



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 12:30 pm BST

PDB ID : 28JW / pdb_000028jw
EMDB ID : EMD-56567
Title : Structure of the Chlamydomonas reinhardtii chlororibosome with P-site tRNA
Authors : Waltz, F.; Kater, L.; Engel, B.D.
Deposited on : 2026-02-04
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

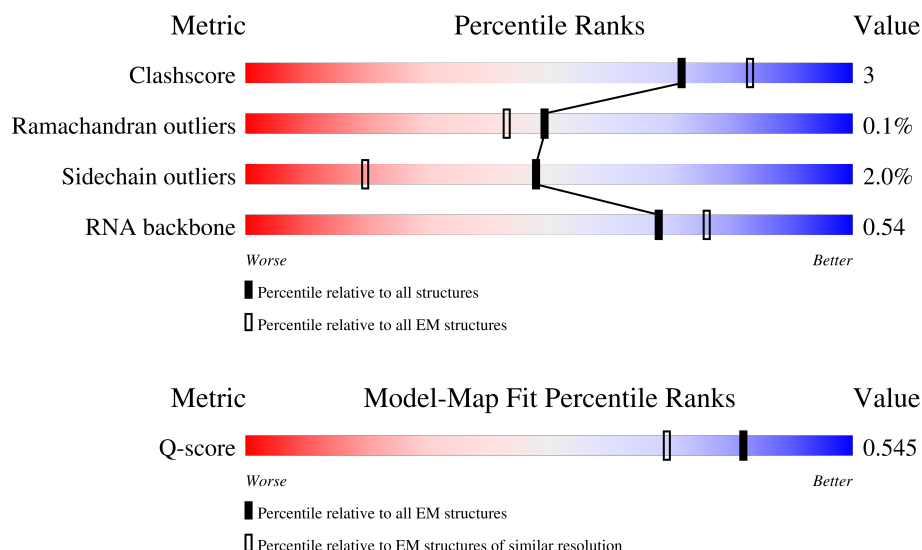
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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.



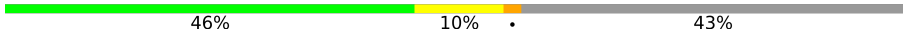
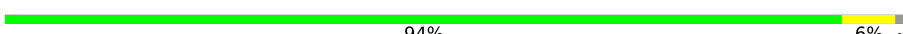
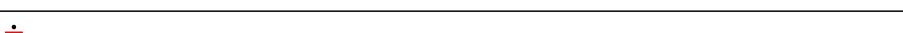
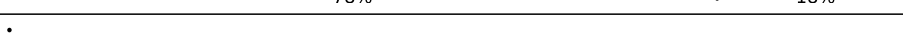
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11884 (2.34 - 3.34)

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

Mol	Chain	Length	Quality of chain
1	0	66	
2	3	121	
3	5	47	

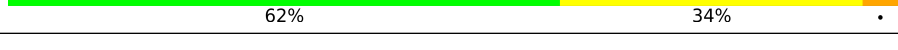
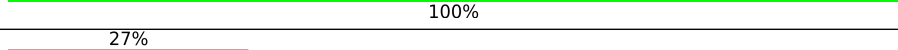
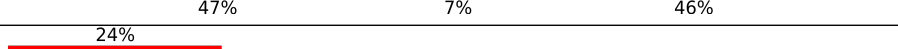
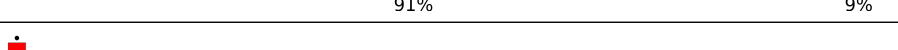
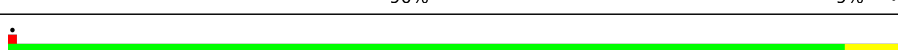
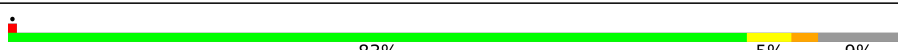
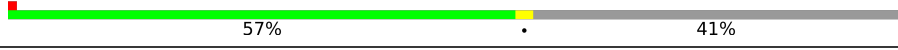
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Mol	Chain	Length	Quality of chain
4	6	101	
5	7	124	
6	8	114	
7	9	37	
8	B	278	
9	C	259	
10	D	243	
11	E	179	
12	F	207	
13	G	200	
14	H	235	
15	I	176	
16	J	225	
17	K	122	
18	L	241	
19	M	136	
20	N	173	
21	O	145	
22	P	153	
23	Q	112	
24	R	179	
25	S	175	
26	T	111	
27	U	170	
28	V	161	

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Mol	Chain	Length	Quality of chain
29	W	195	
30	X	134	
31	Z	98	
32	Y	136	
33	1	2375	
34	4	272	
35	y	76	
36	xx	5	
37	a	436	
38	d	257	
39	f	171	
40	g	168	
41	h	141	
42	j	169	
43	k	130	
44	l	133	
45	m	164	
46	n	100	
47	o	141	
48	p	128	
49	q	105	
50	r	137	
51	s	92	
52	t	166	
53	u	184	

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Mol	Chain	Length	Quality of chain
54	v	298	
55	x	120	
56	w	560	
57	2	1470	
58	b	910	
59	c	712	
60	e	673	
61	i	191	
62	A	6	

2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 160214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called cL38/PSRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	47	Total	C	N	O	0	0
			369	233	76	60		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	17	SER	THR	conflict	UNP A0A835SZL0
0	37	ARG	ALA	conflict	UNP A0A835SZL0
0	38	ALA	SER	conflict	UNP A0A835SZL0
0	41	ASN	ARG	conflict	UNP A0A835SZL0
0	63	ALA	GLY	conflict	UNP A0A835SZL0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	121	Total	C	N	O	P	0	0
			2571	1148	449	853	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	47	Total	C	N	O	P	0	0
			1006	450	185	324	47		

- Molecule 4 is a protein called bL33c.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	58	Total	C	N	O	S	0	0
			473	293	91	86	3		

- Molecule 5 is a protein called bL34c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	60	Total	C	N	O	S	0	0
			455	271	104	77	3		

- Molecule 6 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	68	Total	C	N	O	S	0	0
			520	322	104	91	3		

- Molecule 7 is a protein called Large ribosomal subunit protein bL36c.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	37	Total	C	N	O	S	0	0
			292	177	63	46	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL2c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	276	Total	C	N	O	S	0	0
			2159	1347	431	377	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	223	Total	C	N	O	S	0	0
			1681	1057	310	305	9		

- Molecule 10 is a protein called Large ribosomal subunit protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	216	Total	C	N	O	S	0	0
			1599	997	290	306	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	178	Total	C	N	O	S	0	0
			1413	900	247	260	6		

- Molecule 12 is a protein called Plastid ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	177	Total	C	N	O	S	0	0
			1338	845	245	244	4		

- Molecule 13 is a protein called Large ribosomal subunit protein bL9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	54	Total	C	N	O	S	0	0
			418	272	72	73	1		

- Molecule 14 is a protein called uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	141	Total	C	N	O	S	0	0
			1114	711	189	209	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL11c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	132	Total	C	N	O	S	0	0
			980	623	171	181	5		

- Molecule 16 is a protein called uL13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	173	Total	C	N	O	S	0	0
			1346	857	243	243	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	122	Total	C	N	O	S	0	0
			942	588	180	169	5		

- Molecule 18 is a protein called uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	198	Total	C	N	O	S	0	0
			1484	921	282	276	5		

- Molecule 19 is a protein called Large ribosomal subunit protein uL16c.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	135	Total	C	N	O	S	0	0
			1080	689	211	173	7		

- Molecule 20 is a protein called Large ribosomal subunit protein bL17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	117	Total	C	N	O	S	0	0
			937	585	185	162	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	118	Total	C	N	O	S	0	0
			902	557	173	168	4		

- Molecule 22 is a protein called bL19c.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	130	Total	C	N	O	S	0	0
			995	620	199	174	2		

- Molecule 23 is a protein called Large ribosomal subunit protein bL20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	111	Total	C	N	O	S	0	0
			943	592	193	152	6		

- Molecule 24 is a protein called bL21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	115	Total	C	N	O	S	0	0
			907	585	161	157	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL22c.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	115	Total	C	N	O	S	0	0
			903	564	174	157	8		

- Molecule 26 is a protein called uL23c, Large ribosomal subunit protein uL23c.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	107	Total	C	N	O	S	0	0
			837	542	148	146	1		

- Molecule 27 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	132	Total	C	N	O	S	0	0
			1020	650	189	178	3		

- Molecule 28 is a protein called bL27c.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	114	Total	C	N	O	S	0	0
			869	535	172	159	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	138	Total	C	N	O	S	0	0
			1104	700	205	193	6		

- Molecule 30 is a protein called uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	106	Total	C	N	O	S	0	0
			843	518	169	153	3		

- Molecule 31 is a protein called bL32c.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	41	Total	C	N	O	0	0
			323	213	57	53		

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	65	Total	C	N	O	S	0	0
			521	331	90	98	2		

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1	2375	Total	C	N	O	P	0	0
			50934	22751	9345	16463	2375		

- Molecule 34 is a RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4	272	Total	C	N	O	P	0	0
			5856	2616	1106	1862	272		

- Molecule 35 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	y	76	Total	C	N	O	P	S	0	0
			1627	726	296	528	76	1		

- Molecule 36 is a RNA chain called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	xx	5	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 37 is a protein called Ribosomal protein S1 homologue.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	236	Total	C	N	O	S	0	0
			1868	1175	285	395	13		

- Molecule 38 is a protein called Small ribosomal subunit protein uS4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	256	Total	C	N	O	S	0	0
			2107	1356	403	341	7		

- Molecule 39 is a protein called bS6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	103	Total	C	N	O	S	0	0
			850	543	148	156	3		

- Molecule 40 is a protein called Small ribosomal subunit protein uS7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	167	Total	C	N	O	S	0	0
			1334	846	253	229	6		

- Molecule 41 is a protein called Small ribosomal subunit protein uS8c.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	141	Total	C	N	O	S	0	0
			1113	698	206	203	6		

- Molecule 42 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	122	Total	C	N	O	S	0	0
			957	597	173	178	9		

- Molecule 43 is a protein called Small ribosomal subunit protein uS11c.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	117	Total	C	N	O	S	0	0
			894	560	179	151	4		

- Molecule 44 is a protein called Small ribosomal subunit protein uS12c.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	121	Total	C	N	O	S	0	0
			941	591	190	157	3		

- Molecule 45 is a protein called uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	114	Total	C	N	O	S	0	0
			924	569	181	172	2		

- Molecule 46 is a protein called Small ribosomal subunit protein uS14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	99	Total	C	N	O	S	0	0
			814	513	163	132	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	101	Total	C	N	O	S	0	0
			813	502	156	151	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	80	Total	C	N	O	S	0	0
			666	433	120	112	1		

- Molecule 49 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	78	Total	C	N	O	S	0	0
			621	386	117	116	2		

- Molecule 50 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	81	Total	C	N	O	S	0	0
			664	434	123	106	1		

- Molecule 51 is a protein called Small ribosomal subunit protein uS19c.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	81	Total	C	N	O	S	0	0
			645	414	122	106	3		

- Molecule 52 is a protein called bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	119	Total	C	N	O	S	0	0
			935	592	172	167	4		

- Molecule 53 is a protein called bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	92	Total	C	N	O	S	0	0
			789	494	144	147	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	652	ARG	ASP	conflict	UNP A8HPN4

- Molecule 54 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	181	Total	C	N	O	S	0	0
			1430	907	245	276	2		

- Molecule 55 is a protein called cS26/PSRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	60	Total	C	N	O	S	0	0
			462	299	80	81	2		

- Molecule 56 is a protein called Plastid-specific ribosomal protein-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	365	Total	C	N	O	S	0	0
			2786	1749	429	598	10		

- Molecule 57 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	2	1470	Total	C	N	O	P	0	0
			31537	14077	5779	10211	1470		

- Molecule 58 is a protein called Small ribosomal subunit protein uS2c.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	b	685	Total	C	N	O	S	0	0
			5545	3581	1010	934	20		

- Molecule 59 is a protein called Small ribosomal subunit protein uS3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	c	607	Total	C	N	O	S	0	0
			4939	3179	905	844	11		

- Molecule 60 is a protein called uS5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	e	536	Total	C	N	O	S	0	0
			3988	2477	658	838	15		

- Molecule 61 is a protein called Small ribosomal subunit protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	i	155	Total	C	N	O	S	0	0
			1209	762	225	219	3		

- Molecule 62 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	A	6	Total	C	N	O	P	0	0
			128	58	24	40	6		

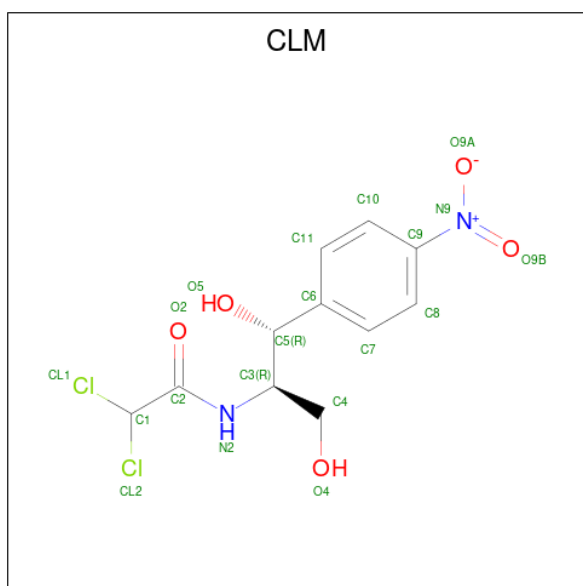
- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
63	3	5	Total	Mg	0
			5	5	
63	5	4	Total	Mg	0
			4	4	
63	D	1	Total	Mg	0
			1	1	
63	L	1	Total	Mg	0
			1	1	
63	N	2	Total	Mg	0
			2	2	
63	1	202	Total	Mg	0
			202	202	
63	4	7	Total	Mg	0
			7	7	
63	n	1	Total	Mg	0
			1	1	
63	q	1	Total	Mg	0
			1	1	
63	2	95	Total	Mg	0
			95	95	

- Molecule 64 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
64	5	1	Total	K	0
			1	1	
64	D	1	Total	K	0
			1	1	
64	1	81	Total	K	0
			81	81	
64	4	4	Total	K	0
			4	4	
64	2	43	Total	K	0
			43	43	

- Molecule 65 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).

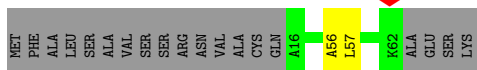


Mol	Chain	Residues	Atoms					AltConf
65	1	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

3 Residue-property plots

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

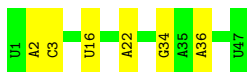
- Molecule 1: cL38/PSRP6



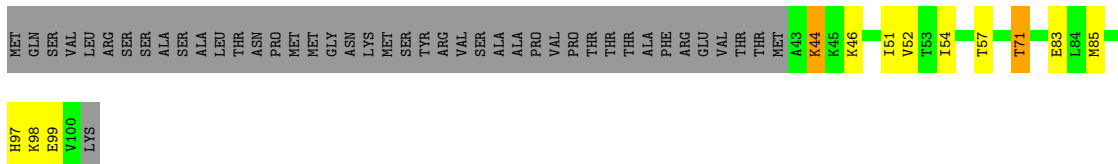
- Molecule 2: 5S rRNA



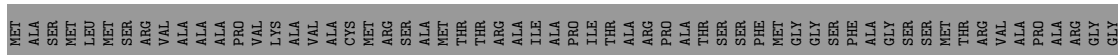
- Molecule 3: 3S rRNA

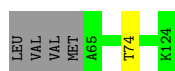


- Molecule 4: bL33c

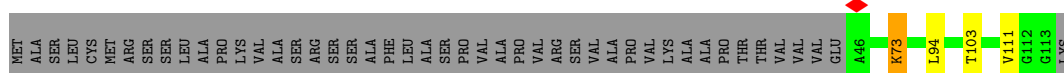


- Molecule 5: bL34c

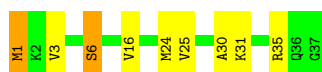
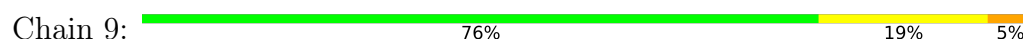




- Molecule 6: 50S ribosomal protein L35



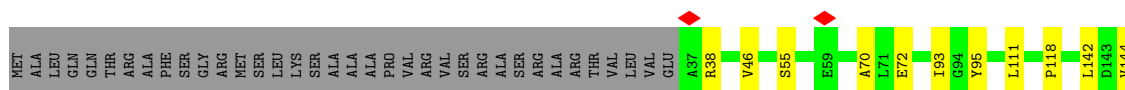
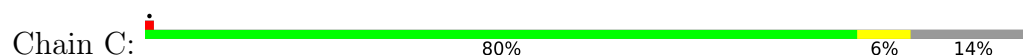
- Molecule 7: Large ribosomal subunit protein bL36c



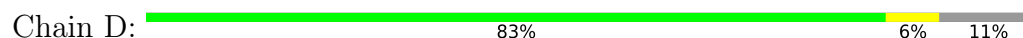
- Molecule 8: Large ribosomal subunit protein uL2c



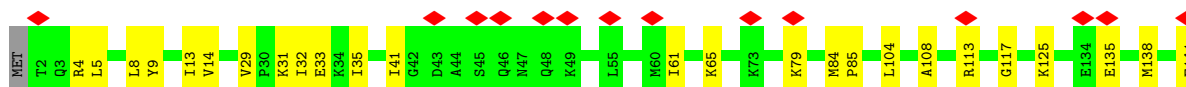
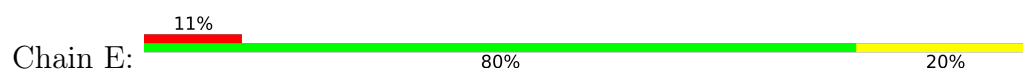
- Molecule 9: Large ribosomal subunit protein uL3c

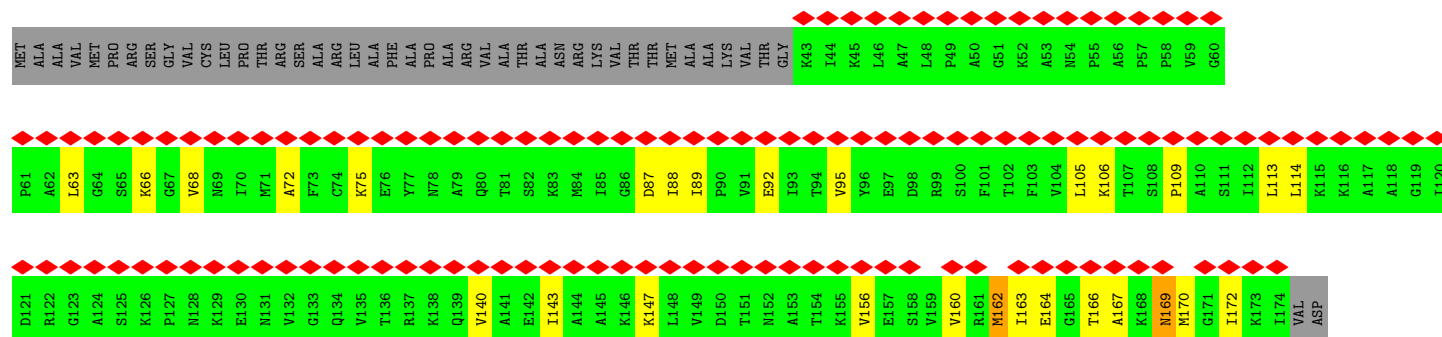


- Molecule 10: Large ribosomal subunit protein uL4c



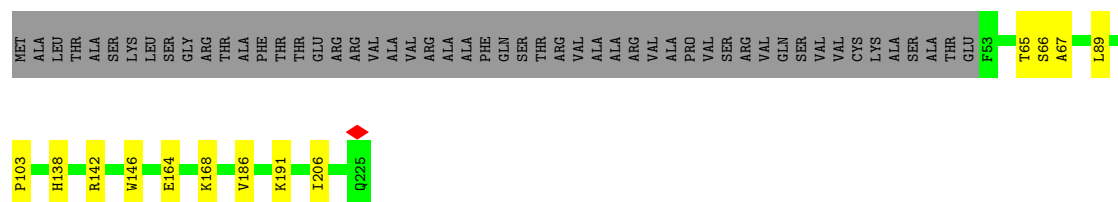
- Molecule 11: Large ribosomal subunit protein uL5c





• Molecule 16: uL13c

Chain J: 71% 6% 23%



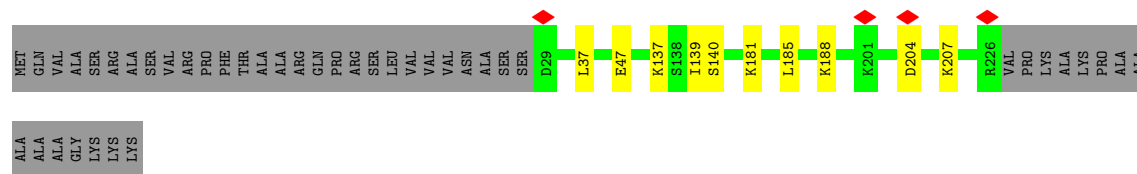
• Molecule 17: Large ribosomal subunit protein uL14c

Chain K: 89% 11%



• Molecule 18: uL15c

Chain L: 78% 18%



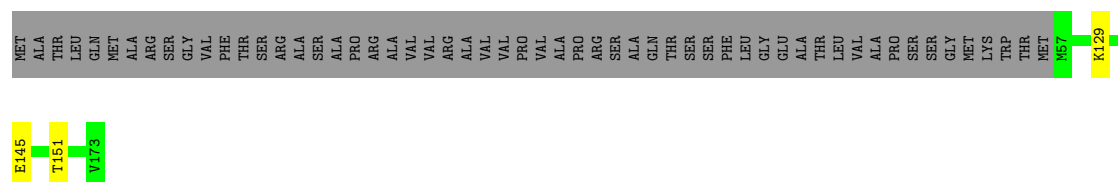
• Molecule 19: Large ribosomal subunit protein uL16c

Chain M: 90% 9%



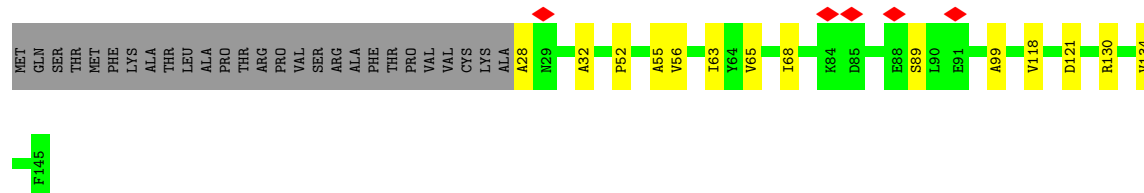
• Molecule 20: Large ribosomal subunit protein bL17c

Chain N: 66% 32%



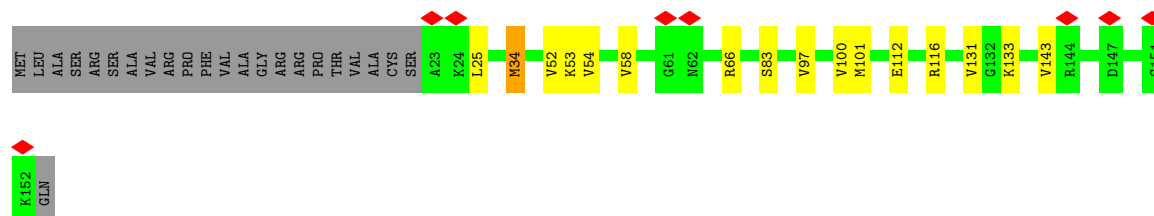
- Molecule 21: Large ribosomal subunit protein uL18c

Chain O: 72% 10% 19%



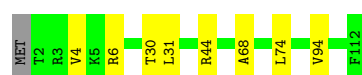
- Molecule 22: bL19c

Chain P: 5% 75% 10% 15%



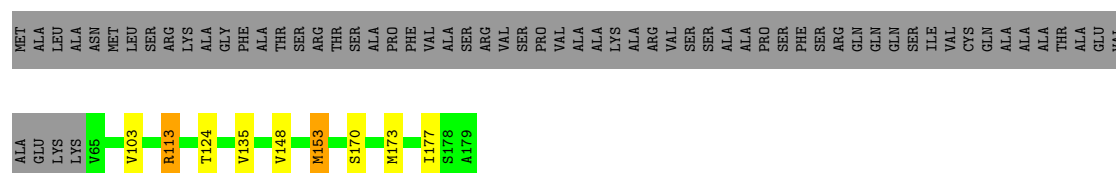
- Molecule 23: Large ribosomal subunit protein bL20c

Chain Q: 92% 7%



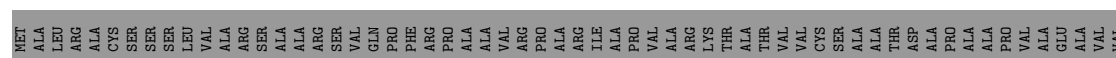
- Molecule 24: bL21c

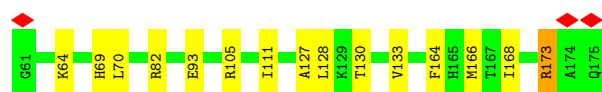
Chain R: 59% 36%



- Molecule 25: Large ribosomal subunit protein uL22c

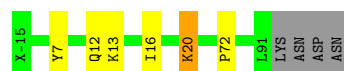
Chain S: 57% 8% 34%





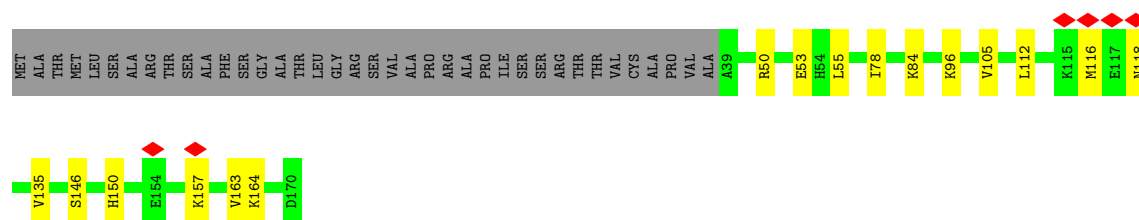
- Molecule 26: uL23c, Large ribosomal subunit protein uL23c

Chain T: 91% 5% . .



