Full wwPDB EM Validation Report

Sep 16, 2026 – 02:27 AM EDT

PDB ID	:	9NO7 / pdb_00009no7
EMDB ID	:	EMD-49594
Title	:	Cryo-EM structure of the wild-type Thermus thermophilus 70S ribosome in complex with mRNA, A-site Q230-N5-methylated Release Factor 1, and P-site 2'-deoxy-A76-fMEAAAKC-peptidyl-tRNAcys at 2.13A resolution
Authors	:	Aleksandrova, E.V.; Syroegin, E.A.; Basu, R.S.; Vassilevski, A.A.; Gagnon, M.G.; Polikanov, Y.S.
Deposited on	:	2025-03-08
Resolution	:	2.13 Å(reported)
Based on initial model	:	9MTP

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:

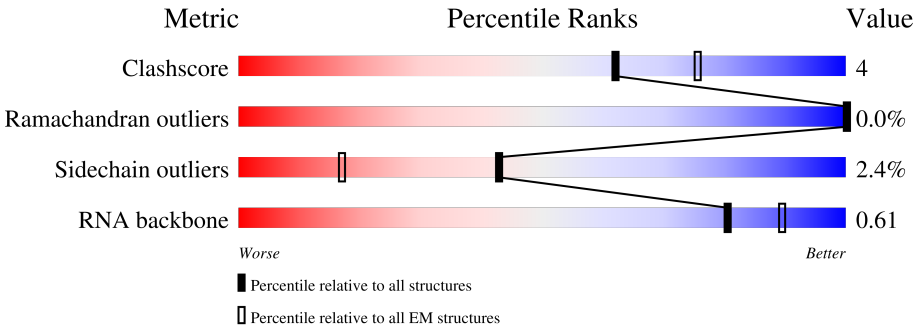
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

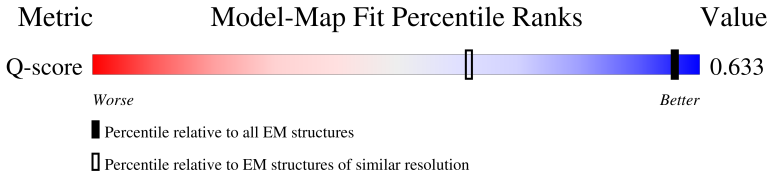
1 Overall quality at a glance

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

The reported resolution of this entry is 2.13 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	2439 (1.64 - 2.63)

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	A	2915	71% 20% • 6%
2	B	121	79% 17% • •

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Mol	Chain	Length	Quality of chain
3	D	276	90% 9%
4	E	206	95%
5	F	210	86% 10%
6	G	182	79% 19%
7	H	180	77% 18%
8	I	148	87% 11%
9	N	140	88% 10%
10	O	122	88% 12%
11	P	150	91% 9%
12	Q	141	94% 6%
13	R	118	92% 8%
14	S	112	87% 12%
15	T	146	82% 8% 10%
16	U	118	92% 7%
17	V	101	92% 7%
18	W	113	89% 8%
19	X	96	88% 10%
20	Y	110	88% 8%
21	Z	206	28% 56% 16% 26%
22	0	85	86% 5% 9%
23	1	98	81% 18%
24	2	72	86% 11%
25	3	60	87% 8% 5%
26	4	71	82% 14%
27	5	60	82% 17%

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Mol	Chain	Length	Quality of chain
28	6	54	89% 9%
29	7	49	84% 12%
30	8	65	80% 18%
31	9	37	78% 19%
32	a	1521	64% 31%
33	b	256	67% 23% 10%
34	c	239	73% 12% 14%
35	d	209	84% 16%
36	e	162	73% 19% 8%
37	f	101	83% 16%
38	g	156	83% 15%
39	h	138	84% 15%
40	i	128	73% 25%
41	j	105	78% 14% 8%
42	k	129	78% 9% 12%
43	l	132	83% 8% 8%
44	m	126	81% 13% 6%
45	n	61	97%
46	o	89	84% 15%
47	p	88	82% 11% 7%
48	q	105	80% 14% 6%
49	r	88	58% 19% 23%
50	s	93	72% 16% 11%
51	t	106	77% 12% 10%
52	u	27	74% 11% 15%

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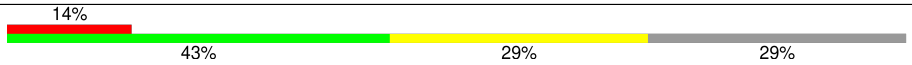
Mol	Chain	Length	Quality of chain
53	v	24	
54	w	354	
55	x	74	
56	z	7	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2734	58906	26221	11028	18923	2734	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2577	1146	476	835	120	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	273	2117	1337	419	358	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	204	1559	985	298	270	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	202	1583	1009	297	275	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	181	1429	916	256	253	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	174	Total	C	N	O	S	0	0
			1330	845	248	236	1		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	146	Total	C	N	O	S	0	0
			952	608	166	177	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	140	Total	C	N	O	S	0	0
			1111	715	207	185	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	122	Total	C	N	O	S	0	0
			922	581	170	168	3		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	149	Total	C	N	O	S	0	0
			1088	677	220	188	3		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0
			1110	709	206	188	7		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	118	Total	C	N	O	S	0	0
			964	602	203	158	1		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	110	Total 865	C 545	N 173	O 147	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	131	Total 1084	C 676	N 223	O 184	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	116	Total 959	C 608	N 201	O 149	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	101	Total 771	C 495	N 140	O 135	S 1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	110	Total 863	C 545	N 167	O 149	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	95	Total 750	C 488	N 135	O 126	S 1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	107	Total 792	C 508	N 150	O 128	S 6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	153	Total	C	N	O	S	0	0
			1236	792	221	221	2		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	77	Total	C	N	O	S	0	0
			608	375	129	103	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	97	Total	C	N	O	S	0	0
			747	470	147	129	1		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	70	Total	C	N	O	S	0	0
			588	365	118	103	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	3	57	Total	C	N	O	0	0
			452	288	88	76		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	69	Total	C	N	O	S	0	0
			462	290	80	87	5		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	59	Total	C	N	O	S	0	0
			455	285	89	76	5		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	53	Total	C	N	O	S	0	0
			453	281	91	77	4		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	47	Total	C	N	O	S	0	0
			409	251	102	54	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			517	331	102	82	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1487	Total	C	N	O	P	0	0
			31971	14236	5931	10317	1487		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	231	Total	C	N	O	S	0	0
			1825	1168	327	326	4		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1524	957	297	269	1		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	208	Total	C	N	O	S	0	0
			1634	1029	314	284	7		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	149	Total	C	N	O	S	0	0
			1130	714	213	199	4		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			810	514	144	149	3		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	154	Total	C	N	O	S	0	0
			1184	737	232	209	6		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	137	Total	C	N	O	S	0	0
			1084	687	207	188	2		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	i	127	Total	C	N	O	0	0
			976	617	192	167		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	j	97	Total	C	N	O	0	0
			695	431	137	127		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	114	Total	C	N	O	S	0	0
			825	514	154	154	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	121	Total	C	N	O	S	0	0
			927	583	184	158	2		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	118	Total	C	N	O	S	0	0
			919	566	190	161	2		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	60	Total	C	N	O	S	0	0
			474	300	98	72	4		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			718	451	141	124	2		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	82	Total	C	N	O	S	0	0
			670	424	132	113	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			815	523	150	140	2		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	r	68	Total	C	N	O	0	0
			545	350	105	90		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	83	Total	C	N	O	S	0	0
			631	404	115	111	1		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	95	Total	C	N	O	S	0	0
			688	424	150	112	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
52	u	23	Total	C	N	O	0	0
			199	122	48	29		

- Molecule 53 is a RNA chain called CYS-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	9	Total	C	N	O	P	0	0
			191	86	34	62	9		

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	249	Total	C	N	O	S	0	0
			1939	1199	360	371	9		

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	x	73	Total	C	N	O	P	S	0	0
			1556	695	278	509	73	1		

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	5	Total 30	C 18	N 6	O 5	S 1	0	0

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

Mol	Chain	Residues	Atoms		AltConf
57	A	1296	Total 1296	Mg 1296	0
57	B	15	Total 15	Mg 15	0
57	D	22	Total 22	Mg 22	0
57	E	22	Total 22	Mg 22	0
57	F	15	Total 15	Mg 15	0
57	G	1	Total 1	Mg 1	0
57	N	4	Total 4	Mg 4	0
57	O	5	Total 5	Mg 5	0
57	P	8	Total 8	Mg 8	0
57	Q	4	Total 4	Mg 4	0
57	R	7	Total 7	Mg 7	0
57	S	1	Total 1	Mg 1	0
57	T	2	Total 2	Mg 2	0
57	U	7	Total 7	Mg 7	0
57	V	5	Total 5	Mg 5	0
57	W	3	Total 3	Mg 3	0
57	X	5	Total 5	Mg 5	0
57	Y	1	Total 1	Mg 1	0
57	0	6	Total 6	Mg 6	0

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Mol	Chain	Residues	Atoms	AltConf
57	1	4	Total Mg 4 4	0
57	3	2	Total Mg 2 2	0
57	5	11	Total Mg 11 11	0
57	6	2	Total Mg 2 2	0
57	7	5	Total Mg 5 5	0
57	8	5	Total Mg 5 5	0
57	a	205	Total Mg 205 205	0
57	e	1	Total Mg 1 1	0
57	h	1	Total Mg 1 1	0
57	k	1	Total Mg 1 1	0
57	m	1	Total Mg 1 1	0
57	n	1	Total Mg 1 1	0
57	q	2	Total Mg 2 2	0
57	v	4	Total Mg 4 4	0
57	w	1	Total Mg 1 1	0
57	x	10	Total Mg 10 10	0

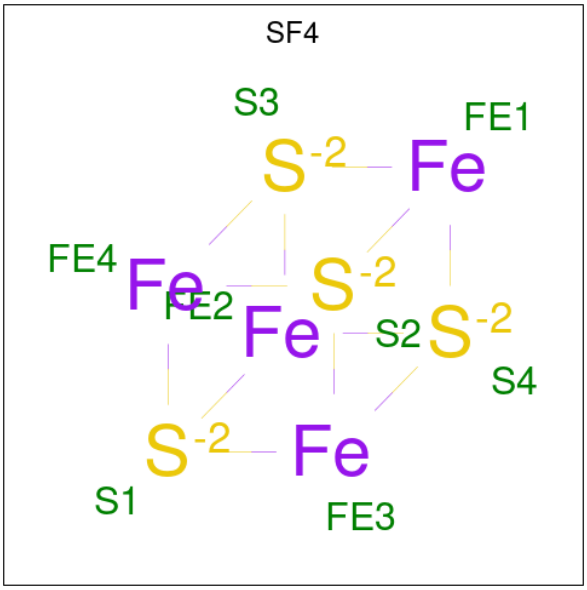
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
58	A	51	Total K 51 51	0
58	Q	1	Total K 1 1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	Y	1	Total Zn 1 1	0
59	4	1	Total Zn 1 1	0
59	5	1	Total Zn 1 1	0
59	6	1	Total Zn 1 1	0
59	9	1	Total Zn 1 1	0
59	n	1	Total Zn 1 1	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
60	d	1	Total Fe S 8 4 4	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	A	3537	Total O 3537 3537	0
61	B	19	Total O 19 19	0
61	D	74	Total O 74 74	0

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Mol	Chain	Residues	Atoms	AltConf
61	E	35	Total O 35 35	0
61	F	39	Total O 39 39	0
61	I	1	Total O 1 1	0
61	N	14	Total O 14 14	0
61	O	15	Total O 15 15	0
61	P	46	Total O 46 46	0
61	Q	22	Total O 22 22	0
61	R	24	Total O 24 24	0
61	S	3	Total O 3 3	0
61	T	13	Total O 13 13	0
61	U	37	Total O 37 37	0
61	V	12	Total O 12 12	0
61	W	19	Total O 19 19	0
61	X	13	Total O 13 13	0
61	Y	1	Total O 1 1	0
61	Z	3	Total O 3 3	0
61	0	13	Total O 13 13	0
61	1	6	Total O 6 6	0
61	2	4	Total O 4 4	0
61	3	5	Total O 5 5	0
61	5	16	Total O 16 16	0

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Mol	Chain	Residues	Atoms	AltConf
61	6	3	Total O 3 3	0
61	7	15	Total O 15 15	0
61	8	16	Total O 16 16	0
61	9	5	Total O 5 5	0
61	a	648	Total O 648 648	0
61	b	1	Total O 1 1	0
61	d	3	Total O 3 3	0
61	e	4	Total O 4 4	0
61	g	1	Total O 1 1	0
61	h	3	Total O 3 3	0
61	i	2	Total O 2 2	0
61	j	2	Total O 2 2	0
61	k	1	Total O 1 1	0
61	l	17	Total O 17 17	0
61	n	1	Total O 1 1	0
61	o	1	Total O 1 1	0
61	q	3	Total O 3 3	0
61	r	1	Total O 1 1	0
61	t	1	Total O 1 1	0
61	v	10	Total O 10 10	0
61	w	20	Total O 20 20	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
61	x	30	30	30	0

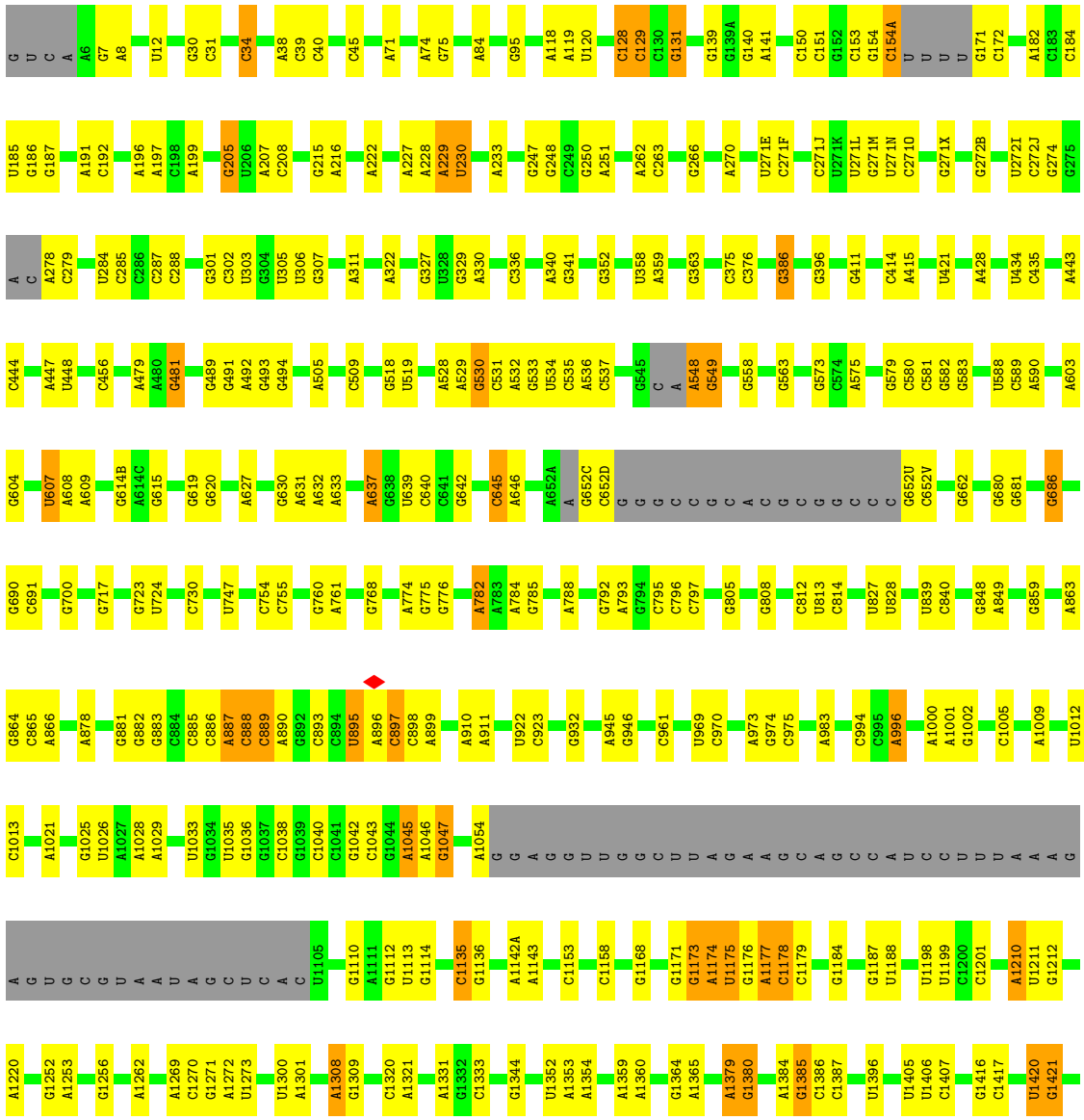
3 Residue-property plots (i)

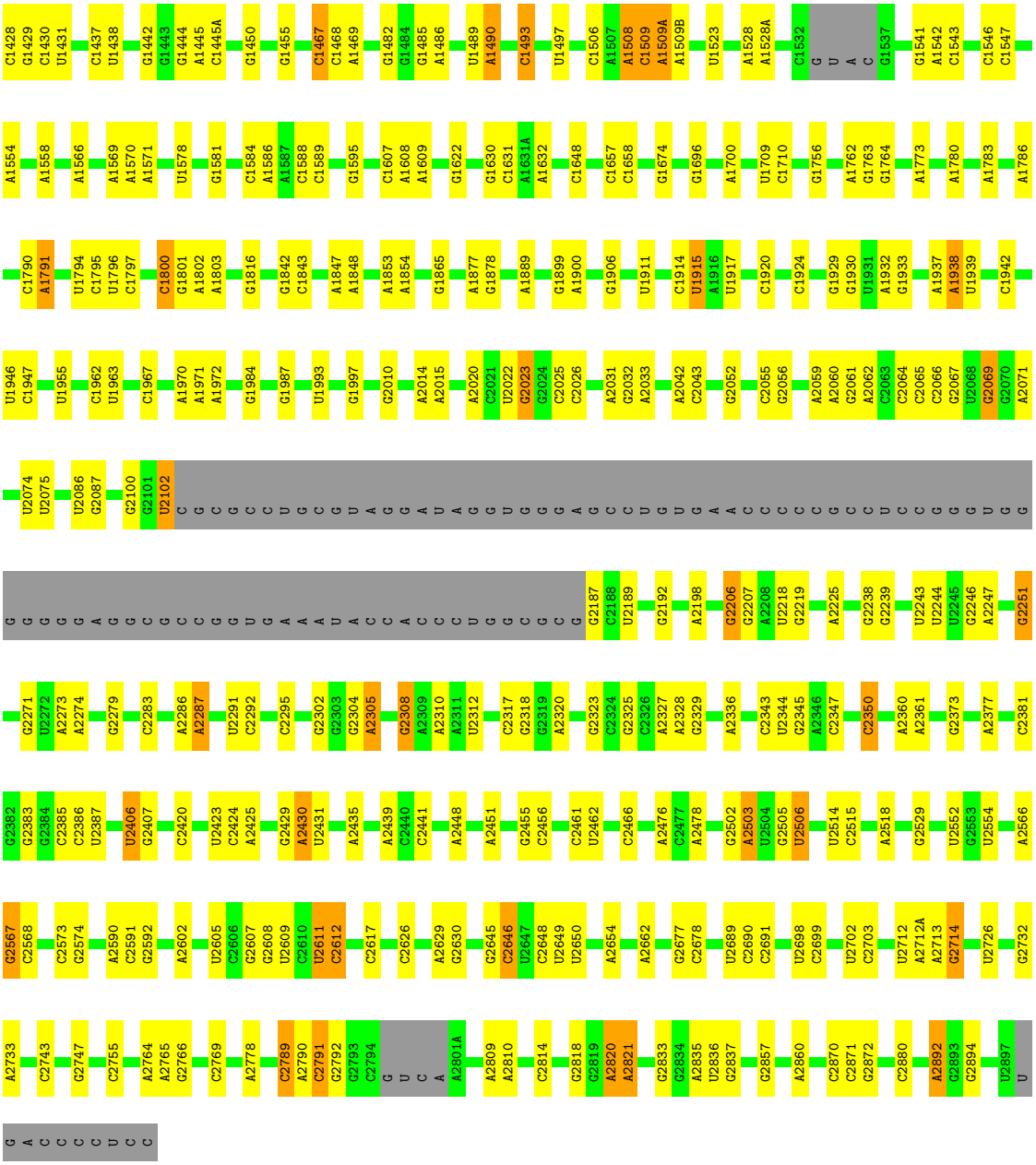
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S Ribosomal RNA

Chain A:



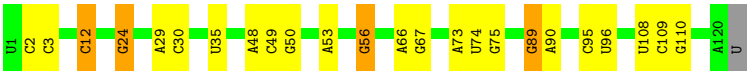




• Molecule 2: 5S Ribosomal RNA

Chain B:





• Molecule 3: 50S ribosomal protein L2

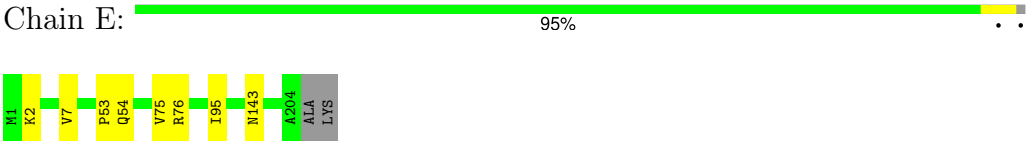
Chain D:





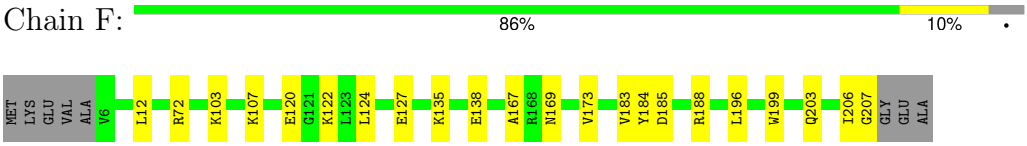
• Molecule 4: 50S ribosomal protein L3

Chain E:



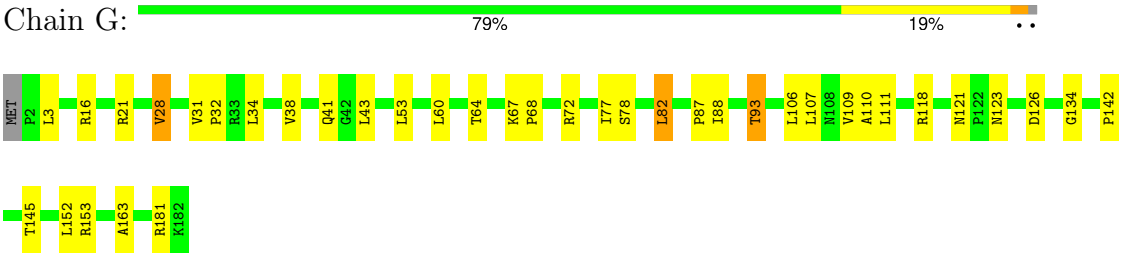
• Molecule 5: 50S ribosomal protein L4

Chain F:



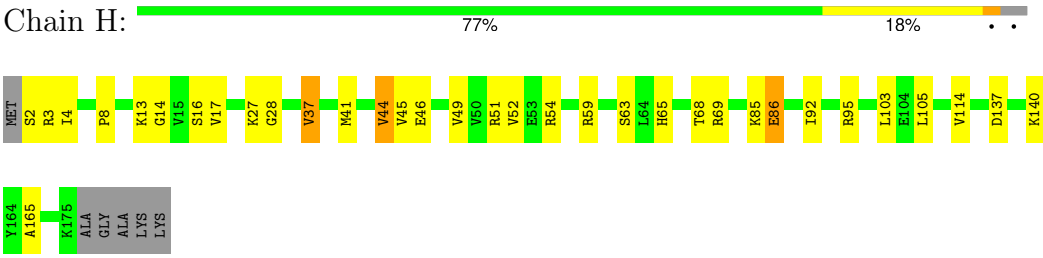
• Molecule 6: 50S ribosomal protein L5

Chain G:



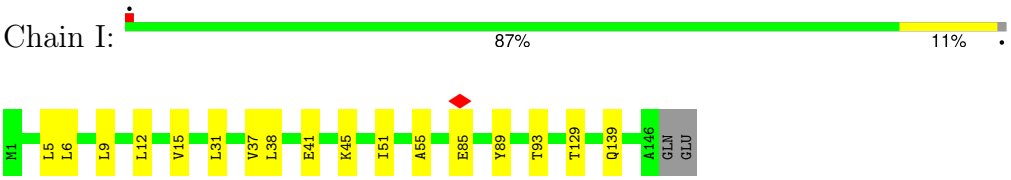
• Molecule 7: 50S ribosomal protein L6

Chain H:



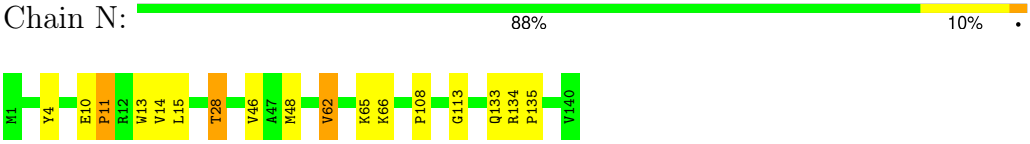
• Molecule 8: 50S ribosomal protein L9

Chain I:



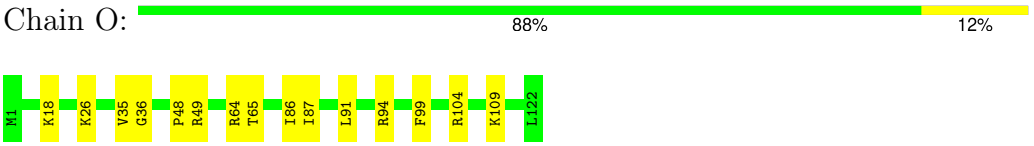
• Molecule 9: 50S ribosomal protein L13

Chain N:



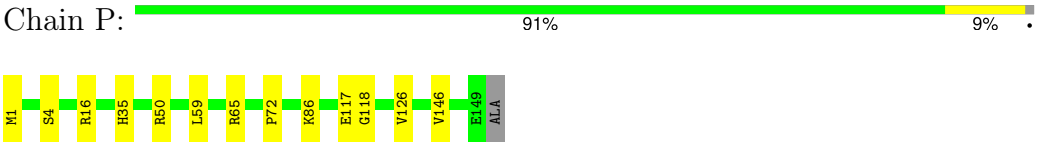
• Molecule 10: 50S ribosomal protein L14

Chain O:



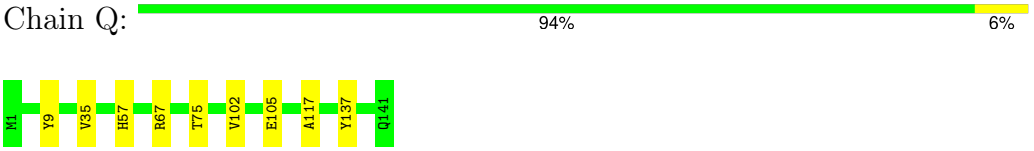
• Molecule 11: 50S ribosomal protein L15

Chain P:



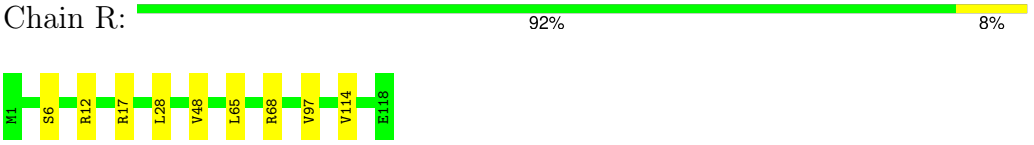
• Molecule 12: 50S ribosomal protein L16

Chain Q:



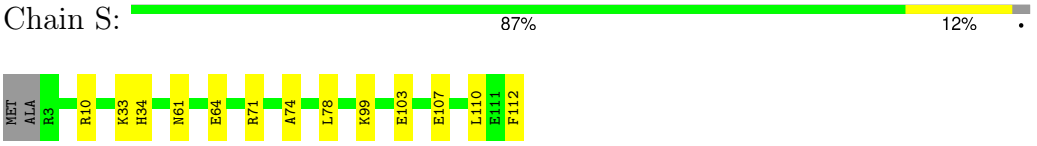
• Molecule 13: 50S ribosomal protein L17

