251	28,29	23,26,27	0.33	0	32,38,41	0.37	0
29	PSU	a	2457	29	18,21,22	1.03	1 (5%)	21,30,33	0.81	0
29	H2U	a	2449	29	18,21,22	0.51	0	19,30,33	0.86	2 (10%)
29	G7M	a	2069	29	23,26,27	1.54	4 (17%)	34,39,42	1.71	5 (14%)
29	PSU	a	2580	29	18,21,22	1.06	2 (11%)	21,30,33	0.82	1 (4%)
6	PSU	A	516	57,6	18,21,22	1.01	1 (5%)	21,30,33	0.79	1 (4%)
6	UR3	A	1498	6	19,22,23	0.29	0	26,32,35	0.85	2 (7%)
29	5MU	a	1939	29	19,22,23	0.31	0	27,32,35	0.45	0
29	PSU	a	746	57,29	18,21,22	1.07	1 (5%)	21,30,33	0.62	0
6	MA6	A	1519	6	23,26,27	1.51	5 (21%)	33,38,41	2.15	10 (30%)
29	PSU	a	2604	29	18,21,22	1.02	1 (5%)	21,30,33	0.85	0
6	MA6	A	1518	6	23,26,27	1.48	4 (17%)	33,38,41	2.10	10 (30%)
17	D2T	L	89	17	8,9,10	3.29	3 (37%)	6,11,13	1.61	2 (33%)
29	PSU	a	1917	29	18,21,22	1.01	1 (5%)	21,30,33	0.70	0
29	PSU	a	955	29	18,21,22	0.99	1 (5%)	21,30,33	0.78	0
29	2MG	a	1835	29	23,26,27	0.37	0	33,38,41	0.47	0
40	4D4	l	81	40	9,11,12	1.93	2 (22%)	7,13,15	1.03	1 (14%)
29	PSU	a	1911	29	18,21,22	1.01	1 (5%)	21,30,33	0.74	0
29	6MZ	a	2030	29	22,25,26	0.30	0	29,36,39	0.62	0
29	3TD	a	1915	29	19,22,23	1.59	5 (26%)	23,32,35	2.15	5 (21%)
32	MEQ	d	150	32	8,9,10	0.48	0	5,10,12	0.15	0
29	2MG	a	2445	29	23,26,27	0.39	0	33,38,41	0.48	0
29	5MC	a	1962	29	19,22,23	0.71	1 (5%)	26,32,35	0.54	0
29	PSU	a	2504	29	18,21,22	1.05	1 (5%)	21,30,33	0.73	0
29	OMC	a	2498	57,29	19,22,23	0.35	0	25,31,34	0.64	1 (4%)
6	2MG	A	1516	6	23,26,27	0.37	0	33,38,41	0.52	0
6	2MG	A	966	6	23,26,27	0.37	0	33,38,41	0.46	0
29	OMU	a	2552	29	19,22,23	0.33	0	25,31,34	0.82	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	G7M	A	527	6	23,26,27	1.52	3 (13%)	34,39,42	1.69	5 (14%)
40	MS6	l	82	40	5,7,8	0.23	0	2,7,9	0.32	0
29	5MU	a	747	29	19,22,23	0.31	0	27,32,35	0.43	0
29	1MG	a	745	29	23,26,27	0.60	0	33,39,42	0.72	1 (3%)
6	4OC	A	1402	6	20,23,24	0.36	0	25,32,35	0.46	0
29	PSU	a	2605	29	18,21,22	0.97	1 (5%)	21,30,33	0.85	0
29	2MA	a	2503	57,29	22,25,26	0.85	1 (4%)	32,37,40	1.16	4 (12%)

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
16	IAS	K	119	16	-	1/7/7/8	-
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	0/9/27/28	0/3/3/3
6	2MG	A	1207	6	-	0/9/27/28	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
29	OMG	a	2251	28,29	-	1/9/27/28	0/3/3/3
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
29	G7M	a	2069	29	-	0/7/25/26	0/3/3/3
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2
6	PSU	A	516	57,6	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
29	5MU	a	1939	29	-	0/7/25/26	0/2/2/2
29	PSU	a	746	57,29	-	4/7/25/26	0/2/2/2
6	MA6	A	1519	6	-	2/11/29/30	0/3/3/3
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
17	D2T	L	89	17	-	3/7/12/14	-
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
29	2MG	a	1835	29	-	0/9/27/28	0/3/3/3
40	4D4	l	81	40	-	1/11/12/14	-
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	6MZ	a	2030	29	-	2/9/27/28	0/3/3/3
29	3TD	a	1915	29	-	2/7/25/26	0/2/2/2
32	MEQ	d	150	32	-	2/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	2MG	a	2445	29	-	0/9/27/28	0/3/3/3
29	5MC	a	1962	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2504	29	-	0/7/25/26	0/2/2/2
29	OMC	a	2498	57,29	-	0/9/27/28	0/2/2/2
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
6	2MG	A	966	6	-	1/9/27/28	0/3/3/3
29	OMU	a	2552	29	-	0/9/27/28	0/2/2/2
6	G7M	A	527	6	-	1/7/25/26	0/3/3/3
40	MS6	l	82	40	-	1/4/6/8	-
29	5MU	a	747	29	-	1/7/25/26	0/2/2/2
29	1MG	a	745	29	-	0/7/25/26	0/3/3/3
6	4OC	A	1402	6	-	0/9/29/30	0/2/2/2
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
29	2MA	a	2503	57,29	-	1/7/25/26	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	89	D2T	CB-CA	7.35	1.57	1.54
29	a	2069	G7M	C5-N7	-5.05	1.33	1.39
6	A	527	G7M	C5-N7	-4.73	1.33	1.39
6	A	1518	MA6	C5-C4	4.57	1.47	1.39
6	A	1519	MA6	C5-C4	4.56	1.47	1.39
17	L	89	D2T	CB-CG	4.31	1.59	1.52
40	l	81	4D4	CZ-NE	4.00	1.41	1.33
29	a	2504	PSU	C6-C5	3.79	1.39	1.35
29	a	746	PSU	C6-C5	3.73	1.39	1.35
29	a	2580	PSU	C6-C5	3.68	1.39	1.35
29	a	1917	PSU	C6-C5	3.67	1.39	1.35
29	a	2604	PSU	C6-C5	3.65	1.39	1.35
29	a	2457	PSU	C6-C5	3.56	1.39	1.35
29	a	1911	PSU	C6-C5	3.54	1.39	1.35
29	a	955	PSU	C6-C5	3.49	1.39	1.35
6	A	516	PSU	C6-C5	3.48	1.39	1.35
29	a	1915	3TD	C4-N3	-3.45	1.33	1.40
29	a	2605	PSU	C6-C5	3.41	1.39	1.35
17	L	89	D2T	CB-SB	3.15	1.85	1.82
6	A	527	G7M	C5-C4	3.12	1.46	1.38
29	a	1915	3TD	C6-C5	3.11	1.38	1.35
29	a	2069	G7M	C5-C4	3.09	1.46	1.38
6	A	1519	MA6	C5-C6	3.02	1.49	1.41
6	A	1518	MA6	C5-C6	2.91	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1915	3TD	C10-N3	2.90	1.52	1.47
6	A	967	5MC	C5-C4	-2.89	1.41	1.44
29	a	1962	5MC	C5-C4	-2.83	1.42	1.44
6	A	1407	5MC	C5-C4	-2.76	1.42	1.44
40	l	81	4D4	CZ-NH2	2.74	1.42	1.32
6	A	527	G7M	C6-N1	-2.48	1.34	1.38
16	K	119	IAS	CB-CG	2.47	1.56	1.50
29	a	2069	G7M	C6-N1	-2.42	1.34	1.38
29	a	2503	2MA	C6-N6	-2.41	1.28	1.34
29	a	1915	3TD	C2-N1	-2.31	1.34	1.37
29	a	1915	3TD	C2-N3	-2.28	1.33	1.38
29	a	2069	G7M	C4-N9	-2.19	1.32	1.38
29	a	2580	PSU	O4'-C1'	-2.19	1.40	1.43
6	A	1519	MA6	C8-N7	2.18	1.35	1.31
6	A	1518	MA6	C5-N7	-2.15	1.35	1.39
6	A	1519	MA6	C4-N9	-2.13	1.33	1.37
6	A	1519	MA6	C5-N7	-2.12	1.35	1.39
6	A	1518	MA6	C4-N9	-2.06	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	1915	3TD	N1-C2-N3	8.09	122.01	116.13
6	A	1519	MA6	C5-C4-N3	-5.44	119.22	126.72
6	A	1518	MA6	C5-C4-N3	-5.37	119.32	126.72
29	a	2069	G7M	N9-C4-N3	5.05	136.05	125.95
6	A	527	G7M	C5-C4-N3	-5.03	118.65	128.15
6	A	527	G7M	N9-C4-N3	5.02	135.98	125.95
29	a	2069	G7M	C5-C4-N3	-4.97	118.75	128.15
29	a	2069	G7M	C2-N3-C4	4.88	120.70	112.30
6	A	527	G7M	C2-N3-C4	4.67	120.34	112.30
6	A	1519	MA6	C4-C5-N7	-4.49	105.45	110.58
6	A	1518	MA6	C2-N1-C6	4.39	122.56	111.83
6	A	1519	MA6	C2-N1-C6	4.28	122.29	111.83
6	A	1518	MA6	N3-C4-N9	4.21	134.33	127.17
6	A	1518	MA6	C4-C5-N7	-3.94	106.07	110.58
6	A	1519	MA6	N3-C4-N9	3.92	133.84	127.17
6	A	1519	MA6	C2-N3-C4	3.72	120.93	111.83
6	A	1518	MA6	C2-N3-C4	3.71	120.90	111.83
6	A	1518	MA6	N1-C2-N3	-3.62	123.10	128.58
29	a	1915	3TD	C4-N3-C2	-3.50	120.91	124.61
6	A	1519	MA6	N1-C2-N3	-3.36	123.50	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	2552	OMU	C2'-C1'-N1	-3.28	108.02	114.24
6	A	1519	MA6	C5-N7-C8	3.12	108.36	103.45
6	A	1518	MA6	C4-N9-C8	2.95	108.84	105.74
29	a	1915	3TD	C1'-C5-C4	2.93	122.06	117.61
6	A	1519	MA6	C4-N9-C8	2.86	108.75	105.74
6	A	1518	MA6	C5-N7-C8	2.84	107.92	103.45
29	a	2503	2MA	C5-C4-N3	-2.84	124.18	127.18
6	A	1519	MA6	C6-C5-N7	2.81	137.92	133.43
29	a	2503	2MA	C2-N1-C6	2.77	122.36	118.10
29	a	2503	2MA	CM2-C2-N1	2.60	121.03	117.13
17	L	89	D2T	OD1-CG-CB	-2.55	117.10	122.44
6	A	527	G7M	O6-C6-C5	-2.52	122.39	128.01
29	a	2503	2MA	N3-C2-N1	-2.48	121.39	125.77
6	A	1519	MA6	N9-C8-N7	-2.43	110.49	113.94
29	a	2498	OMC	C2'-C1'-N1	-2.43	109.64	114.24
29	a	745	1MG	N2-C2-N1	-2.42	116.84	118.79
29	a	2449	H2U	O2-C2-N1	-2.41	120.21	123.10
29	a	2580	PSU	O4'-C1'-C2'	2.39	108.45	105.15
6	A	1518	MA6	C6-C5-N7	2.36	137.21	133.43
29	a	2069	G7M	O6-C6-C5	-2.28	122.92	128.01
29	a	2069	G7M	C5-C6-N1	2.28	116.55	111.84
6	A	516	PSU	O4'-C1'-C2'	2.26	108.28	105.15
29	a	2449	H2U	N3-C2-N1	2.25	118.91	116.65
6	A	1518	MA6	N9-C8-N7	-2.20	110.81	113.94
29	a	1915	3TD	O2-C2-N3	-2.17	118.75	121.82
6	A	1498	UR3	C6-N1-C2	-2.17	120.03	121.80
6	A	527	G7M	C5-C6-N1	2.15	116.29	111.84
29	a	1915	3TD	C5-C6-N1	-2.15	119.16	122.14
40	l	81	4D4	CG-CD-NE	-2.13	106.03	111.88
6	A	1498	UR3	C4-N3-C2	-2.06	122.92	124.58
17	L	89	D2T	OD2-CG-CB	2.02	117.52	113.15