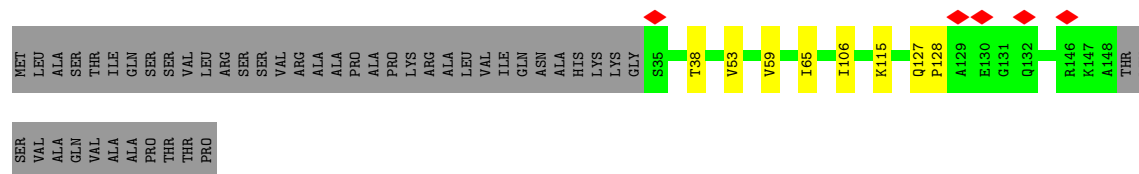
- Molecule 27: KOW domain-containing protein

Chain U: 68% 9% 22%



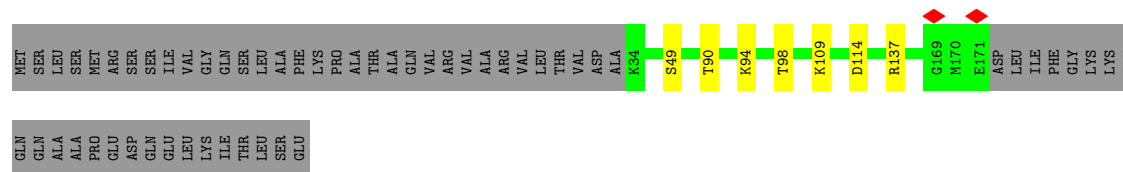
- Molecule 28: bL27c

Chain V: 66% 5% 29%



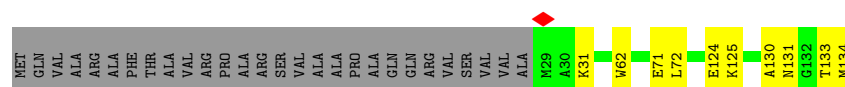
- Molecule 29: Large ribosomal subunit protein bL28c

Chain W: 67% . 29%

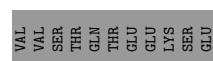
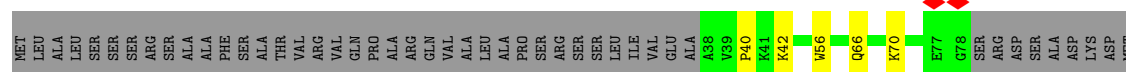
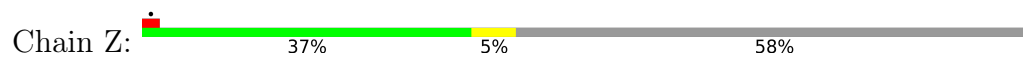


- Molecule 30: uL29c

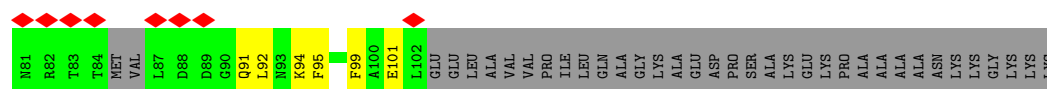
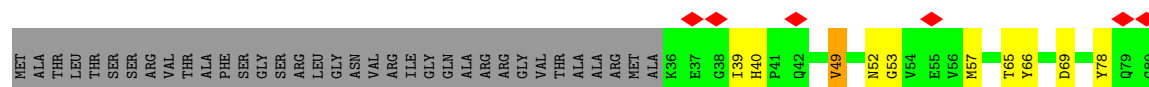
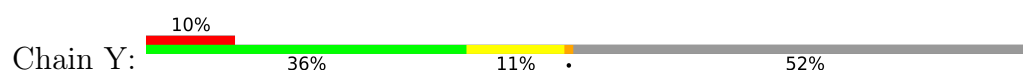
Chain X: 72% 7% 21%



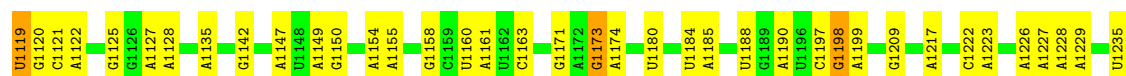
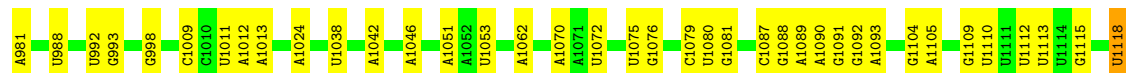
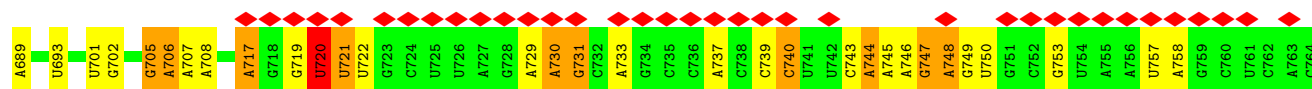
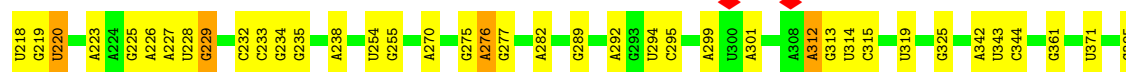
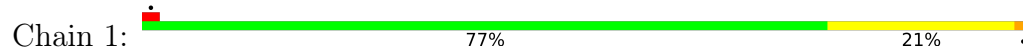
- Molecule 31: bL32c

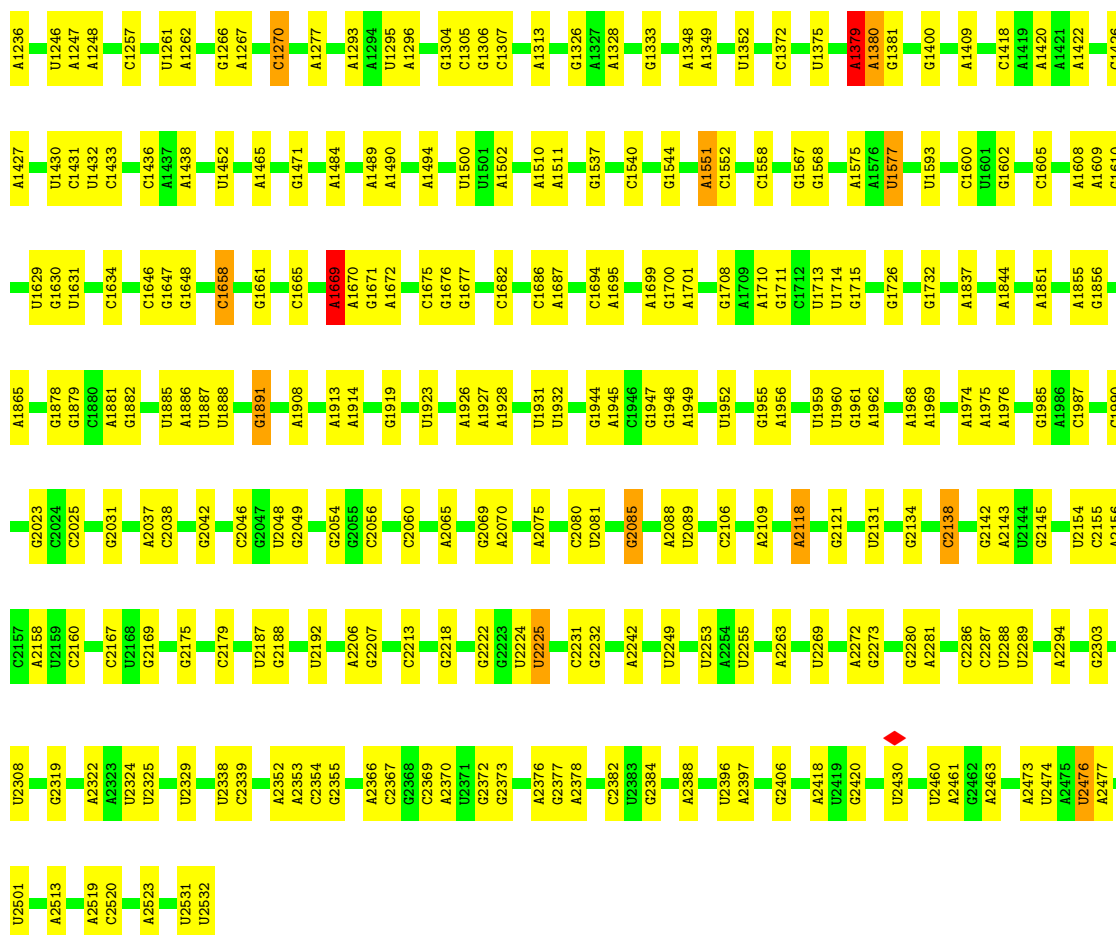


• Molecule 32: 50S ribosomal protein L31



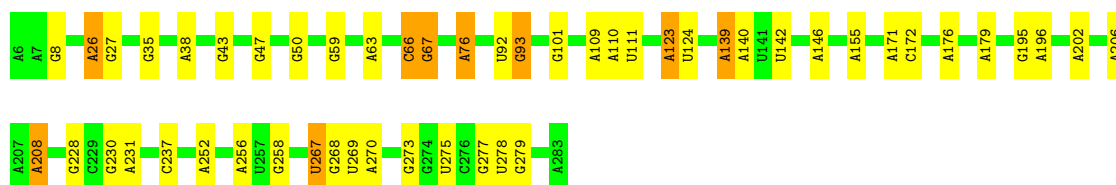
• Molecule 33: 23S rRNA





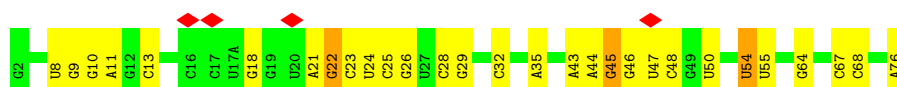
• Molecule 34: 7S RNA

Chain 4: 81% 15%



• Molecule 35: P-site tRNA

Chain y: 5% 62% 34%

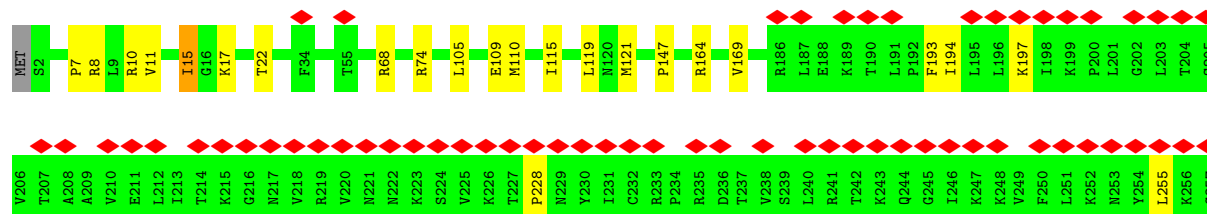
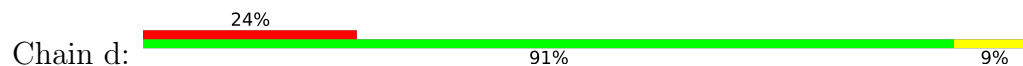


• Molecule 36: Nascent peptide

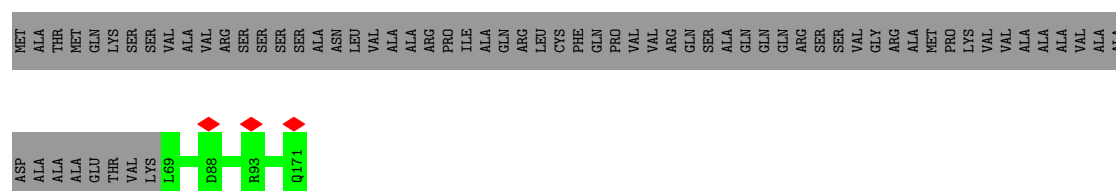
Chain xx: 100%

There are no outlier residues recorded for this chain.

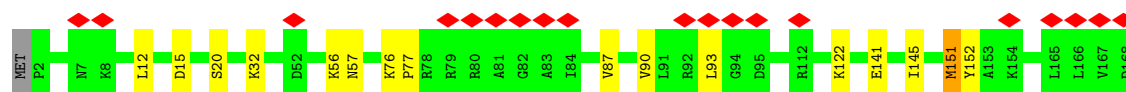
Chain a:



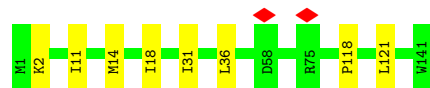
Chain f:



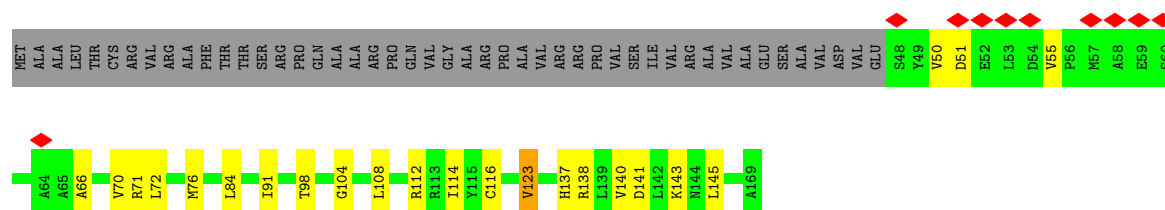
Chain g: 11% 90% 9%



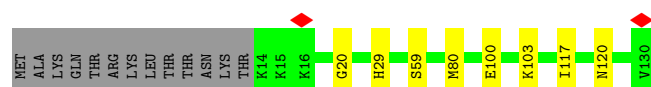
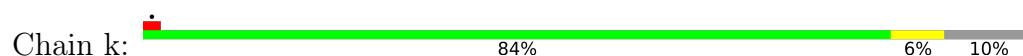
- Molecule 41: Small ribosomal subunit protein uS8c



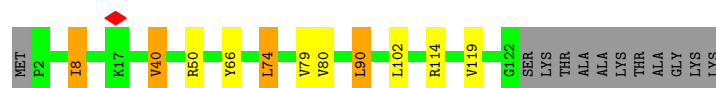
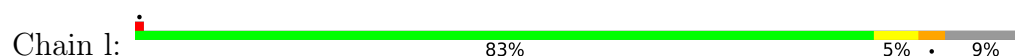
- Molecule 42: Small ribosomal subunit protein uS10 domain-containing protein



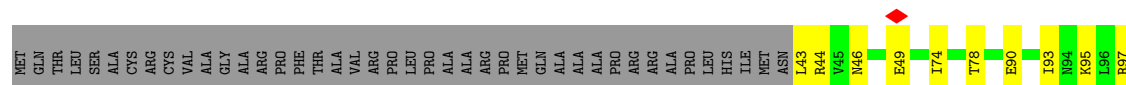
- Molecule 43: Small ribosomal subunit protein uS11c



- Molecule 44: Small ribosomal subunit protein uS12c



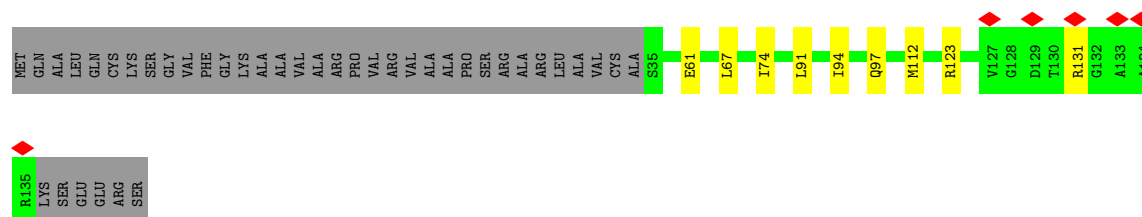
- Molecule 45: uS13c



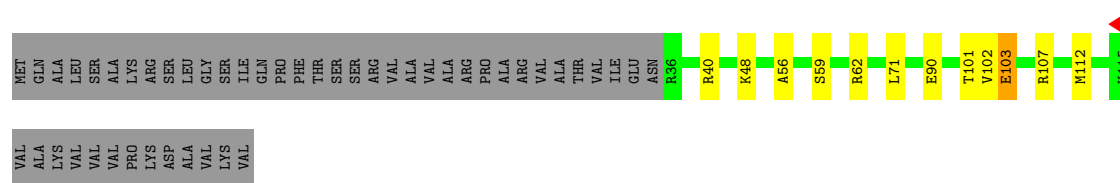
- Molecule 46: Small ribosomal subunit protein uS14c

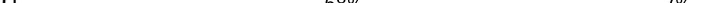
Category	Count
MET	1
A2	1
K3	1
K4	1
S5	1
M6	1
V17	1
L27	1
K38	1
N53	1
V57	1
R58	1
L59	1
W100	1

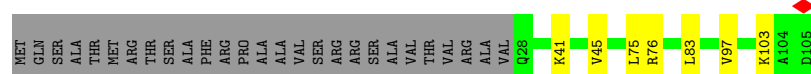
- Chain o: 65% 6% 28%

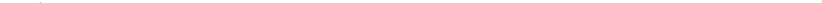


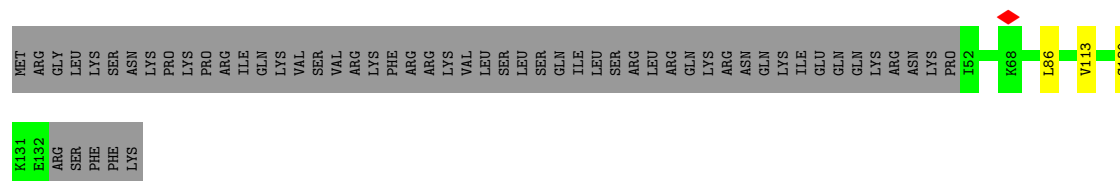
- Chain p: 53% 9% 38%

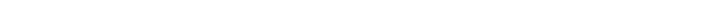


- Chain q: 



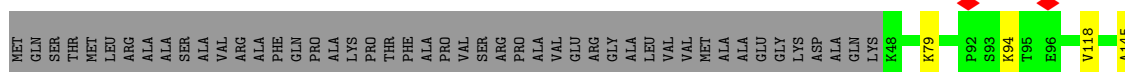
- Chain r:  57% 41%



- Chain s: 



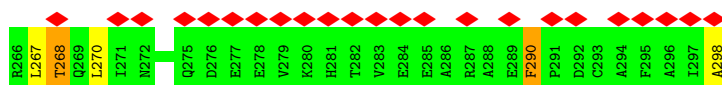
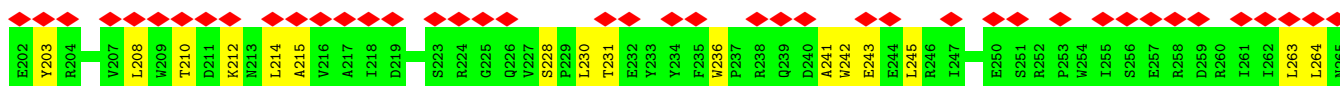
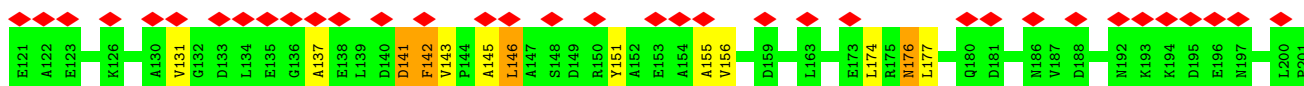
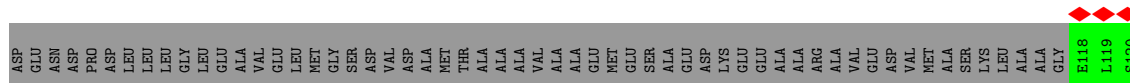
• Molecule 52: bS20c



• Molecule 53: bS21c

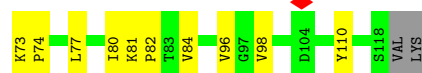


• Molecule 54: 30S ribosomal protein 3, chloroplastic

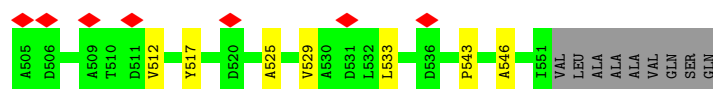
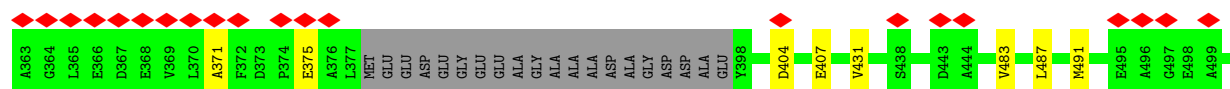
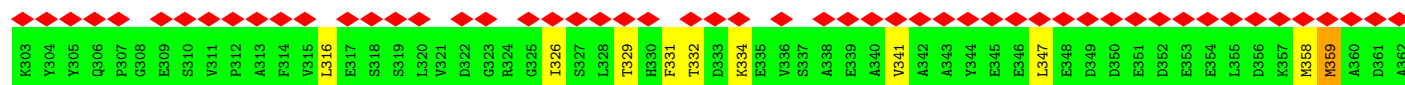
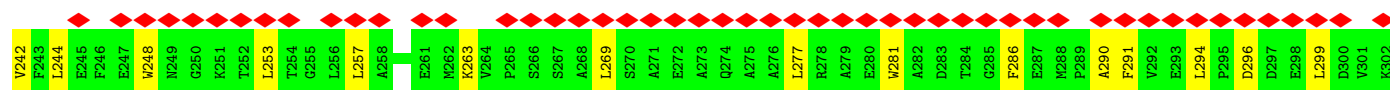
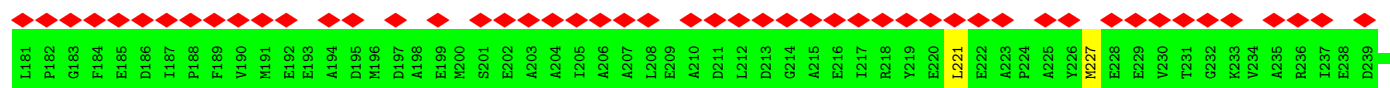
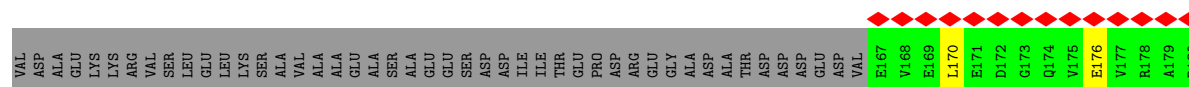


• Molecule 55: cS26/PSRP8

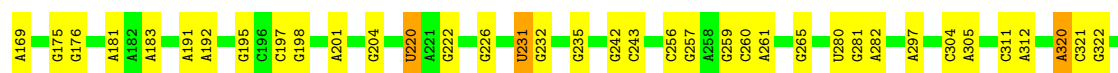


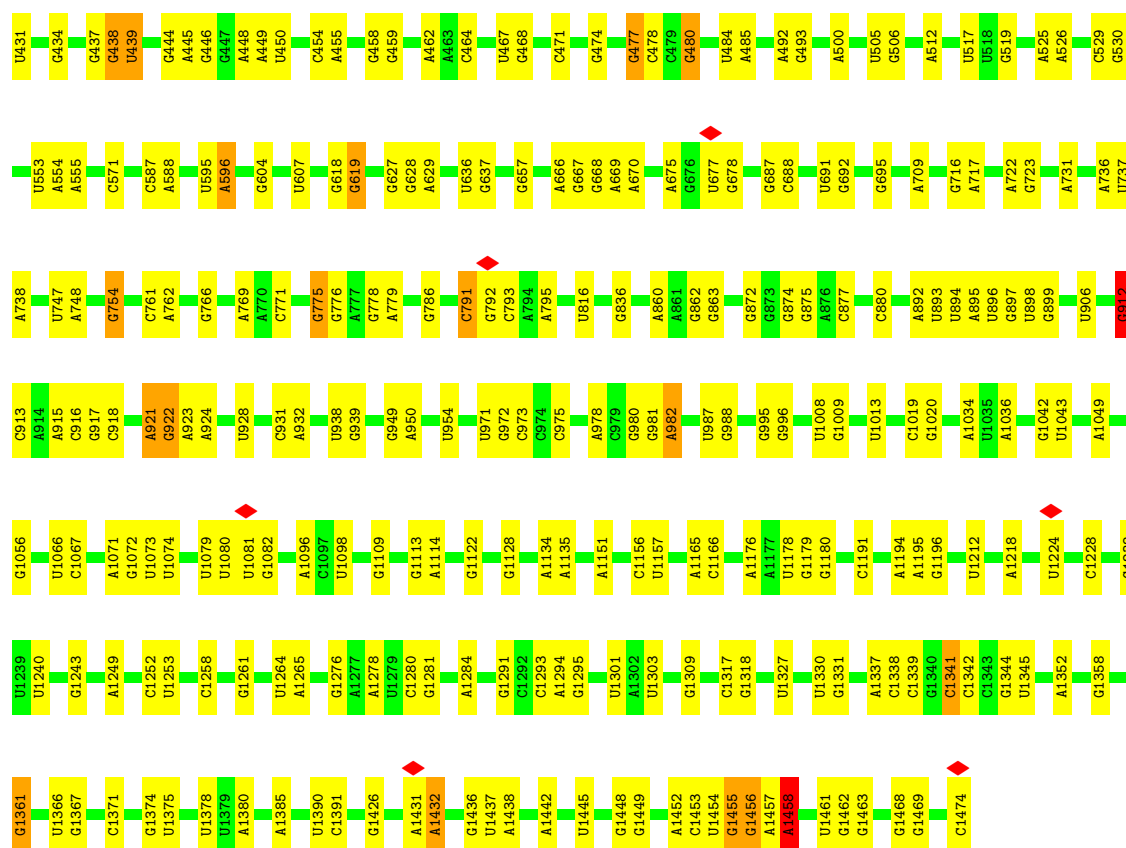


- Molecule 56: Plastid-specific ribosomal protein-7

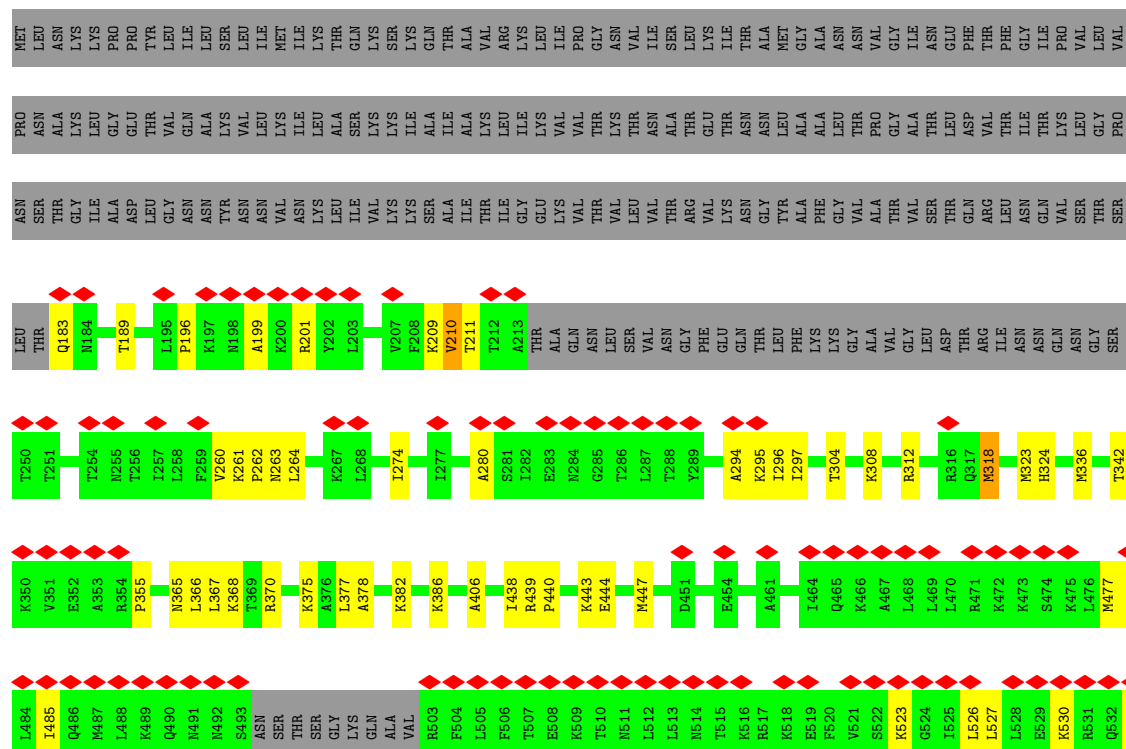


- Molecule 57: 16S rRNA

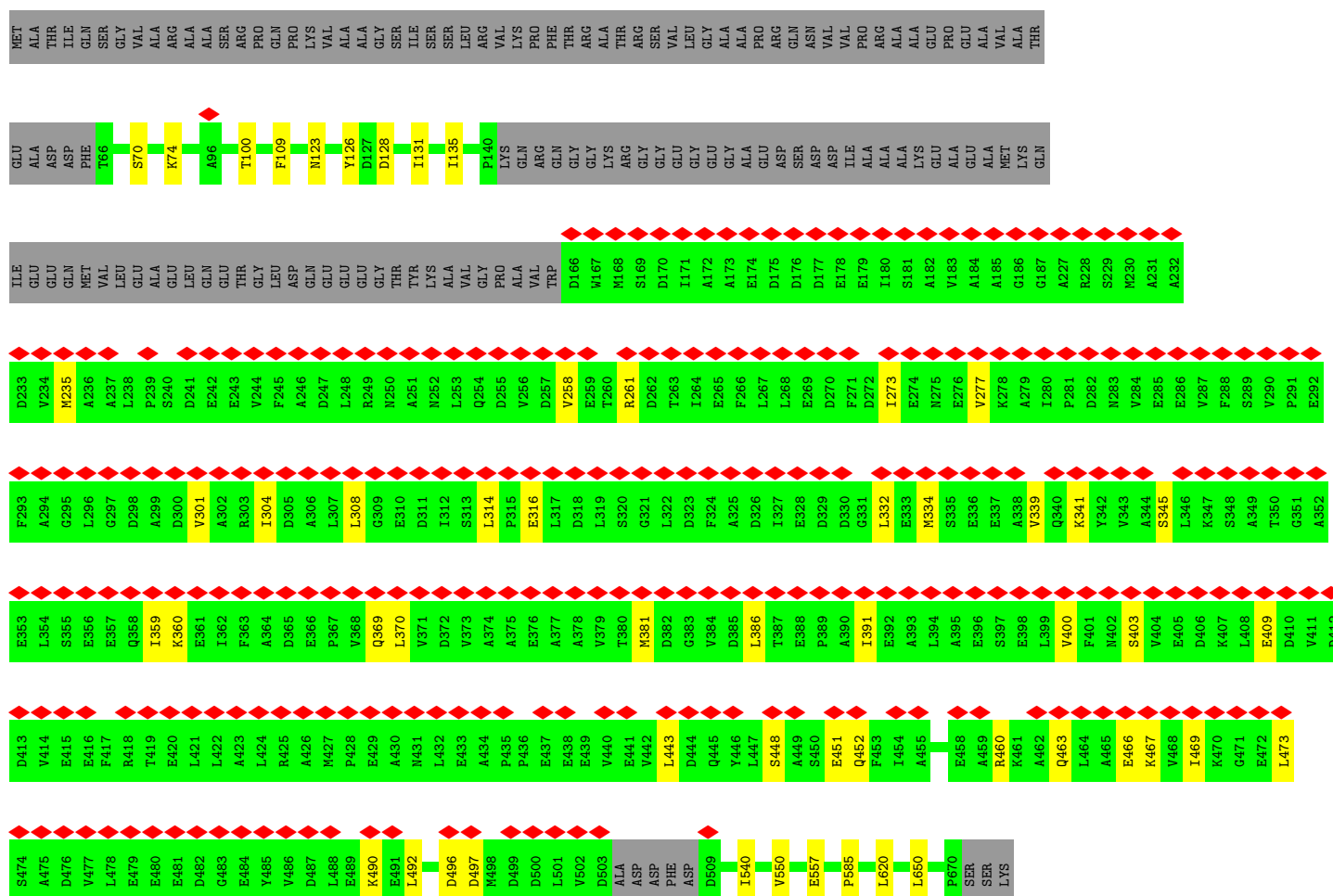
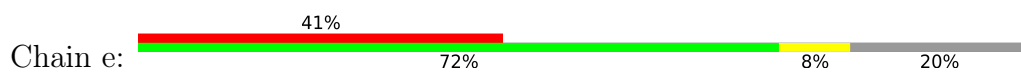