Chain R:



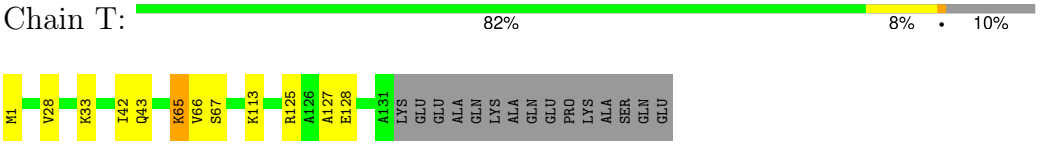
• Molecule 14: 50S ribosomal protein L18

Chain S:



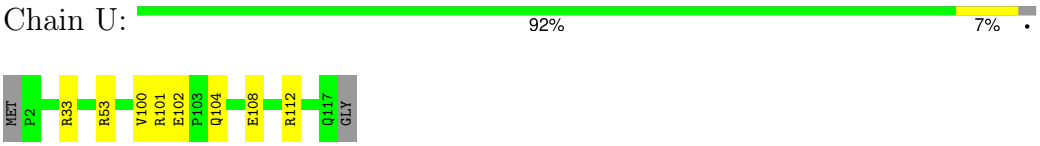
• Molecule 15: 50S ribosomal protein L19

Chain T:



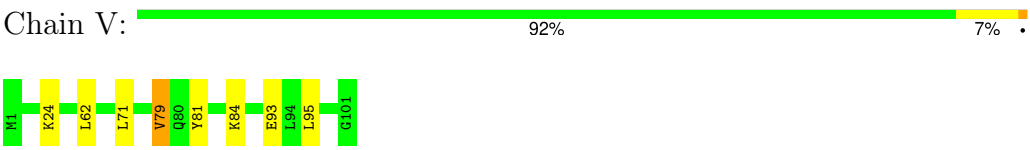
• Molecule 16: 50S ribosomal protein L20

Chain U:



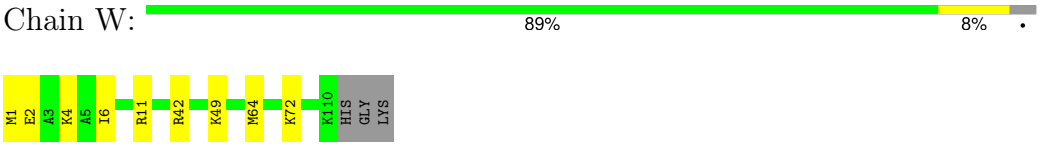
• Molecule 17: 50S ribosomal protein L21

Chain V:



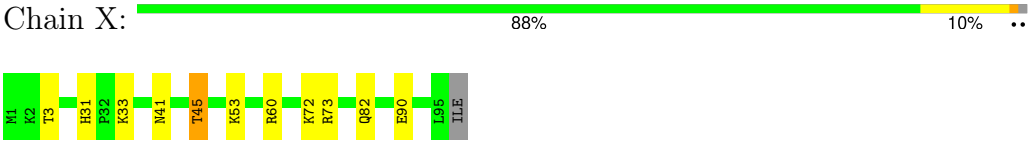
• Molecule 18: 50S ribosomal protein L22

Chain W:



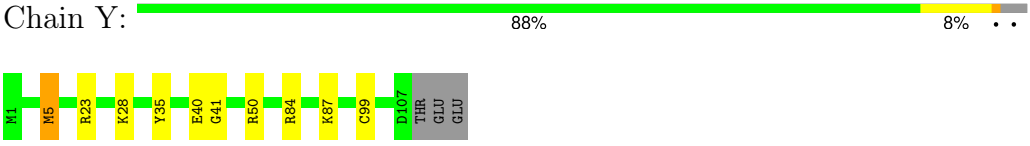
• Molecule 19: 50S ribosomal protein L23

Chain X:



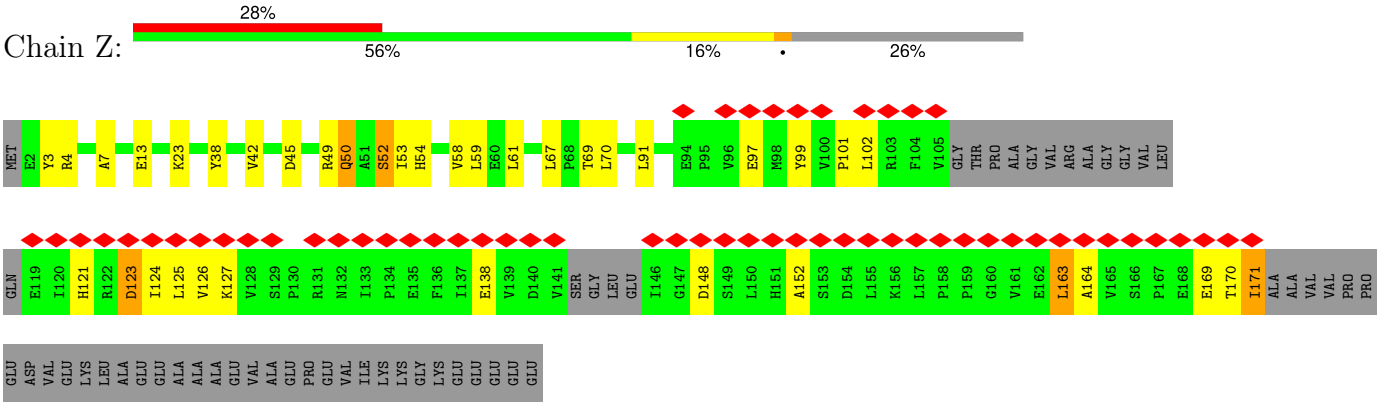
• Molecule 20: 50S ribosomal protein L24

Chain Y:



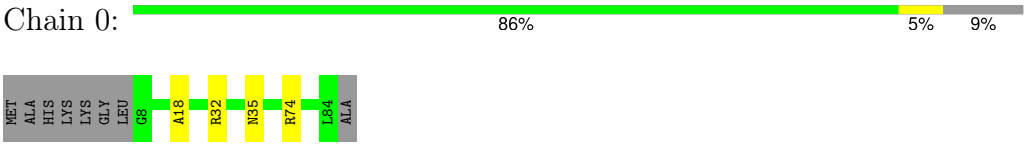
• Molecule 21: 50S ribosomal protein L25

Chain Z:



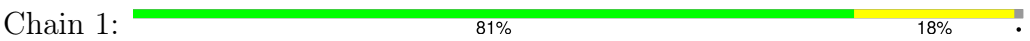
• Molecule 22: 50S ribosomal protein L27

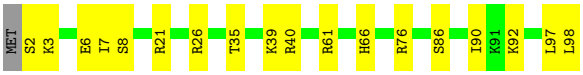
Chain 0:



• Molecule 23: 50S ribosomal protein L28

Chain 1:





• Molecule 24: 50S ribosomal protein L29

Chain 2: 



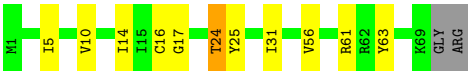
• Molecule 25: 50S ribosomal protein L30

Chain 3: 



• Molecule 26: 50S ribosomal protein L31

Chain 4: 



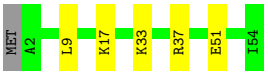
• Molecule 27: 50S ribosomal protein L32

Chain 5: 



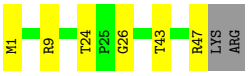
• Molecule 28: 50S ribosomal protein L33

Chain 6: 



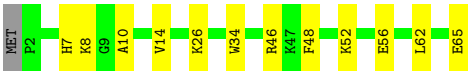
• Molecule 29: 50S ribosomal protein L34

Chain 7: 



• Molecule 30: 50S ribosomal protein L35

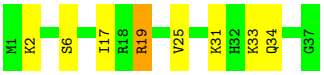
Chain 8: 



• Molecule 31: 50S ribosomal protein L36

Chain 9:

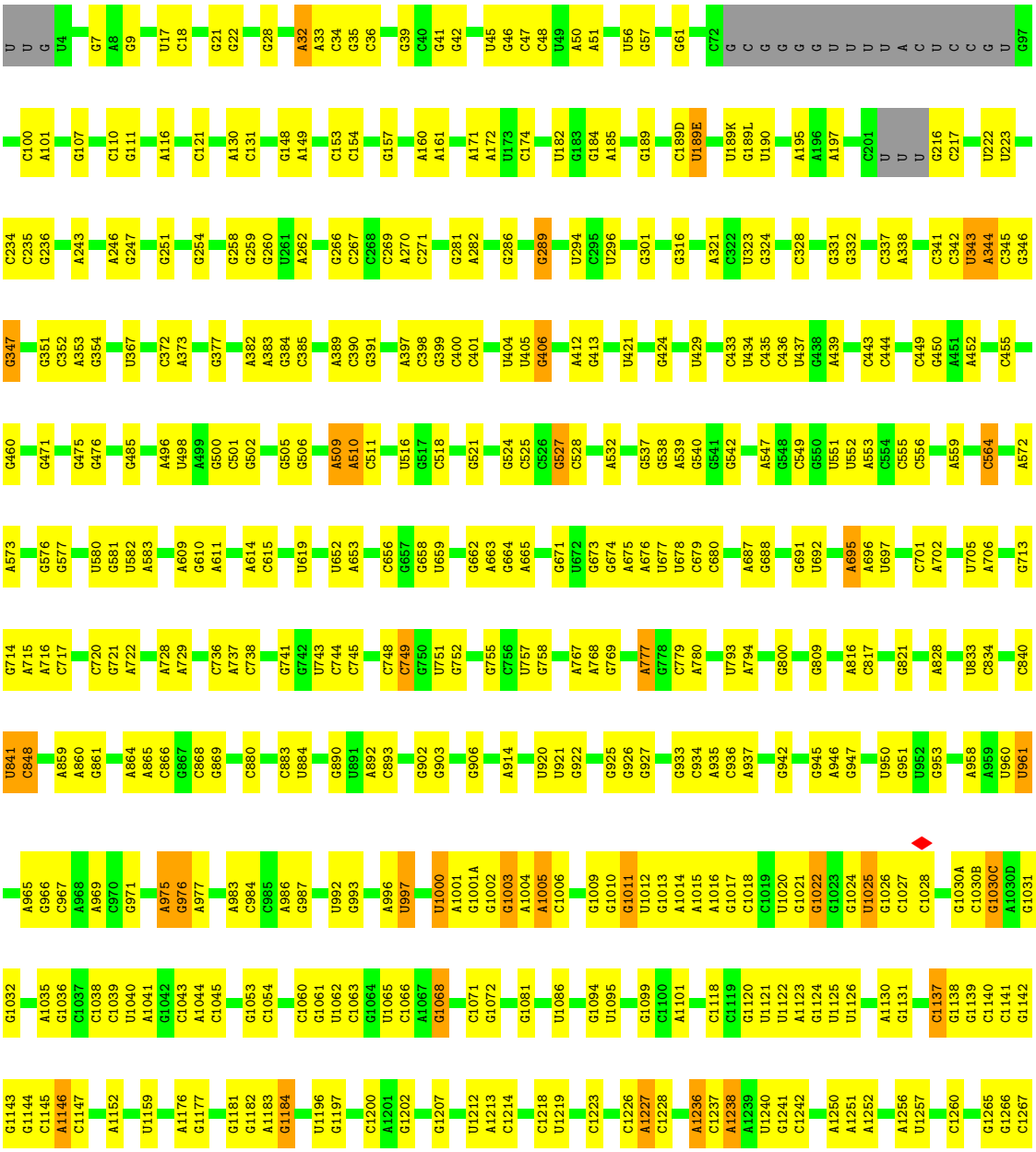


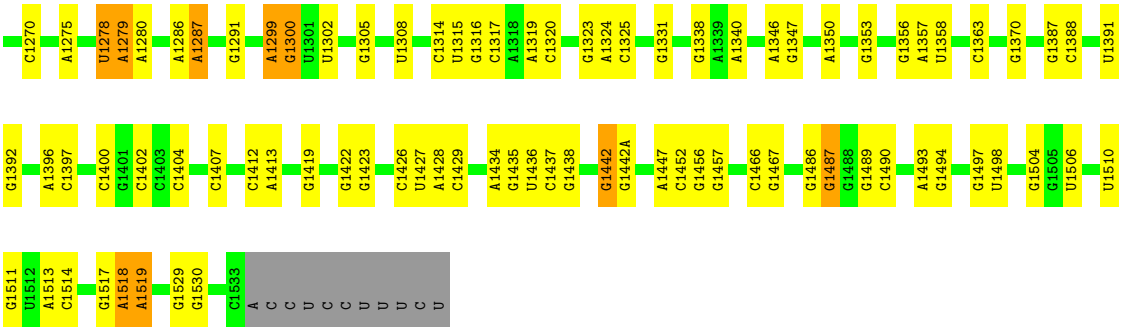


• Molecule 32: 16S Ribosomal RNA

Chain a:



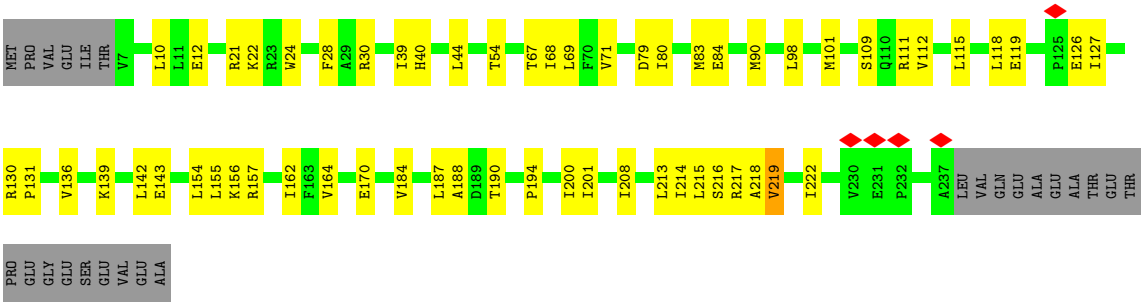




• Molecule 33: 30S ribosomal protein S2

Chain b:

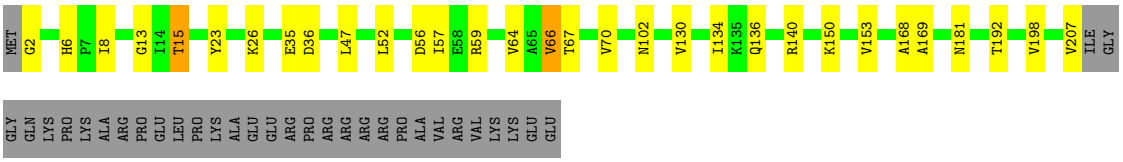




• Molecule 34: 30S ribosomal protein S3

Chain c:

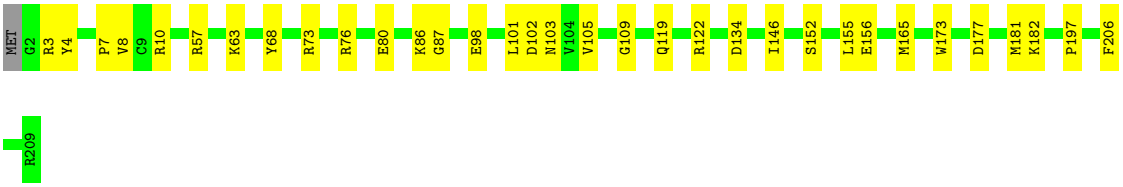




• Molecule 35: 30S ribosomal protein S4

Chain d:



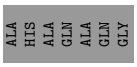


• Molecule 36: 30S ribosomal protein S5

Chain e:







• Molecule 37: 30S ribosomal protein S6

Chain f:





• Molecule 38: 30S ribosomal protein S7

Chain g:





• Molecule 39: 30S ribosomal protein S8

Chain h:





• Molecule 40: 30S ribosomal protein S9

Chain i:

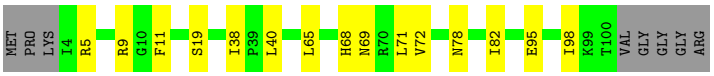




• Molecule 41: 30S ribosomal protein S10

Chain j:





• Molecule 42: 30S ribosomal protein S11

Chain k:

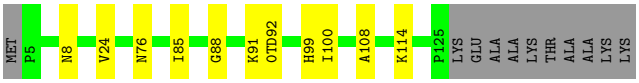




• Molecule 43: 30S ribosomal protein S12

Chain l:

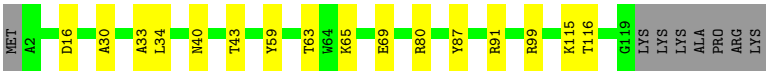




• Molecule 44: 30S ribosomal protein S13

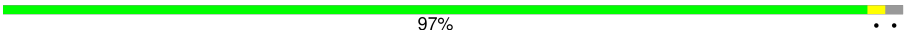
Chain m:





• Molecule 45: 30S ribosomal protein S14 type Z

Chain n:

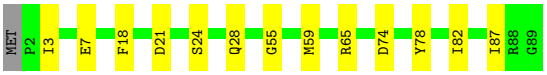




• Molecule 46: 30S ribosomal protein S15

Chain o:





• Molecule 47: 30S ribosomal protein S16

Chain p:

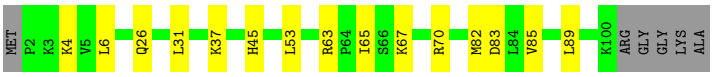




• Molecule 48: 30S ribosomal protein S17

Chain q:

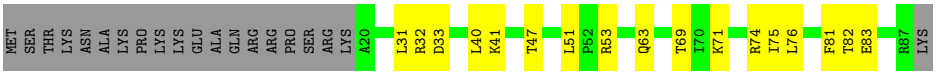




• Molecule 49: 30S ribosomal protein S18

Chain r:

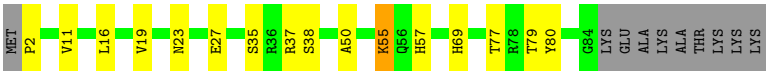




• Molecule 50: 30S ribosomal protein S19

Chain s:

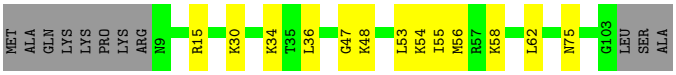




• Molecule 51: 30S ribosomal protein S20

Chain t:

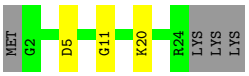




• Molecule 52: 30S ribosomal protein Thx

Chain u:





• Molecule 53: CYS-Stop mRNA

Chain v:

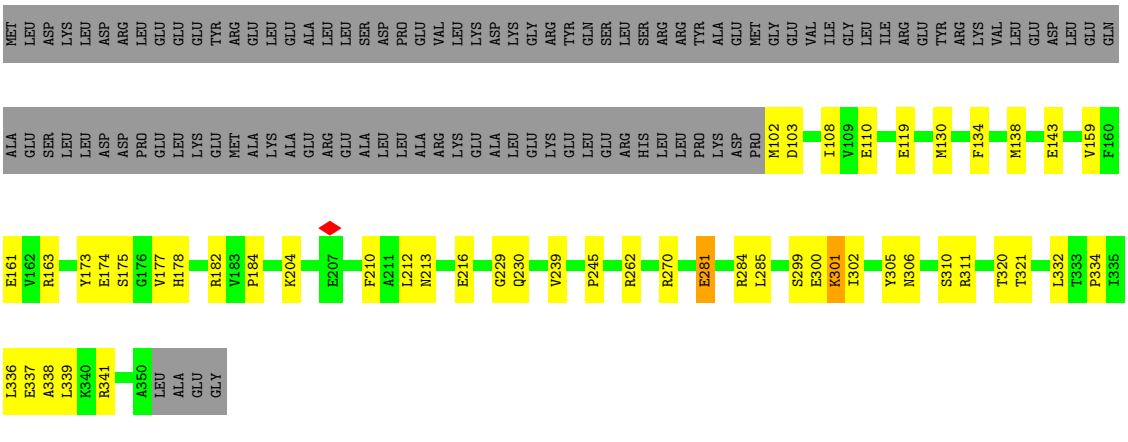




• Molecule 54: Peptide chain release factor 1

Chain w:

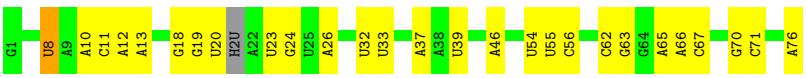




• Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part

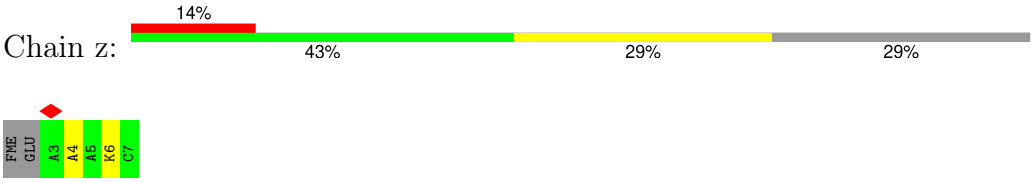
Chain x:





• Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	617938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.7153	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.441	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	431.2576, 431.2576, 431.2576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8423, 0.8423, 0.8423	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: OMG, G7M, MIA, OMU, MEQ, 4OC, 2MG, 0TD, PSU, OMC, H2U, 5MC, 2MA, K, MA6, MG, 5MU, M2G, UR3, 4SU, SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.20	1/65713 (0.0%)	0.33	0/102569
2	B	0.14	0/2882	0.25	0/4494
3	D	0.15	0/2167	0.34	0/2922
4	E	0.15	0/1592	0.34	0/2149
5	F	0.17	0/1618	0.31	0/2191
6	G	0.11	0/1454	0.27	0/1964
7	H	0.13	0/1356	0.30	0/1834
8	I	0.11	0/965	0.29	0/1331
9	N	0.17	0/1138	0.40	1/1535 (0.1%)
10	O	0.14	0/932	0.30	0/1257
11	P	0.15	0/1104	0.35	0/1475
12	Q	0.15	0/1131	0.30	0/1513
13	R	0.14	0/978	0.29	0/1307
14	S	0.11	0/875	0.27	0/1167
15	T	0.13	0/1098	0.29	0/1469
16	U	0.14	0/977	0.28	0/1301
17	V	0.14	0/782	0.29	0/1049
18	W	0.13	0/873	0.28	0/1174
19	X	0.14	0/764	0.30	0/1025
20	Y	0.12	0/805	0.31	0/1078
21	Z	0.11	0/1263	0.29	0/1712
22	0	0.12	0/616	0.26	0/821
23	1	0.15	0/754	0.30	0/1005
24	2	0.11	0/590	0.22	0/781
25	3	0.12	0/456	0.29	0/612
26	4	0.11	0/471	0.41	0/644
27	5	0.15	0/469	0.35	0/635
28	6	0.13	0/460	0.29	0/613
29	7	0.16	0/417	0.33	0/550
30	8	0.15	0/525	0.31	0/691
31	9	0.14	0/310	0.27	0/407