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	746	PSU	C2'-C1'-C5-C4
29	a	746	PSU	C2'-C1'-C5-C6
29	a	746	PSU	O4'-C1'-C5-C6
29	a	1915	3TD	O4'-C4'-C5'-O5'
29	a	2251	OMG	C1'-C2'-O2'-CM2
6	A	1519	MA6	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	d	150	MEQ	OE1-CD-CG-CB
32	d	150	MEQ	NE2-CD-CG-CB
29	a	747	5MU	C3'-C4'-C5'-O5'
29	a	1915	3TD	C3'-C4'-C5'-O5'
29	a	2030	6MZ	O4'-C4'-C5'-O5'
6	A	1519	MA6	C3'-C4'-C5'-O5'
29	a	2030	6MZ	C3'-C4'-C5'-O5'
40	l	82	MS6	CA-CB-CG-SD
29	a	746	PSU	O4'-C1'-C5-C4
17	L	89	D2T	SB-CB-CG-OD2
6	A	527	G7M	C4'-C5'-O5'-P
6	A	966	2MG	C3'-C4'-C5'-O5'
17	L	89	D2T	CA-CB-CG-OD2
17	L	89	D2T	CG-CB-SB-CB1
40	l	81	4D4	O-C-CA-CB
16	K	119	IAS	N-CA-CB-CG
29	a	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	2251	OMG	1	0
6	A	1498	UR3	1	0
29	a	1939	5MU	1	0
6	A	1519	MA6	3	0
29	a	2604	PSU	1	0
6	A	1518	MA6	1	0
29	a	2030	6MZ	2	0
32	d	150	MEQ	1	0
6	A	1516	2MG	1	0
29	a	2552	OMU	1	0
29	a	747	5MU	2	0
6	A	1402	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 292 ligands modelled in this entry, 270 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SPD	a	6196	-	9,9,9	0.16	0	8,8,8	0.31	0
60	SPM	a	6205	-	13,13,13	0.17	0	12,12,12	0.21	0
58	SPD	a	6194	-	9,9,9	0.16	0	8,8,8	0.15	0
59	8AN	Y	101	61,28	21,24,25	0.86	1 (4%)	26,35,38	0.34	0
56	PAR	A	1601	-	44,45,45	0.50	0	63,67,67	0.80	0
61	MET	a	6207	59	6,7,8	0.48	0	2,7,9	0.34	0
58	SPD	a	6198	-	9,9,9	0.18	0	8,8,8	0.32	0
58	SPD	A	1670	-	9,9,9	0.16	0	8,8,8	0.19	0
58	SPD	a	6195	-	9,9,9	0.30	0	8,8,8	0.70	0
58	SPD	a	6202	-	9,9,9	0.16	0	8,8,8	0.17	0
58	SPD	a	6201	-	9,9,9	0.18	0	8,8,8	0.34	0
59	8AN	Z	101	61,28	21,24,25	0.73	1 (4%)	26,35,38	0.54	0
61	MET	a	6206	59	6,7,8	0.56	0	2,7,9	0.22	0
58	SPD	A	1669	-	9,9,9	0.13	0	8,8,8	0.34	0
58	SPD	a	6191	-	9,9,9	0.16	0	8,8,8	0.23	0
58	SPD	a	6204	-	9,9,9	0.13	0	8,8,8	0.19	0
58	SPD	a	6197	-	9,9,9	0.15	0	8,8,8	0.31	0
58	SPD	a	6203	-	9,9,9	0.15	0	8,8,8	0.33	0
58	SPD	a	6200	-	9,9,9	0.17	0	8,8,8	0.18	0
58	SPD	a	6199	-	9,9,9	0.18	0	8,8,8	0.26	0
58	SPD	a	6193	-	9,9,9	0.15	0	8,8,8	0.16	0
58	SPD	a	6192	-	9,9,9	0.16	0	8,8,8	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPD	a	6196	-	-	2/7/7/7	-
60	SPM	a	6205	-	-	1/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPD	a	6194	-	-	2/7/7/7	-
59	8AN	Y	101	61,28	-	0/7/25/26	0/3/3/3
56	PAR	A	1601	-	-	3/18/94/94	0/4/4/4
61	MET	a	6207	59	-	2/5/6/8	-
58	SPD	a	6198	-	-	0/7/7/7	-
58	SPD	A	1670	-	-	2/7/7/7	-
58	SPD	a	6195	-	-	3/7/7/7	-
58	SPD	a	6202	-	-	0/7/7/7	-
58	SPD	a	6201	-	-	1/7/7/7	-
59	8AN	Z	101	61,28	-	1/7/25/26	0/3/3/3
61	MET	a	6206	59	-	1/5/6/8	-
58	SPD	A	1669	-	-	1/7/7/7	-
58	SPD	a	6191	-	-	0/7/7/7	-
58	SPD	a	6204	-	-	1/7/7/7	-
58	SPD	a	6197	-	-	0/7/7/7	-
58	SPD	a	6203	-	-	1/7/7/7	-
58	SPD	a	6200	-	-	0/7/7/7	-
58	SPD	a	6199	-	-	1/7/7/7	-
58	SPD	a	6193	-	-	0/7/7/7	-
58	SPD	a	6192	-	-	0/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Y	101	8AN	C3'-N3'	-3.58	1.41	1.47
59	Z	101	8AN	C3'-N3'	-2.86	1.43	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	Z	101	8AN	C4'-C5'-O5'-P
61	a	6207	MET	N-CA-CB-CG
61	a	6207	MET	C-CA-CB-CG
58	a	6195	SPD	C3-C4-C5-N6
58	a	6199	SPD	C2-C3-C4-C5
58	A	1670	SPD	C2-C3-C4-C5
58	a	6201	SPD	C4-C5-N6-C7
61	a	6206	MET	CA-CB-CG-SD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	a	6196	SPD	C3-C4-C5-N6
58	A	1669	SPD	C2-C3-C4-C5
58	a	6195	SPD	C7-C8-C9-N10
60	a	6205	SPM	C3-C4-N5-C6
56	A	1601	PAR	C52-C42-O11-C11
56	A	1601	PAR	O54-C54-C64-N64
58	a	6194	SPD	C3-C4-C5-N6
58	a	6195	SPD	C4-C5-N6-C7
58	A	1670	SPD	C3-C4-C5-N6
58	a	6203	SPD	C8-C7-N6-C5
58	a	6204	SPD	C2-C3-C4-C5
56	A	1601	PAR	C23-C33-O33-C14
58	a	6194	SPD	C2-C3-C4-C5
58	a	6196	SPD	C4-C5-N6-C7