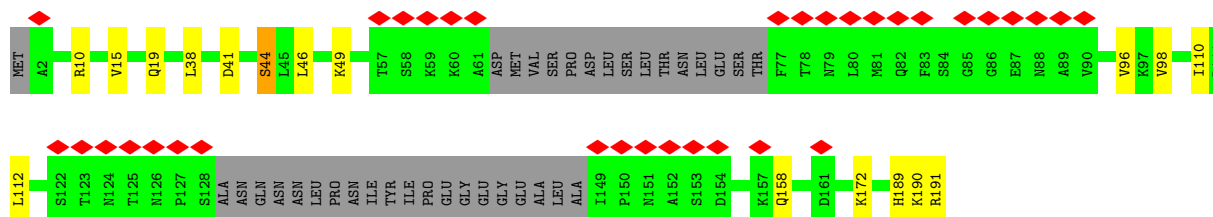
• Molecule 58: Small ribosomal subunit protein uS2c



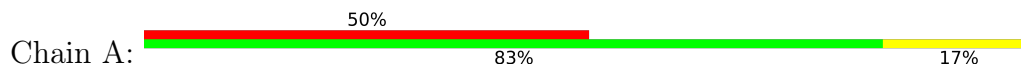




- Molecule 61: Small ribosomal subunit protein uS9c



- Molecule 62: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	75000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.778	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0707	Depositor
Map size (Å)	544.3072, 544.3072, 544.3072	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0631, 1.0631, 1.0631	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MA6, 4OC, 5MU, 6MZ, 2MA, 4SU, H2U, OMC, PSU, 2MG, G7M, K, MG, OMG, OMU, 5MC, CLM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.22	0/382	0.39	0/518
2	3	0.19	0/2871	0.36	0/4471
3	5	0.23	0/1126	0.38	0/1753
4	6	0.23	0/479	0.40	0/640
5	7	0.28	0/457	0.45	0/595
6	8	0.23	0/528	0.39	0/702
7	9	0.25	0/292	0.41	0/379
8	B	0.26	0/2200	0.44	0/2965
9	C	0.26	0/1711	0.45	0/2304
10	D	0.24	0/1619	0.41	0/2183
11	E	0.27	0/1433	0.63	1/1920 (0.1%)
12	F	0.19	0/1354	0.41	0/1821
13	G	0.21	0/424	0.45	0/570
14	H	0.25	0/1131	0.58	0/1520
15	I	2.22	3/992 (0.3%)	1.01	5/1336 (0.4%)
16	J	0.24	0/1375	0.44	0/1855
17	K	0.26	0/952	0.47	0/1280
18	L	0.25	0/1505	0.52	0/2009
19	M	0.24	0/1105	0.39	0/1482
20	N	0.23	0/951	0.43	0/1275
21	O	0.21	0/913	0.49	0/1222
22	P	0.24	0/1005	0.47	0/1351
23	Q	0.28	0/958	0.45	0/1272
24	R	0.25	0/927	0.41	0/1247
25	S	0.25	0/915	0.47	0/1221
26	T	0.26	0/772	0.47	0/1043
27	U	0.23	0/1036	0.44	0/1381
28	V	0.23	0/884	0.47	0/1187
29	W	0.25	0/1126	0.44	0/1507
30	X	0.23	0/853	0.43	0/1141
31	Z	0.25	0/328	0.42	0/436

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.30	0/532	0.70	0/715
33	1	0.54	6/56765 (0.0%)	0.38	3/88499 (0.0%)
34	4	0.26	0/6566	0.37	0/10240
35	y	0.23	0/1728	0.37	0/2694
37	a	0.24	0/1899	0.63	0/2570
38	d	0.19	0/2144	0.46	0/2867
39	f	0.14	0/868	0.34	0/1172
40	g	0.22	0/1354	0.54	1/1820 (0.1%)
41	h	0.16	0/1125	0.39	0/1505
42	j	0.23	0/974	0.61	0/1316
43	k	0.17	0/908	0.43	0/1210
44	l	0.17	0/955	0.43	0/1282
45	m	0.20	0/931	0.49	0/1246
46	n	0.16	0/827	0.37	1/1097 (0.1%)
47	o	0.19	0/822	0.42	0/1098
48	p	0.20	0/682	0.47	0/917
49	q	0.19	0/626	0.46	0/836
50	r	0.18	0/676	0.41	0/907
51	s	0.17	0/661	0.43	0/887
52	t	0.23	0/948	0.51	0/1269
53	u	0.20	0/801	0.51	0/1070
54	v	0.25	0/1463	0.68	4/1994 (0.2%)
55	x	0.18	0/472	0.40	0/637
56	w	0.20	0/2835	0.50	0/3845
57	2	0.15	0/35103	0.31	0/54745
58	b	0.24	0/5616	0.60	3/7512 (0.0%)
59	c	0.19	0/5008	0.47	2/6698 (0.0%)
60	e	0.18	0/4029	0.50	3/5461 (0.1%)
61	i	0.24	0/1222	0.62	0/1630
62	A	0.11	0/143	0.30	0/220
All	All	0.39	9/171287 (0.0%)	0.42	23/252545 (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
18	L	0	1
33	1	2	0
54	v	0	1
56	w	0	1
All	All	2	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	162	MET	CA-C	68.70	2.44	1.52
33	1	720	U	N3-C4	51.15	2.40	1.38
33	1	720	U	C2-N3	48.05	2.33	1.37
33	1	720	U	N1-C2	47.63	2.33	1.38
33	1	720	U	N1-C6	45.80	2.29	1.38
33	1	720	U	C4-C5	40.61	2.24	1.43
33	1	720	U	C5-C6	38.44	2.11	1.34
15	I	162	MET	CA-CB	5.53	1.63	1.53
15	I	162	MET	C-N	5.43	1.40	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	162	MET	O-C-N	-18.92	97.64	122.42
15	I	162	MET	CB-CA-C	14.60	135.06	109.65
15	I	162	MET	N-CA-C	9.29	124.81	113.38
15	I	162	MET	N-CA-CB	-9.29	96.69	110.53
15	I	162	MET	CA-C-O	8.99	129.40	119.15
59	c	410	LEU	CA-CB-CG	7.35	142.01	116.30
33	1	1379	A	O4'-C1'-N9	6.67	118.51	108.50
58	b	667	PHE	CA-C-N	6.59	124.39	120.24
58	b	667	PHE	C-N-CA	6.59	124.39	120.24
33	1	312	A	O4'-C1'-N9	6.18	117.77	108.50
54	v	141	ASP	CA-C-N	6.06	133.11	121.54
54	v	141	ASP	C-N-CA	6.06	133.11	121.54
59	c	440	LYS	CA-CB-CG	5.89	125.89	114.10
33	1	1379	A	N9-C1'-C2'	5.77	120.66	112.00
54	v	142	PHE	N-CA-C	5.67	122.88	110.80
40	g	151	MET	CA-CB-CG	5.59	125.28	114.10
60	e	496	ASP	CA-C-N	5.41	132.89	123.91
60	e	496	ASP	C-N-CA	5.41	132.89	123.91
11	E	135	GLU	CA-CB-CG	5.25	124.60	114.10
58	b	562	LEU	CA-CB-CG	5.20	134.51	116.30
46	n	6	MET	CB-CG-SD	5.18	128.25	112.70
60	e	381	MET	CB-CG-SD	5.18	128.23	112.70
54	v	143	VAL	CA-CB-CG2	5.08	119.03	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	1	312	A	C1'

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Mol	Chain	Res	Type	Atom
33	1	1379	A	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	L	204	ASP	Peptide
54	v	141	ASP	Peptide
56	w	286	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	369	0	381	2	0
2	3	2571	0	1300	13	0
3	5	1006	0	507	2	0
4	6	473	0	498	9	0
5	7	455	0	500	1	0
6	8	520	0	543	2	0
7	9	292	0	332	8	0
8	B	2159	0	2239	6	0
9	C	1681	0	1736	6	0
10	D	1599	0	1659	8	0
11	E	1413	0	1479	23	0
12	F	1338	0	1434	9	0
13	G	418	0	456	2	0
14	H	1114	0	1149	11	0
15	I	980	0	1056	42	0
16	J	1346	0	1389	6	0
17	K	942	0	998	9	0
18	L	1484	0	1530	6	0
19	M	1080	0	1143	5	0
20	N	937	0	978	0	0
21	O	902	0	920	6	0
22	P	995	0	1057	10	0
23	Q	943	0	992	6	0
24	R	907	0	951	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S	903	0	948	8	0
26	T	837	0	823	5	0
27	U	1020	0	1097	9	0
28	V	869	0	882	3	0
29	W	1104	0	1151	3	0
30	X	843	0	884	6	0
31	Z	323	0	367	5	0
32	Y	521	0	500	83	0
33	1	50934	0	25630	231	0
34	4	5856	0	2946	18	0
35	y	1627	0	828	16	0
36	xx	25	0	8	0	0
37	a	1868	0	1762	19	0
38	d	2107	0	2303	15	0
39	f	850	0	852	0	0
40	g	1334	0	1441	7	0
41	h	1113	0	1184	5	0
42	j	957	0	968	11	0
43	k	894	0	956	5	0
44	l	941	0	1029	6	0
45	m	924	0	969	42	0
46	n	814	0	877	30	0
47	o	813	0	828	6	0
48	p	666	0	697	8	0
49	q	621	0	658	5	0
50	r	664	0	743	0	0
51	s	645	0	677	42	0
52	t	935	0	1008	5	0
53	u	789	0	794	2	0
54	v	1430	0	1333	23	0
55	x	462	0	480	7	0
56	w	2786	0	2612	26	0
57	2	31537	0	15887	165	0
58	b	5545	0	6140	73	0
59	c	4939	0	5339	38	0
60	e	3988	0	3837	30	0
61	i	1209	0	1269	10	0
62	A	128	0	65	0	0
63	1	202	0	0	0	0
63	2	95	0	0	0	0
63	3	5	0	0	0	0
63	4	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	5	4	0	0	0	0
63	D	1	0	0	0	0
63	L	1	0	0	0	0
63	N	2	0	0	0	0
63	n	1	0	0	0	0
63	q	1	0	0	0	0
64	1	81	0	0	0	0
64	2	43	0	0	0	0
64	4	4	0	0	0	0
64	5	1	0	0	0	0
64	D	1	0	0	0	0
65	1	20	0	11	0	0
All	All	160214	0	116010	920	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 3.