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	a	0.16	0/35488	0.30	0/55383
33	b	0.13	0/1860	0.34	0/2517
34	c	0.11	0/1548	0.27	0/2097
35	d	0.12	0/1664	0.27	0/2238
36	e	0.15	0/1146	0.36	0/1546
37	f	0.13	0/823	0.33	0/1115
38	g	0.16	0/1201	0.37	1/1619 (0.1%)
39	h	0.12	0/1104	0.28	0/1488
40	i	0.13	0/995	0.32	0/1338
41	j	0.12	0/707	0.32	0/961
42	k	0.12	0/840	0.28	0/1140
43	l	0.13	0/932	0.32	0/1253
44	m	0.11	0/929	0.30	0/1250
45	n	0.12	0/483	0.27	0/645
46	o	0.13	0/729	0.26	0/973
47	p	0.13	0/686	0.33	0/927
48	q	0.13	0/828	0.31	0/1108
49	r	0.11	0/550	0.24	0/734
50	s	0.13	0/646	0.34	0/877
51	t	0.16	0/689	0.34	0/911
52	u	0.09	0/203	0.19	0/266
53	v	0.19	0/213	0.39	0/329
54	w	0.15	0/1956	0.31	0/2634
55	x	0.19	0/1578	0.28	0/2452
56	z	0.17	0/29	0.45	0/37
All	All	0.17	1/153362 (0.0%)	0.32	2/229113 (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
11	P	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2552	OMU	O3'-P	5.01	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	11	PRO	CA-N-CD	-8.75	99.75	112.00
38	g	71	PRO	CA-N-CD	-6.23	103.28	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	P	35	HIS	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	A	58906	0	29692	290	0
2	B	2577	0	1305	13	0
3	D	2117	0	2191	18	0
4	E	1559	0	1618	5	0
5	F	1583	0	1625	13	0
6	G	1429	0	1447	21	0
7	H	1330	0	1407	21	0
8	I	952	0	852	9	0
9	N	1111	0	1173	10	0
10	O	922	0	974	9	0
11	P	1088	0	1135	9	0
12	Q	1110	0	1157	5	0
13	R	964	0	1029	4	0
14	S	865	0	912	8	0
15	T	1084	0	1136	7	0
16	U	959	0	1019	6	0
17	V	771	0	830	6	0
18	W	863	0	916	5	0
19	X	750	0	814	6	0
20	Y	792	0	853	7	0
21	Z	1236	0	1232	23	0
22	0	608	0	622	3	0
23	1	747	0	811	12	0
24	2	588	0	643	4	0
25	3	452	0	504	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	4	462	0	384	6	0
27	5	455	0	465	7	0
28	6	453	0	473	4	0
29	7	409	0	454	4	0
30	8	517	0	582	8	0
31	9	307	0	335	6	0
32	a	31971	0	16158	291	0
33	b	1825	0	1835	33	0
34	c	1524	0	1487	20	0
35	d	1634	0	1637	26	0
36	e	1130	0	1176	20	0
37	f	810	0	804	11	0
38	g	1184	0	1170	15	0
39	h	1084	0	1121	14	0
40	i	976	0	966	23	0
41	j	695	0	622	9	0
42	k	825	0	819	9	0
43	l	927	0	979	6	0
44	m	919	0	951	11	0
45	n	474	0	485	1	0
46	o	718	0	745	8	0
47	p	670	0	666	5	0
48	q	815	0	876	10	0
49	r	545	0	603	9	0
50	s	631	0	618	10	0
51	t	688	0	747	8	0
52	u	199	0	208	2	0
53	v	191	0	97	0	0
54	w	1939	0	1927	28	0
55	x	1556	0	790	14	0
56	z	30	0	32	2	0
57	0	6	0	0	0	0
57	1	4	0	0	0	0
57	3	2	0	0	0	0
57	5	11	0	0	0	0
57	6	2	0	0	0	0
57	7	5	0	0	0	0
57	8	5	0	0	0	0
57	A	1296	0	0	0	0
57	B	15	0	0	0	0
57	D	22	0	0	0	0
57	E	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	F	15	0	0	0	0
57	G	1	0	0	0	0
57	N	4	0	0	0	0
57	O	5	0	0	0	0
57	P	8	0	0	0	0
57	Q	4	0	0	0	0
57	R	7	0	0	0	0
57	S	1	0	0	0	0
57	T	2	0	0	0	0
57	U	7	0	0	0	0
57	V	5	0	0	0	0
57	W	3	0	0	0	0
57	X	5	0	0	0	0
57	Y	1	0	0	0	0
57	a	205	0	0	0	0
57	e	1	0	0	0	0
57	h	1	0	0	0	0
57	k	1	0	0	0	0
57	m	1	0	0	0	0
57	n	1	0	0	0	0
57	q	2	0	0	0	0
57	v	4	0	0	0	0
57	w	1	0	0	0	0
57	x	10	0	0	0	0
58	A	51	0	0	0	0
58	Q	1	0	0	0	0
59	4	1	0	0	0	0
59	5	1	0	0	0	0
59	6	1	0	0	0	0
59	9	1	0	0	0	0
59	Y	1	0	0	0	0
59	n	1	0	0	0	0
60	d	8	0	0	0	0
61	0	13	0	0	0	0
61	1	6	0	0	1	0
61	2	4	0	0	0	0
61	3	5	0	0	0	0
61	5	16	0	0	0	0
61	6	3	0	0	0	0
61	7	15	0	0	0	0
61	8	16	0	0	0	0
61	9	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	A	3537	0	0	16	0
61	B	19	0	0	0	0
61	D	74	0	0	1	0
61	E	35	0	0	0	0
61	F	39	0	0	1	0
61	I	1	0	0	0	0
61	N	14	0	0	0	0
61	O	15	0	0	0	0
61	P	46	0	0	0	0
61	Q	22	0	0	0	0
61	R	24	0	0	0	0
61	S	3	0	0	0	0
61	T	13	0	0	0	0
61	U	37	0	0	0	0
61	V	12	0	0	0	0
61	W	19	0	0	0	0
61	X	13	0	0	1	0
61	Y	1	0	0	0	0
61	Z	3	0	0	0	0
61	a	648	0	0	8	0
61	b	1	0	0	0	0
61	d	3	0	0	0	0
61	e	4	0	0	0	0
61	g	1	0	0	0	0
61	h	3	0	0	0	0
61	i	2	0	0	1	0
61	j	2	0	0	0	0
61	k	1	0	0	0	0
61	l	17	0	0	0	0
61	n	1	0	0	0	0
61	o	1	0	0	0	0
61	q	3	0	0	0	0
61	r	1	0	0	0	0
61	t	1	0	0	0	0
61	v	10	0	0	0	0
61	w	20	0	0	0	0
61	x	30	0	0	0	0
All	All	148436	0	96109	1025	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1025) 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)
40:i:26:VAL:HG23	40:i:61:ALA:HB3	1.51	0.93
1:A:881:G:H1	1:A:895:U:H3	1.09	0.88
49:r:53:ARG:HG2	49:r:63:GLN:HG3	1.60	0.83
1:A:2100:G:H1	1:A:2189:U:H3	1.24	0.81
1:A:2102:U:H3	1:A:2187:G:H1	1.27	0.80
32:a:1086:U:H3	32:a:1099:G:H22	1.25	0.80
43:l:76:ASN:HD21	43:l:108:ALA:H	1.32	0.77
32:a:953:G:H5'	32:a:965:A:H61	1.50	0.77
32:a:1027:C:N4	32:a:1028:C:N4	2.35	0.74
4:E:54:GLN:HB2	4:E:76:ARG:HG3	1.68	0.74
23:1:26:ARG:NH1	61:1:201:HOH:O	2.20	0.74
32:a:673:G:H2'	32:a:674:G:C8	2.23	0.74
36:e:10:MET:HE1	36:e:13:ILE:HB	1.69	0.73
32:a:664:G:H22	32:a:741:G:H1	1.36	0.72
44:m:65:LYS:HE3	44:m:69:GLU:HG2	1.69	0.72
40:i:10:ARG:NH1	40:i:75:ASP:OD2	2.23	0.72
32:a:975:A:H4'	32:a:976:G:H5"	1.71	0.71
1:A:2305:A:H5"	6:G:134:GLY:HA3	1.72	0.71
1:A:2102:U:O2	1:A:2187:G:N2	2.23	0.70
32:a:714:G:H2'	32:a:715:A:C8	2.27	0.70
1:A:548:A:O2'	1:A:549:G:O5'	2.08	0.70
54:w:143:GLU:OE2	54:w:163:ARG:NH1	2.25	0.70
1:A:2646:C:OP2	1:A:2732:G:O2'	2.07	0.69
18:W:4:LYS:HD3	18:W:6:ILE:HD11	1.75	0.69
23:1:76:ARG:NH2	23:1:97:LEU:O	2.26	0.69
21:Z:121:HIS:HB2	21:Z:171:ILE:HG22	1.74	0.69
28:6:9:LEU:HD13	28:6:51:GLU:HG3	1.74	0.69
14:S:71:ARG:NH1	14:S:107:GLU:OE1	2.25	0.68
4:E:7:VAL:HG11	15:T:1:MET:HE1	1.76	0.68
32:a:1035:A:H2'	32:a:1036:G:H21	1.60	0.67
39:h:34:GLU:OE1	39:h:37:ARG:NH1	2.26	0.67
32:a:674:G:H2'	32:a:675:A:H8	1.60	0.67
32:a:713:G:H2'	32:a:714:G:C8	2.30	0.67
5:F:72:ARG:NH2	61:F:402:HOH:O	2.27	0.67
13:R:97:VAL:HG22	13:R:114:VAL:HG22	1.77	0.67
32:a:656:C:O2'	46:o:28:GLN:NE2	2.27	0.67
42:k:14:VAL:HG22	42:k:16:SER:H	1.60	0.67
34:c:136:GLN:HE22	34:c:140:ARG:HE	1.43	0.66
1:A:131:G:N7	61:A:4429:HOH:O	2.29	0.66
1:A:1800:C:OP1	3:D:260:ARG:NH2	2.28	0.66
20:Y:23:ARG:NH2	20:Y:41:GLY:O	2.28	0.66
32:a:1435:G:H2'	32:a:1436:U:C6	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:i:9:ARG:HG2	40:i:14:VAL:HG22	1.76	0.66
36:e:83:GLU:HG2	36:e:88:LYS:HG2	1.77	0.66
7:H:95:ARG:HG2	7:H:95:ARG:HH11	1.61	0.66
32:a:738:C:H5"	37:f:69:GLU:HB3	1.77	0.66
32:a:1015:A:H2'	32:a:1016:A:C8	2.31	0.66
50:s:50:ALA:HB1	50:s:57:HIS:HB3	1.76	0.66
7:H:3:ARG:HH22	7:H:65:HIS:HB3	1.61	0.65
21:Z:99:TYR:HB3	21:Z:123:ASP:HB2	1.76	0.65
32:a:800:G:N7	61:a:1917:HOH:O	2.29	0.65
1:A:1344:G:N7	61:A:4439:HOH:O	2.30	0.65
32:a:343:U:O2'	32:a:345:C:N4	2.26	0.65
54:w:210:PHE:O	54:w:270:ARG:NH1	2.29	0.65
32:a:1513:A:H2'	32:a:1514:C:C6	2.33	0.64
38:g:122:HIS:HA	38:g:125:MET:HE2	1.78	0.64
54:w:230:MEQ:HE2	56:z:6:LYS:HE3	1.78	0.64
61:A:7684:HOH:O	29:7:1:MET:SD	2.55	0.64
11:P:86:LYS:HB3	11:P:118:GLY:HA3	1.79	0.64
33:b:218:ALA:O	33:b:222:ILE:HG13	1.98	0.64
3:D:220:HIS:ND1	61:D:403:HOH:O	2.30	0.64
1:A:631:A:OP1	11:P:65:ARG:NH1	2.28	0.64
32:a:925:G:N7	61:a:1923:HOH:O	2.30	0.64
30:8:62:LEU:HB3	30:8:65:GLU:HG2	1.78	0.63
17:V:71:LEU:HD11	17:V:84:LYS:HE3	1.81	0.63
1:A:642:G:N2	1:A:645:C:OP2	2.27	0.63
33:b:30:ARG:HH21	33:b:194:PRO:HB2	1.64	0.63
6:G:78:SER:OG	55:x:56:C:O2	2.15	0.63
35:d:109:GLY:HA3	35:d:165:MET:HE3	1.81	0.63
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.32	0.62
33:b:12:GLU:OE1	33:b:44:LEU:HD12	1.99	0.62
1:A:1405:U:H2'	1:A:1406:U:C6	2.34	0.62
10:O:36:GLY:HA3	10:O:109:LYS:HD2	1.81	0.62
46:o:78:TYR:O	46:o:82:ILE:HG12	1.99	0.62
32:a:662:G:H2'	32:a:663:A:C8	2.35	0.62
32:a:1031:G:H2'	32:a:1032:G:C8	2.35	0.62
32:a:1125:U:H4'	41:j:5:ARG:HH12	1.65	0.62
1:A:1865:G:N2	1:A:1877:A:OP2	2.30	0.62
9:N:46:VAL:HG23	9:N:48:MET:HG2	1.82	0.62
32:a:1291:G:OP1	38:g:41:ARG:NH1	2.28	0.62
35:d:156:GLU:CD	35:d:156:GLU:H	2.08	0.62
1:A:2052:G:H4'	4:E:143:ASN:O	1.99	0.61
6:G:67:LYS:HD3	26:4:5:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1068:G:H8	32:a:1068:G:OP2	1.83	0.61
1:A:558:G:N7	61:A:4463:HOH:O	2.31	0.61
20:Y:28:LYS:HG3	20:Y:40:GLU:HG2	1.81	0.61
34:c:153:VAL:HG22	34:c:198:VAL:HG22	1.81	0.61
32:a:269:C:H2'	32:a:270:A:H8	1.65	0.61
50:s:19:VAL:O	50:s:23:ASN:ND2	2.28	0.61
6:G:38:VAL:HG22	6:G:93:THR:HG23	1.81	0.60
32:a:1143:G:H2'	32:a:1144:G:H8	1.66	0.60
32:a:1356:G:H2'	32:a:1357:A:C8	2.35	0.60
32:a:946:A:H2'	32:a:947:G:C8	2.36	0.60
32:a:524:G:H2'	32:a:525:C:C6	2.36	0.60
54:w:281:GLU:HG3	54:w:284:ARG:HH21	1.66	0.60
32:a:331:G:N7	61:a:1925:HOH:O	2.31	0.60
1:A:530:G:N1	1:A:2023:G:OP1	2.30	0.60
3:D:122:ASP:OD1	3:D:122:ASP:N	2.34	0.60
32:a:1145:C:H4'	32:a:1146:A:H5'	1.83	0.60
34:c:150:LYS:HG3	34:c:169:ALA:HB2	1.84	0.60
47:p:14:ASN:HD22	47:p:42:ARG:HH12	1.49	0.60
1:A:2611:U:C4	27:5:3:LYS:HG2	2.37	0.60
32:a:342:C:H2'	32:a:343:U:H5'	1.83	0.60
32:a:1323:G:H2'	32:a:1324:A:C8	2.36	0.59
50:s:27:GLU:H	50:s:27:GLU:CD	2.10	0.59
32:a:1286:A:H2'	32:a:1287:A:H4'	1.84	0.59
1:A:2344:U:OP1	28:6:37:ARG:NH1	2.33	0.59
31:9:25:VAL:HB	31:9:34:GLN:HB2	1.85	0.59
47:p:4:ILE:HG12	47:p:21:VAL:HG22	1.84	0.59
1:A:1354:A:H5"	3:D:38:LYS:HE3	1.85	0.59
32:a:1027:C:N4	32:a:1028:C:H41	1.98	0.59
39:h:86:ILE:HD11	39:h:136:GLU:HG2	1.84	0.59
35:d:122:ARG:NH1	35:d:134:ASP:OD2	2.36	0.59
1:A:782:A:C2	3:D:226:MET:HG2	2.38	0.59
38:g:113:GLU:N	38:g:113:GLU:OE2	2.35	0.59
33:b:98:LEU:HG	33:b:101:MET:HE3	1.84	0.59
36:e:20:GLN:NE2	36:e:21:ALA:O	2.36	0.59
26:4:24:THR:OG1	26:4:25:TYR:N	2.37	0.58
33:b:40:HIS:HB2	33:b:190:THR:HG21	1.84	0.58
35:d:86:LYS:HD3	35:d:87:GLY:H	1.69	0.58
38:g:62:PHE:O	38:g:66:VAL:HG23	2.03	0.58
1:A:2291:U:H2'	1:A:2292:C:C6	2.38	0.58
32:a:1218:C:H2'	32:a:1219:U:C6	2.39	0.58
1:A:1113:U:H2'	1:A:1114:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:G:O2'	1:A:1396:U:O2	2.20	0.58
13:R:28:LEU:HD23	13:R:48:VAL:HG21	1.85	0.58
24:2:17:SER:OG	24:2:20:GLU:OE1	2.18	0.58
32:a:619:U:N3	35:d:134:ASP:OD1	2.35	0.58
37:f:36:ARG:HG2	37:f:36:ARG:HH11	1.68	0.58
1:A:1444:G:H2'	1:A:1445(A):C:C5	2.38	0.58
32:a:677:U:H3	32:a:713:G:H22	1.50	0.58
32:a:717:C:H4'	42:k:117:ASN:HD22	1.69	0.58
44:m:80:ARG:HH12	50:s:69:HIS:HE1	1.52	0.58
1:A:2042:A:N3	61:A:4468:HOH:O	2.32	0.58
32:a:17:U:H2'	32:a:18:C:C6	2.38	0.57
32:a:56:U:H2'	32:a:57:G:C8	2.39	0.57
38:g:121:ALA:O	38:g:125:MET:HG3	2.04	0.57
1:A:548:A:O2'	1:A:549:G:O4'	2.23	0.57
54:w:108:ILE:HD13	54:w:161:GLU:HG2	1.85	0.57
32:a:539:A:H2'	32:a:540:G:C8	2.40	0.57
35:d:173:TRP:H	35:d:173:TRP:CD1	2.22	0.57
48:q:53:LEU:HB3	48:q:82:MET:HE1	1.86	0.57
1:A:994:C:OP1	16:U:53:ARG:NH2	2.37	0.57
1:A:2607:G:N7	61:A:4476:HOH:O	2.33	0.57
1:A:38:A:H2'	1:A:39:C:C6	2.40	0.57
12:Q:35:VAL:HG22	12:Q:102:VAL:HG22	1.86	0.57
32:a:35:G:H2'	32:a:36:C:C6	2.39	0.57
1:A:1429:G:H2'	1:A:1430:C:C6	2.40	0.57
6:G:106:LEU:HA	6:G:110:ALA:HB3	1.87	0.57
32:a:715:A:H2'	32:a:716:A:C8	2.40	0.56
32:a:538:G:H5"	43:l:114:LYS:HB2	1.87	0.56
26:4:16:CYS:SG	26:4:17:GLY:N	2.77	0.56
32:a:1391:U:H2'	32:a:1392:G:C8	2.40	0.56
34:c:130:VAL:O	34:c:134:ILE:HG12	2.05	0.56
39:h:46:LYS:HG3	39:h:64:LYS:HB2	1.87	0.56
9:N:4:TYR:HD1	16:U:101:ARG:HH11	1.51	0.56
32:a:1137:C:H4'	32:a:1138:G:C2	2.39	0.56
1:A:881:G:N2	1:A:895:U:O2	2.33	0.56
1:A:1174:A:H4'	1:A:1175:U:OP1	2.05	0.56
13:R:12:ARG:O	13:R:17:ARG:NH1	2.38	0.56
12:Q:67:ARG:HD2	12:Q:105:GLU:OE2	2.05	0.56
32:a:976:G:OP2	32:a:1358:U:O2'	2.24	0.56
1:A:1607:C:N4	1:A:1622:G:OP2	2.33	0.56
39:h:111:ILE:HG22	39:h:134:ILE:HD12	1.88	0.56
32:a:269:C:H2'	32:a:270:A:C8	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:21:ARG:HA	33:b:39:ILE:HA	1.86	0.55
1:A:1353:A:H2'	1:A:1354:A:C8	2.40	0.55
32:a:736:C:H2'	32:a:737:A:H8	1.72	0.55
1:A:895:U:H2'	1:A:897:C:H5	1.72	0.55
32:a:1238:A:H2	32:a:1241:G:N3	2.05	0.55
1:A:2064:C:H2'	1:A:2065:C:C6	2.41	0.55
48:q:83:ASP:OD1	48:q:83:ASP:N	2.37	0.55
1:A:2789:C:H1'	1:A:2892:A:C2	2.42	0.55
32:a:1323:G:H2'	32:a:1324:A:H8	1.72	0.55
1:A:270:A:OP2	1:A:271(X):G:N1	2.31	0.55
1:A:2478:A:OP2	31:9:2:LYS:NZ	2.34	0.55
1:A:2789:C:H1'	1:A:2892:A:H2	1.72	0.55
1:A:2074:U:H2'	1:A:2075:U:C6	2.42	0.54
1:A:2350:C:OP1	30:8:46:ARG:NH2	2.40	0.54
32:a:189(K):U:H2'	32:a:189(L):G:H8	1.73	0.54
1:A:589:C:H2'	1:A:590:A:C8	2.42	0.54
1:A:1005:C:O2'	9:N:28:THR:HG21	2.07	0.54
1:A:2323:G:N7	61:A:4482:HOH:O	2.33	0.54
7:H:137:ASP:HB3	7:H:140:LYS:HB2	1.88	0.54
21:Z:126:VAL:HG12	21:Z:163:LEU:HA	1.89	0.54
32:a:1030(C):G:N7	32:a:1031:G:N2	2.55	0.54
33:b:84:GLU:HG2	33:b:215:LEU:HB3	1.88	0.54
40:i:42:ARG:NH1	40:i:71:SER:OG	2.39	0.54
1:A:1178:C:H2'	1:A:1179:C:C6	2.43	0.54
19:X:31:HIS:HD2	19:X:33:LYS:H	1.56	0.54
32:a:1147:C:O2'	40:i:5:TYR:OH	2.25	0.54
1:A:2870:C:H2'	1:A:2871:C:O4'	2.07	0.54
32:a:390:C:H2'	32:a:391:G:C8	2.42	0.54
1:A:639:U:H2'	1:A:640:C:C6	2.43	0.54
8:I:51:ILE:O	8:I:55:ALA:N	2.33	0.54
44:m:16:ASP:OD1	44:m:16:ASP:N	2.40	0.54
34:c:36:ASP:OD1	34:c:59:ARG:NH2	2.29	0.54
1:A:588:U:H2'	1:A:589:C:C6	2.42	0.54
1:A:1364:G:OP2	23:1:3:LYS:HG3	2.08	0.54
32:a:45:U:H2'	32:a:46:G:C8	2.43	0.54
33:b:54:THR:HG21	33:b:201:ILE:HD11	1.89	0.54
32:a:1152:A:OP1	41:j:68:HIS:ND1	2.41	0.54
32:a:316:G:OP2	32:a:351:G:O2'	2.26	0.53
32:a:130:A:H5'	48:q:63:ARG:HH11	1.73	0.53
32:a:705:U:C2	32:a:706:A:C8	2.95	0.53
32:a:728:A:H2'	32:a:729:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:542:G:OP1	35:d:10:ARG:NH2	2.38	0.53
34:c:136:GLN:HE22	34:c:140:ARG:NE	2.05	0.53
36:e:6:PHE:HD1	36:e:36:ASP:HB3	1.73	0.53
1:A:414:C:H2'	1:A:415:A:C8	2.44	0.53
34:c:6:HIS:HD2	34:c:8:ILE:H	1.57	0.53
1:A:1467:C:H5	1:A:1546:C:H2'	1.72	0.53
16:U:100:VAL:HG13	16:U:101:ARG:HG2	1.90	0.53
32:a:56:U:H2'	32:a:57:G:H8	1.74	0.53
32:a:1025:U:O2	32:a:1036:G:C6	2.61	0.53
32:a:1316:G:N1	32:a:1319:A:OP2	2.40	0.53
51:t:47:GLY:N	51:t:48:LYS:HB2	2.23	0.53
54:w:334:PRO:O	54:w:337:GLU:HG3	2.09	0.53
1:A:1113:U:H2'	1:A:1114:G:H8	1.72	0.53
21:Z:52:SER:OG	21:Z:53:ILE:N	2.38	0.53
6:G:41:GLN:HE22	6:G:153:ARG:HB3	1.74	0.53
32:a:404:U:H2'	32:a:405:U:H6	1.73	0.53
32:a:1317:C:O2	50:s:37:ARG:NH2	2.40	0.53
46:o:55:GLY:O	46:o:59:MET:HG3	2.09	0.53
7:H:54:ARG:HD3	7:H:65:HIS:CG	2.44	0.53
32:a:1518:MA6:N6	32:a:1519:MA6:H103	2.24	0.53
33:b:130:ARG:HG3	33:b:131:PRO:HD2	1.91	0.53
37:f:2:ARG:HH21	37:f:69:GLU:CD	2.16	0.53
8:I:9:LEU:HD13	8:I:12:LEU:HD23	1.91	0.53
5:F:135:LYS:HB2	5:F:138:GLU:HG3	1.90	0.52
32:a:748:C:H4'	32:a:749:C:O5'	2.10	0.52
1:A:1528(A):A:H2	1:A:1541:G:H21	1.56	0.52
36:e:105:VAL:HB	36:e:106:PRO:HD3	1.92	0.52
39:h:119:LEU:HB3	39:h:123:GLU:HB3	1.90	0.52
42:k:48:ILE:O	42:k:50:TYR:N	2.41	0.52
1:A:1035:U:H2'	1:A:1036:G:C8	2.44	0.52
1:A:1173:G:O2'	1:A:1174:A:O4'	2.23	0.52
34:c:64:VAL:HG22	34:c:66:VAL:HG23	1.92	0.52
35:d:86:LYS:HD3	35:d:87:GLY:N	2.25	0.52
1:A:2286:A:H4'	1:A:2287:A:O4'	2.09	0.52
5:F:12:LEU:HD12	5:F:124:LEU:HD21	1.90	0.52
32:a:399:G:H2'	32:a:400:C:C6	2.43	0.52
32:a:1060:C:H3'	34:c:2:GLY:HA3	1.91	0.52
1:A:813:U:H2'	1:A:814:C:C6	2.44	0.52
1:A:1467:C:C5	1:A:1546:C:H2'	2.44	0.52
1:A:1025:G:C4	1:A:1135:C:H1'	2.45	0.52
21:Z:70:LEU:HD12	21:Z:91:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:t:36:LEU:HD12	51:t:62:LEU:HD12	1.92	0.52
1:A:2506:U:O4	56:z:4:ALA:HB3	2.10	0.52
32:a:389:A:H3'	32:a:390:C:H6	1.75	0.52
32:a:1118:C:OP1	40:i:104:ARG:NE	2.41	0.52
35:d:165:MET:O	35:d:165:MET:HG3	2.10	0.52
1:A:768:G:O2'	1:A:1379:A:N1	2.40	0.52
1:A:2649:U:H2'	1:A:2650:U:C6	2.45	0.52
32:a:343:U:O2'	32:a:344:A:OP2	2.24	0.52
1:A:848:G:H2'	1:A:849:A:C8	2.44	0.52
9:N:11:PRO:HD2	9:N:11:PRO:O	2.08	0.52
32:a:737:A:H2'	32:a:738:C:C6	2.45	0.52
33:b:69:LEU:HB3	33:b:162:ILE:HG22	1.91	0.52
32:a:1428:A:H2'	32:a:1429:C:C6	2.46	0.51
55:x:8:4SU:H6	55:x:8:4SU:O5'	2.10	0.51
21:Z:7:ALA:HB2	21:Z:59:LEU:HD22	1.92	0.51
32:a:809:G:N7	61:a:1928:HOH:O	2.33	0.51
32:a:986:A:H2'	32:a:987:G:C8	2.45	0.51
7:H:8:PRO:O	7:H:69:ARG:NH2	2.34	0.51
10:O:87:ILE:HD12	10:O:91:LEU:HA	1.92	0.51
21:Z:54:HIS:CD2	21:Z:101:PRO:HG3	2.45	0.51
21:Z:54:HIS:CE1	21:Z:123:ASP:HB3	2.45	0.51
32:a:460:G:N1	32:a:471:G:OP2	2.40	0.51
1:A:2478:A:H5'	31:9:31:LYS:HE2	1.92	0.51
32:a:737:A:H2'	32:a:738:C:H6	1.76	0.51
32:a:1004:A:N6	32:a:1036:G:H1	2.09	0.51
1:A:518:G:H2'	1:A:519:U:C6	2.46	0.51
1:A:881:G:O6	1:A:895:U:O4	2.29	0.51
1:A:2430:A:N3	1:A:2430:A:H2'	2.26	0.51
1:A:2791:C:H2'	1:A:2792:G:O4'	2.11	0.51
41:j:5:ARG:HD3	41:j:71:LEU:HD21	1.92	0.51
1:A:1796:U:H2'	1:A:1797:C:C6	2.46	0.51
3:D:122:ASP:HB3	8:I:89:TYR:CZ	2.46	0.51
32:a:1125:U:H4'	41:j:5:ARG:NH1	2.26	0.51
33:b:118:LEU:HB3	33:b:142:LEU:HD13	1.92	0.51
36:e:41:VAL:HG13	36:e:136:MET:HE1	1.92	0.51
1:A:1430:C:H2'	1:A:1431:U:C6	2.46	0.51
1:A:2015:A:N3	27:5:4:HIS:HE1	2.09	0.51
1:A:1252:G:N3	16:U:33:ARG:HG2	2.25	0.51
2:B:48:A:H2'	2:B:49:C:C6	2.46	0.51
10:O:48:PRO:HB3	32:a:1422:G:H5'	1.92	0.51
32:a:1251:A:H2'	32:a:1252:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:i:110:GLU:OE1	40:i:113:LYS:NZ	2.44	0.51
1:A:662:G:H5”	11:P:16:ARG:HG3	1.93	0.51
1:A:1405:U:H2’	1:A:1406:U:H6	1.76	0.51
32:a:1009:G:C2	32:a:1010:G:C8	2.99	0.51
22:0:32:ARG:H	22:0:35:ASN:ND2	2.09	0.51
32:a:736:C:H2’	32:a:737:A:C8	2.46	0.51
32:a:1308:U:OP2	44:m:99:ARG:HG3	2.10	0.51
42:k:82:VAL:HB	42:k:108:ILE:HG23	1.93	0.51
1:A:2612:C:OP2	27:5:2:ALA:N	2.44	0.50
41:j:40:LEU:HB2	41:j:69:ASN:HB2	1.94	0.50
54:w:110:GLU:HG2	54:w:159:VAL:HG22	1.94	0.50
35:d:76:ARG:O	35:d:80:GLU:HG2	2.11	0.50
42:k:69:ALA:C	42:k:73:MET:HE3	2.36	0.50
1:A:1379:A:H4’	1:A:1380:G:OP2	2.12	0.50
7:H:95:ARG:HG2	7:H:95:ARG:NH1	2.27	0.50
32:a:28:G:O2’	32:a:296:U:OP1	2.28	0.50
32:a:996:A:H2’	32:a:997:U:C6	2.46	0.50
27:5:16:ARG:HG3	27:5:17:ASP:N	2.25	0.50
32:a:100:C:H2’	32:a:101:A:C8	2.46	0.50
32:a:509:A:H2’	32:a:510:A:C8	2.47	0.50
32:a:1218:C:H2’	32:a:1219:U:H6	1.76	0.50
33:b:213:LEU:HD23	33:b:217:ARG:HG3	1.92	0.50
52:u:5:ASP:O	52:u:11:GLY:HA3	2.10	0.50
29:7:9:ARG:HD3	29:7:47:ARG:HB2	1.94	0.50
32:a:401:C:OP2	35:d:73:ARG:NE	2.43	0.50