There are no ring outliers.

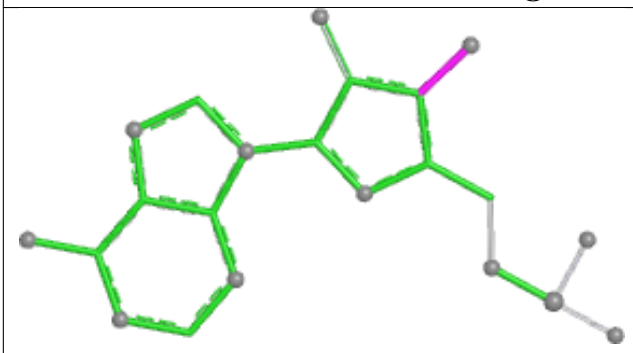
16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	a	6196	SPD	2	0
60	a	6205	SPM	2	0
58	a	6194	SPD	1	0
59	Y	101	8AN	2	0
56	A	1601	PAR	1	0
61	a	6207	MET	2	0
58	a	6198	SPD	2	0
58	A	1670	SPD	1	0
58	a	6201	SPD	2	0
59	Z	101	8AN	2	0
61	a	6206	MET	2	0
58	A	1669	SPD	1	0
58	a	6191	SPD	1	0
58	a	6197	SPD	1	0
58	a	6199	SPD	1	0
58	a	6192	SPD	3	0

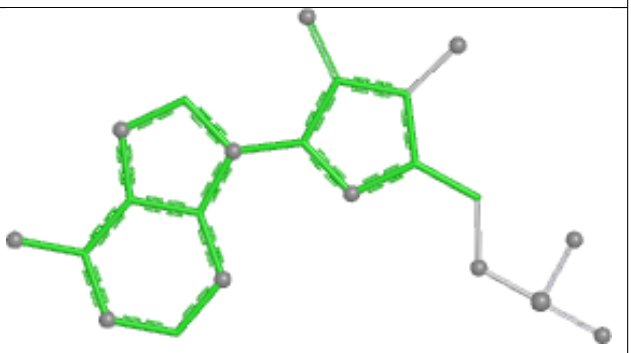
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