All (920) 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)
35:y:54:5MU:C4	35:y:54:5MU:C5	1.82	1.66
33:1:1551:A:H2	57:2:1432:A:C4	1.13	1.65
33:1:1577:5MU:C5	33:1:1577:5MU:C4	1.82	1.64
33:1:404:5MU:C5	33:1:404:5MU:C4	1.82	1.60
32:Y:101:GLU:HG3	46:n:38:LYS:CE	1.23	1.58
33:1:1551:A:C2	57:2:1432:A:C4	1.94	1.56
33:1:1551:A:C2	57:2:1432:A:C5	2.02	1.47
32:Y:101:GLU:HG3	46:n:38:LYS:NZ	1.12	1.41
32:Y:101:GLU:CG	46:n:38:LYS:CE	1.99	1.39
33:1:720:U:C6	33:1:720:U:C5	2.11	1.39
32:Y:101:GLU:CG	46:n:38:LYS:NZ	1.90	1.30
33:1:720:U:C5	33:1:720:U:C4	2.24	1.25
15:I:162:MET:HA	33:1:720:U:C2	1.75	1.22
32:Y:95:PHE:CD2	51:s:42:PRO:HD3	1.76	1.19
32:Y:95:PHE:CE2	51:s:42:PRO:HD3	1.80	1.16
32:Y:95:PHE:CE2	51:s:42:PRO:CD	2.29	1.15
33:1:547:C:C4	45:m:132:ILE:CD1	2.30	1.15
32:Y:92:LEU:HD11	51:s:64:ASP:HB2	1.22	1.12
17:K:93:PRO:HD2	17:K:113:LYS:HD3	1.24	1.12
32:Y:101:GLU:CG	46:n:38:LYS:HE3	1.64	1.12
33:1:547:C:C4	45:m:132:ILE:HD13	1.86	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y:91:GLN:HG2	51:s:65:GLN:NE2	1.69	1.08
32:Y:91:GLN:NE2	45:m:119:ARG:NH2	2.01	1.07
33:1:547:C:C5	45:m:132:ILE:HD13	1.91	1.06
33:1:1551:A:C2	57:2:1432:A:C6	2.44	1.05
33:1:1551:A:N1	57:2:1432:A:C5	2.24	1.03
32:Y:101:GLU:HG3	46:n:38:LYS:HE3	1.17	1.00
32:Y:95:PHE:CE2	51:s:42:PRO:HD2	1.97	1.00
33:1:720:U:C6	33:1:720:U:N1	2.29	1.00
32:Y:92:LEU:HD11	51:s:64:ASP:CB	1.92	1.00
32:Y:101:GLU:HG3	46:n:38:LYS:HZ2	1.20	1.00
33:1:547:C:C4	45:m:132:ILE:HD11	1.96	0.99
33:1:1551:A:N3	57:2:1432:A:C2	2.31	0.99
32:Y:95:PHE:HE2	51:s:42:PRO:CD	1.76	0.98
32:Y:91:GLN:NE2	45:m:119:ARG:HH21	1.61	0.97
32:Y:101:GLU:CB	46:n:38:LYS:CE	2.42	0.97
33:1:753:G:N2	33:1:758:A:H62	1.61	0.97
15:I:162:MET:C	33:1:720:U:C2	2.43	0.97
33:1:720:U:C2	33:1:720:U:N3	2.33	0.96
33:1:1551:A:C2	57:2:1432:A:N3	2.35	0.95
33:1:720:U:C2	33:1:720:U:N1	2.33	0.95
57:2:1352:A:H2	57:2:1426:G:H1	1.06	0.95
32:Y:92:LEU:HD21	51:s:45:ILE:CD1	1.98	0.92
32:Y:95:PHE:CD2	51:s:42:PRO:CD	2.50	0.90
33:1:753:G:H21	33:1:758:A:N6	1.68	0.90
57:2:47:G:H1	57:2:371:A:H2	0.91	0.90
15:I:162:MET:HA	33:1:720:U:N1	1.86	0.90
35:y:50:U:H3	35:y:64:G:H1	1.19	0.90
57:2:47:G:N1	57:2:371:A:C2	2.40	0.90
15:I:162:MET:C	15:I:162:MET:CA	2.44	0.89
33:1:720:U:C4	33:1:720:U:N3	2.40	0.89
33:1:1551:A:C2	57:2:1432:A:C2	2.60	0.88
57:2:47:G:N1	57:2:371:A:H2	1.72	0.88
32:Y:101:GLU:CG	46:n:38:LYS:HZ1	1.72	0.88
33:1:547:C:N3	45:m:132:ILE:HD11	1.88	0.88
35:y:23:C:H2'	35:y:24:U:C6	2.09	0.87
32:Y:101:GLU:CB	46:n:38:LYS:HE2	2.03	0.87
32:Y:101:GLU:CA	46:n:38:LYS:HE2	2.05	0.86
15:I:162:MET:HA	15:I:162:MET:C	2.01	0.85
15:I:162:MET:C	33:1:720:U:N3	2.34	0.85
15:I:162:MET:C	33:1:720:U:C4	2.55	0.84
37:a:75:ALA:O	37:a:79:MET:HB2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1:1551:A:H2	57:2:1432:A:N3	1.69	0.83
32:Y:94:LYS:HE3	57:2:1249:A:OP1	1.79	0.82
32:Y:95:PHE:HD2	51:s:42:PRO:HD3	1.38	0.82
17:K:93:PRO:CD	17:K:113:LYS:HD3	2.07	0.82
32:Y:101:GLU:HG2	46:n:38:LYS:HE3	1.62	0.81
15:I:163:ILE:N	33:1:720:U:C4	2.48	0.81
33:1:540:G:H1	33:1:554:U:H3	1.29	0.81
32:Y:101:GLU:HA	46:n:38:LYS:HE2	1.62	0.81
32:Y:91:GLN:HE22	45:m:119:ARG:NH2	1.79	0.81
32:Y:99:PHE:CE1	51:s:8:GLY:HA2	2.16	0.81
33:1:753:G:H21	33:1:758:A:H62	0.87	0.80
15:I:162:MET:CA	33:1:720:U:C2	2.62	0.80
15:I:162:MET:C	33:1:720:U:C5	2.61	0.79
32:Y:101:GLU:HA	46:n:38:LYS:CE	2.13	0.79
33:1:547:C:C2	45:m:132:ILE:HG12	2.18	0.79
32:Y:99:PHE:HE1	51:s:8:GLY:HA2	1.48	0.78
32:Y:101:GLU:CA	46:n:38:LYS:HZ1	1.96	0.78
15:I:162:MET:C	33:1:720:U:C6	2.62	0.78
32:Y:52:ASN:HA	45:m:90:GLU:OE2	1.84	0.78
32:Y:91:GLN:HG2	51:s:65:GLN:HE21	1.48	0.78
32:Y:101:GLU:HA	46:n:38:LYS:NZ	1.97	0.77
32:Y:91:GLN:CG	51:s:65:GLN:NE2	2.47	0.77
32:Y:69:ASP:OD2	45:m:44:ARG:O	2.03	0.77
32:Y:92:LEU:CD2	51:s:45:ILE:CD1	2.61	0.77
47:o:131:ARG:HG3	49:q:76:ARG:HH22	1.50	0.77
32:Y:95:PHE:CZ	51:s:41:VAL:HG12	2.19	0.76
32:Y:95:PHE:HZ	51:s:41:VAL:HG12	1.50	0.76
32:Y:92:LEU:CD1	51:s:64:ASP:HB2	2.12	0.75
45:m:49:GLU:O	45:m:49:GLU:HG2	1.86	0.75
33:1:1944:G:H22	33:1:1952:U:H3	1.34	0.75
32:Y:95:PHE:CE2	51:s:41:VAL:HA	2.23	0.74
33:1:547:C:N3	45:m:132:ILE:CD1	2.46	0.74
35:y:43:A:H2'	35:y:44:A:C8	2.23	0.74
15:I:162:MET:C	33:1:720:U:N1	2.46	0.73
32:Y:101:GLU:CD	46:n:38:LYS:NZ	2.46	0.73
11:E:138:MET:HE3	11:E:138:MET:H	1.52	0.73
32:Y:95:PHE:HE2	51:s:41:VAL:HA	1.54	0.73
54:v:241:ALA:O	54:v:245:LEU:HB2	1.88	0.73
15:I:162:MET:CA	33:1:720:U:C4	2.72	0.73
32:Y:101:GLU:CA	46:n:38:LYS:CE	2.67	0.72
33:1:1188:U:H3	33:1:1198:G:H1	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2:1352:A:C2	57:2:1426:G:N1	2.48	0.72
57:2:791:C:H42	57:2:795:A:H61	1.37	0.71
57:2:1352:A:H2	57:2:1426:G:N1	1.85	0.71
32:Y:69:ASP:HB2	45:m:97:ARG:NH2	2.06	0.71
34:4:258:G:H1	34:4:267:U:H3	1.37	0.70
15:I:162:MET:CA	33:1:720:U:N3	2.55	0.70
37:a:93:LYS:HD3	54:v:156:VAL:HA	1.74	0.69
15:I:162:MET:O	33:1:720:U:N1	2.26	0.69
32:Y:69:ASP:CG	45:m:97:ARG:CZ	2.65	0.69
33:1:740:C:H41	33:1:747:G:H5''	1.57	0.69
27:U:146:SER:HB3	27:U:164:LYS:HB2	1.73	0.68
33:1:1551:A:N1	57:2:1432:A:N7	2.41	0.68
59:c:52:LEU:HD13	59:c:105:ALA:HB1	1.75	0.68
56:w:227:MET:HE3	56:w:332:THR:HB	1.74	0.68
33:1:219:G:H21	33:1:223:A:H8	1.40	0.68
11:E:4:ARG:HD3	32:Y:57:MET:HE1	1.76	0.68
11:E:113:ARG:HH22	45:m:110:ARG:HD2	1.57	0.67
38:d:193:PHE:O	38:d:197:LYS:HB2	1.93	0.67
7:9:6:SER:HB2	33:1:2106:C:H5''	1.77	0.67
32:Y:92:LEU:CD2	51:s:45:ILE:HD11	2.23	0.66
32:Y:92:LEU:HD21	51:s:45:ILE:HD13	1.77	0.66
27:U:50:ARG:HB2	27:U:53:GLU:HG3	1.76	0.66
33:1:719:G:H2'	33:1:720:U:H3'	1.76	0.66
57:2:1461:U:H2'	57:2:1462:G:H8	1.60	0.65
32:Y:91:GLN:CB	51:s:65:GLN:HA	2.27	0.65
59:c:305:ARG:HD3	59:c:389:LEU:HB2	1.78	0.65
32:Y:101:GLU:HA	46:n:38:LYS:HZ1	1.58	0.65
15:I:164:GLU:HG3	33:1:720:U:H3	1.62	0.64
33:1:1558:C:OP1	57:2:1456:G:C8	2.50	0.64
4:6:71:THR:HG21	33:1:1926:A:H61	1.60	0.64
57:2:47:G:O6	57:2:371:A:N1	2.30	0.64
11:E:84:MET:HE3	11:E:85:PRO:HD2	1.78	0.64
35:y:23:C:H2'	35:y:24:U:H6	1.63	0.64
15:I:162:MET:CA	33:1:720:U:N1	2.61	0.63
15:I:163:ILE:N	33:1:720:U:N3	2.45	0.63
33:1:546:U:C5'	45:m:129:ARG:NH2	2.60	0.63
46:n:3:LYS:HG2	57:2:996:G:H5''	1.81	0.63
16:J:65:THR:HG22	16:J:67:ALA:H	1.64	0.63
11:E:65:LYS:HE2	32:Y:39:ILE:HD12	1.81	0.63
57:2:1352:A:N1	57:2:1426:G:O6	2.32	0.63
37:a:88:GLN:HE21	54:v:174:LEU:HD11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:28:ALA:HB3	21:O:32:ALA:H	1.64	0.63
32:Y:92:LEU:HD11	51:s:64:ASP:CG	2.24	0.63
32:Y:101:GLU:CB	46:n:38:LYS:HZ1	2.12	0.63
35:y:43:A:H2'	35:y:44:A:H8	1.60	0.63
45:m:146:ALA:HB3	45:m:150:LYS:HE2	1.79	0.62
33:1:238:A:H62	33:1:910:A:H2	1.46	0.62
34:4:252:A:H62	34:4:273:G:N2	1.96	0.62
57:2:365:G:H3'	57:2:366:G:H8	1.64	0.62
58:b:377:LEU:HB3	58:b:892:ARG:HD2	1.82	0.62
58:b:644:LEU:HB3	60:e:369:GLN:HB3	1.81	0.62
48:p:40:ARG:HB2	57:2:352:G:H5''	1.82	0.62
10:D:159:ASP:HB3	10:D:161:LYS:HG3	1.81	0.62
15:I:162:MET:HB3	33:1:720:U:C6	2.35	0.61
34:4:252:A:H62	34:4:273:G:H21	1.46	0.61
11:E:41:ILE:HA	11:E:151:ARG:HH21	1.65	0.61
22:P:133:LYS:HB2	57:2:1371:C:OP1	2.00	0.61
54:v:230:LEU:HD13	54:v:231:THR:HG23	1.83	0.61
57:2:736:A:H62	57:2:754:G:H21	1.48	0.61
60:e:585:PRO:HD2	60:e:650:LEU:HD22	1.83	0.61
54:v:208:LEU:H	54:v:215:ALA:HB3	1.65	0.61
32:Y:101:GLU:CD	46:n:38:LYS:HZ1	2.07	0.60
37:a:227:GLU:HG3	37:a:229:ILE:HG12	1.82	0.60
14:H:90:SER:HA	14:H:93:LYS:HD3	1.83	0.60
32:Y:92:LEU:HD23	51:s:45:ILE:HD11	1.83	0.60
52:t:94:LYS:HD2	52:t:145:ALA:HB2	1.83	0.60
57:2:628:G:H2'	57:2:629:A:H8	1.66	0.60
56:w:341:VAL:HG21	56:w:371:ALA:H	1.66	0.60
32:Y:52:ASN:C	45:m:90:GLU:OE2	2.44	0.60
24:R:135:VAL:HG13	24:R:177:ILE:HG12	1.84	0.60
37:a:106:LEU:HD11	58:b:386:LYS:HG3	1.84	0.60
40:g:15:ASP:HB2	40:g:20:SER:H	1.67	0.60
33:1:220:U:H1'	33:1:1669:6MZ:H9C1	1.83	0.60
12:F:162:ASP:HB3	12:F:165:LYS:HB2	1.83	0.59
33:1:1551:A:N3	57:2:1432:A:N1	2.50	0.59
49:q:41:LYS:HD2	57:2:231:U:H5'	1.83	0.59
32:Y:91:GLN:CD	45:m:119:ARG:CZ	2.76	0.59
33:1:546:U:H5'	45:m:129:ARG:CZ	2.32	0.59
58:b:600:LEU:HD22	58:b:657:LEU:HD11	1.84	0.59
22:P:66:ARG:NH2	57:2:322:G:OP1	2.28	0.59
32:Y:53:GLY:N	45:m:90:GLU:OE2	2.35	0.59
33:1:1551:A:C2	57:2:1432:A:N1	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:62:VAL:HA	51:s:66:MET:HE2	1.84	0.59
54:v:176:ASN:O	54:v:176:ASN:ND2	2.32	0.59
56:w:491:MET:HG2	57:2:975:C:H4'	1.85	0.59
59:c:407:LEU:HD23	59:c:410:LEU:HD13	1.85	0.59
12:F:42:VAL:HG13	12:F:51:VAL:HG22	1.85	0.58
58:b:894:ARG:HH22	60:e:492:LEU:HD22	1.68	0.58
32:Y:52:ASN:CA	45:m:90:GLU:OE2	2.51	0.58
46:n:4:LYS:HD3	57:2:995:G:H5''	1.85	0.58
11:E:117:GLY:HA3	11:E:179:LYS:HB3	1.85	0.58
15:I:162:MET:CA	33:1:720:U:C5	2.86	0.58
33:1:765:U:H2'	33:1:766:G:H8	1.67	0.58
43:k:20:GLY:HA3	43:k:80:MET:HE2	1.86	0.58
57:2:346:C:H42	57:2:367:A:H61	1.51	0.58
38:d:119:LEU:HD21	55:x:77:LEU:HB3	1.86	0.58
42:j:104:GLY:HA3	57:2:1071:A:H4'	1.84	0.58
38:d:11:VAL:O	38:d:15:ILE:HB	2.03	0.58
35:y:44:A:H2'	35:y:45:G:C8	2.39	0.58
15:I:162:MET:N	33:1:720:U:C4	2.71	0.58
49:q:75:LEU:HD11	49:q:97:VAL:HG11	1.84	0.57
57:2:791:C:N4	57:2:795:A:H61	2.02	0.57
10:D:213:PHE:O	10:D:217:ASN:HB2	2.05	0.57
41:h:11:ILE:HD11	41:h:36:LEU:HD23	1.87	0.57
57:2:352:G:H1	57:2:363:A:H2	1.51	0.57
12:F:42:VAL:HG11	12:F:75:LEU:HD11	1.85	0.57
7:9:31:LYS:HE2	33:1:2118:A:H5'	1.85	0.57
25:S:133:VAL:HG11	25:S:173:ARG:HG2	1.86	0.57
60:e:341:LYS:O	60:e:345:SER:HB3	2.04	0.57
33:1:514:G:H2'	33:1:515:G:C8	2.40	0.57
32:Y:69:ASP:CB	45:m:97:ARG:NH2	2.68	0.57
58:b:260:VAL:HG22	58:b:294:ALA:HB3	1.87	0.57
17:K:93:PRO:HD2	17:K:113:LYS:CD	2.17	0.56
32:Y:91:GLN:CD	45:m:119:ARG:NE	2.63	0.56
33:1:1304:G:H5''	33:1:1305:C:H5'	1.87	0.56
15:I:162:MET:CA	33:1:720:U:C6	2.89	0.56
33:1:729:A:H61	33:1:733:A:H62	1.54	0.56
57:2:668:G:H2'	57:2:669:A:C8	2.41	0.56
59:c:198:LYS:O	59:c:202:MET:HB2	2.05	0.56
37:a:197:GLU:HB2	37:a:206:ILE:HB	1.86	0.56
57:2:618:G:H22	57:2:695:G:H1	1.54	0.56
32:Y:69:ASP:CG	45:m:97:ARG:NH2	2.64	0.56
59:c:678:LEU:HD23	59:c:685:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:4:U:H3	2:3:120:G:H1	1.51	0.56
30:X:130:ALA:HB2	34:4:123:A:H62	1.71	0.56
33:1:540:G:H2'	33:1:541:G:H8	1.70	0.56
58:b:478:LEU:HD13	60:e:451:GLU:HG2	1.87	0.56
33:1:737:A:H2	33:1:748:A:H8	1.54	0.56
37:a:93:LYS:HB2	54:v:156:VAL:HG23	1.87	0.56
61:i:38:LEU:HD13	61:i:44:SER:HB3	1.85	0.56
33:1:1968:A:H2'	33:1:1969:A:C8	2.40	0.55
26:T:72:PRO:HB3	34:4:50:G:H5'	1.88	0.55
30:X:125:LYS:HG3	30:X:134:MET:HE1	1.88	0.55
33:1:32:G:H22	33:1:42:U:H3	1.53	0.55
35:y:24:U:H2'	35:y:25:C:O4'	2.07	0.55
59:c:368:LEU:HD13	59:c:404:LEU:HG	1.88	0.55
2:3:23:U:H2'	2:3:24:G:C8	2.41	0.55
30:X:131:ASN:HB2	30:X:133:THR:HG23	1.89	0.55
58:b:196:PRO:HG2	58:b:199:ALA:HB2	1.89	0.55
32:Y:69:ASP:CG	45:m:97:ARG:NE	2.64	0.55
40:g:141:GLU:O	40:g:145:ILE:HD12	2.07	0.55
57:2:350:A:N6	57:2:366:G:H21	2.05	0.55
57:2:921:A:H4'	57:2:922:G:H5''	1.88	0.55
8:B:134:LEU:HD23	8:B:137:ILE:HD12	1.89	0.55
32:Y:91:GLN:CD	45:m:119:ARG:NH2	2.65	0.55
58:b:788:TYR:HD2	58:b:804:LYS:HD3	1.72	0.55
59:c:106:ILE:HD12	59:c:109:ILE:HD11	1.89	0.55
10:D:66:VAL:HG22	33:1:270:A:H4'	1.87	0.55
19:M:65:TRP:HB2	19:M:105:GLU:HB2	1.89	0.55
54:v:210:THR:HG22	54:v:212:LYS:H	1.71	0.55
59:c:413:LYS:HE2	60:e:409:GLU:HA	1.89	0.55
17:K:122:LEU:HD13	22:P:97:VAL:HG11	1.88	0.54
44:l:79:VAL:HG12	44:l:102:LEU:HD23	1.89	0.54
29:W:90:THR:HG22	29:W:94:LYS:HG3	1.90	0.54
33:1:705:G:H4'	33:1:706:A:H5''	1.88	0.54
37:a:127:VAL:HG21	58:b:367:LEU:HD11	1.89	0.54
52:t:150:PRO:HD2	52:t:160:TYR:CD2	2.41	0.54
21:O:56:VAL:HG22	21:O:65:VAL:HG22	1.87	0.54
10:D:35:ALA:HA	10:D:151:GLU:HG2	1.89	0.54
15:I:140:VAL:HA	15:I:163:ILE:HD11	1.88	0.54
48:p:62:ARG:HG2	57:2:97:G:H5''	1.90	0.54
14:H:58:VAL:HG22	14:H:118:PHE:HA	1.89	0.54
33:1:1053:U:H4'	33:1:1262:A:H4'	1.89	0.54
40:g:56:LYS:HD2	40:g:57:ASN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1:1551:A:H2	57:2:1432:A:N9	1.88	0.54
38:d:7:PRO:HB2	38:d:10:ARG:HG2	1.90	0.54
57:2:1294:A:H2'	57:2:1295:G:C8	2.42	0.54
56:w:341:VAL:HG23	56:w:359:MET:HE1	1.90	0.53
57:2:38:U:H3	57:2:373:G:H1	1.56	0.53
58:b:845:VAL:HG13	58:b:855:MET:HE1	1.90	0.53
61:i:46:LEU:HA	61:i:49:LYS:HZ2	1.73	0.53
44:l:50:ARG:HB3	44:l:66:TYR:HE1	1.72	0.53
56:w:263:LYS:HB2	56:w:291:PHE:HB3	1.90	0.53
38:d:164:ARG:HG2	57:2:413:U:H5'	1.89	0.53
8:B:43:LYS:HD3	8:B:57:GLY:HA2	1.91	0.53
11:E:61:ILE:HA	11:E:141:GLU:HG3	1.91	0.53
37:a:175:PHE:HE2	54:v:228:SER:HA	1.74	0.53
35:y:22:G:H2'	35:y:23:C:C6	2.43	0.53
56:w:404:ASP:HA	56:w:407:GLU:HG2	1.89	0.53
33:1:371:U:OP2	47:o:123:ARG:NE	2.42	0.53
38:d:194:ILE:HD11	38:d:255:LEU:HD11	1.91	0.53
58:b:578:ALA:HB1	60:e:339:VAL:HG21	1.90	0.53
57:2:1008:U:H2'	57:2:1009:G:H8	1.73	0.52
15:I:113:LEU:HD13	15:I:143:ILE:HD11	1.91	0.52
57:2:875:G:H1	57:2:1327:U:H3	1.57	0.52
57:2:1366:U:H2'	57:2:1367:G:H8	1.75	0.52
59:c:48:LEU:HD11	59:c:109:ILE:HD13	1.92	0.52
8:B:169:LYS:HG2	8:B:174:VAL:HG22	1.91	0.52
32:Y:95:PHE:HE2	51:s:42:PRO:HD2	1.47	0.52
57:2:778:G:H2'	57:2:779:A:H8	1.74	0.52
59:c:509:ARG:HG3	59:c:590:LEU:HD21	1.92	0.52
54:v:155:ALA:HB1	58:b:264:LEU:HD11	1.90	0.52
57:2:47:G:C6	57:2:371:A:N1	2.78	0.52
57:2:619:G:H1'	57:2:687:G:H5'	1.91	0.52
57:2:636:U:H2'	57:2:637:G:H8	1.75	0.52
32:Y:91:GLN:HG3	51:s:65:GLN:HA	1.92	0.52
33:1:1551:A:C2	57:2:1432:A:N9	2.70	0.52
57:2:392:G:H2'	57:2:393:G:H8	1.73	0.52
15:I:114:LEU:HD23	15:I:170:MET:HE1	1.90	0.52
15:I:166:THR:O	15:I:170:MET:HB3	2.09	0.52
32:Y:92:LEU:HD11	51:s:64:ASP:OD2	2.10	0.52
34:4:269:U:H2'	34:4:270:A:H8	1.74	0.52
45:m:43:LEU:HD11	45:m:93:ILE:HG13	1.92	0.52
8:B:146:VAL:HB	8:B:156:LEU:HD23	1.91	0.52
21:O:63:ILE:HD11	21:O:130:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:b:274:ILE:HG22	58:b:296:ILE:HA	1.90	0.52
33:1:53:U:H4'	33:1:54:C:H5'	1.91	0.52
57:2:987:U:H2'	57:2:988:G:H8	1.75	0.52
58:b:734:LEU:HA	58:b:737:LYS:HG2	1.92	0.52
33:1:546:U:H4'	33:1:547:C:H5	1.75	0.51
38:d:147:PRO:HD2	57:2:379:C:H5''	1.91	0.51
57:2:365:G:H3'	57:2:366:G:C8	2.44	0.51
2:3:60:A:H2'	2:3:61:A:C8	2.45	0.51
14:H:57:VAL:HG12	14:H:163:MET:HA	1.92	0.51
11:E:165:GLU:HA	11:E:168:LEU:HB3	1.93	0.51
33:1:2155:C:H2'	33:1:2156:A:H8	1.76	0.51
43:k:120:ASN:HA	53:u:601:ARG:HH12	1.75	0.51
55:x:81:LYS:HB2	55:x:84:VAL:HB	1.92	0.51
57:2:1019:C:H2'	57:2:1020:G:H8	1.76	0.51
58:b:617:LEU:HB3	58:b:655:LEU:HD11	1.91	0.51
59:c:221:TYR:HA	59:c:224:ILE:HD12	1.92	0.51
61:i:96:VAL:HG11	61:i:110:ILE:HG12	1.92	0.51
9:C:70:ALA:HB1	22:P:25:LEU:HD21	1.92	0.51
28:V:65:ILE:HG21	28:V:106:ILE:HG21	1.92	0.51
60:e:128:ASP:HB3	60:e:131:ILE:HG12	1.92	0.51
4:6:51:ILE:HD13	33:1:2060:C:H5''	1.93	0.51
14:H:73:LYS:HD2	14:H:76:LYS:HD2	1.92	0.51
29:W:137:ARG:HH12	33:1:1079:C:H6	1.58	0.51
33:1:254:U:H3	33:1:312:A:H61	1.59	0.51
45:m:133:MET:HE3	45:m:135:LEU:HD12	1.91	0.51
15:I:92:GLU:HG2	15:I:106:LYS:HZ3	1.76	0.51
11:E:35:ILE:HG12	11:E:157:ILE:HG12	1.93	0.51
12:F:140:LEU:HD11	12:F:176:GLN:HG3	1.93	0.51
33:1:1072:U:H3	33:1:1248:A:H61	1.58	0.50
18:L:188:LYS:HD2	34:4:208:A:H5'	1.93	0.50
34:4:267:U:H2'	34:4:268:G:H8	1.76	0.50
57:2:1293:C:H2'	57:2:1294:A:H8	1.76	0.50
7:9:16:VAL:HG22	7:9:25:VAL:HG22	1.93	0.50
54:v:137:ALA:HB3	58:b:210:VAL:HA	1.92	0.50
57:2:627:G:H2'	57:2:628:G:C8	2.46	0.50
16:J:89:LEU:HA	16:J:206:ILE:HD12	1.93	0.50
54:v:264:LEU:HA	54:v:267:LEU:HD12	1.93	0.50
57:2:311:C:H2'	57:2:312:A:H8	1.76	0.50
57:2:667:G:H2'	57:2:668:G:C8	2.46	0.50
57:2:1352:A:N1	57:2:1426:G:C6	2.80	0.50
9:C:93:ILE:HG21	9:C:142:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y:92:LEU:CD1	51:s:64:ASP:OD2	2.60	0.50
37:a:92:LEU:HD12	58:b:903:PHE:HE1	1.76	0.50
4:6:83:GLU:HG2	4:6:98:LYS:HE2	1.93	0.50
14:H:134:PHE:HA	14:H:137:ASP:HB3	1.94	0.50
57:2:220:U:O2	57:2:259:G:C6	2.63	0.50
37:a:147:THR:HG22	37:a:149:ILE:HG12	1.93	0.50
43:k:29:HIS:HA	43:k:59:SER:HB3	1.94	0.50
25:S:164:PHE:HE2	25:S:166:MET:HE2	1.76	0.50
33:1:546:U:C5'	45:m:129:ARG:HH22	2.25	0.50
33:1:546:U:H5'	45:m:129:ARG:NH2	2.26	0.50
58:b:438:ILE:HD13	58:b:810:LEU:HB3	1.94	0.50
15:I:162:MET:N	33:1:720:U:N3	2.60	0.49
35:y:25:C:H2'	35:y:26:G:O4'	2.12	0.49
16:J:103:PRO:HB3	23:Q:68:ALA:HB2	1.94	0.49
32:Y:91:GLN:CG	51:s:65:GLN:CD	2.85	0.49
32:Y:91:GLN:HG3	51:s:65:GLN:CG	2.41	0.49
57:2:220:U:O2	57:2:259:G:O6	2.30	0.49
57:2:931:C:H2'	57:2:932:A:C8	2.47	0.49
14:H:41:LYS:O	14:H:45:VAL:HG23	2.12	0.49
32:Y:101:GLU:CG	46:n:38:LYS:HZ2	1.90	0.49
33:1:701:U:H2'	33:1:702:G:H8	1.76	0.49
60:e:123:ASN:H	60:e:126:TYR:HB2	1.76	0.49
16:J:138:HIS:CD2	16:J:146:TRP:HB3	2.46	0.49
33:1:1676:G:H2'	33:1:1677:G:C8	2.46	0.49
32:Y:52:ASN:OD1	45:m:97:ARG:NH1	2.43	0.49
32:Y:91:GLN:HG3	51:s:65:GLN:HG3	1.94	0.49
34:4:59:G:H1	34:4:66:C:H5	1.60	0.49
57:2:1179:G:H2'	57:2:1180:G:H8	1.77	0.49
33:1:765:U:H2'	33:1:766:G:C8	2.46	0.49
15:I:162:MET:O	33:1:720:U:C6	2.65	0.49
33:1:1246:U:H2'	33:1:1247:A:C8	2.48	0.49
46:n:3:LYS:HB2	46:n:6:MET:HG2	1.94	0.49
57:2:1448:G:H2'	57:2:1449:G:H8	1.78	0.49
33:1:1247:A:H2'	33:1:1248:A:H8	1.78	0.49
33:1:547:C:O2	45:m:121:LYS:HD3	2.12	0.49
33:1:688:A:H2'	33:1:689:A:C8	2.48	0.49
40:g:87:VAL:HG22	40:g:152:TYR:HB3	1.95	0.49
55:x:96:VAL:HG12	55:x:98:VAL:H	1.78	0.49
57:2:133:G:H2'	57:2:134:G:C8	2.48	0.49
54:v:208:LEU:HG	54:v:298:ALA:HB2	1.94	0.48
56:w:347:LEU:HG	59:c:204:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2:1194:A:H2'	59:c:27:GLN:HG2	1.94	0.48
57:2:1341:4OC:H2'	57:2:1342:C:O4'	2.12	0.48
25:S:69:HIS:HB2	33:1:144:G:H4'	1.94	0.48
51:s:41:VAL:HG22	51:s:44:MET:HE3	1.94	0.48
57:2:60:A:H5''	57:2:363:A:H5''	1.95	0.48
58:b:566:LEU:HD21	60:e:391:ILE:HG12	1.94	0.48
33:1:1348:A:H2'	33:1:1349:A:H8	1.78	0.48
56:w:543:PRO:HG2	56:w:546:ALA:HB2	1.95	0.48
57:2:467:U:H2'	57:2:468:G:H8	1.79	0.48
58:b:548:LEU:HD11	58:b:702:LYS:HG2	1.94	0.48
28:V:127:GLN:OE1	28:V:128:PRO:HD2	2.12	0.48
58:b:378:ALA:O	58:b:382:LYS:HG3	2.13	0.48
58:b:695:LEU:O	58:b:699:VAL:HG23	2.14	0.48
21:O:99:ALA:HB1	21:O:134:VAL:HG23	1.95	0.48
33:1:184:U:H2'	33:1:185:G:C8	2.48	0.48
33:1:547:C:C2	45:m:132:ILE:CG1	2.94	0.48
33:1:547:C:O4'	45:m:132:ILE:HG23	2.14	0.48
37:a:281:LEU:HD11	37:a:293:SER:HB2	1.95	0.48
60:e:467:LYS:HE2	60:e:473:LEU:HG	1.96	0.48
41:h:14:MET:HG3	41:h:31:ILE:HG21	1.96	0.48
56:w:517:TYR:HB2	59:c:557:LEU:HD21	1.96	0.48
57:2:131:G:H1	57:2:163:C:H5	1.60	0.48
58:b:671:ILE:O	58:b:675:ILE:HD12	2.14	0.48
58:b:788:TYR:HE2	58:b:808:GLN:HG3	1.79	0.48
42:j:72:LEU:HB2	42:j:145:LEU:HD11	1.96	0.48
57:2:874:G:H2'	57:2:875:G:H8	1.79	0.48
59:c:638:GLU:HG2	59:c:642:LEU:HD13	1.95	0.48
33:1:2287:C:H2'	33:1:2288:U:H6	1.79	0.47
34:4:76:A:H62	34:4:93:G:H8	1.61	0.47
57:2:628:G:H2'	57:2:629:A:C8	2.47	0.47
23:Q:31:LEU:HD13	33:1:232:C:H4'	1.96	0.47
32:Y:101:GLU:CD	46:n:38:LYS:HZ2	2.13	0.47
42:j:71:ARG:HE	42:j:143:LYS:HZ1	1.60	0.47
46:n:53:ASN:HA	46:n:58:ARG:HD2	1.96	0.47
54:v:145:ALA:HA	58:b:189:THR:HG22	1.97	0.47
57:2:1294:A:H2'	57:2:1295:G:H8	1.78	0.47
58:b:365:ASN:HB3	58:b:368:LYS:HB2	1.96	0.47
13:G:55:LYS:HA	13:G:55:LYS:HD3	1.75	0.47
25:S:64:LYS:HB3	25:S:127:ALA:HB2	1.95	0.47
33:1:1088:G:H2'	33:1:1089:A:C8	2.49	0.47
33:1:1537:G:H21	33:1:1540:C:H41	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1:1855:A:H2'	33:1:1856:G:C8	2.49	0.47
57:2:553:U:H2'	57:2:554:A:H8	1.79	0.47
11:E:5:LEU:HD12	11:E:8:LEU:HD23	1.95	0.47
15:I:169:ASN:O	15:I:169:ASN:ND2	2.44	0.47
32:Y:101:GLU:HB3	46:n:38:LYS:HE2	1.91	0.47
42:j:91:ILE:HG21	42:j:140:VAL:HG11	1.97	0.47
57:2:931:C:H2'	57:2:932:A:H8	1.77	0.47
58:b:794:ARG:HE	58:b:794:ARG:HB3	1.56	0.47
59:c:519:THR:HG22	59:c:579:ILE:HD13	1.96	0.47
4:6:85:MET:HE3	4:6:85:MET:HB3	1.74	0.47
33:1:969:G:H1'	33:1:1270:C:H5''	1.95	0.47
33:1:1118:U:H4'	33:1:1119:U:H5'	1.97	0.47
38:d:105:LEU:O	38:d:109:GLU:HG2	2.14	0.47
58:b:308:LYS:HB3	58:b:312:ARG:HH21	1.79	0.47
61:i:10:ARG:HG2	61:i:15:VAL:HG22	1.95	0.47
18:L:140:SER:HB2	33:1:277:G:H5''	1.96	0.47
33:1:1372:C:H41	33:1:1381:G:H1	1.62	0.47
57:2:723:G:H4'	57:2:1452:A:H4'	1.97	0.47
58:b:263:ASN:H	58:b:296:ILE:HD12	1.79	0.47
11:E:14:VAL:HG22	11:E:29:VAL:HG11	1.97	0.47
14:H:170:PRO:HA	14:H:173:LEU:HB3	1.95	0.47
15:I:72:ALA:HA	15:I:75:LYS:HG2	1.96	0.47
29:W:109:LYS:HE2	34:4:146:A:H5''	1.95	0.47
33:1:1379:A:HO2'	33:1:1380:A:H8	1.61	0.47
54:v:242:TRP:HD1	54:v:243:GLU:HG2	1.79	0.47
58:b:444:GLU:HA	58:b:447:MET:HG3	1.97	0.47
3:5:3:C:H5''	27:U:150:HIS:HB2	1.97	0.47
21:O:52:PRO:HG2	21:O:118:VAL:HG12	1.96	0.47
33:1:233:C:H2'	33:1:234:G:C8	2.50	0.47
33:1:547:C:N4	45:m:132:ILE:HD11	2.28	0.47
33:1:547:C:C6	45:m:132:ILE:HD13	2.45	0.47
58:b:308:LYS:HB3	58:b:312:ARG:NH2	2.30	0.47
11:E:146:LYS:HE2	11:E:146:LYS:HB2	1.65	0.47
31:Z:42:LYS:HG3	33:1:1658:C:H5	1.79	0.47
33:1:1710:A:H2'	33:1:1711:G:H8	1.79	0.47
58:b:209:LYS:HE2	58:b:211:THR:HG22	1.97	0.47
27:U:55:LEU:HD13	27:U:96:LYS:HD2	1.97	0.47
33:1:1046:A:H5'	33:1:1127:A:H1'	1.97	0.47
58:b:751:LEU:HD22	60:e:443:LEU:HD21	1.97	0.47
7:9:24:MET:HE3	7:9:35:ARG:HB2	1.95	0.46
23:Q:44:ARG:HD2	24:R:153:MET:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:296:ASP:HA	56:w:299:LEU:HB3	1.97	0.46
57:2:347:G:H21	57:2:349:A:N6	2.13	0.46
57:2:438:G:H1'	57:2:439:U:H5	1.80	0.46
30:X:31:LYS:HE3	30:X:31:LYS:HB3	1.73	0.46
41:h:118:PRO:HA	57:2:596:A:N7	2.31	0.46
52:t:79:LYS:NZ	57:2:1378:U:OP1	2.46	0.46
55:x:80:ILE:HG13	55:x:81:LYS:HG2	1.97	0.46
10:D:60:HIS:HB2	18:L:37:LEU:HB3	1.97	0.46
15:I:169:ASN:HD22	15:I:169:ASN:C	2.23	0.46
27:U:78:ILE:HG13	27:U:135:VAL:HG12	1.97	0.46
42:j:66:ALA:HB1	42:j:70:VAL:HG21	1.96	0.46
56:w:487:LEU:HD12	56:w:512:VAL:HG11	1.98	0.46
32:Y:95:PHE:CD2	51:s:67:VAL:HG13	2.51	0.46
33:1:540:G:N2	33:1:554:U:O2	2.38	0.46
33:1:1713:U:H2'	33:1:1714:U:C6	2.50	0.46
43:k:117:ILE:HD11	53:u:594:VAL:HA	1.98	0.46
57:2:454:C:H2'	57:2:455:A:H8	1.80	0.46
57:2:896:U:H2'	57:2:897:G:H8	1.80	0.46
9:C:216:MET:HG2	33:1:2319:G:H5'	1.98	0.46
33:1:314:U:H2'	33:1:315:C:C6	2.51	0.46
33:1:1489:A:H2'	33:1:1490:A:C8	2.50	0.46
2:3:92:G:H22	19:M:38:GLU:HG2	1.80	0.46
4:6:52:VAL:HB	4:6:99:GLU:HG3	1.98	0.46
14:H:44:VAL:HA	14:H:47:VAL:HG22	1.97	0.46
33:1:771:A:H8	33:1:772:G:H1'	1.80	0.46
33:1:2048:U:H2'	33:1:2049:G:C8	2.51	0.46
49:q:76:ARG:HE	49:q:103:LYS:HZ3	1.62	0.46
57:2:1066:U:H2'	57:2:1067:C:H6	1.81	0.46
59:c:615:VAL:HG21	59:c:640:LEU:HD11	1.98	0.46
7:9:1:MET:HE3	33:1:2382:C:H5''	1.97	0.46
57:2:669:A:H2'	57:2:670:A:C8	2.50	0.46
57:2:892:A:H2'	57:2:893:U:C6	2.51	0.46
2:3:60:A:H2'	2:3:61:A:H8	1.79	0.46
22:P:116:ARG:HD2	22:P:143:VAL:HG21	1.98	0.46
56:w:221:LEU:HB2	56:w:248:TRP:HZ2	1.81	0.46
57:2:454:C:H2'	57:2:455:A:C8	2.50	0.46
58:b:336:MET:HE2	58:b:861:THR:HA	1.97	0.46
58:b:549:LYS:HG3	60:e:403:SER:HB3	1.97	0.46
33:1:294:U:H2'	33:1:295:C:C6	2.51	0.46
33:1:1127:A:H2'	33:1:1128:A:C8	2.51	0.46
56:w:296:ASP:H	59:c:202:MET:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:b:558:THR:O	58:b:562:LEU:HD22	2.16	0.46
59:c:567:GLY:HA2	59:c:570:LYS:HG3	1.97	0.46
11:E:9:TYR:HA	11:E:13:ILE:HB	1.98	0.46
15:I:89:ILE:HG21	15:I:105:LEU:HD22	1.98	0.46
33:1:1537:G:H21	33:1:1540:C:N4	2.14	0.46
48:p:40:ARG:HA	48:p:102:VAL:HG21	1.97	0.46
58:b:261:LYS:HG2	58:b:262:PRO:HD2	1.97	0.46
34:4:66:C:H5''	34:4:67:G:O4'	2.16	0.45
57:2:896:U:H2'	57:2:897:G:C8	2.51	0.45
2:3:19:C:H2'	2:3:20:A:H8	1.80	0.45
33:1:1247:A:H2'	33:1:1248:A:C8	2.51	0.45
33:1:1646:C:H2'	33:1:1647:G:H8	1.81	0.45
33:1:1931:U:H2'	33:1:1932:U:C6	2.50	0.45
37:a:271:LEU:HD22	37:a:276:LEU:HD11	1.99	0.45
57:2:862:G:H2'	57:2:863:G:H8	1.80	0.45
58:b:342:THR:HA	58:b:355:PRO:HA	1.98	0.45
2:3:15:U:H4'	2:3:16:G:H5'	1.99	0.45
17:K:97:ARG:HA	17:K:117:LEU:HD22	1.97	0.45
26:T:13:LYS:HD3	33:1:998:G:H5''	1.98	0.45
57:2:22:G:H2'	57:2:23:G:C8	2.52	0.45
57:2:35:C:H2'	57:2:36:G:H8	1.82	0.45
57:2:197:C:H2'	57:2:198:G:H8	1.82	0.45
57:2:334:U:H2'	57:2:335:G:H8	1.82	0.45
57:2:894:U:H2'	57:2:895:A:H8	1.81	0.45
15:I:63:LEU:HB3	15:I:68:VAL:HB	1.97	0.45
16:J:168:LYS:HE3	16:J:168:LYS:HB3	1.74	0.45
37:a:120:TYR:HD2	58:b:367:LEU:HD22	1.81	0.45
58:b:377:LEU:HD21	58:b:888:LYS:HB2	1.99	0.45
60:e:304:ILE:HG23	60:e:308:LEU:HD12	1.99	0.45
33:1:730:A:H2'	33:1:731:G:H8	1.80	0.45
35:y:24:U:H2'	35:y:25:C:C6	2.51	0.45
41:h:2:LYS:HD3	41:h:2:LYS:HA	1.72	0.45
57:2:1366:U:H2'	57:2:1367:G:C8	2.51	0.45
61:i:191:ARG:HB2	61:i:191:ARG:CZ	2.46	0.45
2:3:82:U:H2'	2:3:83:U:C6	2.51	0.45
23:Q:6:ARG:NH2	33:1:910:A:H2'	2.31	0.45
33:1:547:C:C2	45:m:132:ILE:CD1	3.00	0.45
33:1:1228:A:H2'	33:1:1229:A:C8	2.52	0.45
33:1:1955:G:H2'	33:1:1956:A:C8	2.51	0.45
58:b:439:ARG:HG3	58:b:443:LYS:HE2	1.97	0.45
38:d:15:ILE:HG23	38:d:74:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:76:MET:HE3	42:j:138:ARG:HB2	1.97	0.45
48:p:56:ALA:HB2	48:p:71:LEU:HD11	1.99	0.45
56:w:290:ALA:H	59:c:321:ALA:HB3	1.82	0.45
57:2:874:G:H2'	57:2:875:G:C8	2.52	0.45
57:2:987:U:H2'	57:2:988:G:C8	2.51	0.45
60:e:460:ARG:HA	60:e:463:GLN:HG2	1.98	0.45
15:I:162:MET:CB	33:1:720:U:C6	3.00	0.45
16:J:164:GLU:HG2	16:J:186:VAL:HG21	1.98	0.45
33:1:1184:U:H2'	33:1:1185:A:H8	1.82	0.45
33:1:1551:A:N3	57:2:1432:A:C6	2.84	0.45
47:o:74:ILE:HG21	47:o:91:LEU:HB2	1.99	0.45
56:w:375:GLU:HG3	59:c:337:LEU:HD22	1.99	0.45
57:2:1293:C:H2'	57:2:1294:A:C8	2.52	0.45
57:2:1454:U:H2'	57:2:1455:2MG:C8	2.52	0.45
58:b:551:LYS:HZ2	58:b:699:VAL:HG22	1.82	0.45
23:Q:30:THR:HG22	23:Q:31:LEU:HD23	1.98	0.45
34:4:267:U:H2'	34:4:268:G:C8	2.52	0.45
57:2:505:U:H2'	57:2:506:G:H8	1.82	0.45
58:b:295:LYS:HE2	58:b:297:ILE:HD11	1.99	0.45
58:b:440:PRO:HA	58:b:443:LYS:HE3	1.99	0.45
2:3:54:U:H2'	2:3:55:G:H8	1.82	0.45
15:I:66:LYS:HB3	15:I:95:VAL:HG21	1.97	0.45
33:1:2338:U:H2'	33:1:2339:C:C6	2.52	0.45
46:n:17:VAL:HG11	46:n:59:LEU:HD11	1.99	0.45
60:e:360:LYS:HE3	60:e:360:LYS:HB3	1.73	0.45
15:I:114:LEU:HD21	15:I:167:ALA:HB2	1.99	0.44
33:1:576:A:H5''	33:1:1908:A:H61	1.82	0.44
33:1:1184:U:H2'	33:1:1185:A:C8	2.51	0.44
33:1:2287:C:H2'	33:1:2288:U:C6	2.53	0.44
47:o:112:MET:HE2	47:o:112:MET:HB2	1.71	0.44
58:b:530:LYS:HZ3	60:e:301:VAL:HG23	1.80	0.44
59:c:298:LEU:HD21	59:c:384:ILE:HA	1.98	0.44
1:0:57:LEU:HD23	24:R:103:VAL:HG21	2.00	0.44
12:F:58:LEU:HB3	12:F:100:LEU:HD22	1.99	0.44
13:G:45:ILE:HG12	13:G:71:MET:HE3	1.99	0.44
24:R:173:MET:HE2	24:R:173:MET:HB2	1.80	0.44
25:S:173:ARG:HA	25:S:173:ARG:HD3	1.62	0.44
32:Y:91:GLN:HG3	51:s:65:GLN:CA	2.47	0.44
33:1:992:U:H2'	33:1:993:G:H8	1.82	0.44
33:1:1372:C:H5	33:1:1381:G:H22	1.65	0.44
58:b:807:TRP:O	58:b:811:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:c:213:LYS:HA	59:c:213:LYS:HD3	1.64	0.44
60:e:359:ILE:HD12	60:e:359:ILE:HA	1.91	0.44
4:6:46:LYS:HE2	4:6:46:LYS:HB2	1.78	0.44
33:1:608:C:H2'	33:1:609:A:C8	2.52	0.44
33:1:1885:U:H5''	33:1:1886:A:H5'	1.98	0.44
34:4:171:A:H2'	34:4:172:C:C6	2.53	0.44
55:x:82:PRO:HA	60:e:100:THR:HG21	1.98	0.44
56:w:332:THR:HG23	56:w:334:LYS:H	1.83	0.44
57:2:320:A:H5''	57:2:321:C:H5	1.81	0.44
57:2:444:G:H2'	57:2:445:A:H8	1.81	0.44
58:b:545:SER:O	58:b:549:LYS:HG2	2.18	0.44
58:b:590:LYS:HE3	58:b:590:LYS:HB2	1.78	0.44
27:U:116:MET:HG2	27:U:118:ASN:H	1.81	0.44
33:1:228:U:H2'	33:1:229:G:C8	2.53	0.44
33:1:2369:C:H2'	33:1:2370:A:C8	2.52	0.44
38:d:8:ARG:HG2	38:d:22:THR:HB	1.98	0.44
56:w:407:GLU:HG3	59:c:458:LYS:HG2	1.99	0.44
57:2:553:U:H2'	57:2:554:A:C8	2.51	0.44
58:b:443:LYS:HE3	58:b:443:LYS:HB2	1.77	0.44
58:b:482:ARG:HA	58:b:485:ILE:HG12	1.99	0.44
58:b:616:ILE:HG12	58:b:656:ILE:HB	1.99	0.44
58:b:731:ILE:HA	58:b:734:LEU:HG	2.00	0.44
6:8:73:LYS:HE3	6:8:73:LYS:HB3	1.88	0.44
11:E:179:LYS:HB2	11:E:179:LYS:HE2	1.67	0.44
22:P:58:VAL:HB	22:P:66:ARG:HG3	2.00	0.44
33:1:1246:U:H2'	33:1:1247:A:H8	1.81	0.44
14:H:92:MET:HA	14:H:95:ALA:HB3	2.00	0.44
33:1:937:U:H2'	33:1:938:U:C6	2.53	0.44
33:1:1432:U:H2'	33:1:1433:C:C6	2.52	0.44
47:o:67:LEU:HD22	47:o:94:ILE:HG23	1.99	0.44
56:w:242:VAL:HB	56:w:257:LEU:HD23	2.00	0.44
57:2:791:C:H42	57:2:795:A:N6	2.09	0.44
57:2:1156:C:H2'	57:2:1157:U:C6	2.52	0.44
59:c:644:SER:H	59:c:645:ARG:NH2	2.15	0.44
9:C:46:VAL:HG11	9:C:144:VAL:HG22	2.00	0.44
23:Q:4:VAL:HG22	33:1:858:U:H1'	1.99	0.44
28:V:53:VAL:HG21	28:V:59:VAL:HG23	1.99	0.44
35:y:28:C:H2'	35:y:29:G:H8	1.83	0.44
49:q:45:VAL:HG21	49:q:83:LEU:HD21	1.99	0.44
57:2:351:U:H3	57:2:365:G:H1	1.66	0.44
12:F:114:MET:HG2	12:F:187:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2:554:A:H2'	57:2:555:A:C8	2.53	0.44
18:L:207:LYS:HA	18:L:207:LYS:HD2	1.79	0.43
32:Y:95:PHE:HE2	51:s:41:VAL:CA	2.27	0.43
54:v:203:TYR:HB3	54:v:263:LEU:HD11	2.00	0.43
3:5:2:A:H2'	3:5:3:C:C6	2.54	0.43
26:T:20:LYS:HB3	26:T:20:LYS:HE2	1.83	0.43
32:Y:91:GLN:CG	51:s:65:GLN:HA	2.47	0.43
33:1:123:G:H21	34:4:26:A:N6	2.16	0.43
33:1:453:U:H2'	33:1:454:C:C6	2.53	0.43
33:1:857:U:H2'	33:1:858:U:C6	2.53	0.43
33:1:916:U:H2'	33:1:917:C:C6	2.53	0.43
56:w:331:PHE:HE1	59:c:214:ARG:HE	1.65	0.43
60:e:70:SER:O	60:e:74:LYS:HG2	2.18	0.43
11:E:104:LEU:HA	11:E:108:ALA:HB3	1.99	0.43
18:L:47:GLU:HG2	33:1:319:U:H5''	1.99	0.43
19:M:54:LEU:HD21	19:M:118:MET:HG3	2.00	0.43
33:1:1227:A:H2'	33:1:1228:A:C8	2.54	0.43
57:2:1056:G:H5'	59:c:679:GLN:HG3	2.00	0.43
58:b:318:MET:HE2	58:b:370:ARG:HG2	2.00	0.43
60:e:540:ILE:HG12	60:e:550:VAL:HG22	2.00	0.43
2:3:118:U:H2'	2:3:119:A:C8	2.53	0.43
47:o:67:LEU:HD11	47:o:97:GLN:HG2	1.99	0.43
59:c:362:ARG:HA	59:c:365:ILE:HD12	2.00	0.43
2:3:112:U:H5''	2:3:113:A:H4'	2.00	0.43
12:F:150:VAL:HG22	12:F:156:LEU:HD23	2.00	0.43
25:S:70:LEU:HD12	25:S:70:LEU:HA	1.86	0.43
33:1:64:C:H2'	33:1:65:A:C8	2.53	0.43
33:1:717:A:H62	33:1:746:A:H3'	1.84	0.43
33:1:1092:G:H2'	33:1:1093:A:H8	1.83	0.43
33:1:1432:U:H2'	33:1:1433:C:H6	1.83	0.43
43:k:100:GLU:HA	43:k:103:LYS:HB2	2.01	0.43
45:m:78:THR:HB	45:m:95:LYS:HD2	2.00	0.43
48:p:103:GLU:O	48:p:107:ARG:HG3	2.19	0.43
57:2:42:G:H2'	57:2:43:G:H8	1.83	0.43
31:Z:66:GLN:HG2	31:Z:70:LYS:HE3	2.01	0.43
40:g:32:LYS:HA	40:g:32:LYS:HD3	1.83	0.43
45:m:74:ILE:HG12	45:m:99:GLU:HG3	2.00	0.43
57:2:311:C:H2'	57:2:312:A:C8	2.53	0.43
57:2:554:A:H2'	57:2:555:A:H8	1.84	0.43
57:2:775:G:H2'	57:2:776:G:H8	1.83	0.43
26:T:12:GLN:O	26:T:16:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:157:LYS:HE2	27:U:157:LYS:HB2	1.64	0.43
57:2:1113:G:H2'	57:2:1114:A:H8	1.83	0.43
4:6:54:ILE:HB	4:6:97:HIS:HB3	2.01	0.43
14:H:168:LEU:HD12	14:H:172:GLU:HB2	1.99	0.43
25:S:105:ARG:HB2	33:1:1648:G:H5''	2.01	0.43
32:Y:49:VAL:HA	32:Y:66:TYR:HB2	2.00	0.43
33:1:608:C:H2'	33:1:609:A:H8	1.82	0.43
33:1:1173:G:H2'	33:1:1174:A:H8	1.83	0.43
33:1:1551:A:N1	57:2:1432:A:C8	2.86	0.43
33:1:2322:A:H61	33:1:2369:C:H1'	1.82	0.43
38:d:68:ARG:HE	55:x:110:TYR:HD1	1.66	0.43
59:c:520:LYS:HB2	59:c:520:LYS:HE2	1.91	0.43
59:c:655:GLN:HG3	59:c:670:TRP:HB3	2.01	0.43
11:E:79:LYS:HB3	11:E:79:LYS:HE3	1.82	0.43
33:1:442:U:H2'	33:1:443:C:C6	2.54	0.43
33:1:470:U:H2'	33:1:471:C:C6	2.54	0.43
33:1:1091:G:H2'	33:1:1092:G:C8	2.53	0.43
33:1:1887:U:H2'	33:1:1888:U:H6	1.84	0.43
33:1:2231:C:H2'	33:1:2232:G:C8	2.54	0.43
33:1:2288:U:H2'	33:1:2289:U:C6	2.53	0.43
37:a:183:GLU:H	37:a:183:GLU:HG2	1.68	0.43
37:a:295:LYS:HB3	37:a:295:LYS:HE2	1.82	0.43
58:b:183:GLN:HG2	58:b:280:ALA:HA	2.01	0.43
60:e:258:VAL:HG22	60:e:261:ARG:HH22	1.84	0.43
5:7:74:THR:HG22	33:1:344:C:H1'	2.01	0.43
12:F:136:LYS:HB2	12:F:136:LYS:HE3	1.80	0.43
35:y:22:G:H2'	35:y:23:C:H6	1.84	0.43
56:w:269:LEU:HD21	56:w:294:LEU:HD11	2.01	0.43
4:6:44:LYS:HE3	4:6:44:LYS:HB2	1.80	0.42
22:P:34:MET:HE2	22:P:34:MET:HB3	1.62	0.42
31:Z:66:GLN:O	31:Z:70:LYS:HG3	2.19	0.42
33:1:1348:A:H2'	33:1:1349:A:C8	2.53	0.42
33:1:2224:U:H2'	33:1:2225:U:H2'	2.01	0.42
56:w:533:LEU:HD11	59:c:538:PRO:HB3	2.01	0.42
57:2:477:G:H2'	57:2:478:C:C6	2.54	0.42
57:2:973:C:H42	57:2:982:A:H61	1.66	0.42
59:c:106:ILE:HD13	59:c:482:TRP:CD2	2.53	0.42
11:E:125:LYS:HE3	11:E:125:LYS:HB2	1.84	0.42
37:a:94:TRP:CZ2	37:a:102:GLN:HG2	2.54	0.42
42:j:112:ARG:HH11	42:j:114:ILE:HD11	1.83	0.42
57:2:260:C:H2'	57:2:261:A:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2:898:U:H2'	57:2:899:G:H8	1.83	0.42
2:3:93:C:H5'	19:M:18:ARG:HG2	2.00	0.42
8:B:24:LEU:HD21	8:B:92:ARG:HD2	2.01	0.42
9:C:72:GLU:HB2	9:C:95:TYR:CZ	2.54	0.42
10:D:144:THR:HA	10:D:147:MET:HG3	2.00	0.42
33:1:1891:OMG:H1'	33:1:1891:OMG:HM23	1.69	0.42
57:2:392:G:H2'	57:2:393:G:C8	2.54	0.42
59:c:393:ARG:HA	59:c:393:ARG:HD2	1.77	0.42
12:F:67:LYS:HB3	12:F:80:LEU:HD11	2.00	0.42
17:K:48:PRO:HB3	57:2:1361:G:O5'	2.19	0.42
22:P:53:LYS:HB3	22:P:112:GLU:HB2	2.00	0.42
33:1:182:A:H4'	33:1:183:G:C8	2.55	0.42
33:1:1080:U:H2'	33:1:1081:G:H8	1.84	0.42
33:1:1426:C:H2'	33:1:1427:A:C5	2.54	0.42
38:d:17:LYS:HE2	38:d:17:LYS:HB3	1.78	0.42
52:t:162:LYS:HB2	52:t:162:LYS:HE3	1.80	0.42
57:2:46:U:H2'	57:2:47:G:H8	1.84	0.42
57:2:912:2MG:O2'	61:i:190:LYS:O	2.36	0.42
58:b:551:LYS:HD3	60:e:314:LEU:HD13	2.01	0.42
1:0:56:ALA:HA	24:R:113:ARG:HD3	2.01	0.42
15:I:109:PRO:HG3	33:1:721:U:C4	2.54	0.42
15:I:170:MET:HB3	15:I:170:MET:HE3	1.86	0.42
48:p:48:LYS:HD2	48:p:48:LYS:HA	1.80	0.42
57:2:42:G:H2'	57:2:43:G:C8	2.55	0.42
58:b:527:LEU:HD12	58:b:527:LEU:HA	1.88	0.42
22:P:54:VAL:HG21	22:P:101:MET:HE1	2.01	0.42
22:P:100:VAL:HG11	33:1:2324:U:H5''	2.02	0.42
33:1:485:G:H4'	33:1:488:G:N1	2.34	0.42
33:1:2155:C:H2'	33:1:2156:A:C8	2.55	0.42
35:y:35:A:OP1	61:i:191:ARG:NE	2.46	0.42
52:t:149:LYS:HD2	52:t:160:TYR:HE2	1.85	0.42
57:2:57:U:H2'	57:2:58:G:C8	2.54	0.42
58:b:824:LYS:HE2	58:b:824:LYS:HB3	1.80	0.42
11:E:141:GLU:H	11:E:141:GLU:HG2	1.54	0.42
33:1:470:U:H2'	33:1:471:C:H6	1.84	0.42
33:1:823:U:H2'	33:1:824:A:C8	2.54	0.42
33:1:1551:A:C2	57:2:1432:A:C8	3.08	0.42
38:d:121:MET:HG2	38:d:169:VAL:HG13	2.00	0.42
41:h:14:MET:HE2	41:h:18:ILE:HD11	2.02	0.42
42:j:71:ARG:HG2	42:j:141:ASP:HB3	2.02	0.42
56:w:277:LEU:O	56:w:281:TRP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2:691:U:H2'	57:2:692:G:C8	2.54	0.42
57:2:737:U:H2'	57:2:738:A:H8	1.84	0.42
57:2:1374:G:H2'	57:2:1375:U:C6	2.55	0.42
58:b:406:ALA:HA	58:b:890:LEU:HD11	2.01	0.42
33:1:171:U:H2'	33:1:172:G:C8	2.55	0.42
33:1:569:A:H2'	33:1:570:A:C8	2.54	0.42
60:e:620:LEU:HD23	60:e:620:LEU:HA	1.90	0.42
7:9:3:VAL:HG21	33:1:2179:C:H4'	2.01	0.42
9:C:111:LEU:HD13	9:C:118:PRO:HA	2.01	0.42
17:K:35:ILE:HG21	17:K:103:ALA:HB3	2.02	0.42
57:2:458:G:H2'	57:2:459:G:C8	2.55	0.42
57:2:1252:C:H2'	57:2:1253:U:C6	2.55	0.42
57:2:1452:A:H2'	57:2:1453:C:C6	2.54	0.42
15:I:156:VAL:O	15:I:160:VAL:HG23	2.20	0.42
33:1:497:U:H2'	33:1:498:A:C8	2.55	0.42
34:4:230:G:H2'	34:4:231:A:C8	2.55	0.42
51:s:27:LYS:HG2	51:s:29:VAL:HG13	2.02	0.42
54:v:241:ALA:O	54:v:245:LEU:CB	2.65	0.42
54:v:242:TRP:CZ3	54:v:268:THR:HG23	2.55	0.42
56:w:525:ALA:O	56:w:529:VAL:HG12	2.20	0.42
57:2:492:A:H2'	57:2:493:G:C8	2.55	0.42
57:2:587:C:H2'	57:2:588:A:H8	1.84	0.42
61:i:10:ARG:H	61:i:112:LEU:HD23	1.84	0.42
11:E:177:PRO:HG3	32:Y:78:TYR:OH	2.20	0.41
15:I:92:GLU:HG2	15:I:106:LYS:NZ	2.35	0.41
19:M:43:THR:HG22	19:M:94:VAL:HG12	2.02	0.41
30:X:72:LEU:HD23	30:X:72:LEU:HA	1.91	0.41
33:1:2372:G:H2'	33:1:2373:G:C8	2.55	0.41
33:1:2376:A:H2'	33:1:2377:G:C8	2.55	0.41
58:b:774:LYS:HB3	58:b:774:LYS:HE2	1.78	0.41
58:b:787:ILE:H	58:b:787:ILE:HG12	1.71	0.41
58:b:884:PHE:O	58:b:888:LYS:HG2	2.20	0.41
33:1:1430:U:H2'	33:1:1431:C:H6	1.85	0.41
33:1:2037:A:H2'	33:1:2038:C:C6	2.55	0.41
54:v:290:PHE:HD1	54:v:290:PHE:HA	1.78	0.41
57:2:445:A:H2'	57:2:446:G:H8	1.86	0.41
57:2:1455:2MG:HM21	57:2:1458:MA6:N7	2.35	0.41
58:b:324:HIS:HB3	58:b:366:LEU:HD11	2.01	0.41
58:b:479:LYS:HE2	58:b:479:LYS:HB2	1.89	0.41
60:e:235:MET:HE2	60:e:235:MET:HB3	1.87	0.41
10:D:25:VAL:HA	10:D:49:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:172:LYS:HZ3	11:E:178:PHE:HB2	1.85	0.41
38:d:228:PRO:HB2	60:e:109:PHE:HD1	1.85	0.41
45:m:49:GLU:OE1	45:m:49:GLU:N	2.51	0.41
57:2:82:U:H2'	57:2:83:G:C8	2.56	0.41
57:2:334:U:H2'	57:2:335:G:C8	2.56	0.41
10:D:119:LYS:HD3	10:D:119:LYS:HA	1.84	0.41
33:1:161:U:H4'	33:1:894:G:H4'	2.02	0.41
33:1:823:U:H2'	33:1:824:A:H8	1.85	0.41
33:1:1295:U:H2'	33:1:1296:A:C8	2.56	0.41
33:1:1551:A:N3	57:2:1432:A:N3	2.54	0.41
44:l:114:ARG:HG2	44:l:119:VAL:HB	2.02	0.41
56:w:253:LEU:HD11	56:w:326:ILE:HG13	2.01	0.41
57:2:46:U:H2'	57:2:47:G:C8	2.56	0.41
57:2:1019:C:H2'	57:2:1020:G:C8	2.55	0.41
6:8:103:THR:HG23	6:8:111:VAL:HB	2.02	0.41
33:1:233:C:H2'	33:1:234:G:H8	1.85	0.41
42:j:84:LEU:HB3	42:j:138:ARG:HG3	2.02	0.41
48:p:101:THR:HG23	57:2:428:A:H1'	2.03	0.41
57:2:280:U:H2'	57:2:281:G:C8	2.56	0.41
57:2:410:U:H2'	57:2:411:G:C8	2.55	0.41
57:2:916:C:N4	61:i:189:HIS:CD2	2.88	0.41
58:b:689:LEU:HD23	58:b:689:LEU:HA	1.91	0.41
33:1:744:A:H2'	33:1:745:A:C8	2.56	0.41
58:b:323:MET:HE2	58:b:323:MET:HB2	1.98	0.41
11:E:32:ILE:HG12	11:E:159:THR:HG22	2.02	0.41
33:1:125:U:H5''	33:1:160:A:H8	1.86	0.41
33:1:275:G:H4'	33:1:276:A:H5'	2.03	0.41
33:1:1109:G:H2'	33:1:1110:U:C6	2.55	0.41
42:j:108:LEU:HB2	42:j:137:HIS:HB2	2.03	0.41
51:s:22:LEU:HD11	51:s:29:VAL:HG22	2.03	0.41
54:v:151:TYR:HB3	58:b:375:LYS:HE2	2.03	0.41
57:2:41:C:H2'	57:2:42:G:H8	1.86	0.41
58:b:523:LYS:HA	58:b:526:LEU:HG	2.01	0.41
59:c:222:LEU:HA	59:c:225:ILE:HD12	2.02	0.41
59:c:368:LEU:HB3	59:c:404:LEU:HD21	2.03	0.41
2:3:118:U:H2'	2:3:119:A:H8	1.86	0.41
31:Z:40:PRO:HA	33:1:2255:U:C2	2.55	0.41
33:1:218:U:H2'	33:1:219:G:O4'	2.20	0.41
33:1:1160:U:H2'	33:1:1161:A:C8	2.56	0.41
33:1:1710:A:H2'	33:1:1711:G:C8	2.54	0.41
33:1:2377:G:H2'	33:1:2378:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2:716:G:H2'	57:2:717:A:C8	2.56	0.41
57:2:761:C:H2'	57:2:762:A:H8	1.85	0.41
58:b:537:LYS:HA	58:b:540:GLU:HG2	2.03	0.41
58:b:569:SER:HA	58:b:572:LYS:NZ	2.34	0.41
58:b:660:LEU:HB3	58:b:664:PHE:CZ	2.56	0.41
59:c:76:ILE:HD13	59:c:96:SER:HB3	2.02	0.41
59:c:648:ARG:H	59:c:648:ARG:HG2	1.66	0.41
7:9:30:ALA:HB1	33:1:2167:C:H5''	2.02	0.41
14:H:140:VAL:HG23	14:H:143:LYS:HE3	2.02	0.41
17:K:17:ARG:HH11	17:K:47:LEU:HD23	1.85	0.41
25:S:82:ARG:HD2	31:Z:56:TRP:CH2	2.55	0.41
33:1:299:A:H2'	33:1:301:A:C8	2.56	0.41
33:1:489:C:H2'	33:1:490:G:C8	2.55	0.41
33:1:937:U:H2'	33:1:938:U:H6	1.86	0.41
33:1:1012:A:H2'	33:1:1013:A:C8	2.56	0.41
33:1:1686:C:H2'	33:1:1687:A:C8	2.56	0.41
33:1:1913:A:H2'	33:1:1914:A:C8	2.56	0.41
33:1:2154:U:H2'	33:1:2155:C:C6	2.56	0.41
33:1:2272:A:H2'	33:1:2273:G:C8	2.56	0.41
35:y:44:A:H2'	35:y:45:G:H8	1.84	0.41
38:d:110:MET:HE3	38:d:110:MET:HB3	1.85	0.41
40:g:12:LEU:HD12	40:g:12:LEU:HA	1.90	0.41
44:l:8:ILE:HD13	44:l:8:ILE:HA	1.88	0.41
56:w:316:LEU:HD22	56:w:329:THR:HB	2.02	0.41
57:2:467:U:H2'	57:2:468:G:C8	2.56	0.41
57:2:1344:G:H2'	57:2:1345:U:H6	1.86	0.41
59:c:406:GLN:O	59:c:410:LEU:HD12	2.20	0.41
4:6:57:THR:HG21	4:6:98:LYS:HD3	2.01	0.41
21:O:55:ALA:HA	21:O:121:ASP:HB3	2.03	0.41
34:4:206:A:H5'	34:4:237:C:H4'	2.02	0.41
40:g:76:LYS:HA	40:g:77:PRO:HD3	1.95	0.41
51:s:18:LYS:HD2	51:s:31:ILE:HG23	2.03	0.41
54:v:146:LEU:HD23	54:v:146:LEU:HA	1.87	0.41
54:v:214:LEU:HB3	54:v:236:TRP:HD1	1.86	0.41
56:w:170:LEU:HD11	56:w:176:GLU:HB2	2.03	0.41
57:2:336:A:H2'	57:2:337:G:C8	2.56	0.41
11:E:31:LYS:HG3	11:E:33:GLU:OE2	2.21	0.40
15:I:167:ALA:HB1	15:I:172:ILE:HB	2.02	0.40
17:K:10:VAL:HG22	17:K:19:LEU:HG	2.03	0.40
33:1:975:U:H2'	33:1:976:C:C6	2.56	0.40
33:1:1089:A:H2'	33:1:1090:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1:2109:A:H62	33:1:2121:G:H21	1.68	0.40
33:1:2476:U:H2'	33:1:2477:A:C8	2.57	0.40
37:a:84:LEU:HD13	54:v:177:LEU:HD12	2.04	0.40
57:2:175:G:H2'	57:2:176:G:C8	2.56	0.40
58:b:477:MET:HE3	60:e:277:VAL:HG22	2.03	0.40
8:B:260:LEU:HD23	33:1:1433:C:H5''	2.04	0.40
27:U:78:ILE:HD13	27:U:105:VAL:HG21	2.03	0.40
37:a:129:GLU:O	37:a:133:ALA:HB2	2.20	0.40
55:x:73:LYS:HA	55:x:74:PRO:HD3	1.97	0.40
57:2:666:A:H2'	57:2:667:G:C8	2.56	0.40
27:U:78:ILE:HG22	27:U:84:LYS:HA	2.03	0.40
33:1:2187:U:H2'	33:1:2188:G:C8	2.56	0.40
42:j:116:CYS:HB3	57:2:921:A:N6	2.37	0.40
7:9:1:MET:HE2	7:9:1:MET:HB2	1.84	0.40
18:L:137:LYS:HG3	18:L:139:ILE:HD11	2.03	0.40
26:T:7:TYR:HA	30:X:62:TRP:CD1	2.56	0.40
33:1:936:A:H2'	33:1:937:U:C6	2.56	0.40
33:1:1430:U:H2'	33:1:1431:C:C6	2.56	0.40
33:1:2288:U:H2'	33:1:2289:U:H6	1.87	0.40
34:4:139:A:H2'	34:4:140:A:C8	2.56	0.40
35:y:10:G:H2'	35:y:11:A:C8	2.56	0.40
44:l:74:LEU:HD21	44:l:80:VAL:HG11	2.04	0.40
46:n:27:LEU:HD23	46:n:27:LEU:HA	1.98	0.40
57:2:1264:U:H2'	57:2:1265:A:H8	1.86	0.40
57:2:1280:C:H2'	57:2:1281:G:C8	2.56	0.40
58:b:534:LEU:HD12	58:b:720:ILE:HD13	2.04	0.40
61:i:98:VAL:HG21	61:i:110:ILE:HD11	2.03	0.40
33:1:1121:C:H2'	33:1:1122:A:C8	2.57	0.40
33:1:1881:A:H2'	33:1:1882:G:C8	2.56	0.40
44:l:40:VAL:HB	44:l:90:LEU:HD22	2.03	0.40
48:p:103:GLU:HB2	48:p:112:MET:HE1	2.04	0.40
57:2:35:C:H2'	57:2:36:G:C8	2.57	0.40
57:2:361:C:H2'	57:2:362:G:C8	2.56	0.40
57:2:722:A:H5'	57:2:1463:G:H1'	2.03	0.40
57:2:1330:U:H2'	57:2:1331:G:C8	2.55	0.40
60:e:448:SER:O	60:e:452:GLN:HG2	2.20	0.40
60:e:466:GLU:HA	60:e:469:ILE:HG12	2.04	0.40
60:e:490:LYS:HD2	60:e:490:LYS:HA	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	45/66 (68%)	45 (100%)	0	0	100	100
4	6	56/101 (55%)	55 (98%)	1 (2%)	0	100	100
5	7	58/124 (47%)	57 (98%)	1 (2%)	0	100	100
6	8	66/114 (58%)	65 (98%)	1 (2%)	0	100	100
7	9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	B	274/278 (99%)	268 (98%)	6 (2%)	0	100	100
9	C	221/259 (85%)	215 (97%)	6 (3%)	0	100	100
10	D	214/243 (88%)	210 (98%)	4 (2%)	0	100	100
11	E	176/179 (98%)	166 (94%)	10 (6%)	0	100	100
12	F	175/207 (84%)	167 (95%)	8 (5%)	0	100	100
13	G	52/200 (26%)	51 (98%)	1 (2%)	0	100	100
14	H	139/235 (59%)	138 (99%)	1 (1%)	0	100	100
15	I	130/176 (74%)	124 (95%)	6 (5%)	0	100	100
16	J	171/225 (76%)	164 (96%)	7 (4%)	0	100	100
17	K	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
18	L	196/241 (81%)	188 (96%)	8 (4%)	0	100	100
19	M	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
20	N	115/173 (66%)	113 (98%)	2 (2%)	0	100	100
21	O	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
22	P	128/153 (84%)	122 (95%)	6 (5%)	0	100	100
23	Q	109/112 (97%)	109 (100%)	0	0	100	100
24	R	113/179 (63%)	112 (99%)	1 (1%)	0	100	100
25	S	113/175 (65%)	113 (100%)	0	0	100	100
26	T	90/111 (81%)	88 (98%)	2 (2%)	0	100	100
27	U	130/170 (76%)	127 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	V	112/161 (70%)	108 (96%)	4 (4%)	0	100	100
29	W	136/195 (70%)	133 (98%)	3 (2%)	0	100	100
30	X	104/134 (78%)	104 (100%)	0	0	100	100
31	Z	39/98 (40%)	37 (95%)	2 (5%)	0	100	100
32	Y	61/136 (45%)	53 (87%)	7 (12%)	1 (2%)	7	16
37	a	234/436 (54%)	221 (94%)	12 (5%)	1 (0%)	30	48
38	d	254/257 (99%)	246 (97%)	8 (3%)	0	100	100
39	f	101/171 (59%)	100 (99%)	1 (1%)	0	100	100
40	g	165/168 (98%)	160 (97%)	5 (3%)	0	100	100
41	h	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
42	j	120/169 (71%)	115 (96%)	2 (2%)	3 (2%)	4	9
43	k	115/130 (88%)	112 (97%)	3 (3%)	0	100	100
44	l	119/133 (90%)	113 (95%)	6 (5%)	0	100	100
45	m	112/164 (68%)	109 (97%)	3 (3%)	0	100	100
46	n	97/100 (97%)	97 (100%)	0	0	100	100
47	o	99/141 (70%)	96 (97%)	3 (3%)	0	100	100
48	p	78/128 (61%)	78 (100%)	0	0	100	100
49	q	76/105 (72%)	73 (96%)	3 (4%)	0	100	100
50	r	79/137 (58%)	76 (96%)	3 (4%)	0	100	100
51	s	79/92 (86%)	78 (99%)	1 (1%)	0	100	100
52	t	117/166 (70%)	117 (100%)	0	0	100	100
53	u	90/184 (49%)	86 (96%)	4 (4%)	0	100	100
54	v	179/298 (60%)	160 (89%)	16 (9%)	3 (2%)	7	15
55	x	58/120 (48%)	56 (97%)	2 (3%)	0	100	100
56	w	361/560 (64%)	357 (99%)	4 (1%)	0	100	100
58	b	679/910 (75%)	656 (97%)	22 (3%)	1 (0%)	48	69
59	c	597/712 (84%)	582 (98%)	15 (2%)	0	100	100
60	e	528/673 (78%)	500 (95%)	27 (5%)	1 (0%)	43	62
61	i	149/191 (78%)	136 (91%)	12 (8%)	1 (1%)	18	35
All	All	8252/11171 (74%)	7986 (97%)	255 (3%)	11 (0%)	49	69