36:e:33:VAL:HG13	36:e:112:LEU:HD12	1.93	0.50
1:A:1987:G:N7	61:A:4489:HOH:O	2.34	0.50
1:A:2243:U:H2’	1:A:2244:U:C6	2.47	0.50
1:A:2649:U:H2’	1:A:2650:U:H6	1.76	0.50
6:G:107:LEU:HA	6:G:111:LEU:HD12	1.93	0.50
23:1:7:ILE:HA	23:1:98:LEU:HD11	1.93	0.50
23:1:86:SER:O	23:1:90:ILE:HG12	2.11	0.50
32:a:342:C:C2’	32:a:343:U:H5’	2.41	0.50
1:A:2591:C:H2’	1:A:2592:G:C8	2.46	0.50
32:a:433:C:H2’	32:a:434:U:C6	2.46	0.50
32:a:678:U:H2’	32:a:679:C:H6	1.77	0.50
54:w:212:LEU:HD13	54:w:270:ARG:HG3	1.94	0.50
1:A:796:C:H2’	1:A:797:C:C6	2.47	0.50
32:a:148:G:H2’	32:a:149:A:C8	2.47	0.50
34:c:35:GLU:HB3	34:c:59:ARG:HH22	1.77	0.50
44:m:59:TYR:O	44:m:63:THR:OG1	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:G:O6	23:1:39:LYS:NZ	2.45	0.50
1:A:1783:A:H5'	1:A:2608:G:H4'	1.92	0.50
1:A:2350:C:OP2	61:A:4401:HOH:O	2.20	0.50
32:a:743:U:H2'	32:a:744:C:H6	1.77	0.50
1:A:2304:G:H22	1:A:2312:U:H3	1.60	0.49
10:O:64:ARG:NH2	10:O:99:PHE:O	2.45	0.49
1:A:272(I):U:H2'	1:A:272(J):C:H6	1.77	0.49
1:A:1508:A:O2'	1:A:1509:C:OP1	2.27	0.49
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.45	0.49
32:a:377:G:OP1	47:p:3:LYS:HE3	2.12	0.49
40:i:55:ALA:HA	40:i:58:HIS:CD2	2.47	0.49
1:A:881:G:H2'	1:A:882:G:C8	2.47	0.49
1:A:2302:G:H21	6:G:126:ASP:CG	2.19	0.49
6:G:43:LEU:HD12	6:G:53:LEU:HD23	1.92	0.49
6:G:142:PRO:HB2	26:4:31:ILE:HG21	1.95	0.49
11:P:59:LEU:HD11	30:8:10:ALA:HA	1.94	0.49
14:S:61:ASN:HD22	14:S:64:GLU:H	1.60	0.49
21:Z:61:LEU:HD11	21:Z:67:LEU:HD12	1.94	0.49
24:2:65:ASN:ND2	24:2:69:ARG:HH11	2.09	0.49
32:a:1510:U:H2'	32:a:1511:G:C8	2.46	0.49
34:c:67:THR:HG23	34:c:102:ASN:HB2	1.94	0.49
36:e:142:LEU:O	36:e:143:ARG:NH1	2.42	0.49
1:A:1168:G:N7	61:A:4500:HOH:O	2.35	0.49
9:N:13:TRP:CE2	9:N:133:GLN:HG2	2.48	0.49
21:Z:138:GLU:N	21:Z:138:GLU:OE1	2.45	0.49
32:a:1305:G:N2	32:a:1331:G:H1'	2.28	0.49
1:A:1429:G:H2'	1:A:1430:C:H6	1.76	0.49
39:h:10:LEU:HD22	39:h:83:ILE:HD11	1.93	0.49
40:i:17:VAL:HG13	40:i:63:ILE:HG12	1.93	0.49
55:x:70:G:H2'	55:x:71:C:C6	2.48	0.49
1:A:2455:G:H2'	1:A:2456:C:C6	2.48	0.49
8:I:6:LEU:HD11	8:I:37:VAL:HG13	1.95	0.49
32:a:1040:U:O4	32:a:1041:A:N6	2.45	0.49
34:c:13:GLY:HA3	45:n:57:ARG:HH12	1.78	0.49
54:w:299:SER:O	54:w:300:GLU:HG2	2.13	0.49
1:A:1853:A:H2'	1:A:1854:A:C8	2.48	0.49
3:D:37:LEU:HD13	3:D:62:TYR:HB2	1.94	0.49
32:a:21:G:H2'	32:a:22:G:C8	2.48	0.49
32:a:1005:A:N7	32:a:1024:G:C2	2.81	0.49
1:A:187:G:N7	61:A:4492:HOH:O	2.34	0.49
15:T:125:ARG:HA	15:T:125:ARG:NE	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:4:ARG:HD2	21:Z:58:VAL:HB	1.94	0.49
35:d:63:LYS:NZ	35:d:197:PRO:O	2.44	0.49
7:H:3:ARG:HD2	7:H:3:ARG:HA	1.69	0.49
32:a:555:C:H2'	32:a:556:C:C6	2.48	0.49
32:a:674:G:H2'	32:a:675:A:C8	2.46	0.49
32:a:920:U:H2'	32:a:921:U:C6	2.48	0.49
33:b:187:LEU:HD13	33:b:214:ILE:HG21	1.93	0.49
54:w:306:ASN:HD22	54:w:311:ARG:NH2	2.11	0.49
1:A:700:G:O2'	1:A:1632:A:N3	2.38	0.48
1:A:1021:A:OP2	9:N:65:LYS:NZ	2.44	0.48
4:E:2:LYS:HD2	4:E:95:ILE:HD12	1.95	0.48
8:I:41:GLU:HA	8:I:41:GLU:OE1	2.13	0.48
32:a:744:C:H2'	32:a:745:C:H6	1.78	0.48
37:f:28:ARG:O	37:f:31:GLU:HG3	2.11	0.48
39:h:41:ARG:NH2	39:h:123:GLU:OE1	2.46	0.48
32:a:384:G:H2'	32:a:385:C:C6	2.48	0.48
1:A:184:C:H2'	1:A:185:U:C6	2.48	0.48
10:O:86:ILE:HG22	10:O:94:ARG:HD3	1.95	0.48
36:e:81:GLU:HG3	36:e:90:VAL:HG22	1.95	0.48
40:i:128:ARG:NH2	55:x:33:U:OP2	2.46	0.48
1:A:171:G:H2'	1:A:172:C:C6	2.48	0.48
1:A:2312:U:H5'	6:G:88:ILE:HD11	1.94	0.48
1:A:2377:A:O2'	14:S:112:PHE:O	2.18	0.48
1:A:2836:U:H2'	1:A:2837:G:C8	2.47	0.48
32:a:1061:G:N7	34:c:2:GLY:N	2.61	0.48
40:i:25:LYS:N	40:i:60:ASP:OD1	2.47	0.48
54:w:216:GLU:HB2	54:w:245:PRO:HD3	1.95	0.48
1:A:414:C:H2'	1:A:415:A:H8	1.77	0.48
1:A:808:G:OP1	61:A:4402:HOH:O	2.20	0.48
32:a:950:U:H2'	32:a:951:G:C8	2.49	0.48
36:e:78:HIS:HE1	36:e:143:ARG:H	1.61	0.48
48:q:26:GLN:HG2	48:q:37:LYS:HG2	1.94	0.48
1:A:1786:A:H1'	1:A:1938:A:N6	2.28	0.48
28:6:33:LYS:HG3	28:6:51:GLU:HB3	1.95	0.48
32:a:1124:G:N2	32:a:1125:U:O4	2.37	0.48
33:b:115:LEU:O	33:b:119:GLU:HG2	2.13	0.48
34:c:47:LEU:HD12	34:c:52:LEU:HD13	1.95	0.48
20:Y:50:ARG:HG2	20:Y:50:ARG:HH11	1.79	0.48
37:f:1:MET:HA	37:f:1:MET:HE2	1.95	0.48
1:A:774:A:H2'	1:A:774:A:N3	2.28	0.48
1:A:911:A:H2'	12:Q:9:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:167:ALA:HB1	5:F:173:VAL:HG11	1.95	0.48
1:A:2023:G:H5'	1:A:2617:C:H4'	1.96	0.48
1:A:2820:A:O2'	1:A:2821:A:OP1	2.29	0.48
21:Z:97:GLU:HA	21:Z:127:LYS:HA	1.96	0.48
32:a:189(L):G:H2'	32:a:190:U:C6	2.49	0.48
32:a:1267:C:O2	52:u:20:LYS:NZ	2.38	0.48
32:a:1427:U:H2'	32:a:1428:A:C8	2.49	0.48
15:T:65:LYS:HG2	15:T:66:VAL:N	2.29	0.47
32:a:289:G:O6	61:a:1901:HOH:O	2.20	0.47
32:a:677:U:O2	32:a:777:A:O2'	2.30	0.47
32:a:1017:G:H2'	32:a:1018:C:C6	2.49	0.47
32:a:1466:C:H2'	32:a:1467:G:O4'	2.14	0.47
40:i:46:ALA:HA	40:i:78:LYS:HB2	1.95	0.47
44:m:87:TYR:CZ	44:m:91:ARG:HD2	2.49	0.47
7:H:154:PRO:HB3	7:H:163:TYR:CE2	2.49	0.47
30:8:26:LYS:HD3	30:8:48:PHE:HB3	1.96	0.47
35:d:177:ASP:O	35:d:181:MET:N	2.47	0.47
49:r:32:ARG:HA	49:r:69:THR:HG21	1.96	0.47
1:A:863:A:H2'	1:A:864:G:C8	2.49	0.47
8:I:31:LEU:HD21	8:I:38:LEU:HG	1.95	0.47
29:7:24:THR:HG22	29:7:26:GLY:N	2.29	0.47
32:a:580:U:H2'	32:a:581:G:O4'	2.14	0.47
32:a:961:U:OP2	32:a:1223:C:O2'	2.23	0.47
33:b:156:LYS:HD2	33:b:156:LYS:N	2.28	0.47
47:p:69:THR:HG23	47:p:72:ARG:HH21	1.80	0.47
1:A:548:A:H1'	1:A:549:G:OP1	2.15	0.47
8:I:85:GLU:HG2	37:f:21:LEU:HD11	1.95	0.47
32:a:259:G:H2'	32:a:260:G:C8	2.49	0.47
34:c:23:TYR:CZ	41:j:9:ARG:HG3	2.50	0.47
1:A:1174:A:OP1	1:A:1177:A:N6	2.44	0.47
1:A:2345:G:N3	1:A:2381:C:H2'	2.30	0.47
32:a:744:C:H2'	32:a:745:C:C6	2.50	0.47
1:A:12:U:O2	1:A:2626:C:H4'	2.15	0.47
2:B:49:C:H2'	2:B:50:G:C8	2.49	0.47
2:B:49:C:H2'	2:B:50:G:H8	1.80	0.47
5:F:107:LYS:HB3	5:F:107:LYS:HE2	1.63	0.47
6:G:32:PRO:HB3	6:G:163:ALA:HB2	1.96	0.47
29:7:24:THR:HG22	29:7:26:GLY:H	1.80	0.47
32:a:160:A:H2'	32:a:161:A:O4'	2.14	0.47
32:a:903:G:O6	61:a:1902:HOH:O	2.20	0.47
32:a:1486:G:H2'	32:a:1487:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:155:LEU:HD22	33:b:157:ARG:O	2.15	0.47
32:a:382:A:H2'	32:a:383:A:C8	2.50	0.47
50:s:23:ASN:HA	50:s:27:GLU:HB3	1.97	0.47
1:A:207:A:H2'	1:A:208:C:O4'	2.15	0.47
1:A:793:A:OP2	1:A:2071:A:O2'	2.31	0.47
32:a:323:U:H2'	32:a:324:G:O4'	2.15	0.47
33:b:68:ILE:H	33:b:90:MET:HE3	1.80	0.47
1:A:1420:U:O2'	1:A:1421:G:OP1	2.30	0.47
1:A:2251:OMG:HM23	1:A:2251:OMG:H1'	1.67	0.47
1:A:2466:C:H5"	31:9:6:SER:HB2	1.97	0.47
25:3:35:ARG:HH21	25:3:37:LEU:HD21	1.80	0.47
32:a:189(L):G:H2'	32:a:190:U:H6	1.79	0.47
1:A:247:G:H4'	1:A:386:G:C5	2.49	0.46
1:A:608:A:H2'	1:A:609:A:C8	2.50	0.46
1:A:2246:G:H2'	1:A:2247:A:C8	2.50	0.46
2:B:66:A:H61	2:B:108:U:H2'	1.80	0.46
31:9:17:ILE:HD12	31:9:19:ARG:HG2	1.98	0.46
33:b:139:LYS:HG2	33:b:143:GLU:OE1	2.14	0.46
54:w:103:ASP:OD1	54:w:103:ASP:N	2.48	0.46
1:A:2025:C:H2'	1:A:2026:C:C6	2.50	0.46
32:a:259:G:H2'	32:a:260:G:H8	1.80	0.46
32:a:1141:C:H2'	32:a:1142:G:H8	1.80	0.46
55:x:23:U:H2'	55:x:24:G:C8	2.51	0.46
9:N:62:VAL:HG22	9:N:66:LYS:HD2	1.97	0.46
32:a:676:A:H2'	32:a:677:U:H6	1.80	0.46
37:f:36:ARG:HG2	37:f:36:ARG:NH1	2.29	0.46
1:A:1142(A):A:O2'	1:A:1143:A:H3'	2.16	0.46
1:A:1709:U:H2'	1:A:1710:C:C6	2.51	0.46
38:g:75:VAL:HG21	38:g:144:MET:HG2	1.98	0.46
1:A:434:U:H1'	1:A:435:C:H5	1.81	0.46
7:H:3:ARG:HE	7:H:4:ILE:H	1.64	0.46
32:a:384:G:H2'	32:a:385:C:H6	1.80	0.46
33:b:109:SER:O	33:b:112:VAL:HG22	2.15	0.46
1:A:882:G:C2	1:A:883:G:H1'	2.51	0.46
1:A:883:G:H22	1:A:893:C:N4	2.14	0.46
1:A:1406:U:H2'	1:A:1407:C:H6	1.79	0.46
1:A:2273:A:H2'	1:A:2274:A:C8	2.51	0.46
32:a:184:G:H2'	32:a:185:A:H8	1.81	0.46
32:a:294:U:OP1	32:a:610:G:O2'	2.22	0.46
32:a:343:U:HO2'	32:a:344:A:P	2.39	0.46
32:a:346:G:N3	32:a:346:G:H3'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1071:C:H2'	32:a:1072:G:C8	2.50	0.46
32:a:1396:A:H4'	32:a:1397:C:H5"	1.97	0.46
1:A:271(E):U:H2'	1:A:271(F):C:C6	2.50	0.46
1:A:272(I):U:H2'	1:A:272(J):C:C6	2.51	0.46
1:A:1842:G:H2'	1:A:1843:C:C6	2.51	0.46
1:A:2590:A:H2'	1:A:2591:C:C6	2.51	0.46
32:a:234:C:O3'	48:q:70:ARG:NH1	2.49	0.46
32:a:1025:U:C2	32:a:1036:G:O6	2.69	0.46
32:a:1426:C:H2'	32:a:1427:U:C6	2.51	0.46
7:H:27:LYS:HD3	7:H:28:GLY:N	2.31	0.46
32:a:679:C:H2'	32:a:680:C:C6	2.51	0.46
32:a:1009:G:C6	32:a:1021:G:C5	3.03	0.46
32:a:1012:U:H2'	32:a:1013:G:C8	2.51	0.46
32:a:1181:G:O2'	32:a:1182:G:N7	2.45	0.46
32:a:1250:A:H2'	32:a:1251:A:C8	2.51	0.46
32:a:1265:G:H2'	32:a:1266:G:C8	2.51	0.46
1:A:2743:C:OP1	31:9:33:LYS:NZ	2.45	0.46
1:A:2857:G:N2	1:A:2860:A:OP2	2.39	0.46
32:a:769:G:H4'	32:a:1513:A:H4'	1.97	0.46
40:i:55:ALA:HA	40:i:58:HIS:HD2	1.81	0.46
54:w:229:GLY:HA3	55:x:76:A:H3'	1.98	0.46
1:A:534:U:H2'	1:A:535:C:C6	2.50	0.45
1:A:1042:G:H2'	1:A:1043:C:C6	2.51	0.45
1:A:2100:G:O6	1:A:2189:U:O4	2.33	0.45
32:a:1062:U:H2'	32:a:1063:C:C6	2.51	0.45
1:A:489:G:N7	18:W:49:LYS:NZ	2.63	0.45
1:A:2328:A:H2'	1:A:2329:G:C8	2.51	0.45
3:D:35:LYS:HB2	3:D:35:LYS:HE3	1.78	0.45
14:S:99:LYS:O	14:S:103:GLU:HG3	2.16	0.45
32:a:390:C:H2'	32:a:391:G:H8	1.79	0.45
1:A:680:G:H2'	1:A:681:G:C8	2.52	0.45
4:E:53:PRO:HA	4:E:75:VAL:HA	1.99	0.45
14:S:33:LYS:HB3	14:S:34:HIS:CD2	2.50	0.45
32:a:1141:C:H2'	32:a:1142:G:C8	2.51	0.45
1:A:581:C:H2'	1:A:582:G:C8	2.52	0.45
32:a:270:A:H2'	32:a:271:C:C6	2.51	0.45
32:a:880:C:OP1	43:l:8:ASN:ND2	2.47	0.45
35:d:152:SER:HA	35:d:155:LEU:HD13	1.99	0.45
36:e:66:MET:HE3	36:e:66:MET:HB3	1.85	0.45
1:A:7:G:H2'	1:A:8:A:C8	2.52	0.45
1:A:969:U:H2'	1:A:970:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:13:LYS:HD2	7:H:13:LYS:HA	1.72	0.45
32:a:434:U:H2'	32:a:435:C:C6	2.51	0.45
32:a:1437:C:H2'	32:a:1438:G:H8	1.82	0.45
34:c:36:ASP:OD1	34:c:57:ILE:HG21	2.17	0.45
1:A:1187:G:H5"	17:V:81:TYR:CE1	2.51	0.45
5:F:206:ILE:O	5:F:207:GLY:C	2.59	0.45
7:H:13:LYS:NZ	7:H:14:GLY:H	2.15	0.45
25:3:44:ARG:HG2	25:3:48:GLU:OE1	2.16	0.45
36:e:75:THR:HG22	36:e:117:ASP:HB2	1.99	0.45
38:g:83:ALA:HB3	38:g:85:TYR:HE1	1.82	0.45
49:r:41:LYS:HE2	49:r:41:LYS:HB3	1.70	0.45
54:w:108:ILE:HD11	54:w:204:LYS:HG3	1.99	0.45
1:A:229:A:H5'	1:A:230:U:H5'	1.99	0.45
1:A:922:U:H2'	1:A:923:C:C6	2.51	0.45
1:A:1794:U:H2'	1:A:1795:C:H6	1.82	0.45
1:A:1899:G:N3	1:A:1899:G:H2'	2.32	0.45
1:A:1932:A:H2'	1:A:1933:G:O4'	2.17	0.45
7:H:59:ARG:O	7:H:63:SER:OG	2.31	0.45
32:a:1039:C:H2'	32:a:1040:U:H6	1.82	0.45
32:a:1350:A:O2'	38:g:33:ASP:OD2	2.34	0.45
32:a:1456:G:C5	51:t:55:ILE:HD11	2.52	0.45
1:A:197:A:N6	1:A:2430:A:O2'	2.47	0.45
11:P:50:ARG:HD3	30:8:7:HIS:CD2	2.52	0.45
16:U:102:GLU:HG3	16:U:104:GLN:HE22	1.82	0.45
23:1:21:ARG:HD3	23:1:35:THR:HG21	1.99	0.45
32:a:678:U:H2'	32:a:679:C:C6	2.51	0.45
41:j:5:ARG:HG2	41:j:71:LEU:HD11	1.97	0.45
6:G:121:ASN:ND2	6:G:123:ASN:H	2.14	0.45
32:a:958:A:C6	50:s:55:LYS:HB2	2.52	0.45
32:a:1071:C:H2'	32:a:1072:G:H8	1.82	0.45
32:a:1176:A:H2'	32:a:1177:G:C8	2.52	0.45
1:A:336:C:O2'	20:Y:35:TYR:OH	2.32	0.45
1:A:2067:G:O2'	1:A:2069:G:H5'	2.16	0.45
1:A:2343:C:O2'	1:A:2373:G:O2'	2.35	0.45
3:D:16:MET:HG3	3:D:211:ARG:NH1	2.31	0.45
27:5:20:ARG:HG2	27:5:23:HIS:CE1	2.52	0.45
46:o:21:ASP:OD2	46:o:24:SER:HB3	2.17	0.45
1:A:139:G:O6	1:A:140:G:O2'	2.26	0.44
1:A:579:G:H2'	1:A:580:C:C6	2.52	0.44
1:A:589:C:H2'	1:A:590:A:H8	1.81	0.44
2:B:48:A:H2'	2:B:49:C:H6	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:110:LEU:HD23	14:S:110:LEU:HA	1.86	0.44
32:a:1005:A:C5	32:a:1024:G:C2	3.05	0.44
40:i:5:TYR:OH	40:i:7:THR:OG1	2.33	0.44
40:i:19:LEU:HB3	40:i:59:PHE:HD2	1.81	0.44
44:m:30:ALA:O	44:m:34:LEU:HD23	2.17	0.44
48:q:85:VAL:O	48:q:89:LEU:HG	2.16	0.44
49:r:74:ARG:HD3	49:r:81:PHE:CD1	2.52	0.44
1:A:30:G:H2'	1:A:31:C:C6	2.52	0.44
1:A:1262:A:N7	61:A:4507:HOH:O	2.36	0.44
1:A:1490:A:H2'	3:D:99:ASP:OD1	2.17	0.44
1:A:2271:G:OP1	22:0:18:ALA:HB1	2.18	0.44
1:A:2809:A:H2'	1:A:2810:A:C8	2.53	0.44
15:T:33:LYS:HG3	15:T:42:ILE:HD13	1.98	0.44
19:X:53:LYS:HB3	19:X:82:GLN:HB3	2.00	0.44
32:a:434:U:H2'	32:a:435:C:H6	1.82	0.44
32:a:614:A:H2'	32:a:615:C:C6	2.52	0.44
32:a:679:C:H2'	32:a:680:C:H6	1.82	0.44
32:a:1039:C:H2'	32:a:1040:U:C6	2.51	0.44
33:b:67:THR:HA	33:b:90:MET:HE3	1.98	0.44
34:c:136:GLN:NE2	34:c:140:ARG:HE	2.14	0.44
1:A:630:G:N2	1:A:633:A:OP2	2.44	0.44
1:A:886:C:H2'	1:A:887:A:H5"	1.98	0.44
1:A:994:C:O2'	1:A:996:A:OP1	2.31	0.44
3:D:112:GLN:HB2	3:D:115:GLN:OE1	2.17	0.44
12:Q:137:TYR:OH	21:Z:45:ASP:OD2	2.32	0.44
26:4:61:ARG:C	26:4:63:TYR:H	2.26	0.44
39:h:83:ILE:HG13	39:h:137:VAL:HG22	1.99	0.44
42:k:62:GLN:HG2	42:k:97:ALA:HB2	2.00	0.44
43:l:85:ILE:HG22	43:l:100:ILE:HD13	1.98	0.44
55:x:12:A:H2'	55:x:13:A:O4'	2.18	0.44
1:A:375:C:H2'	1:A:376:C:C6	2.52	0.44
1:A:686:G:N2	1:A:788:A:H61	2.15	0.44
1:A:864:G:H2'	1:A:865:C:C6	2.53	0.44
19:X:60:ARG:NE	61:X:201:HOH:O	2.49	0.44
32:a:1387:G:H2'	32:a:1388:C:C6	2.53	0.44
37:f:23:LYS:HE2	37:f:42:GLU:OE2	2.16	0.44
43:l:88:GLY:O	43:l:99:HIS:HD2	2.01	0.44
1:A:128:C:O2'	1:A:129:C:OP1	2.35	0.44
1:A:184:C:H2'	1:A:185:U:H6	1.83	0.44
1:A:581:C:H2'	1:A:582:G:H8	1.82	0.44
1:A:1009:A:N3	1:A:1153:C:O2'	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:G:H2'	1:A:1043:C:H6	1.82	0.44
1:A:1406:U:H2'	1:A:1407:C:C6	2.52	0.44
1:A:1794:U:H2'	1:A:1795:C:C6	2.52	0.44
2:B:95:C:H2'	2:B:96:U:C6	2.53	0.44
23:1:92:LYS:HB2	23:1:92:LYS:HE3	1.61	0.44
36:e:6:PHE:HB2	36:e:34:VAL:HG13	1.99	0.44
1:A:2567:G:H2'	1:A:2568:C:C6	2.53	0.44
1:A:2645:G:N7	61:A:4513:HOH:O	2.36	0.44
5:F:120:GLU:HB2	5:F:122:LYS:HD3	1.98	0.44
21:Z:125:LEU:HG	21:Z:164:ALA:HB3	1.98	0.44
32:a:35:G:H2'	32:a:36:C:H6	1.82	0.44
32:a:551:U:H2'	32:a:552:U:C6	2.53	0.44
32:a:1121:U:H2'	32:a:1122:U:C6	2.53	0.44
35:d:101:LEU:O	35:d:105:VAL:HG13	2.18	0.44
38:g:31:MET:HE2	38:g:36:LYS:HD3	1.99	0.44
38:g:71:PRO:HD2	38:g:71:PRO:O	2.18	0.44
18:W:1:MET:HG3	18:W:64:MET:SD	2.57	0.44
32:a:501:C:H2'	32:a:502:G:C8	2.53	0.44
32:a:1001(A):G:H2'	32:a:1002:G:O4'	2.18	0.44
1:A:754:C:H2'	1:A:755:C:C6	2.52	0.44
1:A:2308:G:O2'	1:A:2310:A:N7	2.37	0.44
2:B:66:A:H61	2:B:109:C:H5'	1.83	0.44
7:H:85:LYS:HE2	7:H:85:LYS:HB2	1.78	0.44
9:N:10:GLU:HG2	9:N:11:PRO:CD	2.48	0.44
32:a:286:G:N7	61:a:1935:HOH:O	2.37	0.44
32:a:715:A:H2'	32:a:716:A:H8	1.82	0.44
32:a:1130:A:H2'	32:a:1131:G:H8	1.83	0.44
32:a:1241:G:H2'	32:a:1242:C:C6	2.53	0.44
36:e:152:ARG:O	39:h:64:LYS:NZ	2.51	0.44
40:i:10:ARG:NE	61:i:201:HOH:O	2.37	0.44
54:w:119:GLU:HG3	54:w:184:PRO:HB3	2.00	0.44
7:H:37:VAL:HG22	7:H:68:THR:HG23	1.99	0.44
21:Z:102:LEU:HD23	21:Z:102:LEU:HA	1.87	0.44
32:a:581:G:OP1	46:o:65:ARG:NH1	2.50	0.44
32:a:701:C:OP1	32:a:702:A:O2'	2.25	0.44
32:a:933:G:OP2	38:g:3:ARG:HB2	2.18	0.44
32:a:1299:A:O2'	32:a:1300:G:H4'	2.18	0.44
32:a:1315:U:H2'	32:a:1316:G:O4'	2.17	0.44
1:A:227:A:C2	1:A:2407:G:H1'	2.53	0.43
1:A:1946:U:H2'	1:A:1947:C:C6	2.53	0.43
3:D:148:GLU:HB2	3:D:151:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:72:ARG:CZ	6:G:87:PRO:HG3	2.48	0.43
7:H:46:GLU:HB2	7:H:49:VAL:HG23	2.00	0.43
11:P:126:VAL:HG22	11:P:146:VAL:HB	2.00	0.43
17:V:24:LYS:HB3	17:V:24:LYS:HE3	1.67	0.43
32:a:501:C:H2'	32:a:502:G:H8	1.83	0.43
32:a:1434:A:H2'	32:a:1435:G:O4'	2.17	0.43
33:b:188:ALA:HB3	33:b:200:ILE:HD11	2.00	0.43
35:d:57:ARG:HB3	35:d:206:PHE:HB2	2.00	0.43
41:j:11:PHE:CE1	41:j:65:LEU:HD11	2.53	0.43
51:t:54:LYS:HE2	51:t:54:LYS:HB3	1.74	0.43
1:A:2698:U:H2'	1:A:2699:C:C6	2.53	0.43
3:D:37:LEU:HD12	3:D:37:LEU:HA	1.81	0.43
7:H:44:VAL:HG23	7:H:51:ARG:HG3	1.99	0.43
9:N:108:PRO:O	9:N:113:GLY:HA3	2.17	0.43
32:a:110:C:H2'	32:a:111:G:O4'	2.18	0.43
32:a:216:G:H2'	32:a:217:C:C6	2.53	0.43
32:a:501:C:H1'	32:a:549:C:H1'	1.99	0.43
32:a:1183:A:O2'	32:a:1184:G:OP1	2.32	0.43
42:k:69:ALA:O	42:k:73:MET:HE3	2.18	0.43
1:A:1158:C:H5"	25:3:30:ARG:HD3	1.99	0.43
1:A:2590:A:H2'	1:A:2591:C:H6	1.83	0.43
13:R:65:LEU:HA	13:R:68:ARG:HD2	1.99	0.43
24:2:1:MET:SD	24:2:56:GLN:NE2	2.92	0.43
32:a:243:A:N7	61:a:1934:HOH:O	2.36	0.43
32:a:346:G:O2'	32:a:347:G:OP1	2.30	0.43
32:a:865:A:H2'	32:a:866:C:C6	2.53	0.43
32:a:976:G:H5'	32:a:1358:U:O2'	2.17	0.43
32:a:1027:C:C4	32:a:1028:C:N4	2.86	0.43
48:q:45:HIS:HB2	48:q:65:ILE:HD13	2.00	0.43
1:A:284:U:H2'	1:A:285:C:H6	1.83	0.43
1:A:306:U:H2'	1:A:307:G:O4'	2.18	0.43
1:A:619:G:O6	5:F:103:LYS:NZ	2.45	0.43
1:A:1485:G:H2'	1:A:1486:A:C8	2.54	0.43
1:A:2291:U:H2'	1:A:2292:C:H6	1.83	0.43
32:a:551:U:H2'	32:a:552:U:H6	1.83	0.43
32:a:695:A:H2'	32:a:696:A:C8	2.53	0.43
32:a:945:G:C2	32:a:946:A:C8	3.06	0.43
33:b:79:ASP:HB3	33:b:83:MET:HE3	2.00	0.43
55:x:11:C:H2'	55:x:12:A:C8	2.53	0.43
1:A:2295:C:OP1	14:S:10:ARG:NH1	2.52	0.43
6:G:109:VAL:HG11	26:4:14:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:41:MET:HE1	7:H:65:HIS:HA	2.00	0.43
32:a:17:U:H2'	32:a:18:C:H6	1.84	0.43
32:a:757:U:H2'	32:a:758:G:O4'	2.17	0.43
36:e:112:LEU:HD23	36:e:112:LEU:HA	1.85	0.43
51:t:30:LYS:O	51:t:34:LYS:HG3	2.18	0.43
54:w:173:TYR:HB3	54:w:339:LEU:HD13	2.00	0.43
1:A:795:C:H2'	1:A:796:C:C6	2.54	0.43
1:A:1308:A:H2'	1:A:1309:G:O4'	2.19	0.43
1:A:1570:A:H2'	1:A:1571:A:C8	2.54	0.43
6:G:118:ARG:O	6:G:181:ARG:HG2	2.17	0.43
10:O:104:ARG:NH2	15:T:43:GLN:OE1	2.52	0.43
32:a:32:A:H2'	32:a:33:A:C8	2.54	0.43
32:a:539:A:H2'	32:a:540:G:H8	1.82	0.43
32:a:610:G:C2	32:a:611:A:C8	3.06	0.43
32:a:868:C:H2'	32:a:869:G:O4'	2.19	0.43
1:A:632:A:H2'	1:A:633:A:C8	2.54	0.43
1:A:1000:A:H2'	1:A:1001:A:C8	2.54	0.43
1:A:1035:U:H2'	1:A:1036:G:H8	1.82	0.43
1:A:2712:U:OP1	1:A:2714:G:H4'	2.19	0.43
32:a:449:C:H2'	32:a:450:G:O4'	2.19	0.43
32:a:1000:U:C2	32:a:1001:A:C8	3.07	0.43
32:a:1125:U:HO2'	32:a:1126:U:P	2.42	0.43
38:g:28:ASN:HD21	38:g:36:LYS:NZ	2.17	0.43
49:r:71:LYS:O	49:r:75:ILE:HG12	2.18	0.43
1:A:191:A:H2'	1:A:192:C:C6	2.53	0.43
1:A:493:G:H2'	1:A:494:G:O4'	2.19	0.43