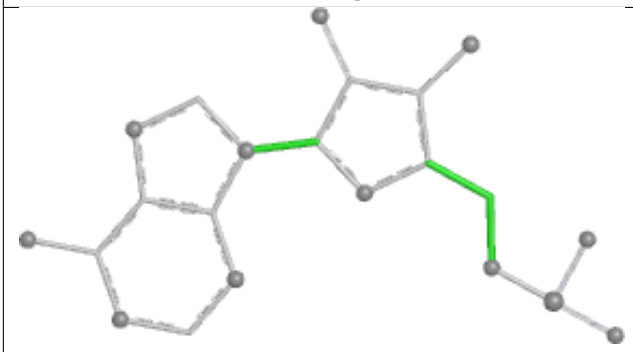
Ligand 8AN Y 101



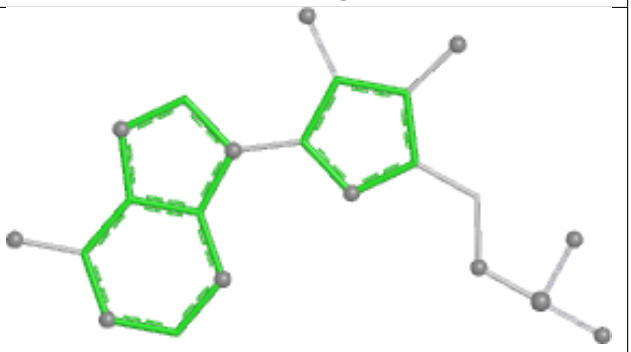
Bond lengths



Bond angles

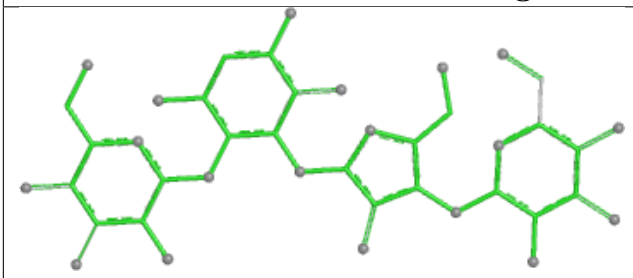


Torsions

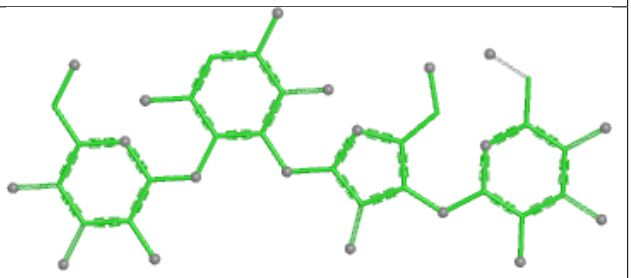


Rings

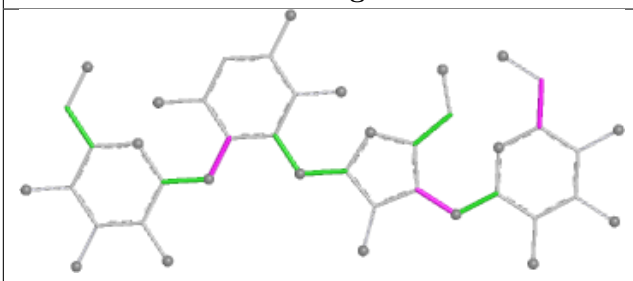
Ligand PAR A 1601



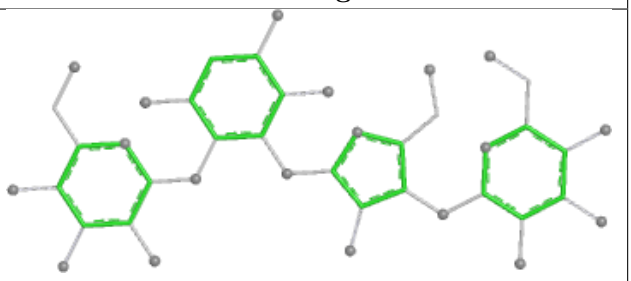
Bond lengths



Bond angles

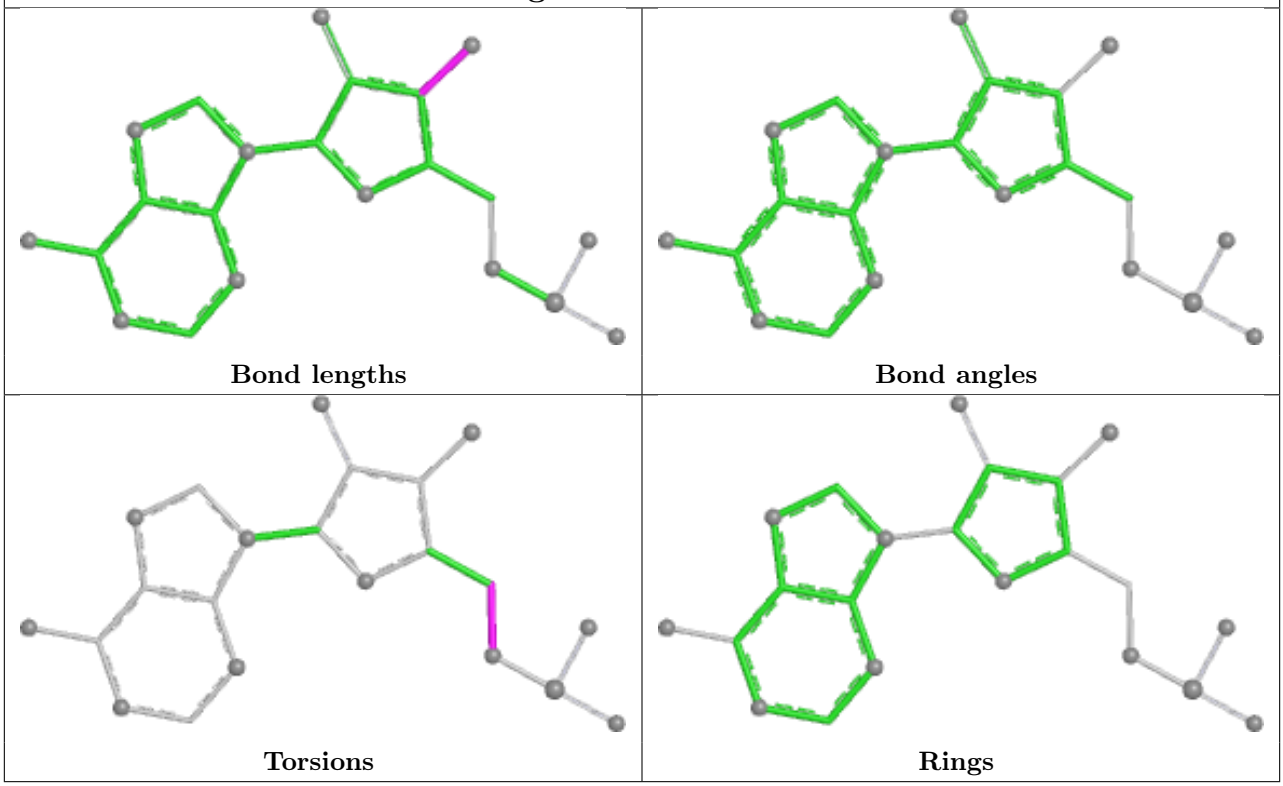


Torsions



Rings

Ligand 8AN Z 101



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.

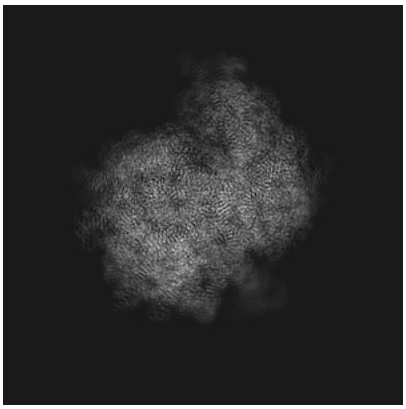
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-28165. These allow visual inspection of the internal detail of the map and identification of artifacts.

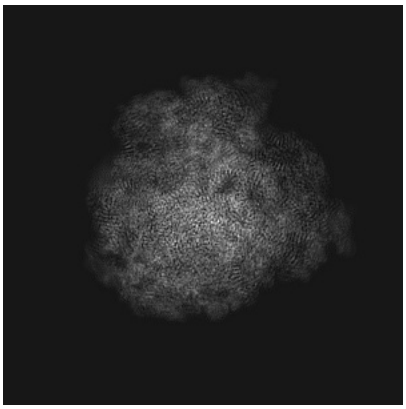
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

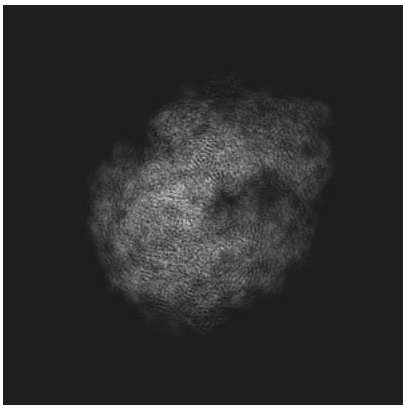
6.1.1 Primary map



X

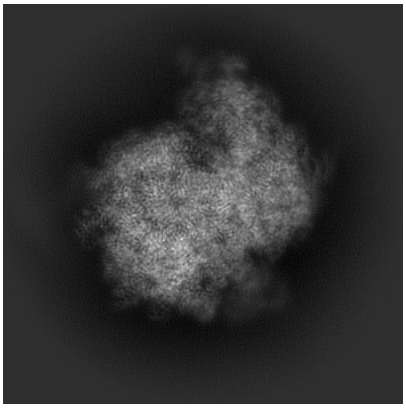


Y

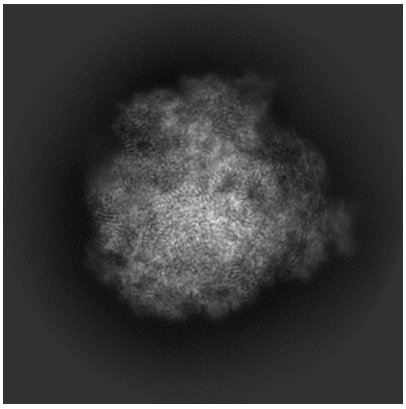


Z

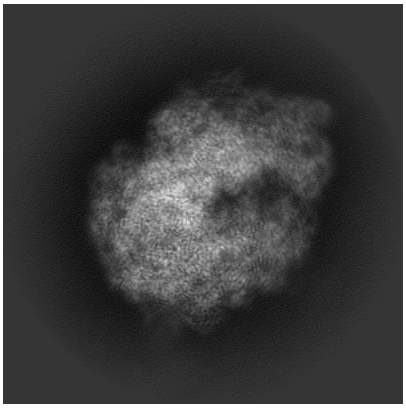
6.1.2 Raw map



X



Y

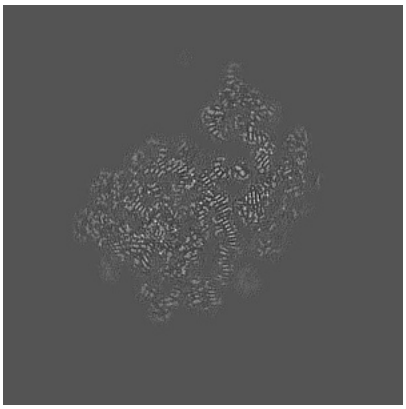


Z

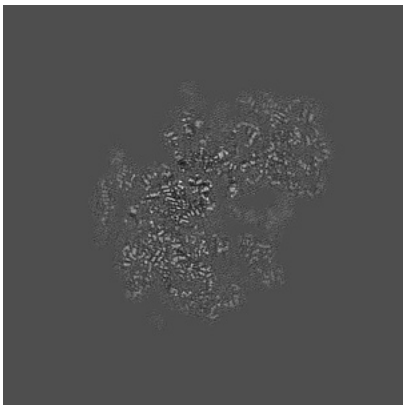
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