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	j	123	VAL
37	a	71	VAL
42	j	50	VAL
54	v	131	VAL
54	v	142	PHE
58	b	347	THR
42	j	51	ASP
54	v	146	LEU
60	e	273	ILE
61	i	41	ASP
32	Y	40	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	39/54 (72%)	39 (100%)	0	100	100
4	6	53/90 (59%)	51 (96%)	2 (4%)	29	54
5	7	45/90 (50%)	45 (100%)	0	100	100
6	8	55/92 (60%)	53 (96%)	2 (4%)	31	56
7	9	33/33 (100%)	31 (94%)	2 (6%)	17	35
8	B	228/230 (99%)	223 (98%)	5 (2%)	45	69
9	C	176/204 (86%)	171 (97%)	5 (3%)	38	62
10	D	167/187 (89%)	166 (99%)	1 (1%)	78	89
11	E	156/157 (99%)	156 (100%)	0	100	100
12	F	145/168 (86%)	142 (98%)	3 (2%)	47	70
13	G	46/167 (28%)	46 (100%)	0	100	100
14	H	122/197 (62%)	119 (98%)	3 (2%)	42	66
15	I	106/138 (77%)	102 (96%)	4 (4%)	29	54
16	J	140/180 (78%)	137 (98%)	3 (2%)	47	70
17	K	101/101 (100%)	99 (98%)	2 (2%)	48	72
18	L	149/180 (83%)	147 (99%)	2 (1%)	61	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	M	110/111 (99%)	106 (96%)	4 (4%)	31	56
20	N	97/140 (69%)	94 (97%)	3 (3%)	35	59
21	O	93/116 (80%)	91 (98%)	2 (2%)	45	69
22	P	104/122 (85%)	100 (96%)	4 (4%)	29	54
23	Q	100/101 (99%)	98 (98%)	2 (2%)	48	72
24	R	97/145 (67%)	92 (95%)	5 (5%)	21	43
25	S	94/136 (69%)	88 (94%)	6 (6%)	16	33
26	T	85/89 (96%)	84 (99%)	1 (1%)	63	80
27	U	109/137 (80%)	107 (98%)	2 (2%)	51	74
28	V	90/127 (71%)	88 (98%)	2 (2%)	45	69
29	W	116/164 (71%)	113 (97%)	3 (3%)	40	65
30	X	89/109 (82%)	87 (98%)	2 (2%)	45	69
31	Z	33/81 (41%)	33 (100%)	0	100	100
32	Y	55/106 (52%)	53 (96%)	2 (4%)	31	56
37	a	206/368 (56%)	201 (98%)	5 (2%)	43	67
38	d	233/234 (100%)	231 (99%)	2 (1%)	70	84
39	f	89/140 (64%)	89 (100%)	0	100	100
40	g	146/147 (99%)	142 (97%)	4 (3%)	39	63
41	h	125/125 (100%)	124 (99%)	1 (1%)	73	86
42	j	107/143 (75%)	104 (97%)	3 (3%)	38	62
43	k	93/105 (89%)	93 (100%)	0	100	100
44	l	103/111 (93%)	99 (96%)	4 (4%)	28	53
45	m	101/138 (73%)	100 (99%)	1 (1%)	68	83
46	n	88/89 (99%)	87 (99%)	1 (1%)	65	81
47	o	86/115 (75%)	85 (99%)	1 (1%)	63	80
48	p	69/108 (64%)	66 (96%)	3 (4%)	26	50
49	q	69/90 (77%)	69 (100%)	0	100	100
50	r	73/128 (57%)	70 (96%)	3 (4%)	27	52
51	s	71/80 (89%)	71 (100%)	0	100	100
52	t	99/133 (74%)	98 (99%)	1 (1%)	68	83
53	u	85/149 (57%)	82 (96%)	3 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	v	143/246 (58%)	139 (97%)	4 (3%)	38	62
55	x	50/95 (53%)	49 (98%)	1 (2%)	48	72
56	w	287/434 (66%)	282 (98%)	5 (2%)	53	75
58	b	620/807 (77%)	610 (98%)	10 (2%)	55	76
59	c	541/634 (85%)	535 (99%)	6 (1%)	65	81
60	e	411/527 (78%)	402 (98%)	9 (2%)	45	69
61	i	128/159 (80%)	124 (97%)	4 (3%)	35	59
All	All	7056/9257 (76%)	6913 (98%)	143 (2%)	48	72