1:A:1657:C:H2'	1:A:1658:C:C6	2.53	0.43
7:H:154:PRO:HB3	7:H:163:TYR:CZ	2.54	0.43
19:X:90:GLU:CD	19:X:90:GLU:H	2.26	0.43
23:1:7:ILE:HG23	23:1:98:LEU:HD21	2.01	0.43
32:a:337:C:H2'	32:a:338:A:C8	2.53	0.43
47:p:58:TYR:O	47:p:62:VAL:HG22	2.19	0.43
17:V:62:LEU:HD11	17:V:95:LEU:HB2	2.00	0.43
32:a:720:C:H2'	32:a:721:G:C8	2.53	0.43
33:b:111:ARG:HD2	33:b:111:ARG:HA	1.75	0.43
35:d:165:MET:HE2	35:d:165:MET:HB2	1.76	0.43
49:r:76:LEU:HD23	49:r:76:LEU:HA	1.83	0.43
1:A:358:U:H2'	1:A:359:A:H8	1.84	0.43
1:A:607:U:C5	1:A:620:G:C5	3.07	0.43
1:A:1028:A:H2'	1:A:1029:A:C8	2.54	0.43
1:A:1210:A:H5"	1:A:1212:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:C:H2'	1:A:1387:C:C6	2.54	0.43
1:A:1588:C:H2'	1:A:1589:C:C6	2.54	0.43
34:c:15:THR:HG21	34:c:181:ASN:HA	2.00	0.43
8:I:129:THR:HG22	8:I:139:GLN:HG3	2.01	0.42
12:Q:57:HIS:HD2	12:Q:117:ALA:HB2	1.84	0.42
17:V:62:LEU:HD12	17:V:93:GLU:HG2	2.01	0.42
19:X:72:LYS:NZ	19:X:73:ARG:O	2.52	0.42
28:6:17:LYS:HA	28:6:17:LYS:HD3	1.71	0.42
32:a:246:A:C2	32:a:282:A:C5	3.07	0.42
32:a:553:A:H5"	43:l:24:VAL:HG21	2.00	0.42
32:a:1227:A:O2'	44:m:115:LYS:NZ	2.52	0.42
33:b:126:GLU:CD	33:b:126:GLU:H	2.27	0.42
40:i:26:VAL:HG13	40:i:33:PHE:HB2	2.00	0.42
44:m:40:ASN:O	44:m:43:THR:HG22	2.19	0.42
54:w:177:VAL:HB	54:w:301:LYS:HA	2.00	0.42
54:w:338:ALA:HA	54:w:341:ARG:HD2	2.01	0.42
1:A:327:G:N7	61:A:4515:HOH:O	2.37	0.42
3:D:146:GLU:HG2	3:D:152:GLY:C	2.43	0.42
5:F:127:GLU:HG2	5:F:196:LEU:HD11	2.01	0.42
32:a:189(K):U:H2'	32:a:189(L):G:C8	2.53	0.42
32:a:890:G:O2'	32:a:906:G:O6	2.24	0.42
32:a:1412:C:H2'	32:a:1413:A:C8	2.55	0.42
1:A:250:G:H2'	1:A:251:A:C8	2.55	0.42
1:A:747:U:O2	1:A:2014:A:H1'	2.19	0.42
1:A:2406:U:C4	11:P:72:PRO:HD2	2.55	0.42
32:a:614:A:H2'	32:a:615:C:H6	1.84	0.42
32:a:691:G:H2'	32:a:692:U:C6	2.54	0.42
32:a:983:A:H5'	32:a:984:C:OP2	2.18	0.42
32:a:1489:G:H2'	32:a:1490:C:O4'	2.19	0.42
1:A:2420:C:OP1	30:8:34:TRP:HB3	2.18	0.42
2:B:89:G:H2'	2:B:90:A:C8	2.53	0.42
6:G:21:ARG:CZ	6:G:21:ARG:HB3	2.50	0.42
32:a:33:A:H2'	32:a:34:C:C6	2.54	0.42
32:a:45:U:H2'	32:a:46:G:H8	1.81	0.42
33:b:28:PHE:CD2	33:b:190:THR:HA	2.54	0.42
54:w:119:GLU:CG	54:w:184:PRO:HB3	2.49	0.42
55:x:10:A:H2'	55:x:11:C:C6	2.54	0.42
1:A:582:G:H2'	1:A:583:G:C8	2.55	0.42
1:A:652(U):G:H2'	1:A:652(V):C:C6	2.55	0.42
1:A:898:C:H2'	1:A:899:A:O4'	2.20	0.42
1:A:2317:C:H2'	1:A:2318:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:C:H2'	2:B:3:C:H6	1.85	0.42
2:B:12:C:O2'	22:0:74:ARG:HG2	2.20	0.42
7:H:103:LEU:HD23	7:H:105:LEU:HD21	2.01	0.42
32:a:1002:G:C5	32:a:1003:G:H1'	2.54	0.42
32:a:1226:C:H4'	50:s:80:TYR:CZ	2.55	0.42
32:a:1314:C:H2'	32:a:1315:U:C6	2.55	0.42
32:a:1324:A:H2'	32:a:1325:C:H6	1.84	0.42
33:b:71:VAL:HG12	33:b:170:GLU:OE2	2.19	0.42
42:k:48:ILE:HD13	42:k:63:LEU:HB3	2.02	0.42
1:A:154:G:H2'	1:A:154(A):C:O4'	2.19	0.42
1:A:1509(A):A:H3'	1:A:1509(B):A:H8	1.83	0.42
32:a:222:U:H2'	32:a:223:U:C6	2.55	0.42
32:a:986:A:H2'	32:a:987:G:H8	1.85	0.42
32:a:1137:C:O2'	32:a:1138:G:N2	2.52	0.42
33:b:22:LYS:O	33:b:24:TRP:HD1	2.03	0.42
33:b:155:LEU:HD23	33:b:155:LEU:HA	1.86	0.42
36:e:151:LEU:HD11	39:h:77:GLU:CD	2.45	0.42
41:j:78:ASN:O	41:j:82:ILE:N	2.52	0.42
49:r:31:LEU:O	49:r:69:THR:HG21	2.20	0.42
1:A:1173:G:N2	1:A:1177:A:OP1	2.53	0.42
1:A:1331:A:H2'	1:A:1333:C:C5	2.55	0.42
7:H:86:GLU:HG2	7:H:165:ALA:HB2	2.01	0.42
32:a:262:A:H4'	51:t:75:ASN:HB2	2.00	0.42
32:a:936:C:C2	32:a:937:A:C8	3.08	0.42
35:d:109:GLY:CA	35:d:165:MET:HE3	2.48	0.42
50:s:11:VAL:HG11	50:s:16:LEU:HB2	2.02	0.42
55:x:66:A:H2'	55:x:67:C:C6	2.54	0.42
1:A:185:U:H2'	1:A:186:G:H8	1.84	0.42
1:A:443:A:H1'	1:A:1201:C:O4'	2.20	0.42
1:A:2010:G:H5"	18:W:42:ARG:HB2	2.02	0.42
1:A:2461:C:H2'	1:A:2462:U:C6	2.55	0.42
2:B:24:G:N7	2:B:56:G:H2'	2.34	0.42
21:Z:3:TYR:CE1	21:Z:50:GLN:HG3	2.54	0.42
32:a:436:C:H2'	32:a:437:U:C6	2.54	0.42
39:h:78:GLN:HE21	39:h:78:GLN:HA	1.84	0.42
1:A:302:C:H2'	1:A:303:U:C6	2.55	0.42
1:A:690:G:H2'	1:A:691:C:C6	2.54	0.42
1:A:839:U:H2'	1:A:840:C:C6	2.54	0.42
1:A:1198:U:H2'	1:A:1199:U:C6	2.54	0.42
1:A:2677:G:H2'	1:A:2678:C:C6	2.55	0.42
5:F:199:TRP:O	5:F:203:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:270:A:H2'	32:a:271:C:H6	1.84	0.42
32:a:722:A:N3	32:a:722:A:H3'	2.35	0.42
32:a:751:U:H2'	32:a:752:G:O4'	2.20	0.42
32:a:1442:G:H2'	32:a:1442:G:N3	2.35	0.42
38:g:37:ASN:OD1	40:i:41:VAL:HG22	2.20	0.42
1:A:39:C:H2'	1:A:40:C:C6	2.55	0.42
1:A:287:C:H2'	1:A:288:C:C6	2.55	0.42
1:A:1796:U:H2'	1:A:1797:C:H6	1.84	0.42
21:Z:53:ILE:HD12	21:Z:99:TYR:HB2	2.02	0.42
32:a:728:A:H2'	32:a:729:A:H8	1.84	0.42
32:a:1236:A:H2'	32:a:1237:C:C6	2.54	0.42
32:a:1314:C:N4	50:s:2:PRO:O	2.49	0.42
51:t:56:MET:HB3	51:t:56:MET:HE2	1.82	0.42
1:A:284:U:H2'	1:A:285:C:C6	2.54	0.41
1:A:1790:C:H2'	1:A:1791:A:C5	2.55	0.41
1:A:2648:C:H2'	1:A:2649:U:H6	1.85	0.41
30:8:52:LYS:O	30:8:56:GLU:HG2	2.20	0.41
32:a:189(D):C:H2'	32:a:189(E):U:O4'	2.20	0.41
32:a:346:G:HO2'	32:a:347:G:P	2.42	0.41
32:a:406:G:H21	35:d:119:GLN:HE22	1.67	0.41
32:a:564:C:C5	48:q:31:LEU:HD11	2.55	0.41
32:a:1324:A:H2'	32:a:1325:C:C6	2.54	0.41
40:i:26:VAL:CG1	40:i:33:PHE:HB2	2.50	0.41
40:i:63:ILE:HG21	40:i:77:ILE:HG12	2.00	0.41
42:k:62:GLN:HG3	42:k:93:GLN:HG3	2.01	0.41
54:w:174:GLU:OE2	54:w:336:LEU:HD11	2.20	0.41
1:A:34:C:N4	1:A:447:A:H61	2.17	0.41
1:A:153:C:H2'	1:A:154:G:C8	2.56	0.41
1:A:479:A:N3	1:A:481:G:H5"	2.35	0.41
1:A:1269:A:H2'	1:A:1270:C:C6	2.55	0.41
1:A:1437:C:H2'	1:A:1438:U:C6	2.55	0.41
1:A:2059:A:H2'	1:A:2503:2MA:HM23	2.02	0.41
8:I:5:LEU:HD22	8:I:9:LEU:HD12	2.02	0.41
21:Z:23:LYS:HD3	21:Z:38:TYR:CE1	2.55	0.41
23:1:8:SER:HB3	23:1:66:HIS:CD2	2.56	0.41
32:a:399:G:H2'	32:a:400:C:H6	1.85	0.41
32:a:537:G:H2'	32:a:538:G:H8	1.85	0.41
32:a:658:G:H2'	32:a:659:U:C6	2.54	0.41
32:a:743:U:H2'	32:a:744:C:C6	2.54	0.41
32:a:1014:A:C2	32:a:1219:U:H1'	2.55	0.41
32:a:1120:G:H2'	32:a:1121:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1427:U:H2'	32:a:1428:A:H8	1.85	0.41
35:d:98:GLU:O	35:d:103:ASN:ND2	2.53	0.41
39:h:14:ARG:HD3	39:h:18:ARG:NH2	2.35	0.41
1:A:686:G:H21	1:A:788:A:H61	1.68	0.41
1:A:888:C:H2'	1:A:889:C:C6	2.55	0.41
1:A:1528:A:OP2	61:A:4404:HOH:O	2.22	0.41
1:A:1802:A:H2'	1:A:1803:A:C8	2.56	0.41
1:A:2065:C:H2'	1:A:2066:C:C6	2.55	0.41
1:A:2386:C:H2'	1:A:2387:U:C6	2.55	0.41
19:X:41:ASN:O	19:X:45:THR:HG22	2.20	0.41
32:a:171:A:H2'	32:a:172:A:C8	2.55	0.41
32:a:779:C:H2'	32:a:780:A:O4'	2.20	0.41
32:a:922:G:H4'	36:e:20:GLN:HA	2.03	0.41
46:o:24:SER:O	46:o:28:GLN:HG3	2.20	0.41
54:w:213:ASN:HB3	54:w:216:GLU:OE2	2.20	0.41
1:A:536:A:H2'	1:A:537:C:C6	2.56	0.41
1:A:723:G:H2'	1:A:724:U:O4'	2.20	0.41
1:A:760:G:H2'	1:A:761:A:O4'	2.20	0.41
1:A:973:A:H8	1:A:973:A:OP1	2.03	0.41
1:A:2451:A:C2	54:w:230:MEQ:HE1	2.55	0.41
15:T:113:LYS:HD2	15:T:113:LYS:HA	1.88	0.41
16:U:108:GLU:O	16:U:112:ARG:HG2	2.20	0.41
18:W:2:GLU:OE2	18:W:72:LYS:NZ	2.37	0.41
32:a:582:U:H2'	32:a:583:A:H8	1.86	0.41
32:a:696:A:H2'	32:a:697:U:H6	1.85	0.41
32:a:883:C:O2'	32:a:884:U:H5'	2.19	0.41
32:a:892:A:H2'	32:a:893:C:C6	2.56	0.41
32:a:1278:U:H5'	32:a:1279:A:O5'	2.21	0.41
54:w:102:MET:HB2	54:w:103:ASP:H	1.62	0.41
1:A:185:U:H2'	1:A:186:G:C8	2.55	0.41
1:A:340:A:H2'	1:A:341:G:O4'	2.20	0.41
1:A:491:G:H2'	1:A:492:A:C8	2.56	0.41
1:A:2747:G:O6	1:A:2755:C:H5"	2.21	0.41
3:D:108:PRO:HD2	3:D:111:LEU:HD22	2.01	0.41
9:N:15:LEU:HB2	9:N:135:PRO:HB2	2.03	0.41
10:O:35:VAL:HG13	10:O:65:THR:HG23	2.02	0.41
33:b:216:SER:O	33:b:219:VAL:HG12	2.21	0.41
46:o:18:PHE:CZ	46:o:21:ASP:HB2	2.56	0.41
1:A:637:A:H2'	11:P:117:GLU:OE1	2.20	0.41
1:A:1001:A:H2'	1:A:1002:G:O4'	2.20	0.41
1:A:1493:C:N4	1:A:2206:G:O2'	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:60:LEU:HB3	6:G:68:PRO:HG3	2.02	0.41
14:S:74:ALA:O	14:S:78:LEU:HD13	2.20	0.41
21:Z:54:HIS:HB3	21:Z:101:PRO:HD3	2.02	0.41
32:a:41:G:H2'	32:a:42:G:H8	1.86	0.41
32:a:1021:G:N3	32:a:1022:G:C8	2.89	0.41
32:a:1024:G:H2'	32:a:1025:U:H5"	2.01	0.41
37:f:6:VAL:HG13	37:f:90:VAL:HG22	2.03	0.41
37:f:24:GLU:OE2	37:f:24:GLU:HA	2.20	0.41
48:q:4:LYS:HE3	48:q:6:LEU:HD21	2.01	0.41
1:A:287:C:H2'	1:A:288:C:H6	1.85	0.41
1:A:1468:C:H2'	1:A:1469:A:C8	2.56	0.41
1:A:2514:U:H2'	1:A:2515:C:C6	2.56	0.41
1:A:2662:A:O5'	1:A:2662:A:H8	2.04	0.41
3:D:141:VAL:HG13	3:D:162:SER:HB2	2.03	0.41
6:G:16:ARG:NH2	6:G:28:VAL:HG22	2.36	0.41
11:P:1:MET:HB2	11:P:1:MET:HE2	1.80	0.41
32:a:406:G:N3	35:d:119:GLN:NE2	2.67	0.41
32:a:406:G:O3'	35:d:3:ARG:NH2	2.51	0.41
32:a:609:A:C5	32:a:610:G:C8	3.09	0.41
32:a:767:A:H2'	32:a:768:A:O4'	2.20	0.41
54:w:134:PHE:CZ	54:w:138:MET:HE2	2.56	0.41
55:x:70:G:H2'	55:x:71:C:H6	1.85	0.41
1:A:7:G:H2'	1:A:8:A:H8	1.86	0.41
1:A:153:C:H2'	1:A:154:G:H8	1.84	0.41
1:A:882:G:H2'	1:A:883:G:O4'	2.21	0.41
1:A:1045:A:H1'	1:A:1047:G:C4	2.55	0.41
20:Y:87:LYS:HD3	20:Y:87:LYS:HA	1.87	0.41
30:8:8:LYS:HA	30:8:8:LYS:HD3	1.80	0.41
32:a:258:G:H2'	32:a:259:G:H8	1.86	0.41
32:a:582:U:H2'	32:a:583:A:C8	2.55	0.41
32:a:1053:G:N7	32:a:1200:C:H5"	2.35	0.41
32:a:1228:C:H4'	44:m:116:THR:HA	2.02	0.41
1:A:322:A:OP2	5:F:169:ASN:HB2	2.21	0.41
1:A:1188:U:H4'	17:V:79:VAL:HG22	2.03	0.41
1:A:1542:A:H8	1:A:1542:A:OP1	2.04	0.41
1:A:2360:A:H2'	1:A:2361:A:O4'	2.21	0.41
1:A:2648:C:H2'	1:A:2649:U:C6	2.56	0.41
10:O:18:LYS:HD2	10:O:18:LYS:HA	1.84	0.41
20:Y:5:MET:HE2	20:Y:5:MET:HB2	1.72	0.41
21:Z:59:LEU:HD12	21:Z:69:THR:HG21	2.03	0.41
32:a:107:G:N7	51:t:15:ARG:NH2	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:652:U:O4	32:a:752:G:O2'	2.27	0.41
32:a:833:U:H2'	32:a:834:C:C6	2.56	0.41
32:a:841:U:H5"	32:a:848:C:C5	2.55	0.41
32:a:860:A:H2'	32:a:861:G:O4'	2.21	0.41
32:a:1014:A:H2	32:a:1219:U:H1'	1.86	0.41
33:b:80:ILE:HD11	33:b:208:ILE:HG23	2.02	0.41
34:c:56:ASP:O	34:c:66:VAL:HA	2.21	0.41
36:e:12:LEU:HB3	36:e:31:LEU:HB3	2.02	0.41
44:m:33:ALA:HA	44:m:59:TYR:HE2	1.86	0.41
49:r:33:ASP:O	49:r:40:LEU:HD11	2.21	0.41
55:x:62:C:H2'	55:x:63:G:H8	1.86	0.41
1:A:150:C:H2'	1:A:151:C:H6	1.86	0.41
1:A:2022:U:O2'	1:A:2617:C:H5'	2.21	0.41
2:B:29:A:H2'	2:B:30:C:C6	2.56	0.41
32:a:610:G:C4	32:a:611:A:C8	3.08	0.41
32:a:1010:G:H2'	32:a:1011:G:H8	1.85	0.41
32:a:1147:C:O2	40:i:16:ARG:NH2	2.53	0.41
33:b:30:ARG:NH2	33:b:194:PRO:HB2	2.31	0.41
40:i:3:GLN:HG2	40:i:20:ARG:NE	2.36	0.41
54:w:119:GLU:OE2	54:w:182:ARG:NH2	2.48	0.41
54:w:239:VAL:HG11	54:w:262:ARG:HA	2.03	0.41
1:A:2086:U:H2'	1:A:2087:G:C8	2.56	0.40
3:D:206:LEU:O	3:D:211:ARG:HD3	2.21	0.40
5:F:184:TYR:CE2	5:F:188:ARG:HD2	2.56	0.40
21:Z:152:ALA:N	21:Z:169:GLU:O	2.38	0.40
25:3:44:ARG:HG3	25:3:44:ARG:NH1	2.37	0.40
32:a:341:C:H2'	32:a:342:C:H6	1.86	0.40
32:a:1240:U:OP1	38:g:119:ARG:NH2	2.40	0.40
35:d:182:LYS:HB3	35:d:182:LYS:HE2	1.85	0.40
38:g:31:MET:HG2	38:g:32:ARG:N	2.36	0.40
46:o:3:ILE:HG23	46:o:7:GLU:HG3	2.04	0.40
1:A:652(C):G:H2'	1:A:652(D):C:C6	2.56	0.40
1:A:883:G:H8	1:A:883:G:O5'	2.05	0.40
1:A:2814:C:O2'	27:5:29:THR:OG1	2.31	0.40
24:2:8:LYS:HB3	24:2:8:LYS:HE2	1.84	0.40
35:d:4:TYR:OH	35:d:7:PRO:O	2.35	0.40
36:e:79:GLU:OE1	39:h:105:ARG:HG2	2.20	0.40
37:f:55:ASP:HA	37:f:56:PRO:HD3	1.95	0.40
49:r:47:THR:O	49:r:83:GLU:N	2.50	0.40
1:A:358:U:H2'	1:A:359:A:C8	2.56	0.40
1:A:2327:A:H2'	1:A:2328:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2406:U:OP2	1:A:2406:U:H2'	2.20	0.40
3:D:245:PRO:HA	3:D:246:PRO:HD3	1.96	0.40
6:G:41:GLN:NE2	6:G:153:ARG:HB3	2.36	0.40
21:Z:45:ASP:O	21:Z:49:ARG:HG3	2.21	0.40
32:a:153:C:H2'	32:a:154:C:C6	2.56	0.40
32:a:443:C:H2'	32:a:444:C:C6	2.57	0.40
32:a:864:A:H2'	32:a:865:A:C8	2.56	0.40
33:b:155:LEU:C	33:b:156:LYS:HD2	2.47	0.40
1:A:1364:G:P	23:1:3:LYS:HG3	2.62	0.40
1:A:1630:G:H2'	1:A:1631:C:C6	2.56	0.40
1:A:1924:C:H4'	55:x:13:A:H4'	2.03	0.40
21:Z:52:SER:C	21:Z:54:HIS:H	2.29	0.40
23:1:6:GLU:HG3	23:1:61:ARG:O	2.22	0.40
27:5:40:LYS:HD3	27:5:46:CYS:HA	2.03	0.40
32:a:235:C:H2'	32:a:236:G:H8	1.87	0.40
32:a:500:G:H2'	32:a:501:C:C6	2.56	0.40
32:a:1121:U:H2'	32:a:1122:U:H6	1.86	0.40
35:d:68:TYR:OH	35:d:98:GLU:OE2	2.25	0.40
36:e:82:VAL:HG21	36:e:138:ALA:HA	2.02	0.40
39:h:41:ARG:NH1	39:h:42:GLU:OE2	2.55	0.40
54:w:178:HIS:HB3	54:w:305:TYR:HE1	1.86	0.40
55:x:65:A:H2'	55:x:66:A:H8	1.86	0.40
1:A:262:A:H2'	1:A:263:C:O4'	2.22	0.40
1:A:305:U:H2'	1:A:306:U:C6	2.56	0.40
1:A:1657:C:H2'	1:A:1658:C:H6	1.85	0.40
1:A:2064:C:H2'	1:A:2065:C:H6	1.85	0.40
2:B:74:U:H2'	2:B:75:G:O4'	2.22	0.40
6:G:77:ILE:H	6:G:82:LEU:HD23	1.87	0.40
10:O:49:ARG:NH2	32:a:1423:G:OP1	2.47	0.40
15:T:127:ALA:O	15:T:128:GLU:HG2	2.22	0.40
32:a:254:G:OP1	48:q:67:LYS:O	2.40	0.40
32:a:475:G:H2'	32:a:476:G:H8	1.87	0.40
32:a:505:G:H2'	32:a:506:G:C8	2.56	0.40
32:a:946:A:H2'	32:a:947:G:H8	1.85	0.40
32:a:1038:C:H2'	32:a:1039:C:H6	1.87	0.40
33:b:126:GLU:HG2	33:b:127:ILE:H	1.87	0.40
34:c:134:ILE:HG22	34:c:168:ALA:HB3	2.04	0.40
35:d:102:ASP:N	35:d:102:ASP:OD1	2.54	0.40
40:i:112:LYS:NZ	40:i:116:LYS:O	2.51	0.40
54:w:130:MET:SD	54:w:332:LEU:HD21	2.62	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	
3	D	271/276 (98%)	267 (98%)	4 (2%)	0	100	100
4	E	202/206 (98%)	195 (96%)	7 (4%)	0	100	100
5	F	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
6	G	179/182 (98%)	169 (94%)	10 (6%)	0	100	100
7	H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
8	I	144/148 (97%)	141 (98%)	3 (2%)	0	100	100
9	N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
10	O	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
11	P	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
12	Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
13	R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
14	S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	T	129/146 (88%)	128 (99%)	1 (1%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
18	W	108/113 (96%)	108 (100%)	0	0	100	100
19	X	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
20	Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	Z	147/206 (71%)	140 (95%)	7 (5%)	0	100	100
22	0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
23	1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	2	68/72 (94%)	68 (100%)	0	0	100	100
25	3	55/60 (92%)	54 (98%)	1 (2%)	0	100	100
26	4	67/71 (94%)	50 (75%)	16 (24%)	1 (2%)	8	3
27	5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	7	45/49 (92%)	45 (100%)	0	0	100	100
30	8	62/65 (95%)	62 (100%)	0	0	100	100
31	9	35/37 (95%)	35 (100%)	0	0	100	100
33	b	229/256 (90%)	213 (93%)	16 (7%)	0	100	100
34	c	204/239 (85%)	196 (96%)	7 (3%)	1 (0%)	24	19
35	d	206/209 (99%)	203 (98%)	3 (2%)	0	100	100
36	e	147/162 (91%)	142 (97%)	5 (3%)	0	100	100
37	f	98/101 (97%)	98 (100%)	0	0	100	100
38	g	152/156 (97%)	143 (94%)	9 (6%)	0	100	100
39	h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
40	i	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
41	j	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
42	k	112/129 (87%)	109 (97%)	3 (3%)	0	100	100
43	l	118/132 (89%)	118 (100%)	0	0	100	100
44	m	116/126 (92%)	111 (96%)	5 (4%)	0	100	100
45	n	58/61 (95%)	58 (100%)	0	0	100	100
46	o	86/89 (97%)	86 (100%)	0	0	100	100
47	p	80/88 (91%)	80 (100%)	0	0	100	100
48	q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
51	t	93/106 (88%)	86 (92%)	7 (8%)	0	100	100
52	u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	w	246/354 (70%)	240 (98%)	6 (2%)	0	100	100
56	z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
All	All	5909/6425 (92%)	5727 (97%)	180 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	c	66	VAL
26	4	56	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
3	D	213/218 (98%)	211 (99%)	2 (1%)	70 77
4	E	164/166 (99%)	164 (100%)	0	100 100
5	F	160/166 (96%)	159 (99%)	1 (1%)	78 84
6	G	144/156 (92%)	135 (94%)	9 (6%)	16 11
7	H	144/148 (97%)	134 (93%)	10 (7%)	14 9
8	I	73/124 (59%)	70 (96%)	3 (4%)	27 24
9	N	116/119 (98%)	112 (97%)	4 (3%)	32 32
10	O	97/100 (97%)	96 (99%)	1 (1%)	68 74
11	P	105/116 (90%)	104 (99%)	1 (1%)	68 74
12	Q	109/111 (98%)	108 (99%)	1 (1%)	70 77
13	R	100/101 (99%)	99 (99%)	1 (1%)	68 74
14	S	84/88 (96%)	84 (100%)	0	100 100
15	T	113/127 (89%)	110 (97%)	3 (3%)	39 41
16	U	93/94 (99%)	93 (100%)	0	100 100
17	V	80/82 (98%)	79 (99%)	1 (1%)	61 67
18	W	87/92 (95%)	86 (99%)	1 (1%)	65 71
19	X	77/78 (99%)	75 (97%)	2 (3%)	40 42
20	Y	81/91 (89%)	79 (98%)	2 (2%)	42 44
21	Z	135/179 (75%)	125 (93%)	10 (7%)	13 8
22	0	61/67 (91%)	61 (100%)	0	100 100
23	1	78/83 (94%)	76 (97%)	2 (3%)	40 42
24	2	65/67 (97%)	64 (98%)	1 (2%)	57 63
25	3	49/52 (94%)	49 (100%)	0	100 100
26	4	39/63 (62%)	37 (95%)	2 (5%)	21 17
27	5	50/52 (96%)	50 (100%)	0	100 100
28	6	51/52 (98%)	51 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	7	40/42 (95%)	39 (98%)	1 (2%)	42 44
30	8	54/55 (98%)	53 (98%)	1 (2%)	50 55
31	9	34/34 (100%)	33 (97%)	1 (3%)	37 38
33	b	187/220 (85%)	181 (97%)	6 (3%)	34 35
34	c	136/188 (72%)	131 (96%)	5 (4%)	30 29
35	d	166/181 (92%)	164 (99%)	2 (1%)	63 69
36	e	112/123 (91%)	111 (99%)	1 (1%)	70 77
37	f	84/90 (93%)	82 (98%)	2 (2%)	43 45
38	g	111/127 (87%)	107 (96%)	4 (4%)	31 30
39	h	112/119 (94%)	111 (99%)	1 (1%)	70 77
40	i	88/99 (89%)	86 (98%)	2 (2%)	44 47
41	j	61/92 (66%)	56 (92%)	5 (8%)	10 6
42	k	81/99 (82%)	79 (98%)	2 (2%)	42 44
43	l	96/108 (89%)	95 (99%)	1 (1%)	68 74
44	m	89/101 (88%)	89 (100%)	0	100 100
45	n	45/50 (90%)	45 (100%)	0	100 100
46	o	76/80 (95%)	74 (97%)	2 (3%)	40 42
47	p	66/74 (89%)	65 (98%)	1 (2%)	57 63
48	q	92/97 (95%)	92 (100%)	0	100 100
49	r	57/77 (74%)	55 (96%)	2 (4%)	32 31
50	s	64/80 (80%)	59 (92%)	5 (8%)	11 7
51	t	61/82 (74%)	59 (97%)	2 (3%)	33 33
52	u	18/22 (82%)	18 (100%)	0	100 100
54	w	203/298 (68%)	195 (96%)	8 (4%)	28 26
56	z	2/3 (67%)	2 (100%)	0	100 100
All	All	4703/5333 (88%)	4592 (98%)	111 (2%)	43 45