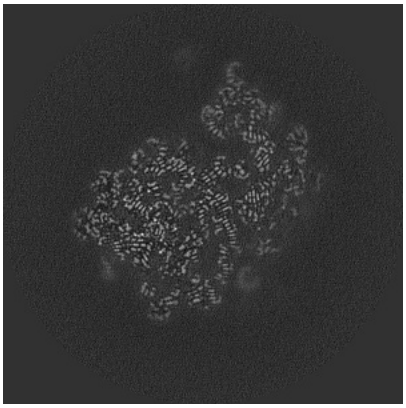
6.2.1 Primary map

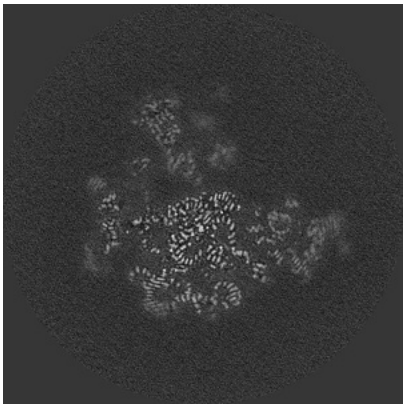

X Index: 220

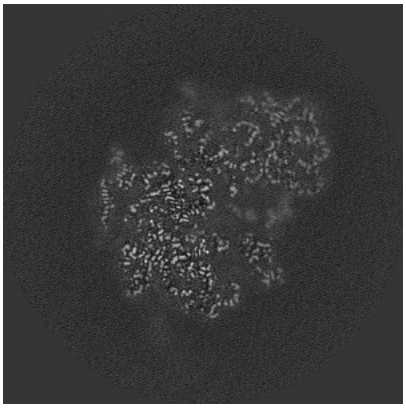
Y Index: 220


Z Index: 220

6.2.2 Raw map


X Index: 220

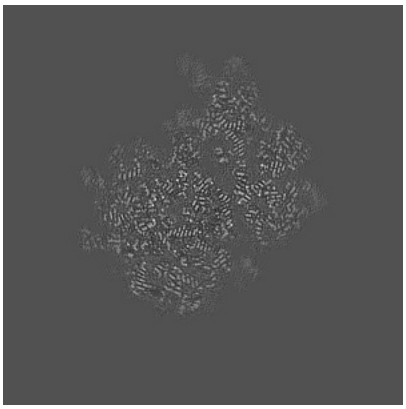

Y Index: 220


Z Index: 220

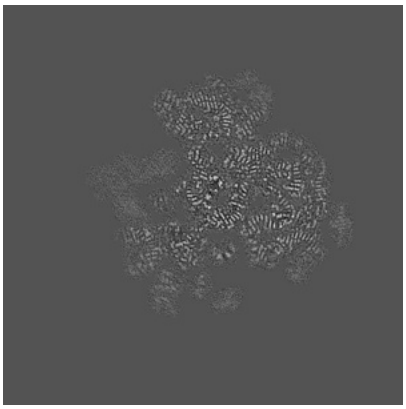
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

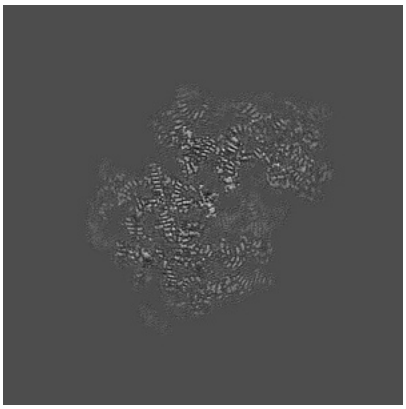
6.3.1 Primary map



X Index: 204

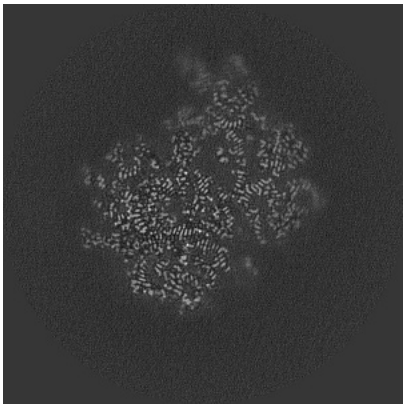


Y Index: 261

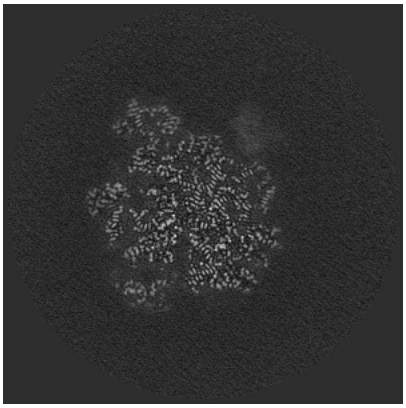


Z Index: 233

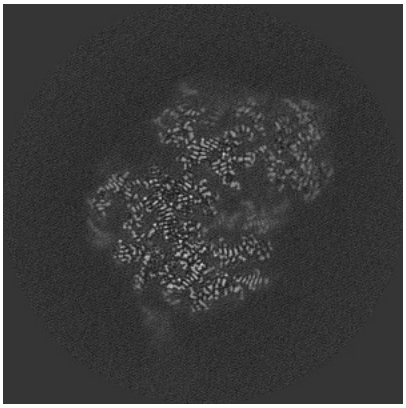
6.3.2 Raw map



X Index: 203



Y Index: 168

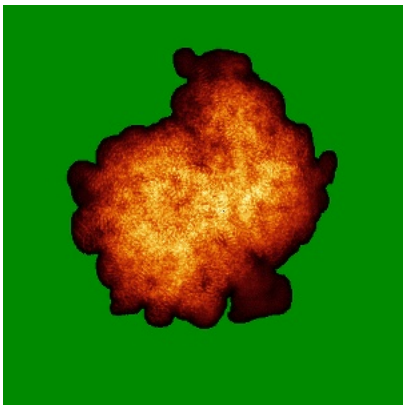


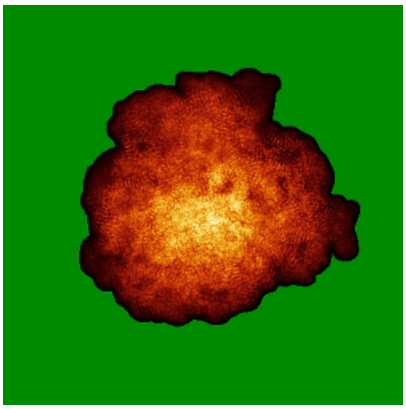
Z Index: 230

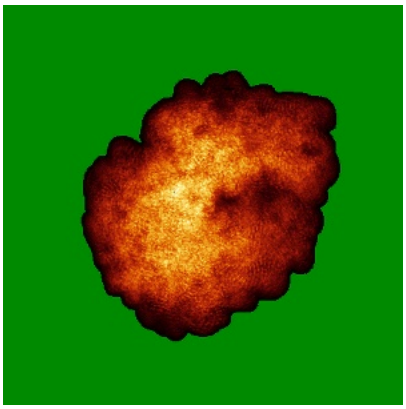
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

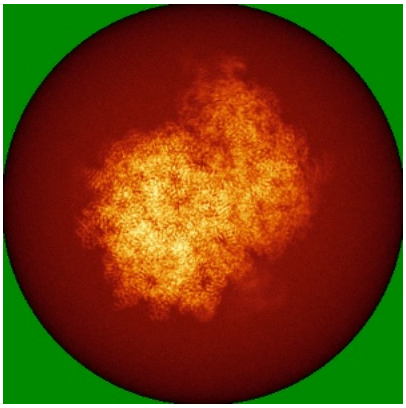
6.4.1 Primary map

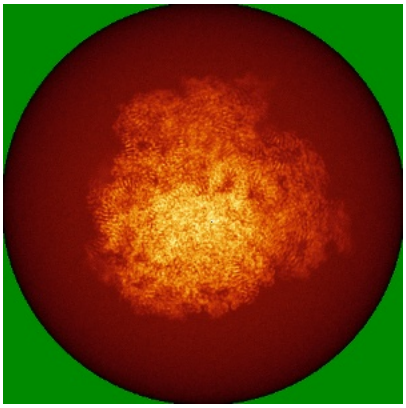

X

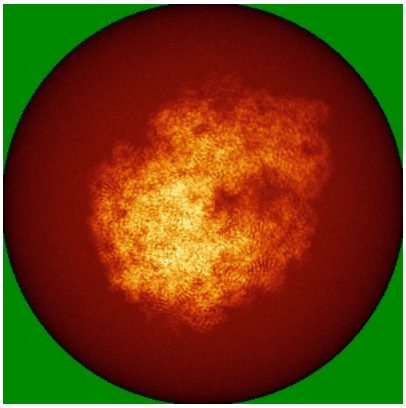

Y


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 0.0329. 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.