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	6	44	LYS
4	6	71	THR
6	8	73	LYS
6	8	94	LEU
7	9	1	MET
7	9	6	SER
8	B	159	SER
8	B	186	VAL
8	B	203	TYR
8	B	205	LEU
8	B	221	THR
9	C	38	ARG
9	C	55	SER
9	C	168	THR
9	C	222	SER
9	C	229	GLU
10	D	142	SER
12	F	44	LEU
12	F	154	THR
12	F	159	SER
14	H	74	PHE
14	H	85	TYR
14	H	124	ILE
15	I	87	ASP
15	I	88	ILE
15	I	147	LYS
15	I	169	ASN
16	J	66	SER

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Mol	Chain	Res	Type
16	J	142	ARG
16	J	191	LYS
17	K	55	SER
17	K	65	THR
18	L	181	LYS
18	L	185	LEU
19	M	6	ARG
19	M	26	LYS
19	M	37	GLN
19	M	91	ASP
20	N	129	LYS
20	N	145	GLU
20	N	151	THR
21	O	68	ILE
21	O	89	SER
22	P	34	MET
22	P	52	VAL
22	P	83	SER
22	P	131	VAL
23	Q	74	LEU
23	Q	94	VAL
24	R	113	ARG
24	R	124	THR
24	R	148	VAL
24	R	153	MET
24	R	170	SER
25	S	93	GLU
25	S	111	ILE
25	S	128	LEU
25	S	130	THR
25	S	168	ILE
25	S	173	ARG
26	T	20	LYS
27	U	112	LEU
27	U	163	VAL
28	V	38	THR
28	V	115	LYS
29	W	49	SER
29	W	98	THR
29	W	114	ASP
30	X	71	GLU
30	X	124	GLU

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Mol	Chain	Res	Type
32	Y	49	VAL
32	Y	65	THR
37	a	110	VAL
37	a	131	LEU
37	a	149	ILE
37	a	278	VAL
37	a	300	THR
38	d	15	ILE
38	d	115	ILE
40	g	90	VAL
40	g	93	LEU
40	g	122	LYS
40	g	151	MET
41	h	121	LEU
42	j	55	VAL
42	j	98	THR
42	j	123	VAL
44	l	8	ILE
44	l	40	VAL
44	l	74	LEU
44	l	90	LEU
45	m	46	ASN
46	n	57	VAL
47	o	61	GLU
48	p	59	SER
48	p	90	GLU
48	p	103	GLU
50	r	86	LEU
50	r	113	VAL
50	r	130	SER
52	t	118	VAL
53	u	586	MET
53	u	592	SER
53	u	627	VAL
54	v	176	ASN
54	v	268	THR
54	v	270	LEU
54	v	290	PHE
55	x	59	VAL
56	w	244	LEU
56	w	358	MET
56	w	359	MET

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Mol	Chain	Res	Type
56	w	431	VAL
56	w	483	VAL
58	b	201	ARG
58	b	210	VAL
58	b	304	THR
58	b	318	MET
58	b	533	GLN
58	b	585	GLU
58	b	589	PHE
58	b	665	SER
58	b	685	GLN
58	b	714	VAL
59	c	82	GLU
59	c	89	GLU
59	c	404	LEU
59	c	455	ILE
59	c	641	MET
59	c	664	GLU
60	e	135	ILE
60	e	316	GLU
60	e	332	LEU
60	e	334	MET
60	e	370	LEU
60	e	386	LEU
60	e	400	VAL
60	e	497	ASP
60	e	557	GLU
61	i	19	GLN
61	i	44	SER
61	i	158	GLN
61	i	172	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	26	HIS
8	B	189	ASN
10	D	44	GLN
10	D	45	GLN
10	D	205	ASN
11	E	3	GLN
11	E	46	GLN

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Mol	Chain	Res	Type
12	F	131	ASN
14	H	72	GLN
15	I	78	ASN
15	I	139	GLN
17	K	9	ASN
20	N	106	HIS
21	O	60	ASN
22	P	59	GLN
23	Q	36	ASN
23	Q	81	ASN
24	R	163	GLN
25	S	124	ASN
28	V	74	ASN
28	V	132	GLN
29	W	67	ASN
32	Y	91	GLN
37	a	86	GLN
37	a	102	GLN
37	a	219	GLN
38	d	46	GLN
39	f	149	GLN
39	f	171	GLN
40	g	100	ASN
41	h	60	GLN
42	j	82	GLN
43	k	120	ASN
46	n	8	GLN
47	o	81	ASN
47	o	97	GLN
51	s	65	GLN
54	v	180	GLN
54	v	197	ASN
56	w	430	GLN
58	b	465	GLN
58	b	514	ASN
58	b	719	GLN
58	b	827	GLN
58	b	843	ASN
59	c	21	GLN
59	c	108	ASN
59	c	316	GLN
59	c	457	GLN

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Mol	Chain	Res	Type
59	c	530	ASN
59	c	679	GLN
60	e	101	ASN
60	e	275	ASN
60	e	452	GLN
61	i	19	GLN
61	i	24	ASN
61	i	187	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	3	120/121 (99%)	20 (16%)	1 (0%)
3	5	46/47 (97%)	4 (8%)	0
33	1	2362/2375 (99%)	333 (14%)	4 (0%)
34	4	270/272 (99%)	35 (12%)	1 (0%)
35	y	75/76 (98%)	12 (16%)	0
36	xx	0/5	-	-
57	2	1468/1470 (99%)	202 (13%)	3 (0%)
62	A	5/6 (83%)	1 (20%)	0
All	All	4346/4372 (99%)	607 (13%)	9 (0%)

All (607) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	3	14	U
2	3	16	G
2	3	19	C
2	3	25	G
2	3	33	C
2	3	35	A
2	3	36	A
2	3	37	U
2	3	42	C
2	3	54	U
2	3	57	G
2	3	66	G
2	3	68	G
2	3	71	G
2	3	78	G
2	3	87	G

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Mol	Chain	Res	Type
2	3	102	A
2	3	107	A
2	3	108	G
2	3	113	A
3	5	16	U
3	5	22	A
3	5	34	G
3	5	36	A
33	1	36	G
33	1	55	A
33	1	61	G
33	1	62	A
33	1	71	U
33	1	86	C
33	1	92	G
33	1	99	A
33	1	105	A
33	1	129	A
33	1	131	G
33	1	139	G
33	1	144	G
33	1	155	A
33	1	158	A
33	1	172	G
33	1	179	A
33	1	181	C
33	1	182	A
33	1	183	G
33	1	215	G
33	1	220	U
33	1	225	G
33	1	226	A
33	1	227	A
33	1	229	G
33	1	235	G
33	1	255	G
33	1	276	A
33	1	282	A
33	1	289	G
33	1	292	A
33	1	313	G
33	1	325	G

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Mol	Chain	Res	Type
33	1	342	A
33	1	343	U
33	1	361	G
33	1	385	G
33	1	386	G
33	1	387	U
33	1	396	A
33	1	404	5MU
33	1	421	A
33	1	428	A
33	1	432	G
33	1	434	G
33	1	439	A
33	1	441	U
33	1	442	U
33	1	446	A
33	1	448	C
33	1	449	G
33	1	462	G
33	1	469	C
33	1	484	U
33	1	502	A
33	1	505	A
33	1	517	G
33	1	523	C
33	1	524	U
33	1	546	U
33	1	547	C
33	1	549	C
33	1	550	G
33	1	554	U
33	1	555	A
33	1	556	C
33	1	566	G
33	1	569	A
33	1	573	C
33	1	574	A
33	1	590	U
33	1	596	A
33	1	597	A
33	1	601	A
33	1	606	G

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Mol	Chain	Res	Type
33	1	621	G
33	1	634	G
33	1	639	A
33	1	643	A
33	1	649	G
33	1	656	A
33	1	665	C
33	1	672	U
33	1	673	G
33	1	682	G
33	1	685	G
33	1	686	A
33	1	693	U
33	1	705	G
33	1	706	A
33	1	707	A
33	1	708	A
33	1	717	A
33	1	720	U
33	1	721	U
33	1	722	U
33	1	730	A
33	1	731	G
33	1	739	C
33	1	740	C
33	1	743	C
33	1	744	A
33	1	747	G
33	1	748	A
33	1	749	G
33	1	750	U
33	1	757	U
33	1	772	G
33	1	782	G
33	1	790	U
33	1	794	C
33	1	795	G
33	1	801	A
33	1	808	C
33	1	847	U
33	1	871	G
33	1	895	G

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Mol	Chain	Res	Type
33	1	909	G
33	1	913	A
33	1	915	G
33	1	930	G
33	1	931	A
33	1	934	A
33	1	959	A
33	1	960	A
33	1	970	G
33	1	980	U
33	1	981	A
33	1	988	U
33	1	1009	C
33	1	1011	U
33	1	1024	A
33	1	1038	U
33	1	1042	A
33	1	1051	A
33	1	1062	A
33	1	1070	A
33	1	1075	U
33	1	1076	G
33	1	1087	C
33	1	1104	G
33	1	1105	A
33	1	1112	U
33	1	1113	U
33	1	1115	G
33	1	1118	U
33	1	1119	U
33	1	1120	G
33	1	1125	G
33	1	1135	A
33	1	1142	G
33	1	1147	A
33	1	1149	A
33	1	1150	G
33	1	1154	A
33	1	1155	A
33	1	1158	G
33	1	1163	C
33	1	1171	G

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Mol	Chain	Res	Type
33	1	1173	G
33	1	1180	U
33	1	1190	A
33	1	1197	C
33	1	1198	G
33	1	1199	A
33	1	1209	G
33	1	1217	A
33	1	1222	C
33	1	1223	A
33	1	1226	A
33	1	1235	U
33	1	1236	A
33	1	1257	C
33	1	1261	U
33	1	1266	G
33	1	1267	A
33	1	1270	C
33	1	1277	A
33	1	1293	A
33	1	1306	G
33	1	1307	C
33	1	1313	A
33	1	1326	G
33	1	1328	A
33	1	1333	G
33	1	1352	U
33	1	1375	U
33	1	1379	A
33	1	1380	A
33	1	1400	G
33	1	1409	A
33	1	1418	C
33	1	1420	A
33	1	1422	A
33	1	1436	C
33	1	1438	A
33	1	1452	U
33	1	1465	A
33	1	1484	A
33	1	1494	A
33	1	1500	U

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Mol	Chain	Res	Type
33	1	1502	A
33	1	1510	A
33	1	1511	A
33	1	1544	G
33	1	1551	A
33	1	1552	C
33	1	1567	G
33	1	1568	G
33	1	1575	A
33	1	1593	U
33	1	1602	G
33	1	1605	C
33	1	1608	A
33	1	1609	A
33	1	1610	G
33	1	1629	U
33	1	1630	G
33	1	1631	U
33	1	1634	C
33	1	1658	C
33	1	1661	G
33	1	1665	C
33	1	1669	6MZ
33	1	1670	A
33	1	1671	G
33	1	1672	A
33	1	1675	C
33	1	1682	C
33	1	1694	C
33	1	1695	A
33	1	1699	A
33	1	1700	G
33	1	1701	A
33	1	1708	G
33	1	1715	G
33	1	1726	G
33	1	1732	G
33	1	1837	A
33	1	1844	A
33	1	1851	A
33	1	1865	A
33	1	1878	G

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Mol	Chain	Res	Type
33	1	1879	G
33	1	1919	G
33	1	1923	U
33	1	1927	A
33	1	1928	A
33	1	1945	A
33	1	1947	G
33	1	1948	G
33	1	1949	A
33	1	1959	U
33	1	1960	U
33	1	1961	G
33	1	1962	A
33	1	1974	A
33	1	1975	A
33	1	1976	A
33	1	1985	G
33	1	1987	C
33	1	1990	C
33	1	2023	G
33	1	2025	C
33	1	2031	G
33	1	2042	G
33	1	2046	C
33	1	2054	G
33	1	2056	C
33	1	2065	A
33	1	2069	G
33	1	2070	A
33	1	2075	A
33	1	2080	C
33	1	2081	U
33	1	2085	2MG
33	1	2088	A
33	1	2118	A
33	1	2131	U
33	1	2134	G
33	1	2138	OMC
33	1	2142	G
33	1	2145	G
33	1	2158	A
33	1	2160	C

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Mol	Chain	Res	Type
33	1	2169	G
33	1	2175	G
33	1	2206	A
33	1	2207	G
33	1	2213	C
33	1	2218	G
33	1	2222	G
33	1	2225	U
33	1	2242	A
33	1	2249	U
33	1	2253	U
33	1	2263	A
33	1	2269	U
33	1	2280	G
33	1	2281	A
33	1	2286	C
33	1	2294	A
33	1	2303	G
33	1	2308	U
33	1	2325	U
33	1	2329	U
33	1	2352	A
33	1	2353	A
33	1	2354	C
33	1	2355	G
33	1	2366	A
33	1	2367	C
33	1	2384	G
33	1	2388	A
33	1	2397	A
33	1	2406	G
33	1	2418	A
33	1	2420	G
33	1	2430	U
33	1	2460	U
33	1	2461	A
33	1	2463	A
33	1	2473	A
33	1	2474	U
33	1	2476	U
33	1	2501	U
33	1	2513	A

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Mol	Chain	Res	Type
33	1	2519	A
33	1	2520	C
33	1	2523	A
33	1	2531	U
33	1	2532	U
34	4	8	G
34	4	26	A
34	4	27	G
34	4	35	G
34	4	38	A
34	4	43	G
34	4	47	G
34	4	63	A
34	4	66	C
34	4	67	G
34	4	76	A
34	4	92	U
34	4	93	G
34	4	101	G
34	4	109	A
34	4	110	A
34	4	111	U
34	4	123	A
34	4	124	U
34	4	139	A
34	4	142	U
34	4	155	A
34	4	176	A
34	4	179	A
34	4	195	G
34	4	196	A
34	4	202	A
34	4	208	A
34	4	228	G
34	4	256	A
34	4	267	U
34	4	275	U
34	4	277	G
34	4	278	U
34	4	279	G
35	y	9	G
35	y	13	C

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Mol	Chain	Res	Type
35	y	18	G
35	y	21	A
35	y	22	G
35	y	45	G
35	y	46	G
35	y	47	U
35	y	48	C
35	y	67	C
35	y	68	C
35	y	76	A
57	2	6	U
57	2	10	G
57	2	23	G
57	2	32	G
57	2	33	A
57	2	40	G
57	2	48	C
57	2	49	U
57	2	52	A
57	2	59	C
57	2	80	U
57	2	86	U
57	2	106	A
57	2	107	C
57	2	116	A
57	2	117	C
57	2	130	G
57	2	149	C
57	2	168	C
57	2	169	A
57	2	181	A
57	2	183	A
57	2	191	A
57	2	192	A
57	2	195	G
57	2	201	A
57	2	204	G
57	2	220	U
57	2	222	G
57	2	226	G
57	2	231	U
57	2	232	G

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Mol	Chain	Res	Type
57	2	235	G
57	2	242	G
57	2	243	C
57	2	256	C
57	2	257	G
57	2	265	G
57	2	282	A
57	2	297	A
57	2	304	C
57	2	305	A
57	2	320	A
57	2	327	G
57	2	328	C
57	2	330	G
57	2	343	U
57	2	348	C
57	2	349	A
57	2	360	G
57	2	382	G
57	2	388	A
57	2	389	G
57	2	397	G
57	2	398	U
57	2	399	G
57	2	400	G
57	2	405	U
57	2	415	U
57	2	429	G
57	2	430	U
57	2	431	U
57	2	434	G
57	2	437	G
57	2	438	G
57	2	439	U
57	2	448	A
57	2	449	A
57	2	450	U
57	2	462	A
57	2	464	C
57	2	471	C
57	2	474	G
57	2	477	G

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Mol	Chain	Res	Type
57	2	480	G7M
57	2	484	U
57	2	485	A
57	2	500	A
57	2	512	A
57	2	517	U
57	2	519	G
57	2	525	A
57	2	526	A
57	2	529	C
57	2	530	G
57	2	571	C
57	2	595	U
57	2	596	A
57	2	604	G
57	2	607	U
57	2	619	G
57	2	657	G
57	2	675	A
57	2	677	U
57	2	678	G
57	2	688	C
57	2	709	A
57	2	731	A
57	2	747	U
57	2	748	A
57	2	754	G
57	2	766	G
57	2	769	A
57	2	771	C
57	2	775	G
57	2	786	G
57	2	791	C
57	2	792	G
57	2	793	C
57	2	816	U
57	2	836	G
57	2	860	A
57	2	872	G
57	2	877	C
57	2	880	C
57	2	906	U

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Mol	Chain	Res	Type
57	2	912	2MG
57	2	915	A
57	2	917	G
57	2	918	C
57	2	921	A
57	2	922	G
57	2	923	A
57	2	924	A
57	2	928	U
57	2	938	U
57	2	939	G
57	2	949	G
57	2	950	A
57	2	954	U
57	2	971	U
57	2	972	G
57	2	978	A
57	2	980	G
57	2	981	G
57	2	982	A
57	2	1013	U
57	2	1034	A
57	2	1036	A
57	2	1042	G
57	2	1043	U
57	2	1049	A
57	2	1072	G
57	2	1073	U
57	2	1074	U
57	2	1079	U
57	2	1080	U
57	2	1081	U
57	2	1082	G
57	2	1096	A
57	2	1098	U
57	2	1109	G
57	2	1122	G
57	2	1128	G
57	2	1134	A
57	2	1135	A
57	2	1151	A
57	2	1165	A

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Mol	Chain	Res	Type
57	2	1166	C
57	2	1176	A
57	2	1178	U
57	2	1191	C
57	2	1195	A
57	2	1196	G
57	2	1212	U
57	2	1218	A
57	2	1224	U
57	2	1228	C
57	2	1238	G
57	2	1240	U
57	2	1243	G
57	2	1258	C
57	2	1261	G
57	2	1276	G
57	2	1278	A
57	2	1284	A
57	2	1291	G
57	2	1301	U
57	2	1303	U
57	2	1309	G
57	2	1317	C
57	2	1318	G
57	2	1337	A
57	2	1338	C
57	2	1339	C
57	2	1358	G
57	2	1361	G
57	2	1380	A
57	2	1385	A
57	2	1390	U
57	2	1391	C
57	2	1431	A
57	2	1432	A
57	2	1436	G
57	2	1438	A
57	2	1442	A
57	2	1445	U
57	2	1456	G
57	2	1458	MA6
57	2	1468	G

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Mol	Chain	Res	Type
57	2	1469	G
57	2	1474	C
62	A	1	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	3	15	U
33	1	1154	A
33	1	1379	A
33	1	1961	G
33	1	2396	U
34	4	277	G
57	2	191	A
57	2	595	U
57	2	980	G

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

23 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
33	5MU	1	404	33	19,22,23	7.67	8 (42%)	28,32,35	3.32	9 (32%)
35	PSU	y	55	35	18,21,22	1.12	1 (5%)	22,30,33	1.65	4 (18%)
33	2MG	1	2085	33	23,26,27	2.69	8 (34%)	32,38,41	2.53	14 (43%)
33	OMU	1	2192	33,64	19,22,23	2.98	8 (42%)	26,31,34	1.77	5 (19%)
33	5MU	1	1577	33,64	19,22,23	7.66	9 (47%)	28,32,35	3.48	10 (35%)
57	MA6	2	1457	57	23,26,27	1.62	5 (21%)	34,38,41	3.40	11 (32%)
33	H2U	1	2089	33	18,21,22	0.57	0	21,30,33	1.01	1 (4%)
33	2MA	1	2143	33,63,64	22,25,26	4.08	7 (31%)	33,37,40	2.44	10 (30%)
57	MA6	2	1458	57	23,26,27	1.68	5 (21%)	34,38,41	3.50	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	OMG	1	1891	33,64,35	23,26,27	2.39	7 (30%)	33,38,41	2.22	9 (27%)
57	G7M	2	480	57,64	23,26,27	2.27	7 (30%)	35,39,42	3.01	10 (28%)
57	2MG	2	912	57	23,26,27	3.03	7 (30%)	32,38,41	3.00	10 (31%)
57	2MG	2	1455	57	23,26,27	2.86	7 (30%)	32,38,41	2.96	11 (34%)
35	4SU	y	8	35	18,21,22	3.94	7 (38%)	26,30,33	2.15	4 (15%)
35	5MU	y	54	35	19,22,23	7.68	9 (47%)	28,32,35	3.22	11 (39%)
33	OMC	1	2138	33,63	19,22,23	2.84	8 (42%)	26,31,34	0.90	0
33	2MG	1	1471	33	23,26,27	2.84	7 (30%)	32,38,41	2.88	11 (34%)
57	UR3	2	1437	57	19,22,23	2.76	8 (42%)	26,32,35	1.32	2 (7%)
35	5MC	y	32	35	18,22,23	3.60	7 (38%)	26,32,35	1.19	2 (7%)
33	5MC	1	1600	33,64	18,22,23	3.45	7 (38%)	26,32,35	1.06	1 (3%)
57	4OC	2	1341	57	20,23,24	3.39	8 (40%)	26,32,35	0.85	1 (3%)
57	5MC	2	913	57	18,22,23	3.57	7 (38%)	26,32,35	1.04	2 (7%)
33	6MZ	1	1669	33	22,25,26	4.41	13 (59%)	30,36,39	2.99	12 (40%)