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	3	VAL
3	D	99	ASP
5	F	183	VAL

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Mol	Chain	Res	Type
6	G	3	LEU
6	G	28	VAL
6	G	31	VAL
6	G	34	LEU
6	G	64	THR
6	G	82	LEU
6	G	93	THR
6	G	145	THR
6	G	152	LEU
7	H	2	SER
7	H	16	SER
7	H	17	VAL
7	H	37	VAL
7	H	44	VAL
7	H	45	VAL
7	H	52	VAL
7	H	86	GLU
7	H	92	ILE
7	H	114	VAL
8	I	15	VAL
8	I	45	LYS
8	I	93	THR
9	N	14	VAL
9	N	28	THR
9	N	62	VAL
9	N	134	ARG
10	O	26	LYS
11	P	4	SER
12	Q	75	THR
13	R	6	SER
15	T	28	VAL
15	T	65	LYS
15	T	67	SER
17	V	79	VAL
18	W	11	ARG
19	X	3	THR
19	X	45	THR
20	Y	5	MET
20	Y	99	CYS
21	Z	13	GLU
21	Z	42	VAL
21	Z	50	GLN

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Mol	Chain	Res	Type
21	Z	52	SER
21	Z	123	ASP
21	Z	124	ILE
21	Z	148	ASP
21	Z	163	LEU
21	Z	170	THR
21	Z	171	ILE
23	1	2	SER
23	1	40	ARG
24	2	68	ARG
26	4	10	VAL
26	4	24	THR
29	7	43	THR
30	8	14	VAL
31	9	19	ARG
33	b	10	LEU
33	b	136	VAL
33	b	154	LEU
33	b	164	VAL
33	b	184	VAL
33	b	219	VAL
34	c	15	THR
34	c	26	LYS
34	c	70	VAL
34	c	192	THR
34	c	207	VAL
35	d	8	VAL
35	d	146	ILE
36	e	50	GLU
37	f	19	LEU
37	f	65	VAL
38	g	49	ILE
38	g	77	SER
38	g	80	VAL
38	g	118	VAL
39	h	26	VAL
40	i	7	THR
40	i	27	THR
41	j	19	SER
41	j	38	ILE
41	j	72	VAL
41	j	95	GLU

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Mol	Chain	Res	Type
41	j	98	ILE
42	k	16	SER
42	k	108	ILE
43	l	91	LYS
46	o	74	ASP
46	o	87	ILE
47	p	34	GLU
49	r	51	LEU
49	r	82	THR
50	s	35	SER
50	s	38	SER
50	s	55	LYS
50	s	77	THR
50	s	79	THR
51	t	53	LEU
51	t	58	LYS
54	w	175	SER
54	w	281	GLU
54	w	285	LEU
54	w	301	LYS
54	w	302	ILE
54	w	310	SER
54	w	320	THR
54	w	321	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	96	HIS
3	D	164	GLN
4	E	35	GLN
4	E	48	GLN
4	E	54	GLN
5	F	69	HIS
5	F	133	ASN
5	F	160	ASN
5	F	204	ASN
6	G	26	GLN
6	G	41	GLN
6	G	79	ASN
6	G	121	ASN
8	I	43	ASN

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Mol	Chain	Res	Type
9	N	131	GLN
10	O	3	GLN
10	O	5	GLN
11	P	128	HIS
12	Q	57	HIS
13	R	24	GLN
13	R	50	HIS
13	R	71	GLN
14	S	34	HIS
14	S	38	GLN
14	S	61	ASN
15	T	58	ASN
16	U	94	ASN
17	V	80	GLN
19	X	31	HIS
19	X	82	GLN
20	Y	43	ASN
21	Z	34	ASN
21	Z	132	ASN
21	Z	151	HIS
22	0	70	GLN
24	2	38	GLN
24	2	56	GLN
24	2	65	ASN
24	2	70	GLN
25	3	19	GLN
26	4	46	GLN
28	6	29	ASN
30	8	43	GLN
31	9	29	ASN
33	b	135	GLN
33	b	140	HIS
33	b	204	ASN
34	c	6	HIS
34	c	28	GLN
34	c	37	GLN
34	c	123	GLN
34	c	136	GLN
34	c	176	HIS
35	d	77	ASN
35	d	116	GLN
35	d	161	ASN

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Mol	Chain	Res	Type
36	e	20	GLN
36	e	56	GLN
36	e	78	HIS
36	e	141	GLN
38	g	28	ASN
38	g	96	GLN
38	g	109	ASN
39	h	78	GLN
40	i	38	GLN
40	i	58	HIS
40	i	73	GLN
40	i	124	GLN
41	j	56	HIS
41	j	69	ASN
42	k	13	GLN
42	k	26	ASN
42	k	93	GLN
42	k	117	ASN
43	l	76	ASN
43	l	99	HIS
44	m	92	HIS
46	o	28	GLN
46	o	62	GLN
47	p	14	ASN
47	p	16	HIS
47	p	76	GLN
48	q	16	GLN
49	r	36	ASN
50	s	14	HIS
50	s	69	HIS
50	s	83	HIS
54	w	129	ASN
54	w	181	GLN
54	w	253	GLN
54	w	258	GLN
54	w	309	GLN
54	w	315	HIS
54	w	347	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2726/2915 (93%)	299 (10%)	13 (0%)
2	B	119/121 (98%)	9 (7%)	0
32	a	1483/1521 (97%)	177 (11%)	0
53	v	8/24 (33%)	1 (12%)	0
55	x	70/74 (94%)	4 (5%)	0
All	All	4406/4655 (94%)	490 (11%)	13 (0%)

All (490) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	34	C
1	A	45	C
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	95	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	128	C
1	A	129	C
1	A	131	G
1	A	141	A
1	A	154(A)	C
1	A	182	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	222	A
1	A	228	A
1	A	229	A
1	A	230	U
1	A	233	A
1	A	248	G
1	A	271(J)	C
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(O)	C
1	A	272(B)	G

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Mol	Chain	Res	Type
1	A	274	G
1	A	279	C
1	A	311	A
1	A	329	G
1	A	330	A
1	A	352	G
1	A	363	G
1	A	386	G
1	A	396	G
1	A	411	G
1	A	421	U
1	A	428	A
1	A	444	C
1	A	448	U
1	A	456	C
1	A	481	G
1	A	505	A
1	A	509	C
1	A	528	A
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	549	G
1	A	563	G
1	A	573	G
1	A	575	A
1	A	603	A
1	A	604	G
1	A	607	U
1	A	614(B)	G
1	A	615	G
1	A	627	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	686	G
1	A	717	G
1	A	730	C
1	A	775	G
1	A	776	G

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Mol	Chain	Res	Type
1	A	782	A
1	A	784	A
1	A	785	G
1	A	792	G
1	A	805	G
1	A	812	C
1	A	827	U
1	A	828	U
1	A	859	G
1	A	866	A
1	A	878	A
1	A	885	C
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	910	A
1	A	932	G
1	A	945	A
1	A	946	G
1	A	961	C
1	A	974	G
1	A	975	C
1	A	983	A
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1026	U
1	A	1033	U
1	A	1038	C
1	A	1040	C
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1054	A
1	A	1110	G
1	A	1112	G
1	A	1135	C
1	A	1136	G

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Mol	Chain	Res	Type
1	A	1171	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1178	C
1	A	1184	G
1	A	1211	U
1	A	1220	A
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	U
1	A	1301	A
1	A	1308	A
1	A	1320	C
1	A	1321	A
1	A	1352	U
1	A	1359	A
1	A	1360	A
1	A	1365	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1416	G
1	A	1417	C
1	A	1421	G
1	A	1428	C
1	A	1445	A
1	A	1450	G
1	A	1455	G
1	A	1467	C
1	A	1482	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1506	C
1	A	1509	C
1	A	1509(A)	A

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Mol	Chain	Res	Type
1	A	1523	U
1	A	1543	C
1	A	1547	C
1	A	1554	A
1	A	1558	A
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1584	C
1	A	1586	A
1	A	1595	G
1	A	1608	A
1	A	1609	A
1	A	1648	C
1	A	1674	G
1	A	1696	G
1	A	1700	A
1	A	1756	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1780	A
1	A	1791	A
1	A	1800	C
1	A	1801	G
1	A	1816	G
1	A	1847	A
1	A	1848	A
1	A	1878	G
1	A	1889	A
1	A	1900	A
1	A	1906	G
1	A	1914	C
1	A	1915	5MU
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1955	U
1	A	1963	U

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Mol	Chain	Res	Type
1	A	1967	C
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1984	G
1	A	1993	U
1	A	1997	G
1	A	2020	A
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2102	U
1	A	2192	G
1	A	2198	A
1	A	2206	G
1	A	2207	G
1	A	2218	U
1	A	2219	G
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2305	A
1	A	2308	G
1	A	2320	A
1	A	2325	G
1	A	2336	A
1	A	2347	C
1	A	2350	C
1	A	2383	G
1	A	2385	C
1	A	2406	U

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Mol	Chain	Res	Type
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2439	A
1	A	2441	C
1	A	2448	A
1	A	2476	A
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2602	A
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2629	A
1	A	2630	G
1	A	2646	C
1	A	2654	A
1	A	2689	U
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2703	C
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2764	A
1	A	2765	A
1	A	2766	G

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Mol	Chain	Res	Type
1	A	2769	C
1	A	2778	A
1	A	2789	C
1	A	2790	A
1	A	2791	C
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2833	G
1	A	2835	A
1	A	2872	G
1	A	2880	C
1	A	2892	A
1	A	2894	G
2	B	12	C
2	B	24	G
2	B	35	U
2	B	53	A
2	B	56	G
2	B	67	G
2	B	73	A
2	B	89	G
2	B	110	G
32	a	7	G
32	a	9	G
32	a	32	A
32	a	39	G
32	a	47	C
32	a	48	C
32	a	50	A
32	a	51	A
32	a	61	G
32	a	116	A
32	a	121	C
32	a	131	C
32	a	157	G
32	a	174	C
32	a	182	U
32	a	189	G
32	a	189(E)	U
32	a	195	A
32	a	197	A

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Mol	Chain	Res	Type
32	a	247	G
32	a	251	G
32	a	266	G
32	a	267	C
32	a	281	G
32	a	289	G
32	a	301	G
32	a	321	A
32	a	328	C
32	a	332	G
32	a	343	U
32	a	344	A
32	a	347	G
32	a	352	C
32	a	353	A
32	a	354	G
32	a	367	U
32	a	372	C
32	a	373	A
32	a	397	A
32	a	398	C
32	a	406	G
32	a	412	A
32	a	413	G
32	a	421	U
32	a	424	G
32	a	429	U
32	a	439	A
32	a	452	A
32	a	455	C
32	a	485	G
32	a	496	A
32	a	498	U
32	a	509	A
32	a	510	A
32	a	511	C
32	a	518	C
32	a	521	G
32	a	527	G7M
32	a	528	C
32	a	532	A
32	a	547	A

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Mol	Chain	Res	Type
32	a	559	A
32	a	564	C
32	a	572	A
32	a	573	A
32	a	576	G
32	a	577	G
32	a	653	A
32	a	665	A
32	a	671	G
32	a	687	A
32	a	688	G
32	a	695	A
32	a	749	C
32	a	755	G
32	a	777	A
32	a	793	U
32	a	794	A
32	a	816	A
32	a	817	C
32	a	821	G
32	a	828	A
32	a	840	C
32	a	841	U
32	a	848	C
32	a	859	A
32	a	902	G
32	a	914	A
32	a	926	G
32	a	927	G
32	a	934	C
32	a	935	A
32	a	942	G
32	a	960	U
32	a	961	U
32	a	969	A
32	a	971	G
32	a	975	A
32	a	976	G
32	a	977	A
32	a	992	U
32	a	993	G
32	a	997	U

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Mol	Chain	Res	Type
32	a	1000	U
32	a	1003	G
32	a	1005	A
32	a	1006	C
32	a	1011	G
32	a	1020	U
32	a	1022	G
32	a	1025	U
32	a	1026	G
32	a	1030(A)	G
32	a	1030(B)	C
32	a	1030(C)	G
32	a	1043	C
32	a	1044	A
32	a	1045	C
32	a	1054	C
32	a	1065	U
32	a	1066	C
32	a	1068	G
32	a	1081	G
32	a	1094	G
32	a	1095	U
32	a	1101	A
32	a	1123	A
32	a	1137	C
32	a	1139	G
32	a	1140	C
32	a	1146	A
32	a	1159	U
32	a	1184	G
32	a	1196	U
32	a	1197	G
32	a	1202	G
32	a	1212	U
32	a	1213	A
32	a	1214	C
32	a	1227	A
32	a	1236	A
32	a	1238	A
32	a	1256	A
32	a	1257	U
32	a	1260	C

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Mol	Chain	Res	Type
32	a	1270	C
32	a	1275	A
32	a	1278	U
32	a	1279	A
32	a	1280	A
32	a	1287	A
32	a	1299	A
32	a	1300	G
32	a	1302	U
32	a	1320	C
32	a	1338	G
32	a	1340	A
32	a	1346	A
32	a	1347	G
32	a	1353	G
32	a	1363	C
32	a	1370	G
32	a	1419	G
32	a	1442	G
32	a	1442(A)	G
32	a	1447	A
32	a	1452	C
32	a	1457	G
32	a	1487	G
32	a	1493	A
32	a	1494	G
32	a	1497	G
32	a	1504	G
32	a	1506	U
32	a	1517	G
32	a	1529	G
32	a	1530	G
53	v	22	U
55	x	18	G
55	x	19	G
55	x	26	A
55	x	46	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	128	C

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Mol	Chain	Res	Type
1	A	196	A
1	A	266	G
1	A	278	A
1	A	548	A
1	A	1210	A
1	A	1379	A
1	A	1420	U
1	A	1442	G
1	A	1489	U
1	A	1508	A
1	A	2430	A
1	A	2689	U

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

32 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	$\#\|Z\| > 2$
32	MA6	a	1518	32	23,26,27	1.52	4 (17%)	33,38,41	2.30	14 (42%)
1	PSU	A	2605	57,1	18,21,22	1.41	3 (16%)	21,30,33	2.14	4 (19%)
32	UR3	a	1498	32	19,22,23	0.92	0	26,32,35	1.82	3 (11%)
55	H2U	x	20	55	18,21,22	0.94	2 (11%)	19,30,33	0.86	1 (5%)
55	MIA	x	37	57,55	21,24,32	1.53	4 (19%)	30,35,47	2.03	9 (30%)
55	5MU	x	54	55	19,22,23	1.42	6 (31%)	27,32,35	2.09	6 (22%)
43	0TD	l	92	43	8,9,10	4.55	1 (12%)	6,11,13	9.05	3 (50%)
32	5MC	a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.12	3 (11%)
54	MEQ	w	230	54	8,9,10	0.57	0	5,10,12	0.58	0
55	PSU	x	39	57,55	18,21,22	1.42	3 (16%)	21,30,33	1.86	3 (14%)
55	PSU	x	32	57,55	18,21,22	1.36	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	a	1519	57,32	23,26,27	1.51	4 (17%)	33,38,41	2.32	12 (36%)
1	PSU	A	1911	1	18,21,22	1.35	3 (16%)	21,30,33	2.04	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	M2G	a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.88	6 (18%)
1	5MC	A	1962	57,1,58	19,22,23	1.73	3 (15%)	26,32,35	1.12	3 (11%)
32	4OC	a	1402	57,32	20,23,24	0.76	0	25,32,35	1.02	2 (8%)
32	5MC	a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.11	2 (7%)
1	OMG	A	2251	57,1,55,58	23,26,27	1.20	3 (13%)	32,38,41	2.16	7 (21%)
1	5MU	A	1915	1	19,22,23	1.44	6 (31%)	27,32,35	2.06	5 (18%)
1	5MU	A	1939	1,58	19,22,23	1.44	5 (26%)	27,32,35	2.05	6 (22%)
32	2MG	a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.20	7 (21%)
32	5MC	a	1404	57,32	19,22,23	1.65	3 (15%)	26,32,35	1.13	3 (11%)
1	5MC	A	1942	57,1	19,22,23	1.68	3 (15%)	26,32,35	1.14	3 (11%)
1	OMU	A	2552	57,1	19,22,23	1.23	3 (15%)	25,31,34	1.81	5 (20%)
1	PSU	A	1917	1	18,21,22	1.43	3 (16%)	21,30,33	2.10	4 (19%)
55	4SU	x	8	55	18,21,22	1.86	4 (22%)	25,30,33	2.03	5 (20%)
1	2MA	A	2503	57,1,58	22,25,26	1.47	3 (13%)	32,37,40	2.36	7 (21%)
32	5MC	a	967	32	19,22,23	1.56	3 (15%)	26,32,35	1.12	3 (11%)
1	OMC	A	1920	1	19,22,23	0.79	0	25,31,34	0.98	1 (4%)
32	G7M	a	527	32	23,26,27	1.52	3 (13%)	34,39,42	1.71	5 (14%)
32	PSU	a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	2.09	4 (19%)
55	PSU	x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)

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
32	MA6	a	1518	32	-	1/11/29/30	0/3/3/3
1	PSU	A	2605	57,1	-	0/7/25/26	0/2/2/2
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2
55	H2U	x	20	55	-	0/7/38/39	0/2/2/2
55	MIA	x	37	57,55	-	0/7/25/34	0/3/3/3
55	5MU	x	54	55	-	0/7/25/26	0/2/2/2
43	0TD	l	92	43	-	2/7/12/14	-
32	5MC	a	1407	32	-	0/7/25/26	0/2/2/2
54	MEQ	w	230	54	-	2/8/9/11	-
55	PSU	x	39	57,55	-	0/7/25/26	0/2/2/2
55	PSU	x	32	57,55	-	0/7/25/26	0/2/2/2
32	MA6	a	1519	57,32	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	A	1962	57,1,58	-	0/7/25/26	0/2/2/2
32	4OC	a	1402	57,32	-	0/9/29/30	0/2/2/2
32	5MC	a	1400	32	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	57,1,55,58	-	1/9/27/28	0/3/3/3
1	5MU	A	1915	1	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1,58	-	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	a	1404	57,32	-	0/7/25/26	0/2/2/2
1	5MC	A	1942	57,1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	57,1	-	0/9/27/28	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	x	8	55	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	57,1,58	-	2/7/25/26	0/3/3/3
32	5MC	a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	A	1920	1	-	0/9/27/28	0/2/2/2
32	G7M	a	527	32	-	3/7/25/26	0/3/3/3
32	PSU	a	516	57,32	-	0/7/25/26	0/2/2/2
55	PSU	x	55	55	-	0/7/25/26	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	l	92	0TD	CB-SB	-12.56	1.69	1.82
1	A	1962	5MC	C5-C4	6.48	1.49	1.44
32	a	1400	5MC	C5-C4	6.12	1.48	1.44
32	a	1407	5MC	C5-C4	6.09	1.48	1.44
1	A	1942	5MC	C5-C4	6.08	1.48	1.44
32	a	1404	5MC	C5-C4	6.02	1.48	1.44
32	a	967	5MC	C5-C4	5.56	1.48	1.44
55	x	8	4SU	C4-S4	-4.98	1.59	1.68
32	a	527	G7M	C5-N7	-4.69	1.33	1.39
32	a	1518	MA6	C5-C4	4.68	1.47	1.39
55	x	37	MIA	C5-C4	4.50	1.47	1.39
32	a	1519	MA6	C5-C4	4.49	1.47	1.39
1	A	2503	2MA	C5-C4	4.46	1.47	1.39
55	x	8	4SU	C4-N3	-3.52	1.34	1.37
55	x	39	PSU	C6-C5	3.50	1.39	1.35
1	A	2605	PSU	C6-C5	3.43	1.39	1.35
55	x	55	PSU	C6-C5	3.37	1.39	1.35
1	A	1917	PSU	C6-C5	3.37	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	516	PSU	C6-C5	3.28	1.38	1.35
32	a	527	G7M	C5-C4	3.26	1.46	1.38
1	A	2251	OMG	C5-C4	3.12	1.47	1.38
1	A	2605	PSU	C4-N3	-3.05	1.33	1.38
55	x	32	PSU	C6-C5	3.05	1.38	1.35
1	A	1942	5MC	C6-C5	3.05	1.39	1.34
1	A	1911	PSU	C6-C5	3.05	1.38	1.35
32	a	966	M2G	C5-C4	3.04	1.47	1.38
32	a	1207	2MG	C5-C4	3.00	1.47	1.38
32	a	1518	MA6	C5-C6	2.94	1.48	1.41
55	x	39	PSU	C4-N3	-2.92	1.33	1.38
55	x	8	4SU	C5-C4	-2.88	1.39	1.42
1	A	1939	5MU	C4-N3	-2.88	1.33	1.38
1	A	1917	PSU	C4-N3	-2.88	1.33	1.38
1	A	1915	5MU	C4-N3	-2.87	1.33	1.38
1	A	2552	OMU	C4-N3	-2.87	1.33	1.38
1	A	1939	5MU	C6-C5	2.86	1.39	1.34
32	a	1519	MA6	C5-C6	2.84	1.48	1.41
32	a	1404	5MC	C6-C5	2.80	1.39	1.34
55	x	32	PSU	C4-N3	-2.80	1.33	1.38
1	A	2251	OMG	C6-N1	-2.78	1.33	1.38
32	a	1400	5MC	C6-C5	2.78	1.39	1.34
55	x	55	PSU	C4-N3	-2.77	1.33	1.38
1	A	1911	PSU	C4-N3	-2.75	1.33	1.38
32	a	967	5MC	C6-C5	2.74	1.39	1.34
32	a	1407	5MC	C6-C5	2.73	1.39	1.34
32	a	966	M2G	C2-N2	2.71	1.40	1.35
32	a	966	M2G	C6-N1	-2.71	1.33	1.38
55	x	54	5MU	C4-N3	-2.71	1.33	1.38
32	a	516	PSU	C4-N3	-2.70	1.33	1.38
55	x	37	MIA	C5-C6	2.70	1.48	1.41
1	A	1962	5MC	C6-C5	2.68	1.39	1.34
1	A	2503	2MA	C5-C6	2.66	1.48	1.41
1	A	1915	5MU	C6-C5	2.61	1.38	1.34
1	A	2503	2MA	C5-N7	-2.53	1.34	1.39
55	x	20	H2U	C2-N3	-2.53	1.33	1.38
32	a	527	G7M	C6-N1	-2.52	1.34	1.38
32	a	1207	2MG	C6-N1	-2.50	1.34	1.38
55	x	54	5MU	C6-C5	2.47	1.38	1.34
1	A	1939	5MU	C2-N3	-2.45	1.33	1.38
1	A	1915	5MU	C2-N1	2.45	1.42	1.38
32	a	1519	MA6	C5-N7	-2.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	5MU	C4-C5	2.41	1.48	1.44
55	x	54	5MU	C4-C5	2.37	1.48	1.44
55	x	37	MIA	C5-N7	-2.36	1.34	1.39
32	a	1518	MA6	C5-N7	-2.35	1.34	1.39
32	a	966	M2G	C5-N7	-2.35	1.34	1.39
55	x	54	5MU	C2-N1	2.34	1.42	1.38
1	A	1962	5MC	C6-N1	-2.30	1.34	1.38
55	x	37	MIA	C8-N7	2.30	1.36	1.31
55	x	54	5MU	C6-N1	-2.30	1.34	1.38
55	x	20	H2U	C4-N3	-2.27	1.33	1.37
1	A	1915	5MU	C6-N1	-2.26	1.34	1.38
32	a	1400	5MC	C6-N1	-2.25	1.34	1.38
1	A	1915	5MU	C2-N3	-2.24	1.34	1.38
1	A	2251	OMG	C5-N7	-2.22	1.34	1.39
32	a	967	5MC	C6-N1	-2.22	1.34	1.38
55	x	54	5MU	C2-N3	-2.21	1.34	1.38
1	A	1939	5MU	C6-N1	-2.21	1.34	1.38
32	a	1404	5MC	C6-N1	-2.20	1.34	1.38
32	a	1407	5MC	C6-N1	-2.20	1.34	1.38
1	A	2552	OMU	C2-N3	-2.18	1.34	1.38
55	x	8	4SU	C2-N3	-2.18	1.34	1.38
1	A	1917	PSU	C2-N3	-2.17	1.33	1.37
1	A	2605	PSU	C2-N3	-2.15	1.33	1.37
1	A	1942	5MC	C6-N1	-2.14	1.34	1.38
1	A	1915	5MU	C4-C5	2.13	1.48	1.44
32	a	1518	MA6	C4-N9	-2.12	1.33	1.37
55	x	39	PSU	C2-N3	-2.11	1.34	1.37
32	a	1519	MA6	C4-N9	-2.10	1.33	1.37
32	a	1207	2MG	C5-N7	-2.08	1.34	1.39
1	A	1911	PSU	C2-N3	-2.07	1.34	1.37
1	A	2552	OMU	C5-C4	-2.04	1.39	1.43