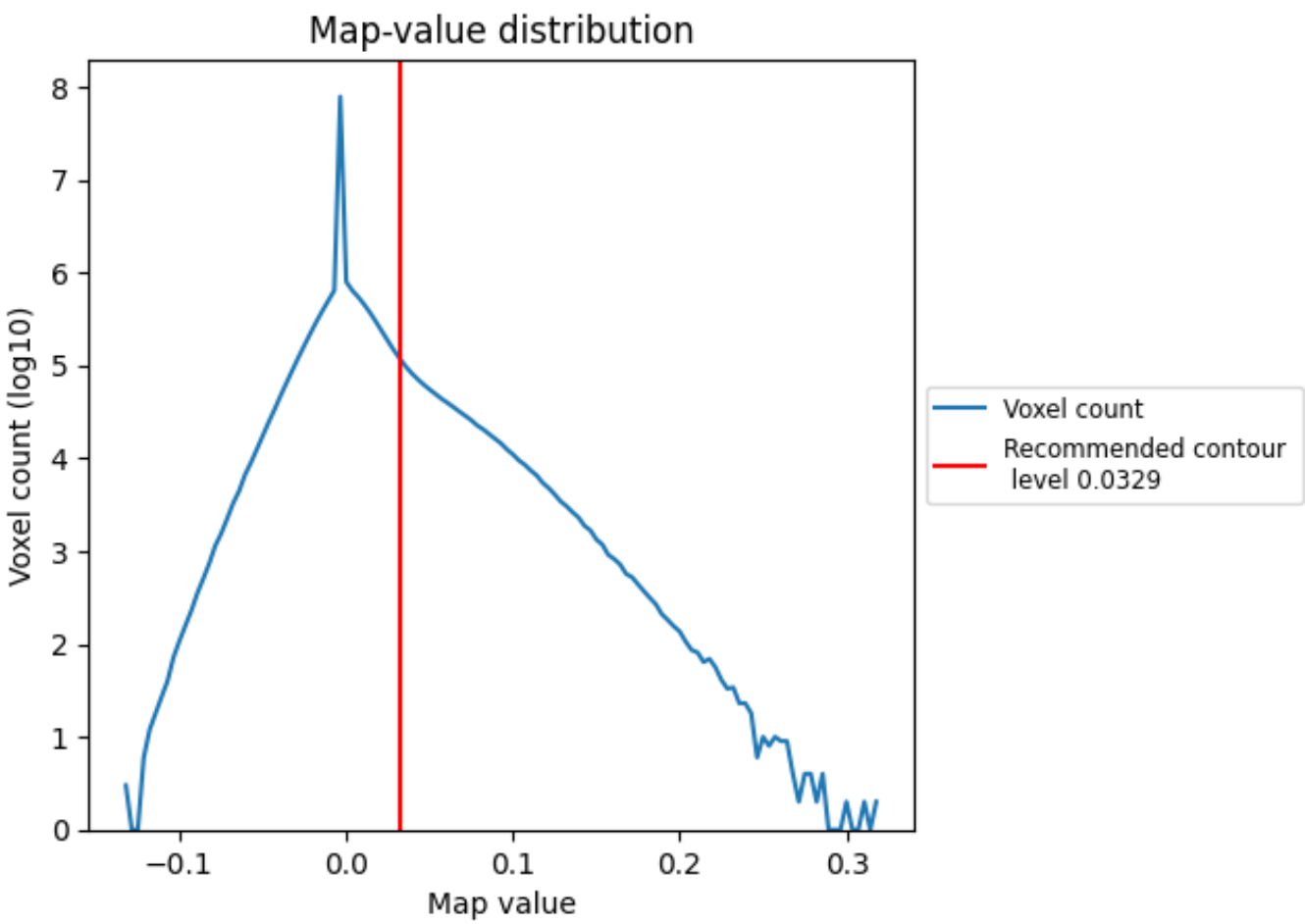
6.6 Mask visualisation (i)

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

7 Map analysis (i)

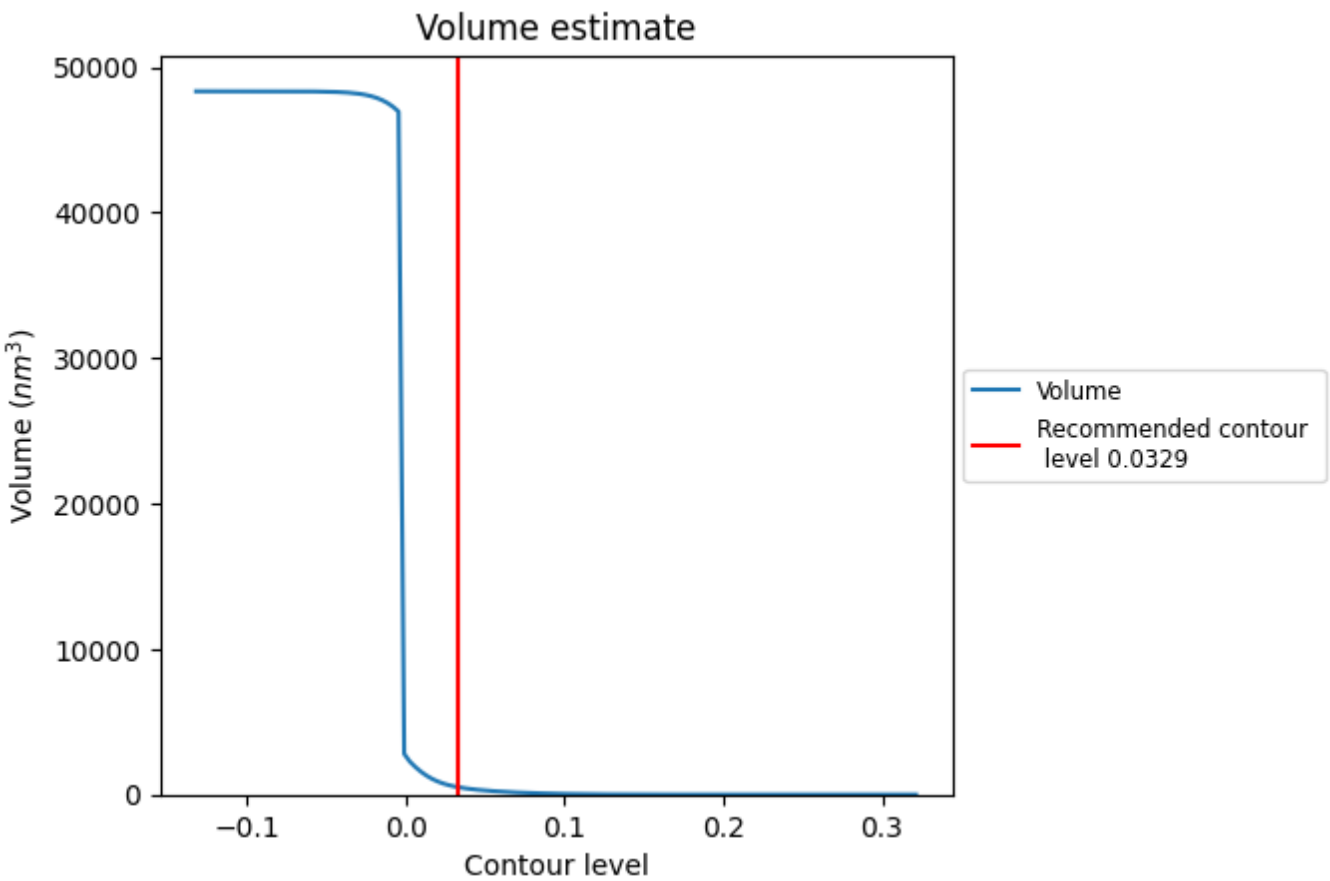
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