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
33	5MU	1	404	33	-	0/7/25/26	0/2/2/2
35	PSU	y	55	35	-	0/7/25/26	0/2/2/2
33	2MG	1	2085	33	-	2/9/27/28	0/3/3/3
33	OMU	1	2192	33,64	-	0/9/27/28	0/2/2/2
33	5MU	1	1577	33,64	-	0/7/25/26	0/2/2/2
57	MA6	2	1457	57	-	0/11/29/30	0/3/3/3
33	H2U	1	2089	33	-	0/7/38/39	0/2/2/2
33	2MA	1	2143	33,63,64	-	1/7/25/26	0/3/3/3
57	MA6	2	1458	57	-	2/11/29/30	0/3/3/3
33	OMG	1	1891	33,64,35	-	3/9/27/28	0/3/3/3
57	G7M	2	480	57,64	-	3/7/25/26	0/3/3/3
57	2MG	2	912	57	-	2/9/27/28	0/3/3/3
57	2MG	2	1455	57	-	0/9/27/28	0/3/3/3
35	4SU	y	8	35	-	0/7/25/26	0/2/2/2
35	5MU	y	54	35	-	0/7/25/26	0/2/2/2
33	OMC	1	2138	33,63	-	0/9/27/28	0/2/2/2
33	2MG	1	1471	33	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	UR3	2	1437	57	-	0/7/25/26	0/2/2/2
35	5MC	y	32	35	-	0/7/25/26	0/2/2/2
33	5MC	1	1600	33,64	-	2/7/25/26	0/2/2/2
57	4OC	2	1341	57	-	2/9/29/30	0/2/2/2
57	5MC	2	913	57	-	0/7/25/26	0/2/2/2
33	6MZ	1	1669	33	-	2/9/27/28	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	1577	5MU	C4-C5	22.76	1.82	1.44
35	y	54	5MU	C4-C5	22.61	1.82	1.44
33	1	404	5MU	C4-C5	22.41	1.82	1.44
35	y	54	5MU	C6-N1	15.66	1.64	1.38
33	1	404	5MU	C6-N1	15.52	1.64	1.38
33	1	1577	5MU	C6-N1	15.41	1.64	1.38
33	1	1669	6MZ	C6-N6	14.05	1.49	1.34
33	1	2143	2MA	C4-N3	13.45	1.51	1.34
33	1	404	5MU	C4-N3	-12.71	1.15	1.38
33	1	1577	5MU	C4-N3	-12.46	1.15	1.38
35	y	54	5MU	C4-N3	-12.36	1.15	1.38
33	1	404	5MU	C6-C5	-12.14	1.14	1.34
33	1	1577	5MU	C6-C5	-11.97	1.14	1.34
35	y	54	5MU	C6-C5	-11.91	1.15	1.34
35	y	32	5MC	C6-C5	8.67	1.48	1.34
57	2	913	5MC	C6-C5	8.58	1.48	1.34
57	2	912	2MG	C2-N3	8.28	1.47	1.31
33	1	1600	5MC	C6-C5	8.17	1.48	1.34
57	2	912	2MG	C2-N2	7.83	1.50	1.33
33	1	2143	2MA	C2-N3	7.70	1.47	1.34
35	y	8	4SU	C2-N3	7.69	1.51	1.38
57	2	1455	2MG	C2-N3	7.66	1.46	1.31
33	1	1471	2MG	C2-N3	7.61	1.46	1.31
33	1	1669	6MZ	O4'-C1'	7.54	1.59	1.42
57	2	1341	4OC	C4-N3	7.51	1.45	1.32
35	y	8	4SU	C2-N1	7.50	1.50	1.38
57	2	1455	2MG	C2-N2	7.32	1.49	1.33
33	1	1471	2MG	C2-N2	7.24	1.49	1.33
33	1	2085	2MG	C2-N2	7.18	1.49	1.33
57	2	913	5MC	C4-N3	7.10	1.46	1.34
57	2	1437	UR3	C2-N1	7.05	1.48	1.38
35	y	8	4SU	C5-C4	7.04	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	1600	5MC	C4-N3	6.97	1.45	1.34
35	y	32	5MC	C4-N3	6.87	1.45	1.34
35	y	8	4SU	C4-N3	6.85	1.45	1.37
33	1	2192	OMU	C2-N1	6.67	1.49	1.38
33	1	2192	OMU	C2-N3	6.64	1.49	1.38
57	2	1341	4OC	C2-N3	6.63	1.49	1.36
57	2	1341	4OC	C6-C5	6.54	1.50	1.35
33	1	2085	2MG	C2-N3	6.43	1.44	1.31
57	2	480	G7M	C4-N3	6.41	1.49	1.34
33	1	1891	OMG	C4-N3	6.40	1.49	1.34
33	1	2143	2MA	C6-N1	6.38	1.44	1.35
57	2	912	2MG	C4-N3	6.24	1.49	1.34
33	1	1669	6MZ	C2'-C1'	-6.16	1.33	1.53
57	2	1437	UR3	C6-C5	6.15	1.49	1.35
57	2	913	5MC	C2-N3	6.15	1.48	1.36
35	y	32	5MC	C2-N3	6.14	1.48	1.36
33	1	1600	5MC	C2-N3	6.04	1.48	1.36
57	2	1341	4OC	C4-N4	5.98	1.48	1.35
33	1	2138	OMC	C2-N3	5.89	1.48	1.36
33	1	1669	6MZ	O4'-C4'	-5.89	1.31	1.45
35	y	8	4SU	C6-C5	5.81	1.48	1.35
33	1	1471	2MG	C4-N3	5.80	1.48	1.34
33	1	2138	OMC	C6-C5	5.66	1.48	1.35
57	2	1455	2MG	C4-N3	5.56	1.47	1.34
33	1	2192	OMU	C6-C5	5.45	1.47	1.35
33	1	1891	OMG	C2-N3	5.41	1.46	1.33
33	1	2143	2MA	C2-N1	5.39	1.43	1.34
35	y	32	5MC	C6-N1	5.29	1.47	1.38
35	y	54	5MU	C2-N3	5.20	1.47	1.38
57	2	913	5MC	C6-N1	5.14	1.46	1.38
57	2	1437	UR3	C2-N3	5.12	1.48	1.39
33	1	2143	2MA	C5-C6	5.09	1.55	1.41
33	1	2085	2MG	C4-N3	5.04	1.46	1.34
33	1	404	5MU	C2-N3	4.95	1.46	1.38
33	1	1600	5MC	C6-N1	4.91	1.46	1.38
33	1	1577	5MU	C2-N3	4.87	1.46	1.38
57	2	1458	MA6	C6-N6	4.81	1.51	1.36
33	1	2138	OMC	C4-N3	4.81	1.44	1.34
57	2	1457	MA6	C6-N6	4.79	1.51	1.36
33	1	2138	OMC	C4-N4	4.55	1.44	1.33
33	1	1891	OMG	C2-N2	4.45	1.44	1.34
57	2	912	2MG	C2-N1	4.45	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	y	8	4SU	C4-S4	-4.43	1.60	1.68
57	2	1455	2MG	C2-N1	4.41	1.43	1.36
35	y	54	5MU	C2-N1	4.40	1.45	1.38
33	1	2138	OMC	C2-N1	4.30	1.49	1.40
33	1	2085	2MG	C2-N1	4.23	1.43	1.36
57	2	913	5MC	C4-N4	4.22	1.45	1.34
35	y	32	5MC	C4-N4	4.21	1.45	1.34
33	1	1471	2MG	C2-N1	4.18	1.43	1.36
57	2	480	G7M	C2-N2	4.17	1.44	1.34
35	y	32	5MC	C2-N1	4.13	1.48	1.40
33	1	1600	5MC	C4-N4	4.04	1.44	1.34
33	1	2192	OMU	C4-N3	4.02	1.45	1.38
33	1	1669	6MZ	C5-C4	-4.01	1.31	1.39
57	2	1341	4OC	C2-N1	3.97	1.48	1.40
57	2	480	G7M	C2-N3	3.96	1.42	1.33
57	2	1341	4OC	C5-C4	3.96	1.49	1.40
33	1	404	5MU	C2-N1	3.88	1.44	1.38
35	y	55	PSU	C6-C5	3.86	1.39	1.35
33	1	1669	6MZ	O3'-C3'	-3.83	1.33	1.43
33	1	1669	6MZ	C8-N9	-3.76	1.30	1.37
57	2	480	G7M	C5-N7	-3.75	1.34	1.39
33	1	1669	6MZ	C5-N7	-3.64	1.32	1.39
33	1	2143	2MA	C6-N6	-3.56	1.25	1.34
57	2	913	5MC	C2-N1	3.46	1.47	1.40
33	1	1577	5MU	C2-N1	3.37	1.43	1.38
35	y	8	4SU	C6-N1	3.35	1.46	1.38
33	1	404	5MU	O4-C4	-3.34	1.17	1.23
33	1	1891	OMG	C5-N7	-3.31	1.32	1.39
33	1	1600	5MC	C2-N1	3.27	1.47	1.40
33	1	1577	5MU	O4-C4	-3.26	1.17	1.23
57	2	1341	4OC	C6-N1	3.25	1.45	1.38
35	y	54	5MU	O4-C4	-3.14	1.17	1.23
33	1	2192	OMU	O4-C4	-3.10	1.18	1.24
33	1	2192	OMU	C6-N1	3.07	1.45	1.38
33	1	2138	OMC	O2-C2	-3.01	1.18	1.23
33	1	404	5MU	O2-C2	-3.00	1.17	1.23
57	2	1458	MA6	C5-N7	-2.98	1.33	1.39
57	2	1437	UR3	C6-N1	2.97	1.45	1.38
33	1	1669	6MZ	C9-N6	2.96	1.50	1.45
33	1	2138	OMC	C6-N1	2.94	1.45	1.38
33	1	1577	5MU	O2-C2	-2.94	1.17	1.23
57	2	480	G7M	C6-N1	2.84	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	2192	OMU	O2-C2	-2.82	1.17	1.23
33	1	2085	2MG	C4-N9	-2.78	1.30	1.38
57	2	480	G7M	C5-C6	2.76	1.51	1.43
33	1	1669	6MZ	C4-N9	-2.75	1.31	1.37
33	1	1600	5MC	O2-C2	-2.72	1.18	1.23
33	1	1891	OMG	O6-C6	-2.71	1.18	1.23
57	2	1458	MA6	C5-C4	-2.70	1.34	1.39
57	2	1455	2MG	C5-C6	2.70	1.54	1.44
33	1	1669	6MZ	C6-N1	-2.65	1.30	1.35
57	2	913	5MC	O2-C2	-2.65	1.18	1.23
57	2	1458	MA6	C10-N6	2.58	1.51	1.45
35	y	54	5MU	O2-C2	-2.57	1.18	1.23
57	2	1457	MA6	C5-C4	-2.52	1.34	1.39
57	2	1457	MA6	C10-N6	2.50	1.51	1.45
57	2	1457	MA6	C5-N7	-2.49	1.34	1.39
35	y	32	5MC	O2-C2	-2.48	1.19	1.23
33	1	1471	2MG	C5-C6	2.47	1.53	1.44
57	2	1455	2MG	C6-N1	2.45	1.43	1.38
57	2	480	G7M	C2-N1	2.45	1.43	1.37
57	2	1341	4OC	O2-C2	-2.44	1.19	1.23
57	2	912	2MG	C5-C6	2.43	1.53	1.44
33	1	2143	2MA	C5-N7	-2.42	1.34	1.39
57	2	1458	MA6	C8-N9	-2.42	1.33	1.37
33	1	1669	6MZ	O2'-C2'	2.41	1.48	1.43
33	1	1891	OMG	C2-N1	2.40	1.43	1.37
57	2	912	2MG	C6-N1	2.35	1.43	1.38
33	1	2085	2MG	C6-N1	2.34	1.43	1.38
57	2	1437	UR3	O2-C2	-2.34	1.18	1.22
33	1	2192	OMU	C5-C4	2.34	1.48	1.43
33	1	2085	2MG	C5-C6	2.32	1.53	1.44
33	1	1891	OMG	C5-C6	2.30	1.52	1.44
57	2	1457	MA6	C8-N9	-2.30	1.33	1.37
57	2	1437	UR3	O4-C4	-2.28	1.18	1.23
57	2	1437	UR3	C5-C4	2.28	1.49	1.43
33	1	1471	2MG	C5-N7	-2.26	1.34	1.39
33	1	1669	6MZ	C8-N7	2.22	1.35	1.31
57	2	912	2MG	C5-N7	-2.16	1.34	1.39
33	1	1471	2MG	C6-N1	2.15	1.42	1.38
57	2	1455	2MG	C5-N7	-2.12	1.35	1.39
57	2	1437	UR3	C4-N3	2.11	1.45	1.40
33	1	2138	OMC	C5-C4	2.11	1.47	1.42
35	y	54	5MU	C5M-C5	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1	1577	5MU	C5M-C5	2.01	1.55	1.50
33	1	2085	2MG	C5-N7	-2.01	1.35	1.39

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2	1458	MA6	N1-C6-N6	-13.46	102.36	117.08
57	2	1457	MA6	N1-C6-N6	-13.27	102.58	117.08
33	1	1577	5MU	C5-C4-N3	10.60	124.36	115.31
35	y	54	5MU	C5-C4-N3	10.08	123.92	115.31
33	1	404	5MU	C5-C4-N3	10.03	123.87	115.31
57	2	480	G7M	CN7-N7-C5	9.45	138.51	126.77
57	2	912	2MG	C1'-N9-C8	-8.76	101.77	126.70
33	1	1577	5MU	C5-C6-N1	-8.69	114.40	123.34
57	2	912	2MG	C1'-N9-C4	8.41	151.50	126.50
33	1	404	5MU	C5-C6-N1	-8.23	114.87	123.34
33	1	2143	2MA	C5-C4-N3	-8.20	117.97	127.19
33	1	1471	2MG	C1'-N9-C8	-8.16	103.47	126.70
33	1	1669	6MZ	C1'-N9-C8	-7.81	109.49	127.14
33	1	1471	2MG	C1'-N9-C4	7.78	149.62	126.50
57	2	1455	2MG	C1'-N9-C4	7.65	149.22	126.50
57	2	1455	2MG	C1'-N9-C8	-7.62	105.01	126.70
35	y	54	5MU	C5-C6-N1	-7.54	115.58	123.34
57	2	1458	MA6	C5-C6-N6	7.36	138.13	125.30
35	y	8	4SU	C4-N3-C2	-7.35	120.20	127.34
33	1	1577	5MU	C4-N3-C2	-7.30	117.90	127.35
33	1	1669	6MZ	N1-C2-N3	-7.26	117.24	128.60
57	2	480	G7M	CN7-N7-C8	-7.22	113.70	124.84
57	2	1457	MA6	C5-C6-N6	7.19	137.83	125.30
33	1	404	5MU	C4-N3-C2	-6.66	118.73	127.35
57	2	480	G7M	C1'-N9-C4	6.61	146.14	126.50
33	1	2085	2MG	C1'-N9-C8	-6.60	107.90	126.70
33	1	1669	6MZ	C4-N9-C1'	6.55	142.21	126.59
35	y	54	5MU	C4-N3-C2	-6.44	119.02	127.35
57	2	912	2MG	C2-N3-C4	6.37	119.93	112.04
57	2	1455	2MG	C2-N3-C4	6.35	119.92	112.04
33	1	1471	2MG	C2-N3-C4	6.15	119.67	112.04
33	1	2085	2MG	C1'-N9-C4	6.05	144.47	126.50
57	2	480	G7M	C1'-N9-C8	-5.93	106.70	126.74
33	1	2085	2MG	C2-N3-C4	5.70	119.11	112.04
33	1	2143	2MA	N3-C4-N9	5.65	134.83	126.99
33	1	1891	OMG	C5-C4-N3	-5.64	119.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	2192	OMU	C4-N3-C2	-5.46	119.37	126.58
57	2	1457	MA6	N1-C2-N3	-5.45	120.08	128.60
57	2	1458	MA6	N1-C2-N3	-5.39	120.17	128.60
35	y	8	4SU	C5-C4-N3	5.35	119.65	114.69
57	2	1458	MA6	C5-C4-N3	-5.35	119.77	126.75
33	1	1891	OMG	C1'-N9-C4	-5.24	110.94	126.50
57	2	1455	2MG	C2-N1-C6	-5.23	118.46	124.48
57	2	912	2MG	C5-C4-N3	-5.21	120.00	128.46
57	2	1458	MA6	N9-C8-N7	-5.20	106.81	113.91
57	2	1455	2MG	C5-C4-N3	-5.06	120.25	128.46
57	2	1457	MA6	N9-C8-N7	-4.99	107.09	113.91
33	1	1891	OMG	C1'-N9-C8	4.94	140.77	126.70
57	2	1457	MA6	C5-C4-N3	-4.92	120.33	126.75
33	1	1669	6MZ	N9-C8-N7	-4.87	107.25	113.91
33	1	1471	2MG	C5-C4-N3	-4.79	120.69	128.46
57	2	1437	UR3	C4-N3-C2	-4.78	120.06	124.56
33	1	1471	2MG	C2-N1-C6	-4.77	118.99	124.48
33	1	1577	5MU	N3-C2-N1	4.61	121.02	114.89
33	1	404	5MU	C5M-C5-C6	-4.50	116.83	122.85
57	2	480	G7M	C2-N3-C4	4.44	120.21	112.30
57	2	912	2MG	C2-N1-C6	-4.41	119.40	124.48
33	1	1577	5MU	C5M-C5-C6	-4.40	116.97	122.85
33	1	1891	OMG	C2-N3-C4	4.39	120.13	112.30
33	1	404	5MU	N3-C2-N1	4.39	120.71	114.89
35	y	55	PSU	C4-N3-C2	-4.38	120.03	126.34
57	2	1455	2MG	CM2-N2-C2	-4.37	114.20	123.86
35	y	54	5MU	C5M-C5-C6	-4.26	117.16	122.85
35	y	55	PSU	N1-C2-N3	4.22	119.92	115.13
35	y	54	5MU	N3-C2-N1	4.14	120.38	114.89
33	1	2192	OMU	N3-C2-N1	4.13	120.37	114.89
57	2	1458	MA6	C4-C5-C6	4.10	120.47	115.88
33	1	2143	2MA	N9-C8-N7	-4.03	108.40	113.91
33	1	1669	6MZ	C2-N3-C4	3.97	121.14	111.75
57	2	480	G7M	C5-C6-N1	3.95	120.03	111.79
35	y	54	5MU	O4-C4-C5	-3.94	120.34	124.90
33	1	1577	5MU	O4-C4-C5	-3.92	120.36	124.90
57	2	1458	MA6	C5-N7-C8	3.88	109.02	103.51
57	2	480	G7M	C5-C4-N3	-3.86	120.74	128.15
35	y	8	4SU	N3-C2-N1	3.81	119.94	114.89
33	1	1891	OMG	N9-C4-N3	3.78	133.52	125.94
57	2	1457	MA6	C2-N1-C6	3.63	120.32	111.75
57	2	1457	MA6	C4-C5-C6	3.62	119.93	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	404	5MU	O4-C4-C5	-3.60	120.73	124.90
57	2	480	G7M	O6-C6-C5	-3.58	119.99	128.06
57	2	1457	MA6	C4-N9-C8	3.55	109.58	105.73
33	1	2192	OMU	C5-C4-N3	3.55	120.15	114.84
57	2	1458	MA6	N3-C4-N9	3.54	132.91	127.08
57	2	1458	MA6	C2-N1-C6	3.53	120.10	111.75
57	2	1457	MA6	N3-C4-N9	3.50	132.86	127.08
33	1	1669	6MZ	C5-C4-N3	-3.50	122.18	126.75
57	2	1458	MA6	C2-N3-C4	3.49	119.99	111.75
35	y	54	5MU	C5M-C5-C4	3.49	122.60	118.77
33	1	2085	2MG	C2-N1-C6	-3.48	120.47	124.48
33	1	2143	2MA	C4-N9-C1'	-3.44	118.39	126.59
57	2	1457	MA6	C2-N3-C4	3.38	119.75	111.75
33	1	2143	2MA	N3-C2-N1	-3.38	119.50	125.72
33	1	1577	5MU	C5M-C5-C4	3.37	122.48	118.77
33	1	2085	2MG	N9-C8-N7	-3.36	107.06	113.39
57	2	1457	MA6	C5-N7-C8	3.35	108.27	103.51
33	1	2143	2MA	C5-N7-C8	3.33	108.25	103.51
33	1	2089	H2U	C5-C4-N3	-3.30	112.94	116.65
33	1	404	5MU	C5M-C5-C4	3.30	122.40	118.77
33	1	404	5MU	C6-C5-C4	3.27	120.76	118.03
57	2	913	5MC	C5-C6-N1	-3.23	120.01	123.34
57	2	1458	MA6	C4-N9-C8	3.15	109.14	105.73
33	1	1669	6MZ	C5-C4-N9	3.13	109.43	105.78
35	y	8	4SU	C5-C4-S4	-3.09	120.48	124.47
33	1	1600	5MC	C5-C6-N1	-3.07	120.18	123.34
33	1	2085	2MG	C5-C4-N3	-3.06	123.50	128.46
33	1	1891	OMG	C2-N1-C6	-3.03	119.57	125.10
33	1	1577	5MU	C6-C5-C4	3.00	120.54	118.03
33	1	2192	OMU	O4-C4-C5	-2.99	119.90	125.16
33	1	1669	6MZ	C5-N7-C8	2.95	107.70	103.51
33	1	2143	2MA	C1'-N9-C8	2.94	133.78	127.14
33	1	2085	2MG	CM2-N2-C2	-2.93	117.39	123.86
35	y	32	5MC	O2-C2-N3	-2.93	117.57	122.33
57	2	480	G7M	C2-N1-C6	-2.92	119.77	125.10
33	1	1669	6MZ	C6-C5-N7	2.86	135.48	132.39
33	1	1471	2MG	C5-C6-N1	2.86	120.45	113.19
33	1	1577	5MU	O2-C2-N1	-2.86	118.99	122.79
57	2	912	2MG	C5-C6-N1	2.83	120.37	113.19
33	1	2085	2MG	N1-C2-N3	-2.77	119.66	123.95
57	2	912	2MG	O6-C6-C5	-2.76	119.28	126.60
57	2	1455	2MG	C5-C6-N1	2.75	120.17	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1	2085	2MG	C6-C5-N7	2.74	135.35	130.25
35	y	32	5MC	C5-C6-N1	-2.73	120.53	123.34
33	1	1891	OMG	N9-C8-N7	-2.72	108.26	113.39
57	2	912	2MG	N9-C4-N3	2.71	131.39	125.94
33	1	2085	2MG	C5-C4-N9	2.71	110.55	105.63
33	1	1669	6MZ	C4-C5-N7	-2.70	107.33	110.62
33	1	1471	2MG	N9-C8-N7	-2.69	108.32	113.39
33	1	1891	OMG	C5-C6-N1	2.68	119.99	113.19
57	2	1455	2MG	C5-C4-N9	2.65	110.43	105.63
35	y	54	5MU	C6-C5-C4	2.63	120.23	118.03
33	1	1577	5MU	O4-C4-N3	-2.52	115.28	120.12
33	1	2085	2MG	C4-C5-N7	-2.51	106.75	110.72
33	1	2143	2MA	C6-C5-C4	2.49	120.53	117.18
33	1	404	5MU	O4-C4-N3	-2.46	115.39	120.12
35	y	55	PSU	O2-C2-N1	-2.44	120.10	122.79
33	1	1471	2MG	O6-C6-C5	-2.44	120.14	126.60
33	1	2085	2MG	C5-C6-N1	2.43	119.36	113.19
57	2	912	2MG	N1-C2-N3	-2.42	120.20	123.95
33	1	1891	OMG	O6-C6-C5	-2.40	120.23	126.60
57	2	1455	2MG	O6-C6-C5	-2.40	120.24	126.60
57	2	1455	2MG	C4-C5-N7	-2.39	106.93	110.72
33	1	2192	OMU	O2-C2-N1	-2.38	119.62	122.79
57	2	1458	MA6	C4-C5-N7	-2.38	107.72	110.62
57	2	912	2MG	N9-C8-N7	-2.37	108.92	113.39
33	1	1669	6MZ	C4-N9-C8	2.37	108.30	105.73
57	2	1455	2MG	N9-C8-N7	-2.31	109.04	113.39
33	1	1471	2MG	CM2-N2-C2	-2.29	118.81	123.86
35	y	54	5MU	O4-C4-N3	-2.28	115.75	120.12
33	1	2085	2MG	O6-C6-C5	-2.27	120.58	126.60
33	1	2143	2MA	CM2-C2-N3	2.25	120.67	117.15
33	1	1669	6MZ	C2-N1-C6	2.24	122.77	115.25
57	2	1341	4OC	C6-C5-C4	2.22	119.68	116.96
57	2	1437	UR3	C1'-N1-C2	2.21	120.72	116.99
57	2	480	G7M	N2-C2-N1	2.21	121.42	116.71
57	2	913	5MC	CM5-C5-C6	-2.17	119.95	122.85
35	y	55	PSU	C6-N1-C2	-2.10	120.54	122.68
35	y	54	5MU	C1'-N1-C2	2.09	121.36	117.57
33	1	2085	2MG	C8-N7-C5	2.09	108.02	104.24
33	1	1471	2MG	N1-C2-N3	-2.09	120.72	123.95
33	1	1471	2MG	C5-C4-N9	2.07	109.38	105.63
33	1	2143	2MA	C2-N3-C4	2.03	121.97	116.99
35	y	54	5MU	C1'-N1-C6	-2.02	117.76	121.12

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	1	1669	6MZ	C3'-C4'-C5'-O5'
33	1	1891	OMG	C1'-C2'-O2'-CM2
57	2	912	2MG	O4'-C4'-C5'-O5'
57	2	1458	MA6	O4'-C4'-C5'-O5'
33	1	1669	6MZ	O4'-C4'-C5'-O5'
57	2	912	2MG	C3'-C4'-C5'-O5'
57	2	1341	4OC	O4'-C4'-C5'-O5'
57	2	1458	MA6	C3'-C4'-C5'-O5'
33	1	2085	2MG	C3'-C4'-C5'-O5'
57	2	480	G7M	C3'-C4'-C5'-O5'
33	1	1891	OMG	O4'-C4'-C5'-O5'
57	2	1341	4OC	C3'-C4'-C5'-O5'
33	1	2085	2MG	O4'-C4'-C5'-O5'
57	2	480	G7M	O4'-C4'-C5'-O5'
33	1	1891	OMG	C3'-C4'-C5'-O5'
57	2	480	G7M	C4'-C5'-O5'-P
33	1	1600	5MC	C2'-C1'-N1-C6
33	1	1600	5MC	O4'-C1'-N1-C6
33	1	2143	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	1	404	5MU	1	0
33	1	1577	5MU	1	0
57	2	1458	MA6	1	0
33	1	1891	OMG	1	0
57	2	912	2MG	1	0
57	2	1455	2MG	2	0
35	y	54	5MU	1	0
57	2	1341	4OC	1	0
33	1	1669	6MZ	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 450 ligands modelled in this entry, 449 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
65	CLM	1	2884	64	19,20,20	1.55	3 (15%)	23,27,27	0.98	2 (8%)

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
65	CLM	1	2884	64	-	5/20/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	1	2884	CLM	C2-N2	4.83	1.44	1.34
65	1	2884	CLM	O9B-N9	-3.15	1.17	1.22
65	1	2884	CLM	O2-C2	-2.60	1.18	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	1	2884	CLM	C3-N2-C2	-2.60	118.48	123.07
65	1	2884	CLM	O2-C2-N2	-2.01	119.21	122.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	1	2884	CLM	CL1-C1-C2-O2
65	1	2884	CLM	CL1-C1-C2-N2
65	1	2884	CLM	CL2-C1-C2-N2