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	l	92	0TD	CSB-SB-CB	-21.70	63.36	102.36
1	A	2503	2MA	C5-C4-N3	-8.52	118.21	127.18
32	a	1498	UR3	C4-N3-C2	-7.34	118.67	124.58
32	a	1207	2MG	C2-N3-C4	7.18	120.98	112.00
1	A	2251	OMG	C5-C4-N3	-6.96	117.32	128.39
1	A	2503	2MA	N3-C4-N9	6.74	135.55	126.99
1	A	2605	PSU	N1-C2-N3	6.72	122.26	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1917	PSU	N1-C2-N3	6.68	122.22	115.17
55	x	55	PSU	N1-C2-N3	6.42	121.94	115.17
32	a	516	PSU	N1-C2-N3	6.34	121.86	115.17
55	x	32	PSU	N1-C2-N3	6.34	121.86	115.17
1	A	1911	PSU	N1-C2-N3	6.31	121.82	115.17
32	a	966	M2G	C5-C4-N3	-6.15	118.60	128.39
32	a	1207	2MG	C5-C4-N3	-5.91	118.98	128.39
55	x	39	PSU	N1-C2-N3	5.78	121.27	115.17
55	x	8	4SU	C4-N3-C2	-5.76	121.79	127.31
1	A	2251	OMG	C2-N3-C4	5.66	122.05	112.30
55	x	37	MIA	C5-C4-N3	-5.58	119.04	126.72
32	a	527	G7M	N9-C4-N3	5.46	136.87	125.95
32	a	1519	MA6	C5-C4-N3	-5.45	119.21	126.72
32	a	1518	MA6	C5-C4-N3	-5.33	119.37	126.72
55	x	8	4SU	C5-C4-N3	5.28	119.66	114.75
32	a	527	G7M	C5-C4-N3	-5.27	118.19	128.15
1	A	1939	5MU	N3-C2-N1	5.26	121.74	114.89
1	A	2251	OMG	N9-C4-N3	5.25	136.45	125.95
1	A	1915	5MU	N3-C2-N1	5.12	121.56	114.89
55	x	54	5MU	C4-N3-C2	-5.05	120.72	127.34
1	A	1939	5MU	C4-N3-C2	-4.99	120.80	127.34
1	A	1915	5MU	C4-N3-C2	-4.97	120.83	127.34
32	a	966	M2G	N9-C4-N3	4.89	135.74	125.95
55	x	54	5MU	N3-C2-N1	4.86	121.21	114.89
1	A	2552	OMU	C4-N3-C2	-4.71	120.76	126.61
32	a	527	G7M	C2-N3-C4	4.69	120.38	112.30
1	A	2552	OMU	N3-C2-N1	4.57	120.85	114.89
32	a	1518	MA6	C2-N1-C6	4.48	122.78	111.83
55	x	54	5MU	C5-C4-N3	4.47	119.21	115.32
32	a	1519	MA6	C2-N1-C6	4.43	122.64	111.83
32	a	966	M2G	C2-N3-C4	4.39	120.63	112.51
1	A	2605	PSU	C4-N3-C2	-4.36	120.37	126.37
32	a	1519	MA6	N3-C4-N9	4.33	134.54	127.17
1	A	1917	PSU	C4-N3-C2	-4.31	120.44	126.37
55	x	37	MIA	N3-C4-N9	4.28	134.45	127.17
1	A	1939	5MU	C5-C4-N3	4.20	118.97	115.32
1	A	1911	PSU	C4-N3-C2	-4.18	120.61	126.37
32	a	1518	MA6	C9-N6-C6	-4.15	109.95	120.52
55	x	55	PSU	C4-N3-C2	-4.15	120.66	126.37
32	a	1207	2MG	N9-C4-N3	4.14	134.24	125.95
32	a	1518	MA6	N3-C4-N9	4.13	134.19	127.17
1	A	1915	5MU	C5-C4-N3	4.10	118.89	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	516	PSU	C4-N3-C2	-4.09	120.73	126.37
32	a	1519	MA6	C9-N6-C6	-4.07	110.18	120.52
55	x	32	PSU	C4-N3-C2	-4.06	120.78	126.37
55	x	54	5MU	O4-C4-C5	-3.99	120.35	124.92
32	a	1518	MA6	C4-C5-N7	-3.97	106.04	110.58
55	x	8	4SU	N3-C2-N1	3.81	119.85	114.89
32	a	1519	MA6	C4-C5-N7	-3.77	106.27	110.58
55	x	37	MIA	N3-C2-N1	-3.75	122.90	128.58
55	x	37	MIA	C2-N3-C4	3.74	120.98	111.83
32	a	516	PSU	O2-C2-N1	-3.74	118.93	122.79
1	A	1939	5MU	C5-C6-N1	-3.70	119.30	123.31
1	A	1915	5MU	O4-C4-C5	-3.69	120.69	124.92
55	x	39	PSU	C4-N3-C2	-3.67	121.32	126.37
55	x	37	MIA	C4-C5-N7	-3.60	106.46	110.58
32	a	1207	2MG	C6-C5-N7	3.60	136.83	130.29
32	a	1518	MA6	C2-N3-C4	3.59	120.60	111.83
1	A	2552	OMU	C5-C4-N3	3.58	119.82	114.80
1	A	1915	5MU	C5-C6-N1	-3.57	119.44	123.31
55	x	8	4SU	C5-C4-S4	-3.56	120.24	124.31
32	a	1519	MA6	C2-N3-C4	3.55	120.51	111.83
1	A	1911	PSU	O2-C2-N1	-3.53	119.15	122.79
1	A	2503	2MA	C4-C5-N7	-3.52	106.56	110.58
32	a	1498	UR3	C5-C4-N3	3.51	119.66	115.04
43	l	92	0TD	OD2-CG-CB	3.48	120.66	113.15
1	A	2605	PSU	O2-C2-N1	-3.46	119.22	122.79
55	x	32	PSU	O2-C2-N1	-3.46	119.22	122.79
55	x	54	5MU	C5-C6-N1	-3.45	119.56	123.31
32	a	1518	MA6	N1-C2-N3	-3.43	123.39	128.58
1	A	1939	5MU	O4-C4-C5	-3.42	121.01	124.92
32	a	1519	MA6	N1-C2-N3	-3.42	123.41	128.58
1	A	1917	PSU	O2-C2-N1	-3.25	119.44	122.79
1	A	1942	5MC	C5-C6-N1	-3.24	119.79	123.31
32	a	1407	5MC	C5-C6-N1	-3.23	119.80	123.31
1	A	1962	5MC	C5-C6-N1	-3.20	119.84	123.31
55	x	55	PSU	O2-C2-N1	-3.19	119.50	122.79
32	a	1400	5MC	C5-C6-N1	-3.18	119.86	123.31
32	a	1404	5MC	C5-C6-N1	-3.18	119.86	123.31
1	A	1942	5MC	C5-C4-N3	-3.14	118.54	121.75
1	A	2251	OMG	C6-C5-N7	3.12	135.97	130.29
32	a	967	5MC	C5-C6-N1	-3.01	120.04	123.31
32	a	1519	MA6	N1-C6-N6	2.98	120.49	116.86
1	A	2503	2MA	N6-C6-N1	2.97	121.04	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	1518	MA6	C10-N6-C6	-2.94	113.04	120.52
32	a	1519	MA6	C4-N9-C8	2.93	108.81	105.74
1	A	1962	5MC	C5-C4-N3	-2.89	118.79	121.75
32	a	1400	5MC	C5-C4-N3	-2.89	118.80	121.75
32	a	1518	MA6	C5-N7-C8	2.87	107.97	103.45
1	A	2552	OMU	O4-C4-C5	-2.87	120.21	125.16
32	a	1518	MA6	C4-N9-C8	2.83	108.71	105.74
32	a	1519	MA6	C5-N7-C8	2.82	107.89	103.45
32	a	966	M2G	C6-C5-N7	2.82	135.43	130.29
32	a	1207	2MG	C4-C5-N7	-2.82	106.20	110.67
32	a	967	5MC	C5-C4-N3	-2.82	118.87	121.75
32	a	1407	5MC	C5-C4-N3	-2.79	118.90	121.75
32	a	1404	5MC	C5-C4-N3	-2.76	118.93	121.75
32	a	1207	2MG	N1-C2-N2	2.65	119.26	116.56
32	a	1519	MA6	C10-N6-C6	-2.63	113.84	120.52
1	A	2503	2MA	C5-N7-C8	2.62	107.57	103.45
55	x	39	PSU	O2-C2-N1	-2.62	120.09	122.79
55	x	37	MIA	C4-N9-C8	2.60	108.46	105.74
55	x	37	MIA	C5-N7-C8	2.58	107.51	103.45
1	A	2251	OMG	C4-C5-N7	-2.57	106.59	110.67
32	a	1402	4OC	C6-C5-C4	2.54	120.06	117.00
1	A	1920	OMC	O2-C2-N3	-2.53	118.34	122.33
1	A	2503	2MA	C2-N1-C6	2.52	121.97	118.10
1	A	1939	5MU	O2-C2-N1	-2.50	119.54	122.80
43	l	92	0TD	OD1-CG-CB	-2.50	117.21	122.44
32	a	516	PSU	O4'-C1'-C2'	2.49	108.59	105.15
1	A	2605	PSU	C5-C6-N1	-2.46	118.72	122.14
1	A	1917	PSU	C5-C6-N1	-2.36	118.86	122.14
55	x	20	H2U	C5-C6-N1	-2.36	104.38	111.52
1	A	2503	2MA	C4-N9-C8	2.34	108.19	105.74
1	A	2552	OMU	O2-C2-N1	-2.34	119.75	122.80
32	a	1404	5MC	O2-C2-N3	-2.33	118.66	122.33
32	a	527	G7M	O6-C6-C5	-2.31	122.85	128.01
32	a	1518	MA6	C6-C5-N7	2.31	137.12	133.43
32	a	1519	MA6	N9-C8-N7	-2.24	110.76	113.94
1	A	1911	PSU	C5-C6-N1	-2.23	119.04	122.14
32	a	966	M2G	C4-C5-N7	-2.23	107.14	110.67
32	a	966	M2G	O6-C6-C5	-2.22	120.66	126.53
55	x	55	PSU	C5-C6-N1	-2.22	119.05	122.14
55	x	37	MIA	C6-C5-N7	2.20	136.34	132.09
32	a	1518	MA6	N9-C8-N7	-2.18	110.84	113.94
32	a	1498	UR3	C3U-N3-C4	2.18	120.89	117.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2251	OMG	C5-C6-N1	2.18	118.79	113.25
32	a	967	5MC	O2-C2-N3	-2.16	118.92	122.33
32	a	1518	MA6	N1-C6-N6	2.14	119.46	116.86
32	a	1518	MA6	C10-N6-C9	-2.12	109.36	116.18
32	a	527	G7M	C5-C6-N1	2.12	116.23	111.84
1	A	1962	5MC	O2-C2-N3	-2.08	119.05	122.33
1	A	1942	5MC	O2-C2-N3	-2.07	119.07	122.33
55	x	54	5MU	O2-C2-N1	-2.06	120.12	122.80
32	a	1402	4OC	O2-C2-N3	-2.06	119.09	122.33
55	x	8	4SU	C1'-N1-C2	2.04	121.26	117.59
55	x	37	MIA	N9-C8-N7	-2.03	111.06	113.94
32	a	1407	5MC	O2-C2-N3	-2.02	119.15	122.33
1	A	1911	PSU	O4'-C1'-C2'	2.02	107.94	105.15
32	a	1207	2MG	N2-C2-N3	-2.00	117.96	120.51
1	A	2251	OMG	C2-N1-C6	-2.00	121.48	125.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2251	OMG	C1'-C2'-O2'-CM2
1	A	1915	5MU	C3'-C4'-C5'-O5'
1	A	1915	5MU	O4'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
32	a	527	G7M	C3'-C4'-C5'-O5'
32	a	1519	MA6	C3'-C4'-C5'-O5'
32	a	1518	MA6	C5-C6-N6-C10
32	a	1519	MA6	C5-C6-N6-C10
32	a	527	G7M	C4'-C5'-O5'-P
1	A	2503	2MA	C4'-C5'-O5'-P
54	w	230	MEQ	OE1-CD-CG-CB
54	w	230	MEQ	NE2-CD-CG-CB
43	l	92	0TD	SB-CB-CG-OD2
43	l	92	0TD	CG-CB-SB-CSB
1	A	2503	2MA	O4'-C4'-C5'-O5'
32	a	527	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	1518	MA6	1	0
54	w	230	MEQ	2	0
32	a	1519	MA6	1	0
1	A	2251	OMG	1	0
55	x	8	4SU	1	0
1	A	2503	2MA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1744 ligands modelled in this entry, 1743 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
60	SF4	d	501	35	0,12,12	-	-	-		

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
60	SF4	d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

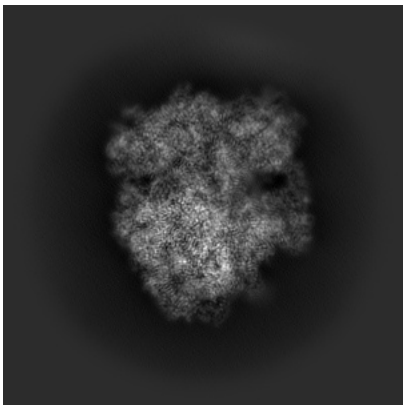
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49594. These allow visual inspection of the internal detail of the map and identification of artifacts.

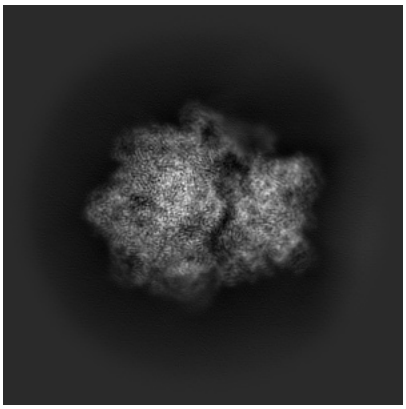
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

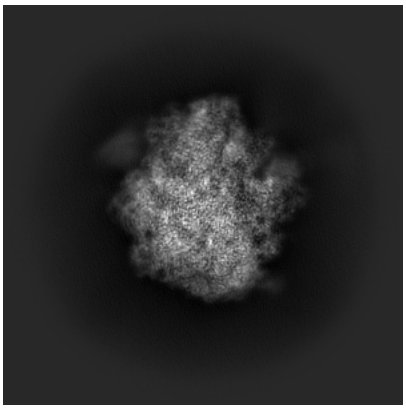
6.1.1 Primary map



X

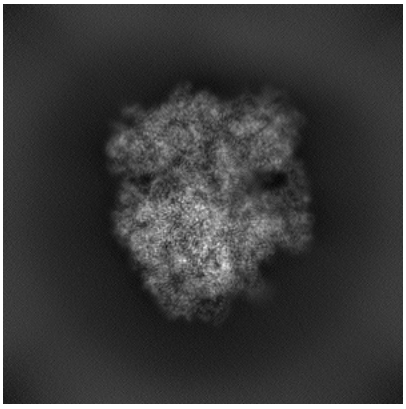


Y

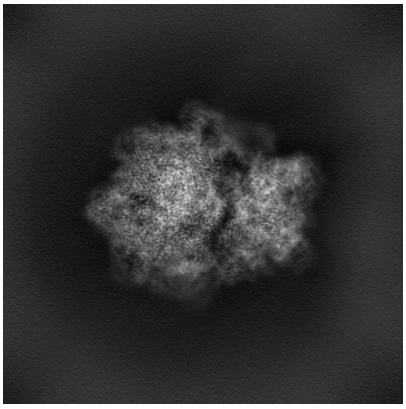


Z

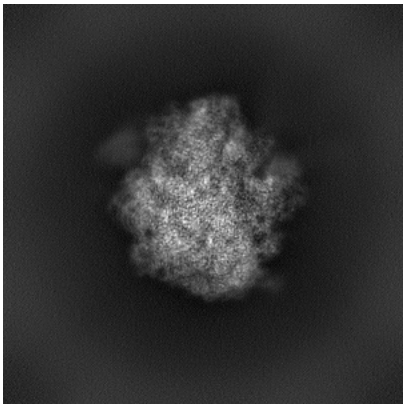
6.1.2 Raw map



X



Y

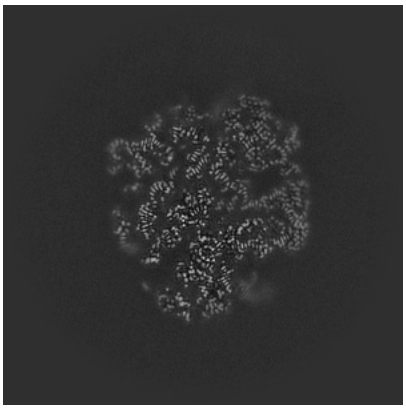


Z

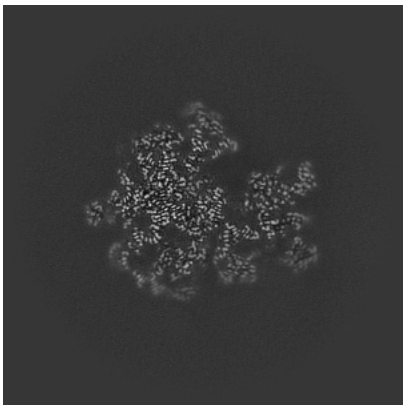
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

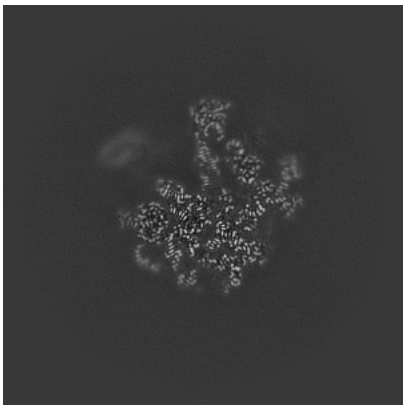
6.2.1 Primary map



X Index: 256

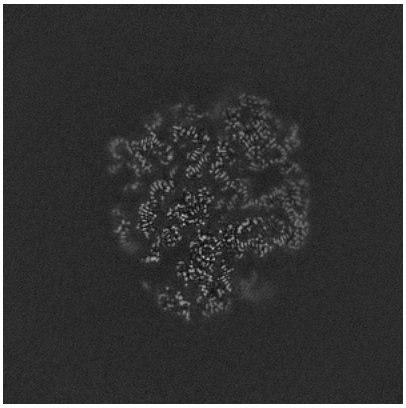


Y Index: 256

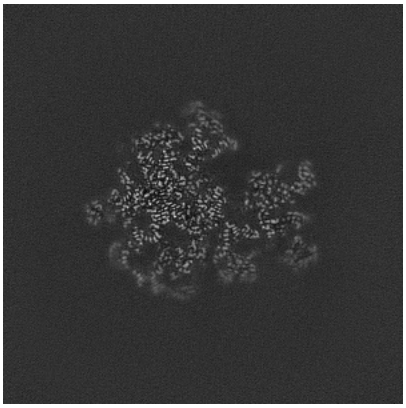


Z Index: 256

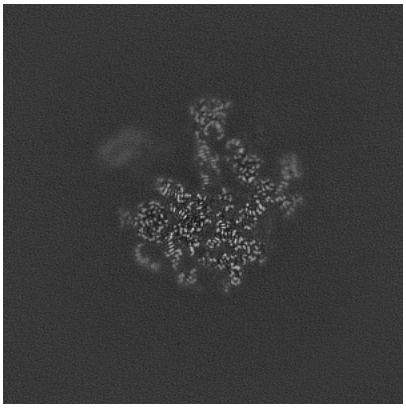
6.2.2 Raw map



X Index: 256



Y Index: 256

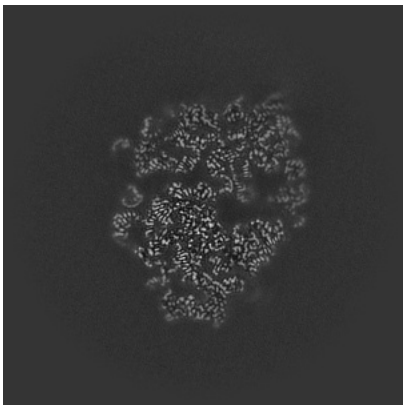


Z Index: 256

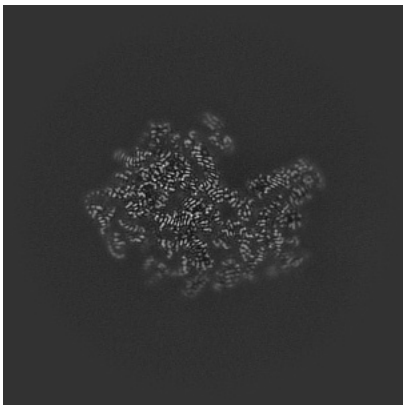
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

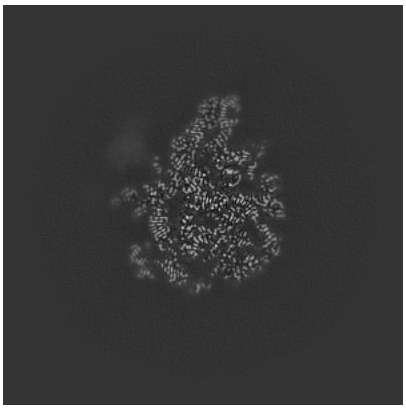
6.3.1 Primary map



X Index: 243

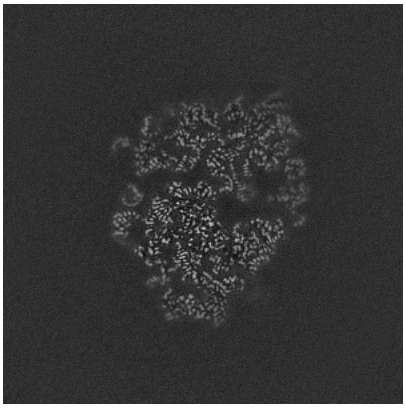


Y Index: 240

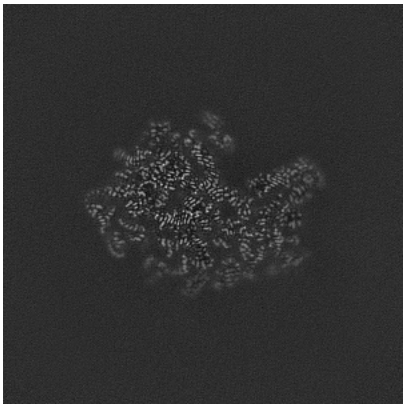


Z Index: 212

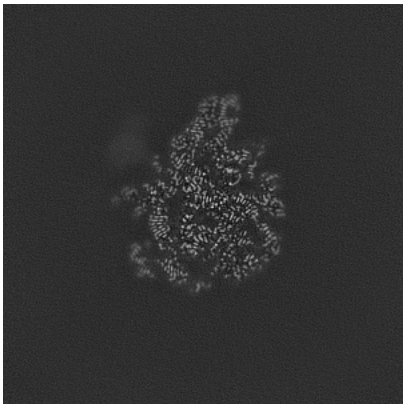
6.3.2 Raw map



X Index: 243



Y Index: 240

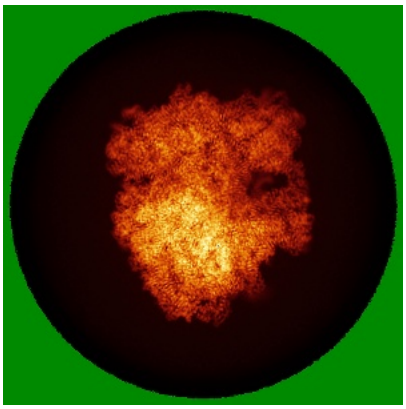


Z Index: 212

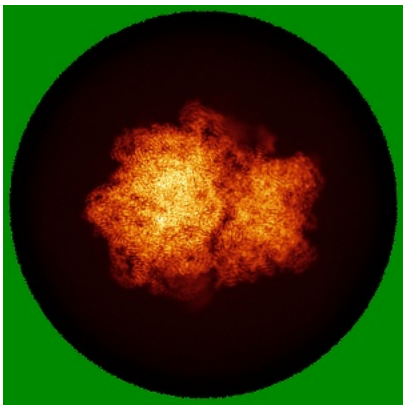
The images above show the largest variance slices of the map in three orthogonal directions.