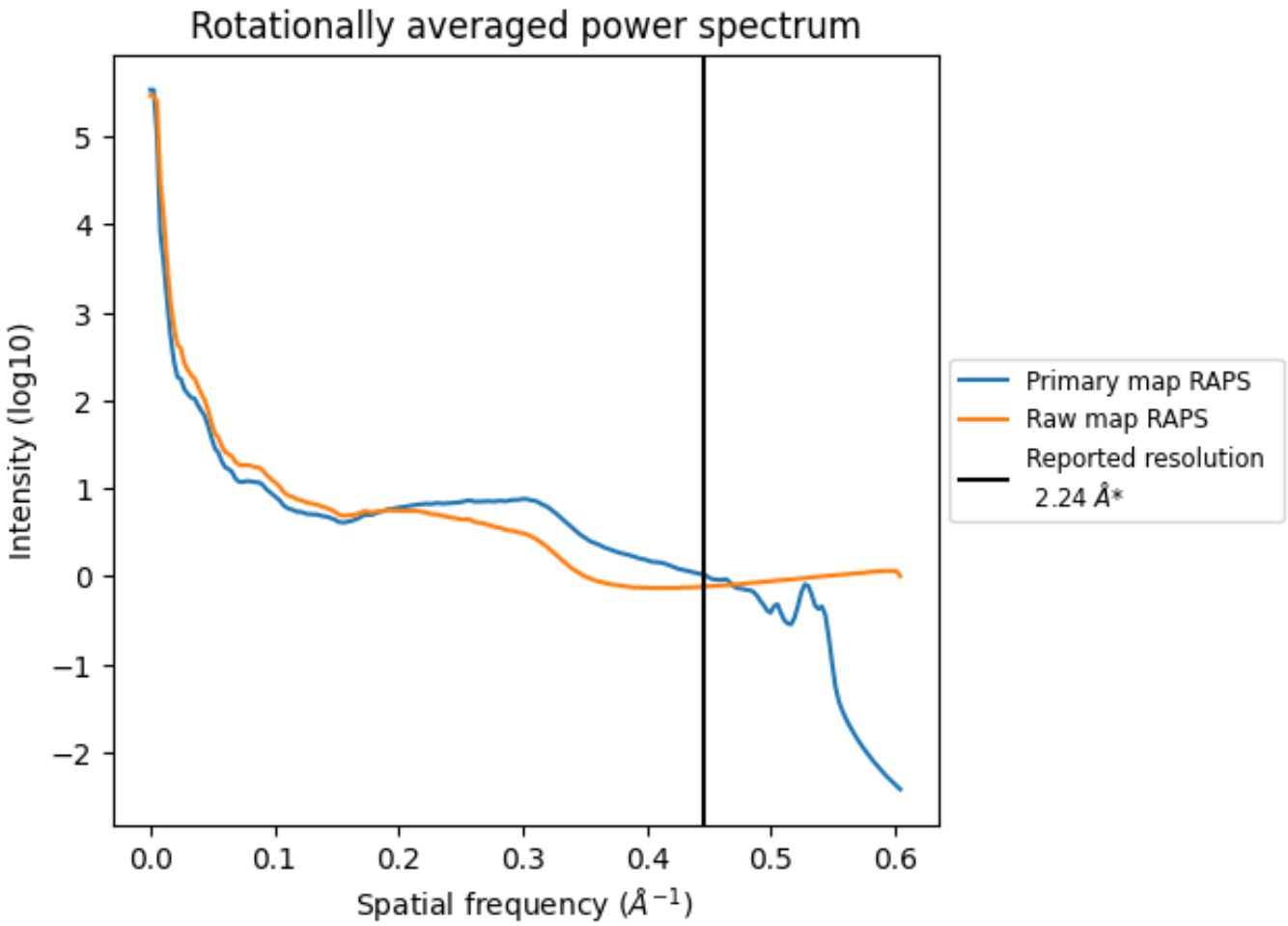
7.2 Volume estimate (i)



The volume at the recommended contour level is 516 nm^3; this corresponds to an approximate mass of 466 kDa.

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

7.3 Rotationally averaged power spectrum (i)

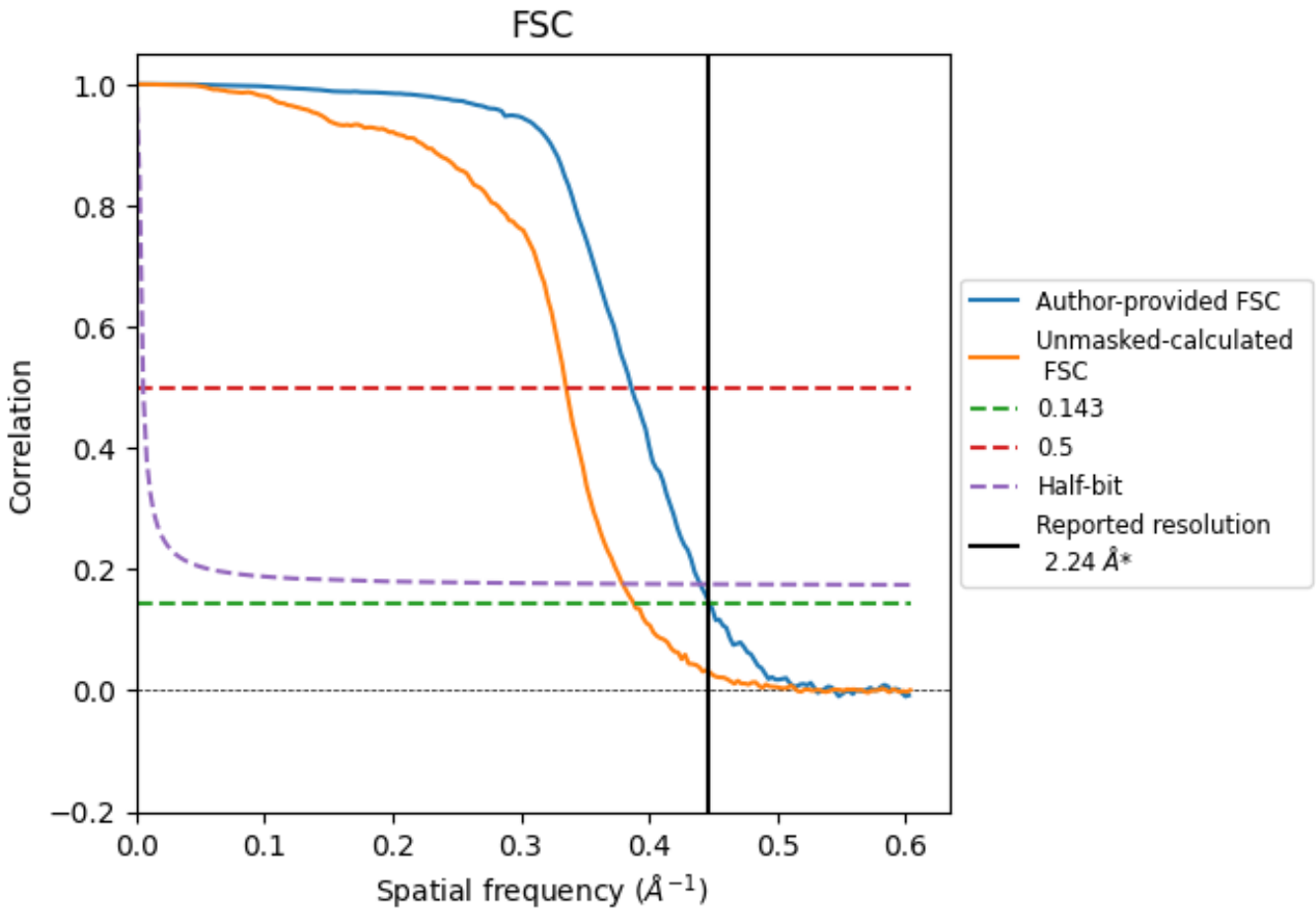


*Reported resolution corresponds to spatial frequency of 0.446 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.446 Å^{-1}

8.2 Resolution estimates (i)

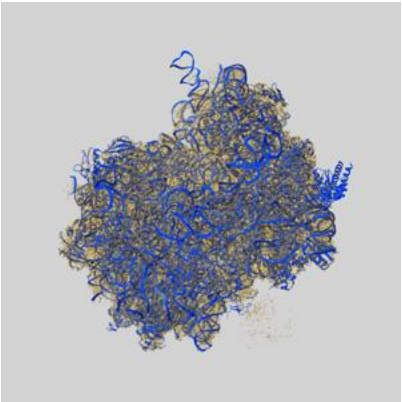
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.23	2.59	2.27
Unmasked-calculated*	2.58	2.98	2.64

*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 2.58 differs from the reported value 2.24 by more than 10 %

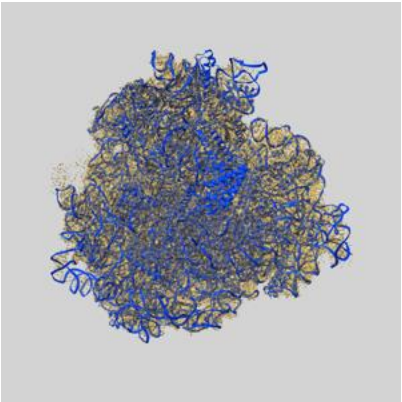
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-28165 and PDB model 8EIU. Per-residue inclusion information can be found in section 3 on page 21.

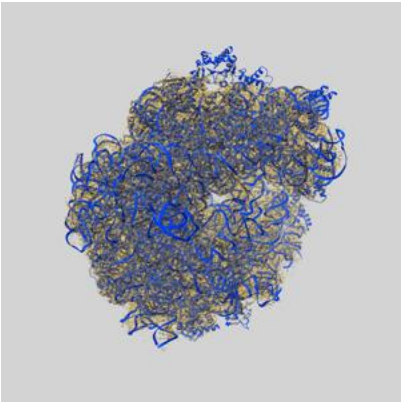
9.1 Map-model overlay (i)



X



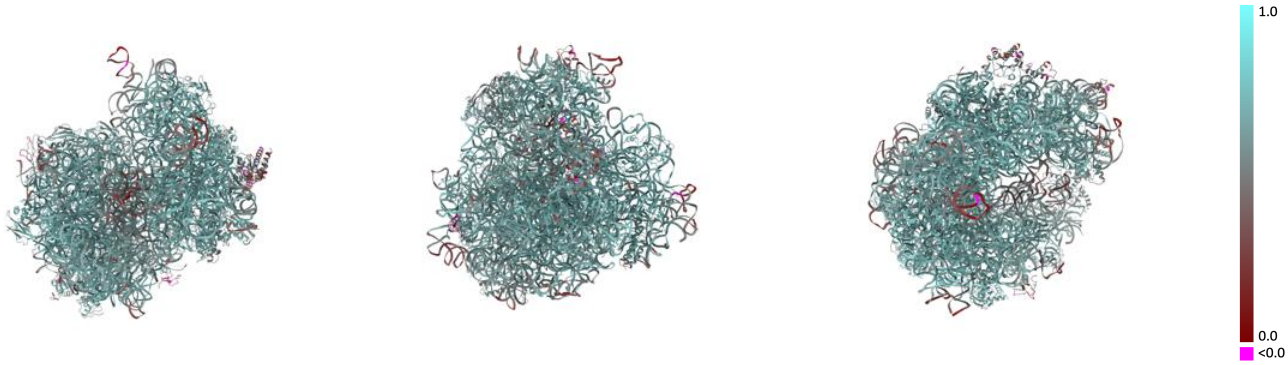
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0329 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.

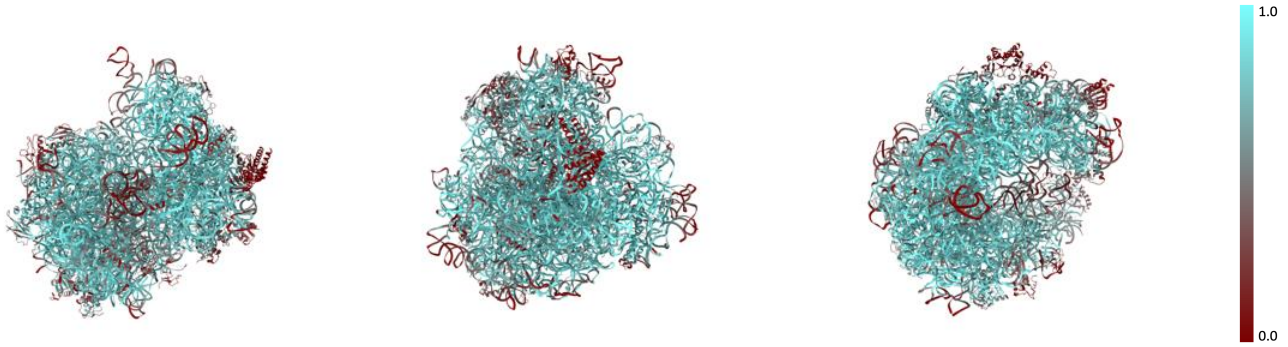
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

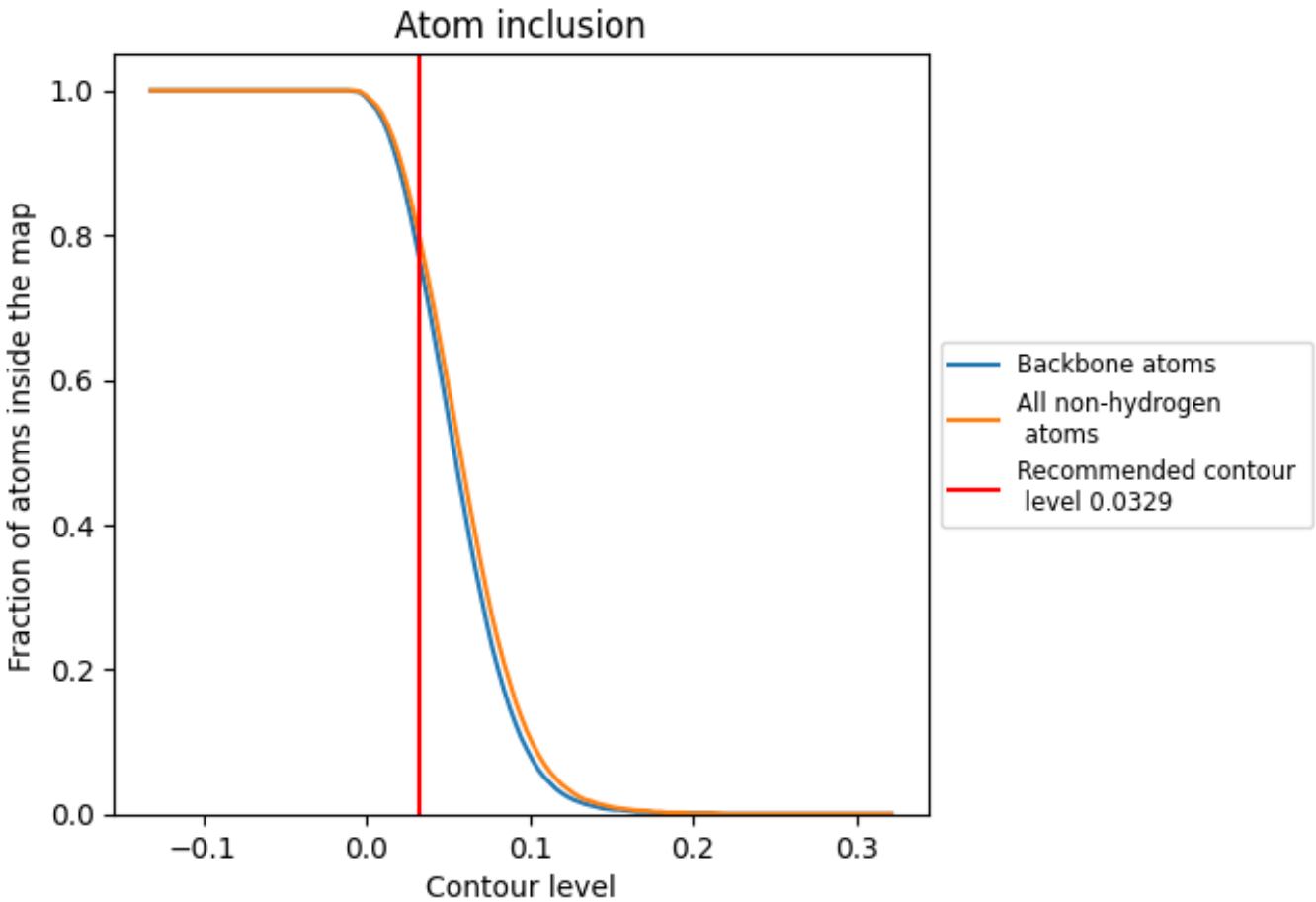
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0329).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0329) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.6580
0	0.7020	0.6640
1	0.9490	0.7350
2	0.9470	0.7410
3	0.7640	0.6790
4	0.2050	0.4610
A	0.8470	0.6590
B	0.1430	0.4580
C	0.6710	0.6550
D	0.7010	0.6540
E	0.8300	0.6890
F	0.5530	0.6040
G	0.5010	0.5930
H	0.8400	0.6880
I	0.6100	0.6340
J	0.4130	0.5370
K	0.7100	0.6550
L	0.8920	0.7120
M	0.6690	0.6410
N	0.7450	0.6740
O	0.7880	0.6770
P	0.8070	0.6830
Q	0.7550	0.6580
R	0.6690	0.6390
S	0.6520	0.6360
T	0.7340	0.6390
U	0.3600	0.5220
X	0.6900	0.6100
Y	0.3840	0.4750
Z	0.6620	0.5610
a	0.8650	0.6750
b	0.7340	0.6210
c	0.8950	0.7120
d	0.8400	0.7100
e	0.6790	0.6600

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.4240	0.5540
g	0.2780	0.4890
h	0.1270	0.2450
i	0.8330	0.7100
j	0.8700	0.7100
k	0.7950	0.6880
l	0.8510	0.7090
m	0.9450	0.7350
n	0.6210	0.6350
o	0.8010	0.6850
p	0.8880	0.7330
q	0.6660	0.6680
r	0.8430	0.7080
s	0.6800	0.6430
t	0.5680	0.6190
u	0.5810	0.6240
v	0.8240	0.6970
w	0.7940	0.6700
x	0.4970	0.6070
y	0.8010	0.6920
z	0.8090	0.6940