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

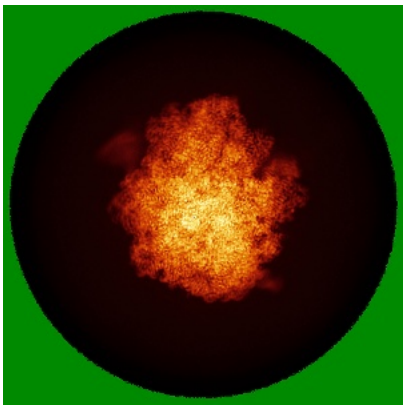
6.4.1 Primary map



X

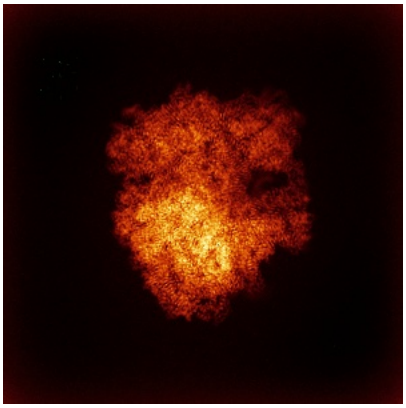


Y

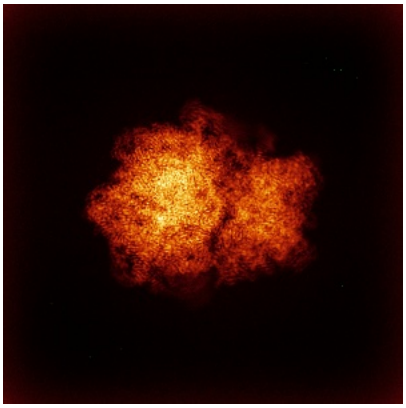


Z

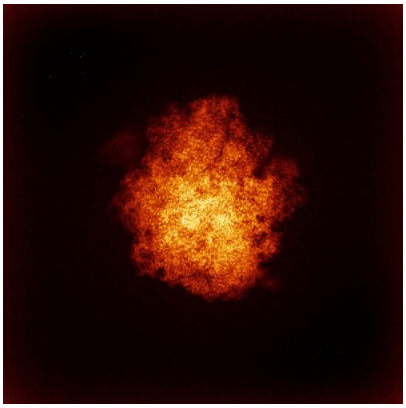
6.4.2 Raw map



X



Y

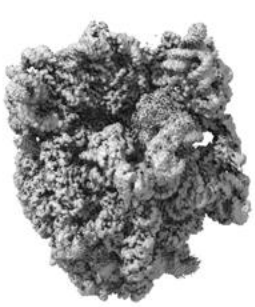


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



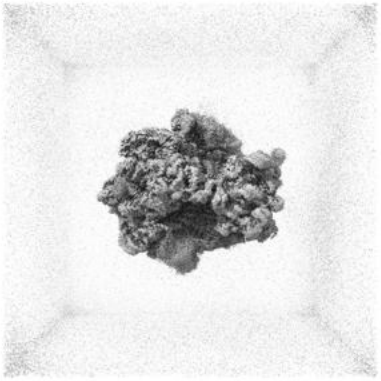
Z

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

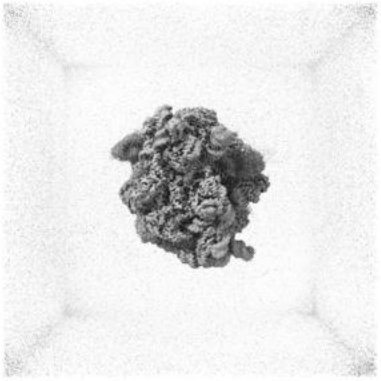
6.5.2 Raw map



X



Y



Z

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

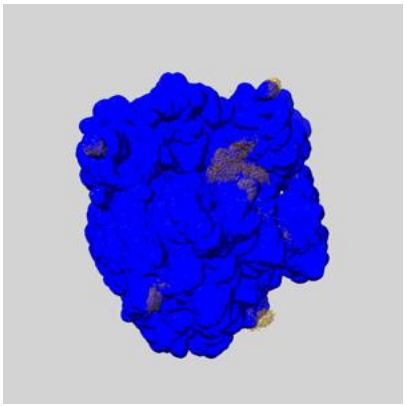
6.6 Mask visualisation (i)

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

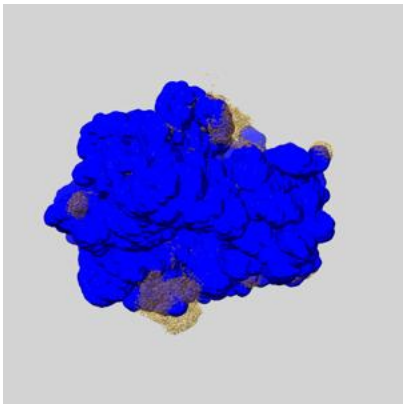
A mask typically either:

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

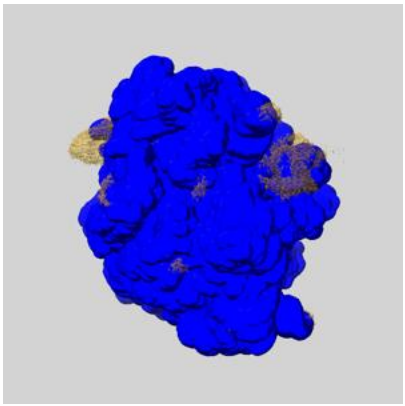
6.6.1 emd_49594_msk_1.map (i)



X



Y

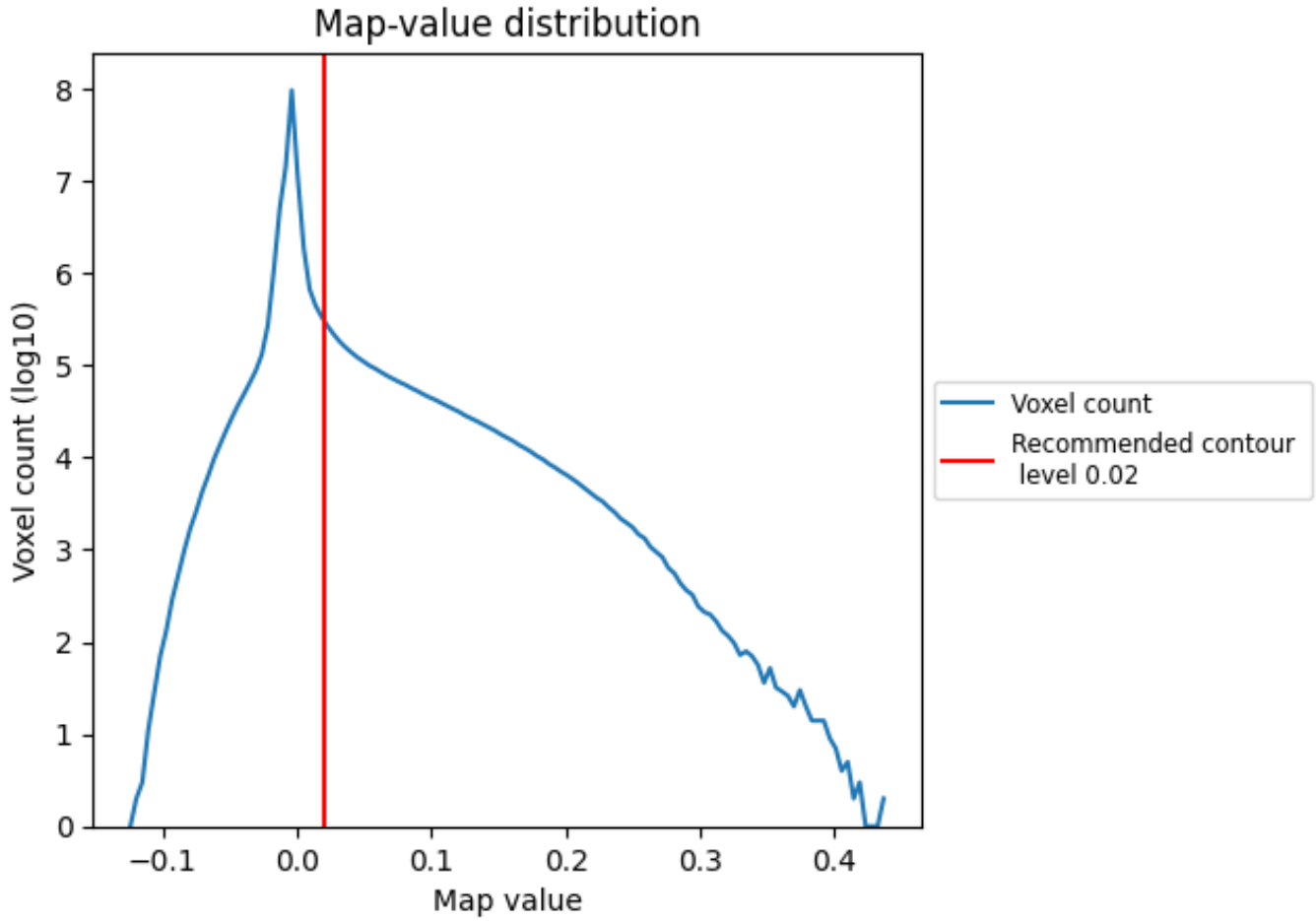


Z

7 Map analysis

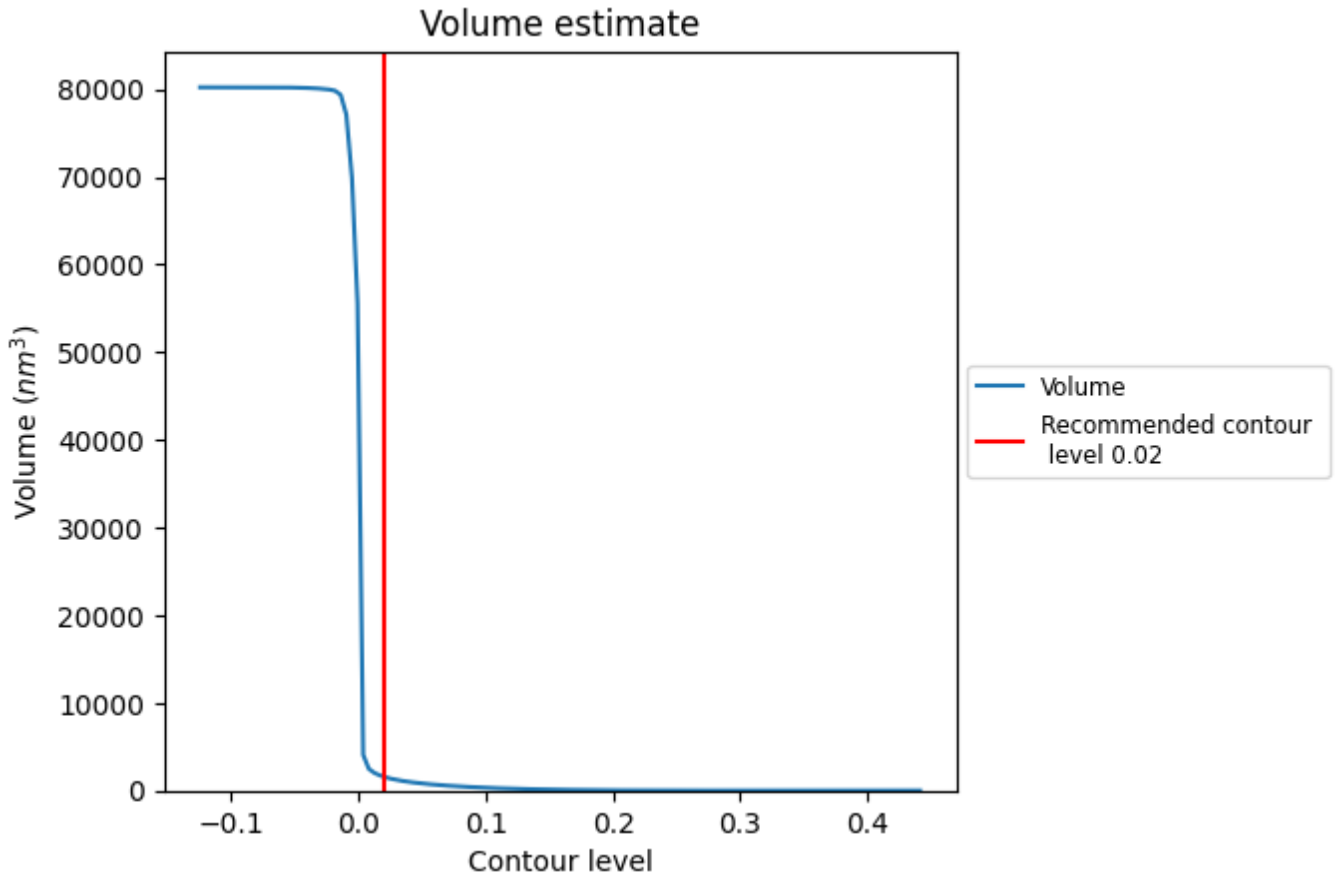
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

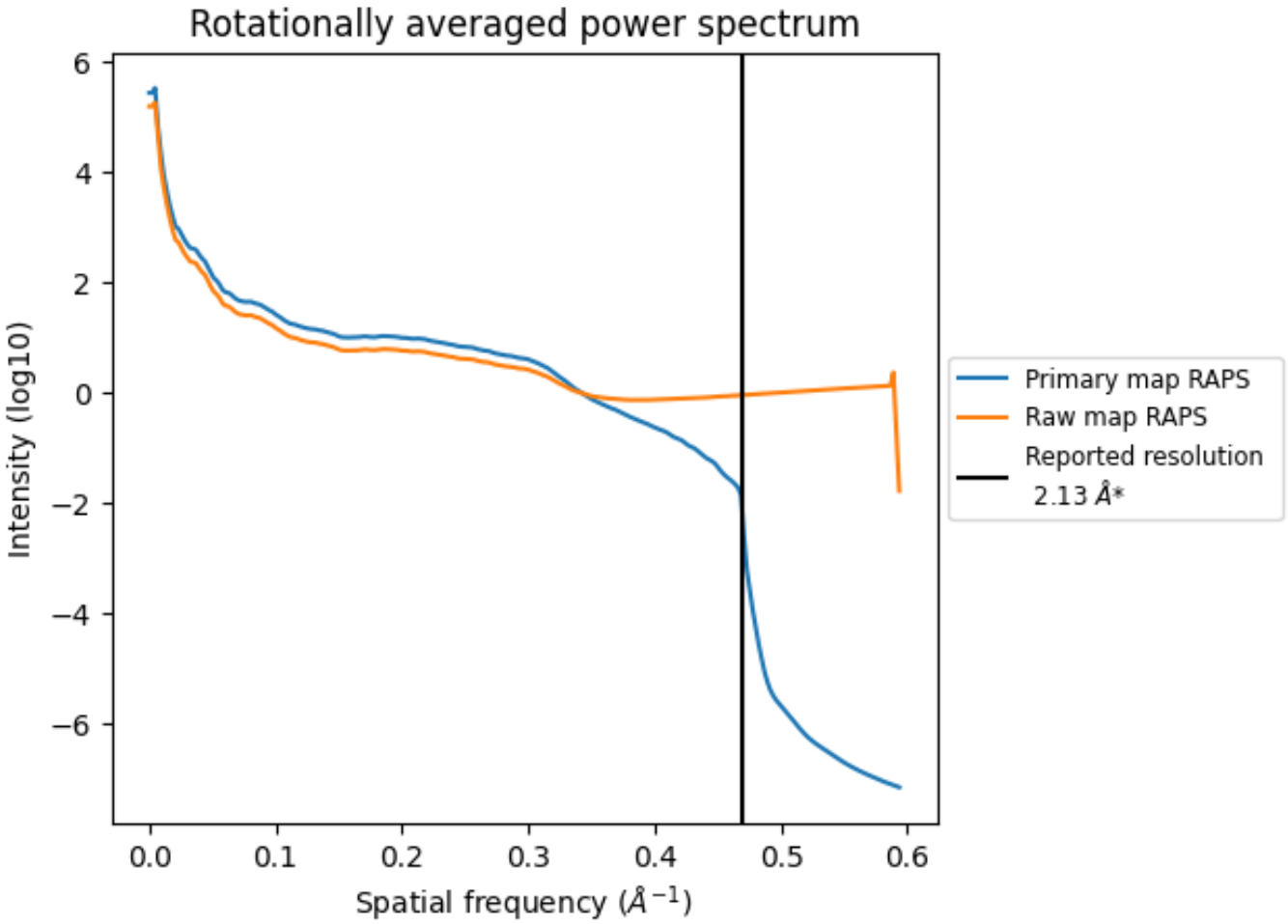
7.2 Volume estimate



The volume at the recommended contour level is 1591 nm^3; this corresponds to an approximate mass of 1437 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)

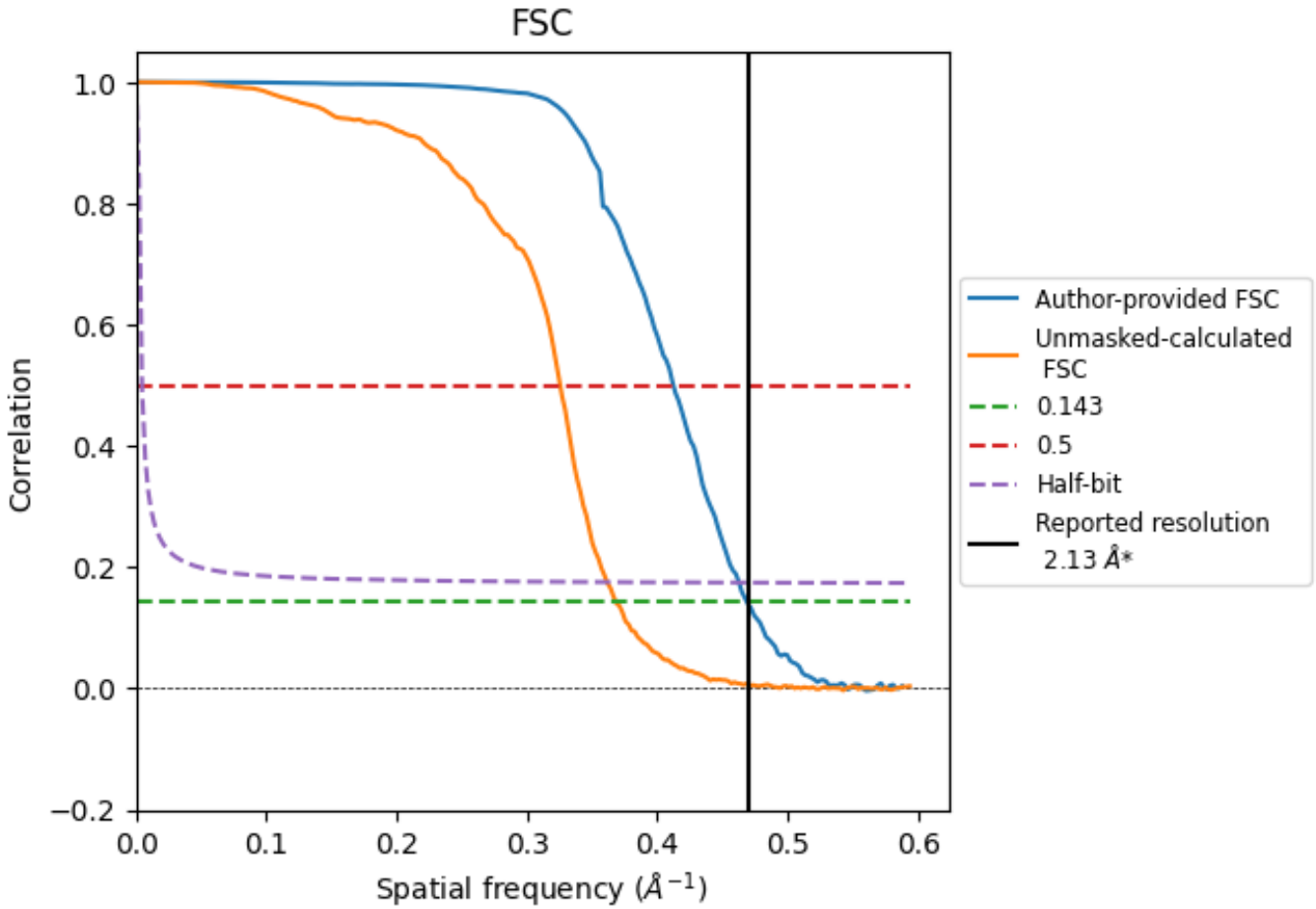


*Reported resolution corresponds to spatial frequency of 0.469 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.469 Å^{-1}

8.2 Resolution estimates (i)

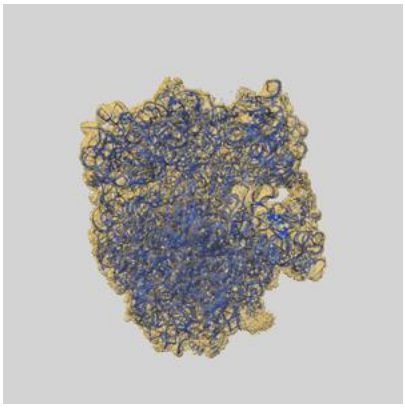
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.43	2.16
Unmasked-calculated*	2.72	3.07	2.77

*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 2.72 differs from the reported value 2.13 by more than 10 %

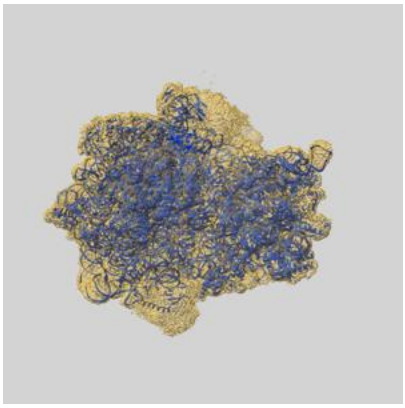
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49594 and PDB model 9NO7. Per-residue inclusion information can be found in section 3 on page 20.

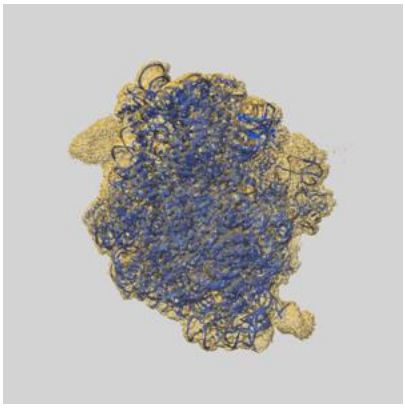
9.1 Map-model overlay



X



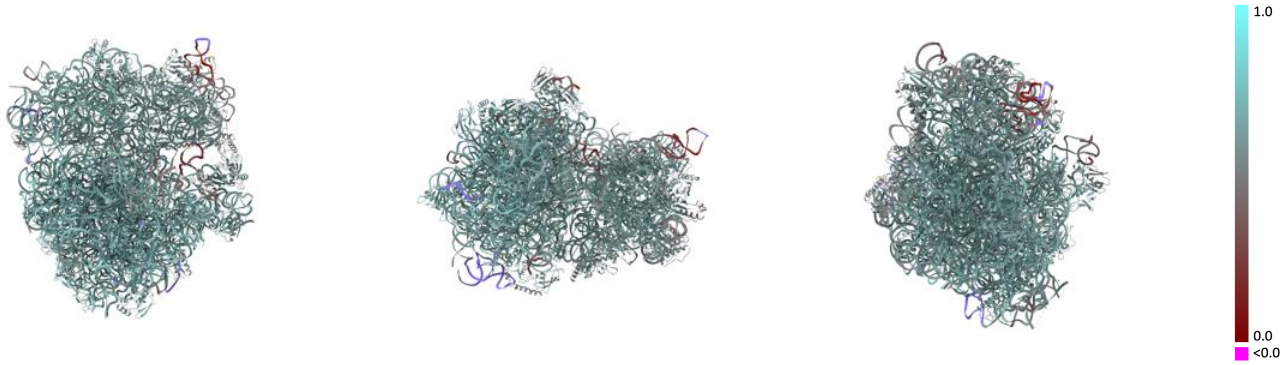
Y



Z

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

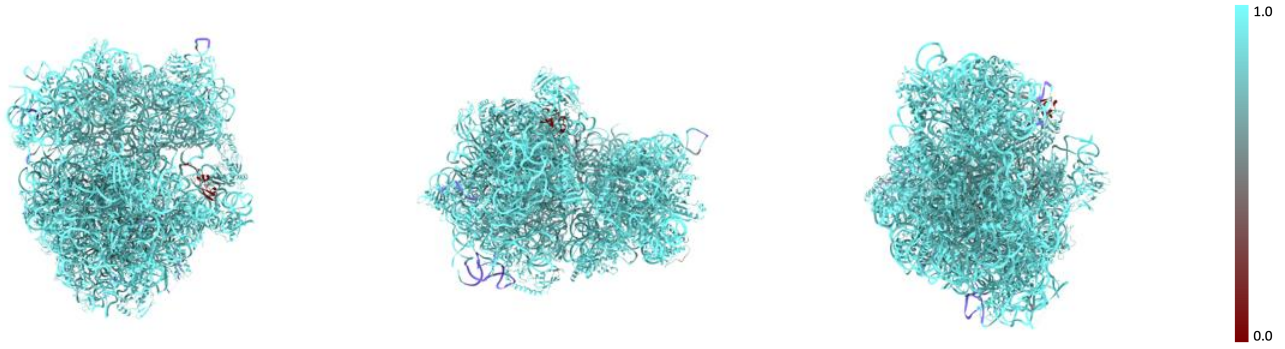
9.2 Q-score mapped to coordinate model (i)



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.

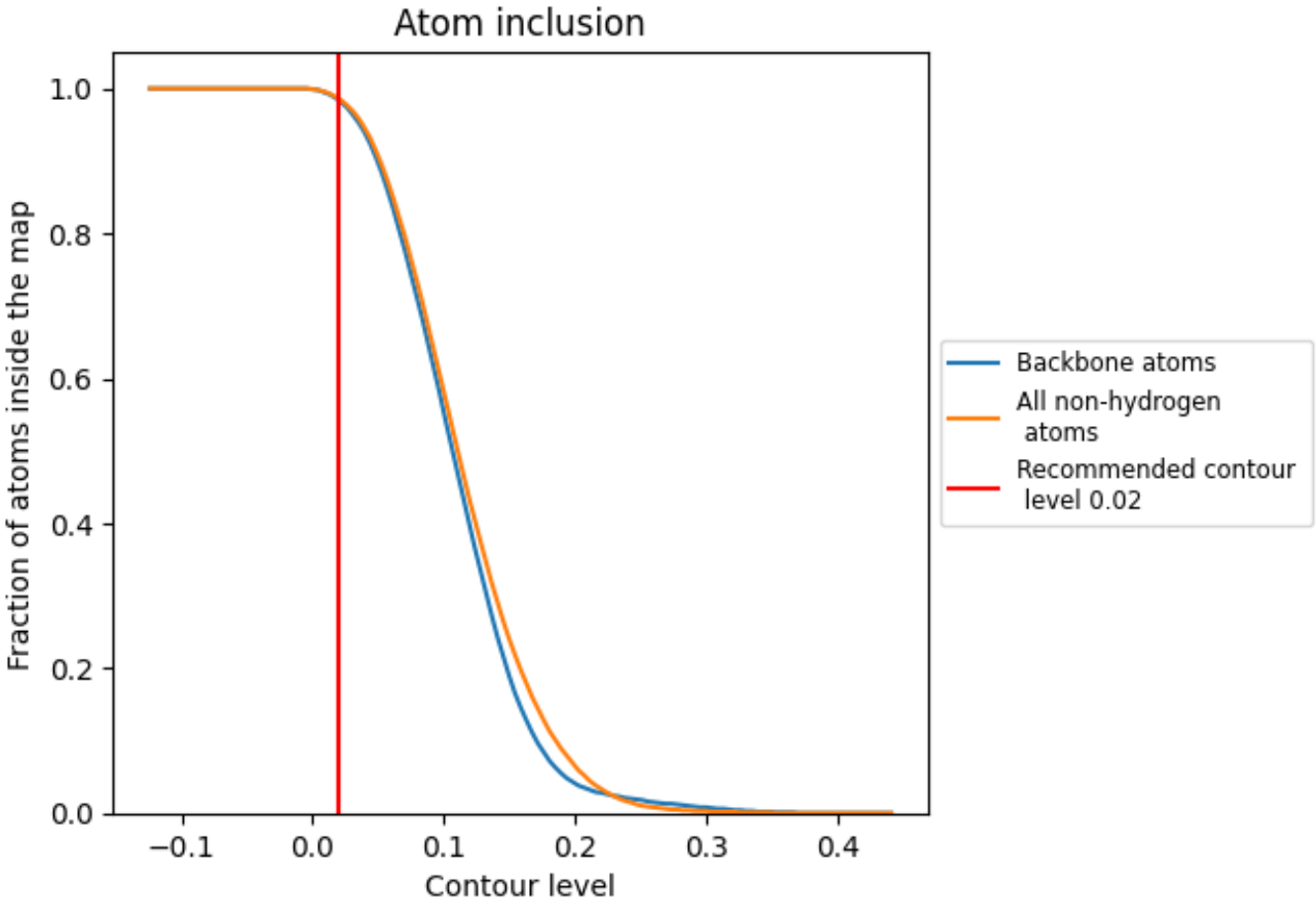
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.9860	0.6330
0	0.9900	0.6690
1	0.9770	0.6400
2	0.9740	0.6110
3	0.9820	0.6570
4	0.9300	0.4970
5	0.9890	0.6780
6	0.9820	0.6590
7	0.9970	0.6980
8	0.9800	0.6800
9	0.9760	0.6520
A	0.9950	0.6550
B	0.9990	0.6160
D	0.9910	0.6770
E	0.9920	0.6700
F	0.9880	0.6540
G	0.9710	0.5810
H	0.9730	0.5620
I	0.9430	0.5540
N	0.9860	0.6530
O	0.9790	0.6670
P	0.9890	0.6570
Q	0.9800	0.6520
R	0.9930	0.6760
S	0.9920	0.6190
T	0.9870	0.6550
U	0.9900	0.6730
V	0.9760	0.6500
W	0.9880	0.6790
X	0.9760	0.6450
Y	0.9900	0.6220
Z	0.6270	0.5370
a	0.9950	0.6120
b	0.9270	0.5410
c	0.9690	0.5950



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Chain	Atom inclusion	Q-score
d	0.9830	0.6010
e	0.9730	0.6220
f	0.9680	0.5550
g	0.9810	0.5840
h	0.9870	0.6250
i	0.9840	0.5700
j	0.9590	0.5480
k	0.9790	0.5840
l	0.9820	0.6600
m	0.9690	0.5750
n	0.9910	0.6180
o	0.9800	0.6050
p	0.9880	0.6130
q	0.9720	0.6280
r	0.9750	0.5670
s	0.9860	0.5660
t	0.9870	0.6000
u	1.0000	0.6300
v	1.0000	0.6240
w	0.9540	0.6240
x	0.9970	0.6330
z	0.8000	0.5770