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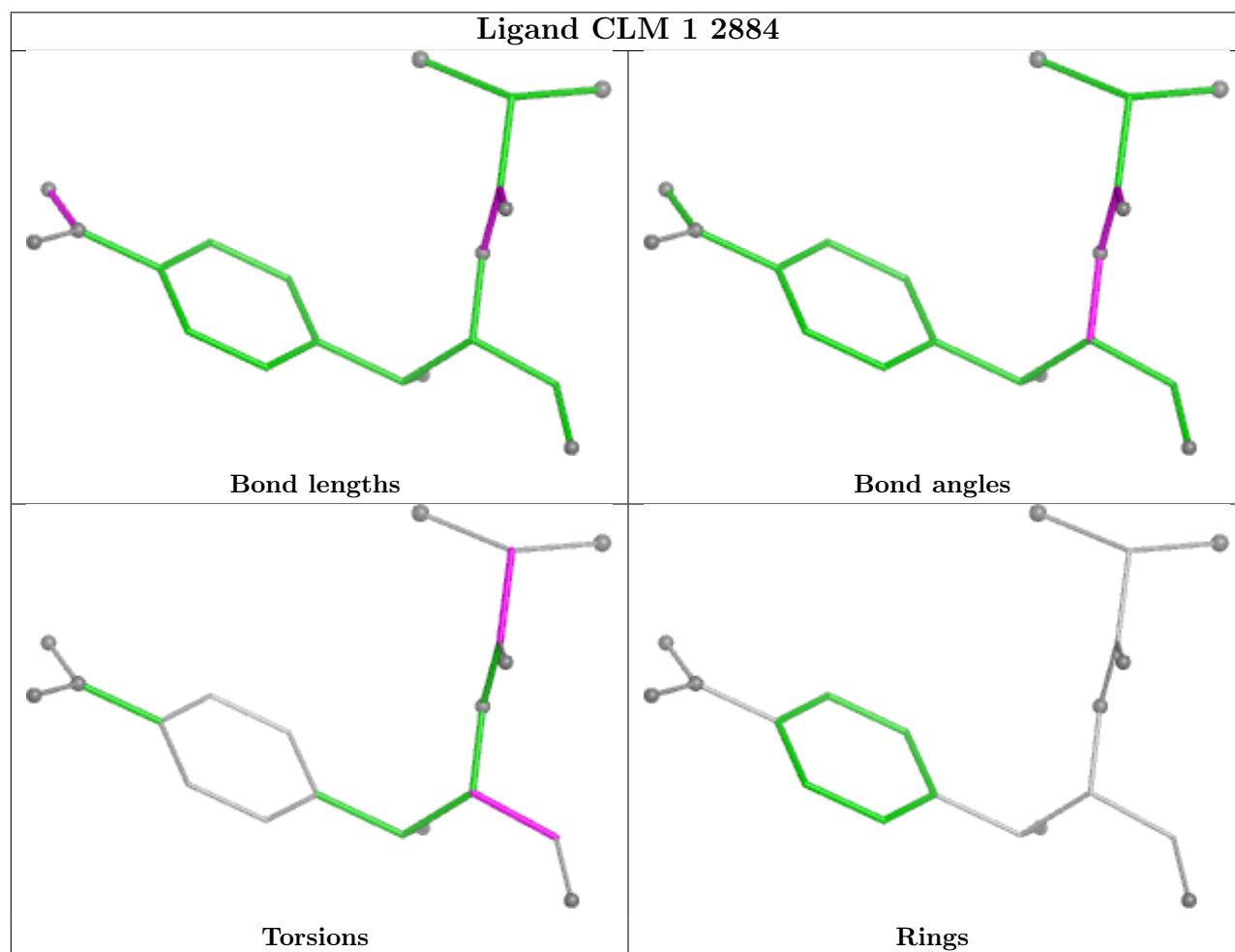
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Mol	Chain	Res	Type	Atoms
65	1	2884	CLM	C5-C3-C4-O4
65	1	2884	CLM	N2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	1	12
57	2	2
60	e	1
34	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	187:GLY	C	227:ALA	N	24.73
1	1	1506:C	O3'	1509:G	P	16.37
1	4	259:U	O3'	266:A	P	16.18
1	1	1190:A	O3'	1196:U	P	16.03
1	1	1738:G	O3'	1830:G	P	15.23
1	1	828:U	O3'	840:U	P	15.13
1	1	194:A	O3'	201:G	P	11.27
1	1	2430:U	O3'	2449:A	P	10.72
1	1	308:A	O3'	312:A	P	9.67
1	1	586:A	O3'	588:U	P	9.23
1	1	590:U	O3'	592:C	P	8.79
1	2	76:G	O3'	79:A	P	8.54
1	1	1242:U	O3'	1245:A	P	7.64
1	1	502:A	O3'	504:G	P	5.81
1	1	139:G	O3'	141:U	P	4.15
1	2	1472:C	O3'	1473:A	P	3.20

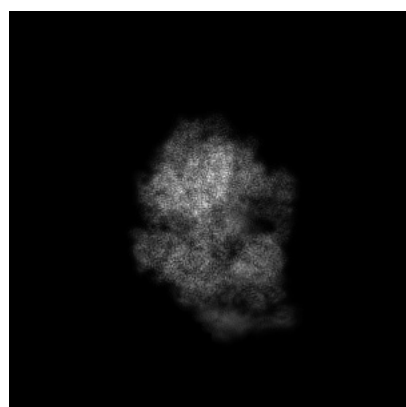
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56567. These allow visual inspection of the internal detail of the map and identification of artifacts.

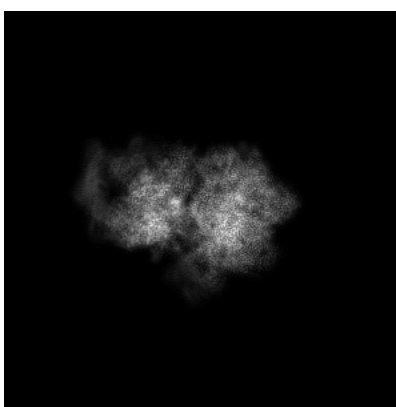
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

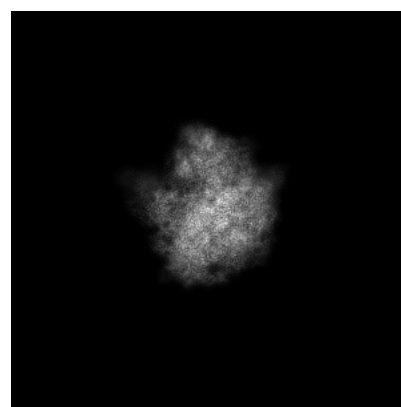
6.1.1 Primary map



X



Y

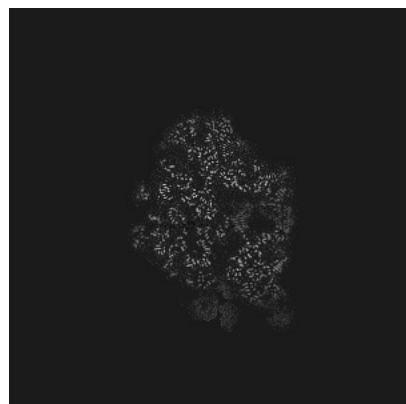


Z

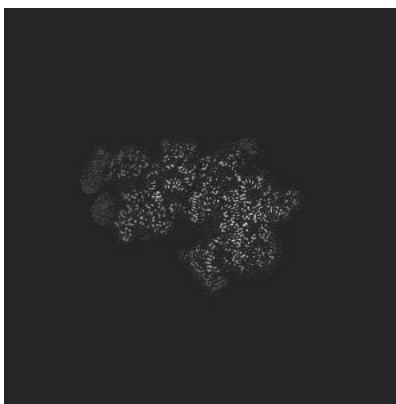
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

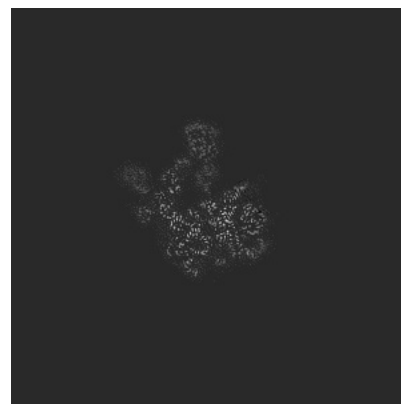
6.2.1 Primary map



X Index: 256



Y Index: 256

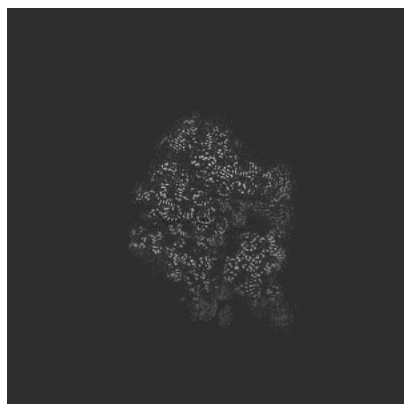


Z Index: 256

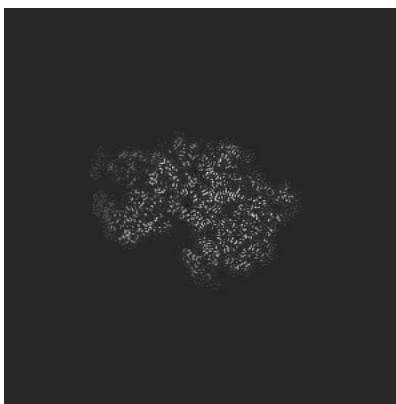
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

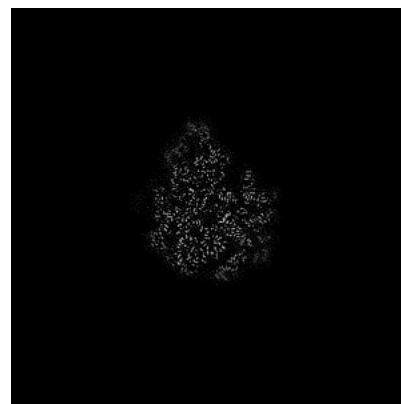
6.3.1 Primary map



X Index: 251



Y Index: 244

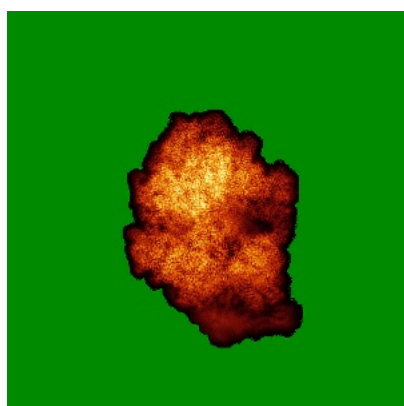


Z Index: 286

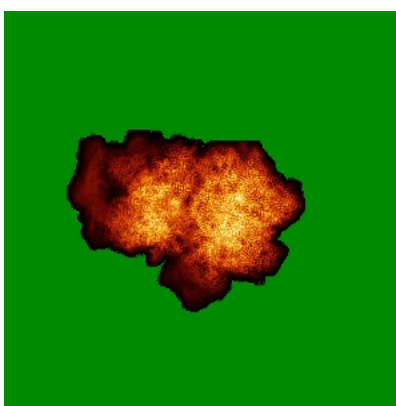
The images above show the largest variance slices of the map in three orthogonal directions.

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

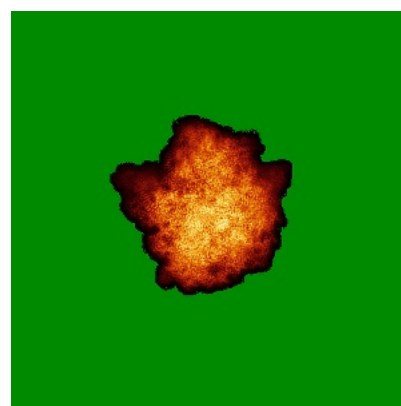
6.4.1 Primary map



X



Y

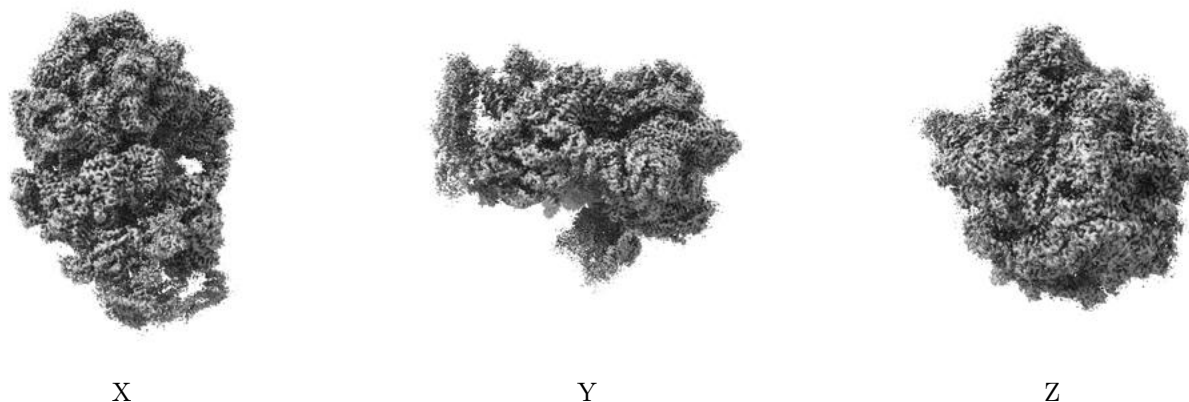


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0707. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

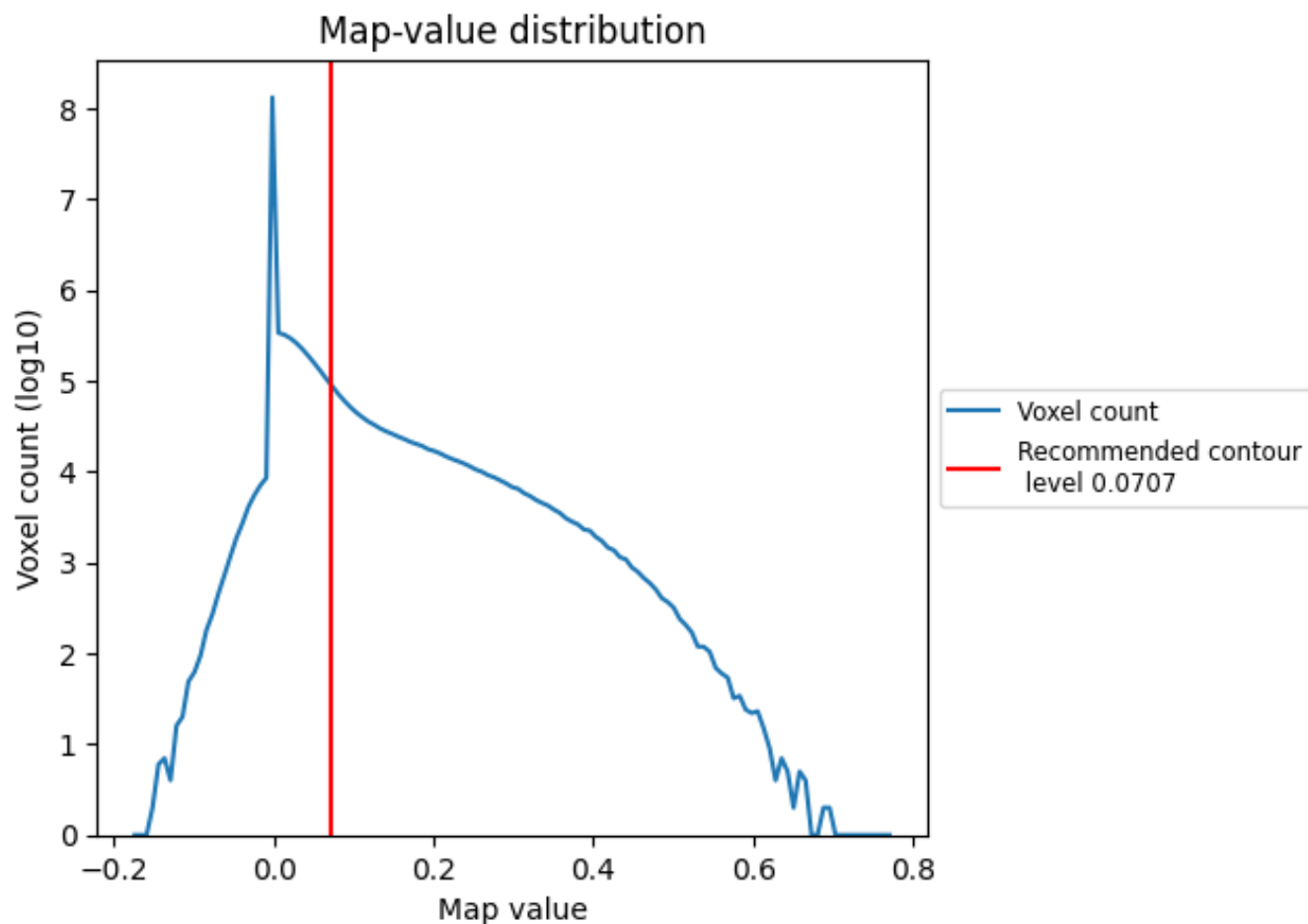
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

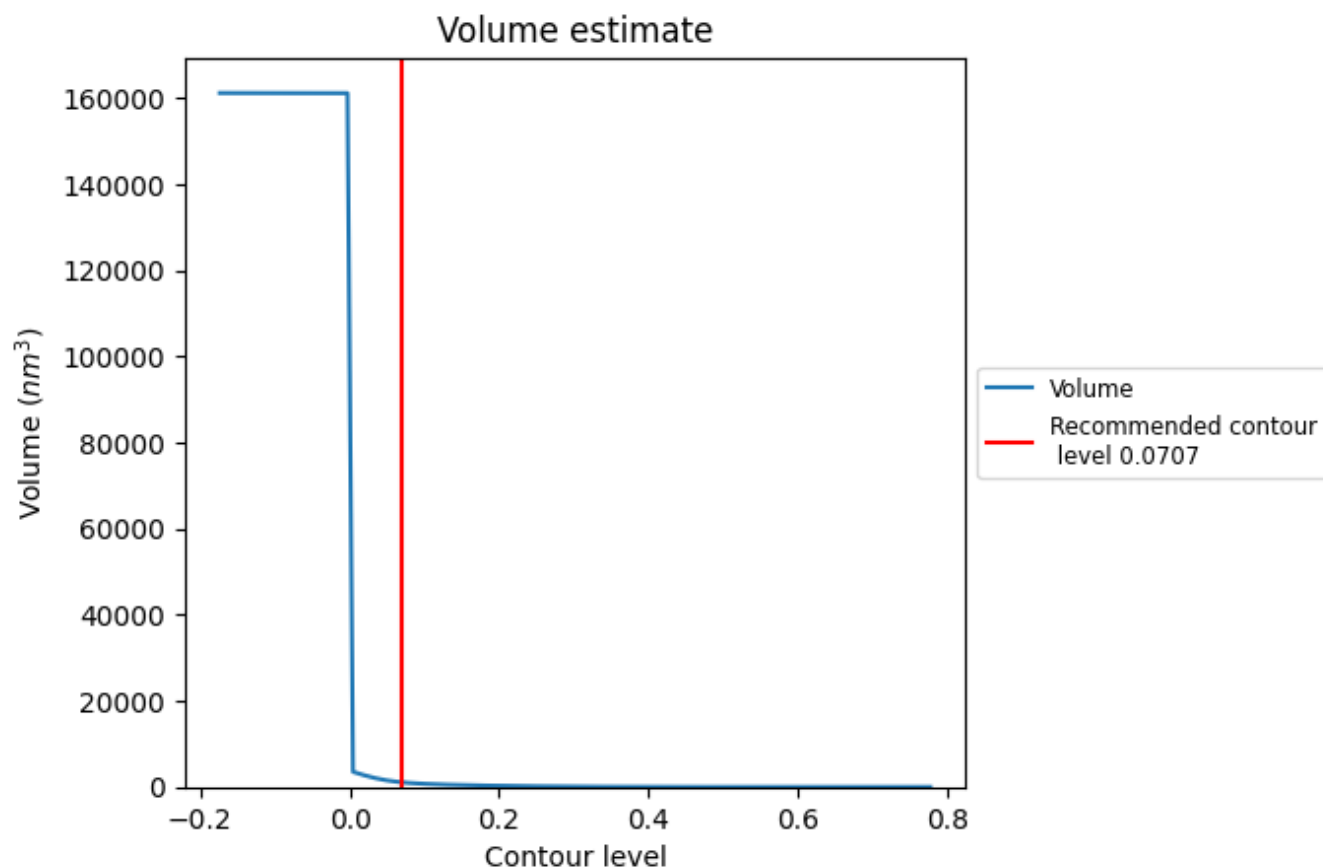
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

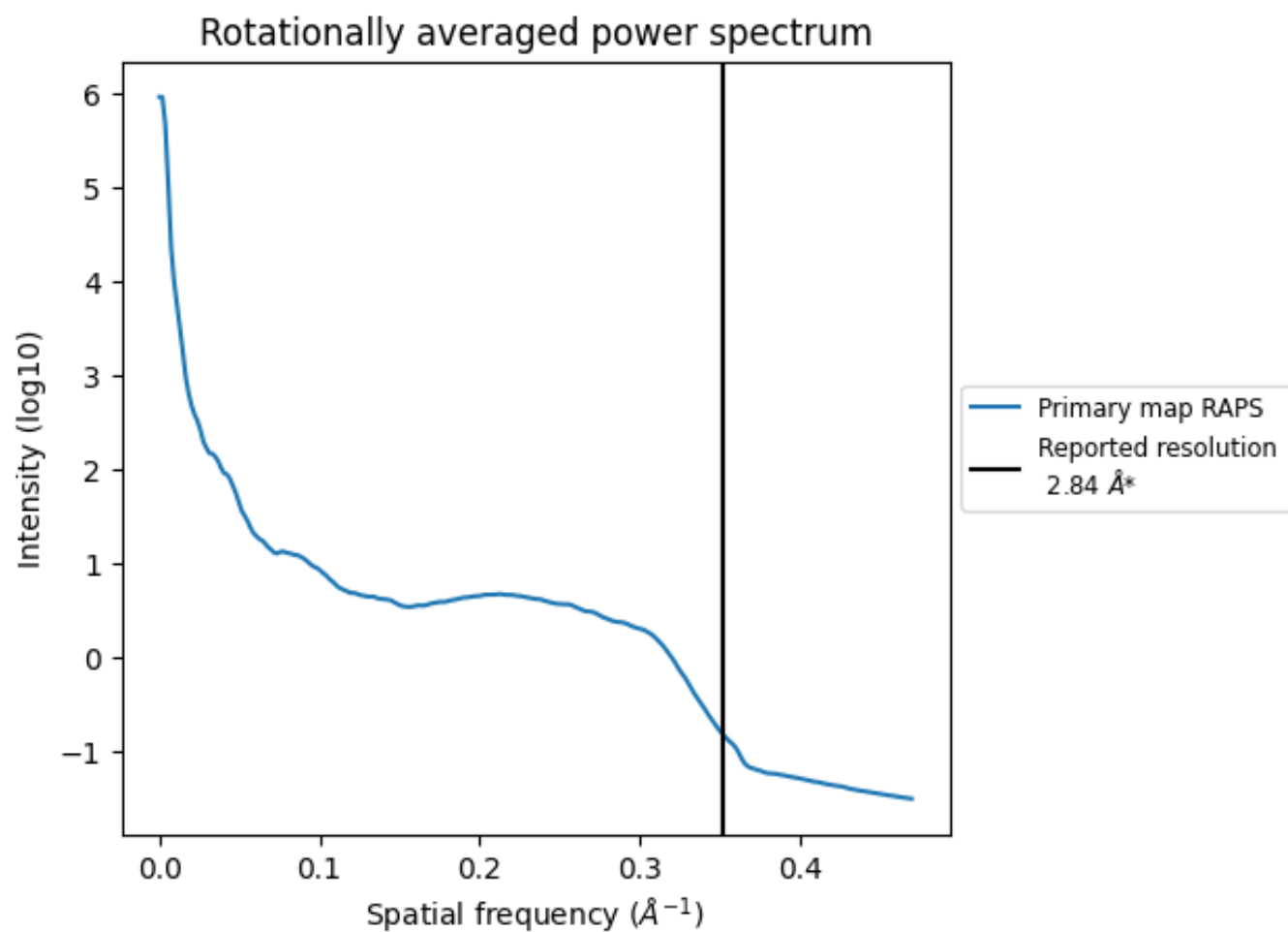
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070 nm^3 ; this corresponds to an approximate mass of 967 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

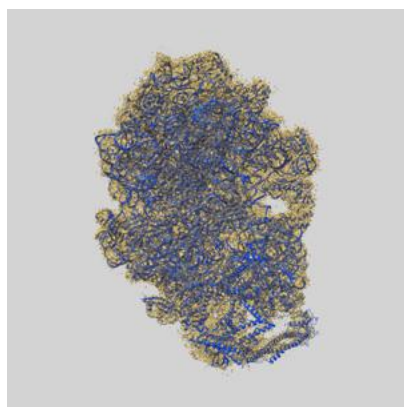
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

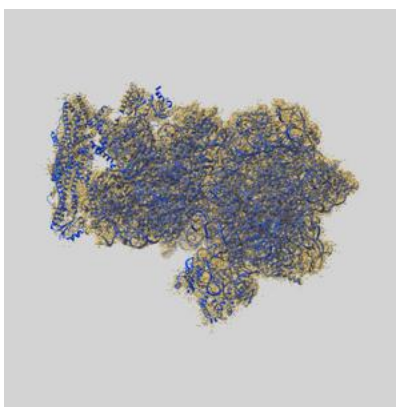
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56567 and PDB model 28JW. Per-residue inclusion information can be found in section 3 on page 17.

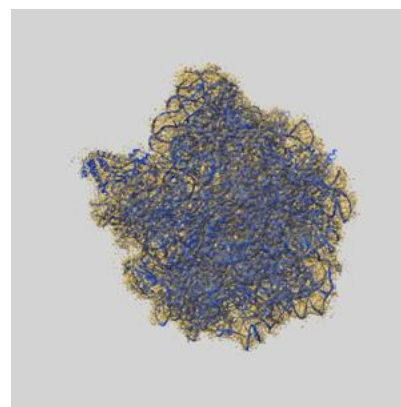
9.1 Map-model overlay [i](#)



X



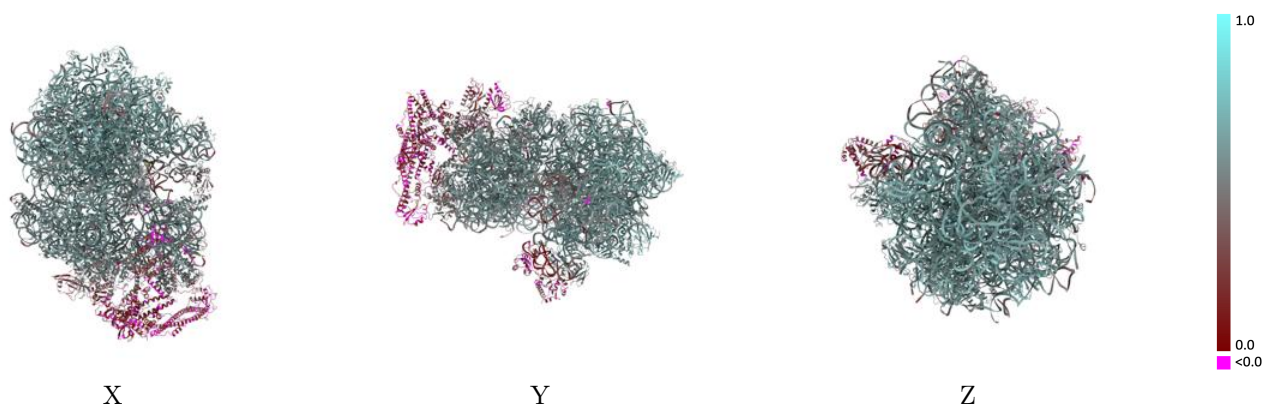
Y



Z

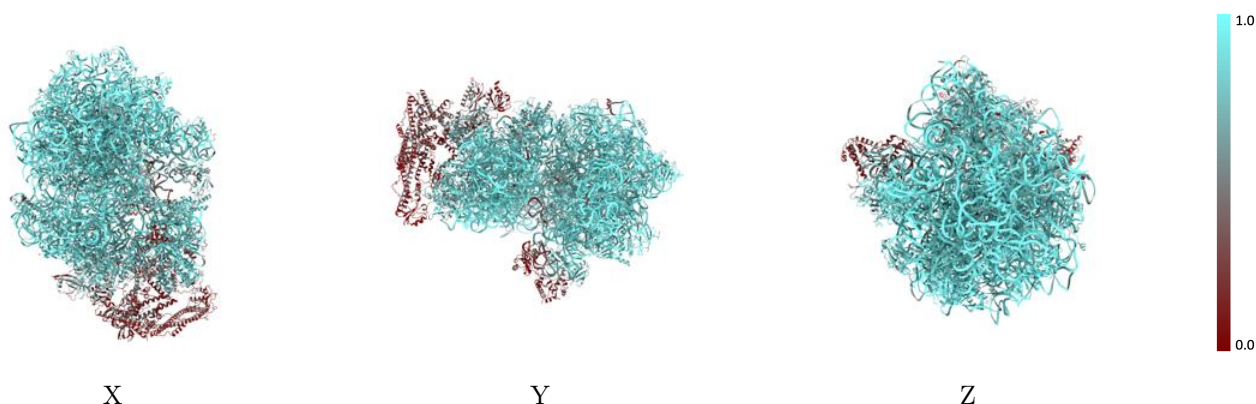
The images above show the 3D surface view of the map at the recommended contour level 0.0707 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



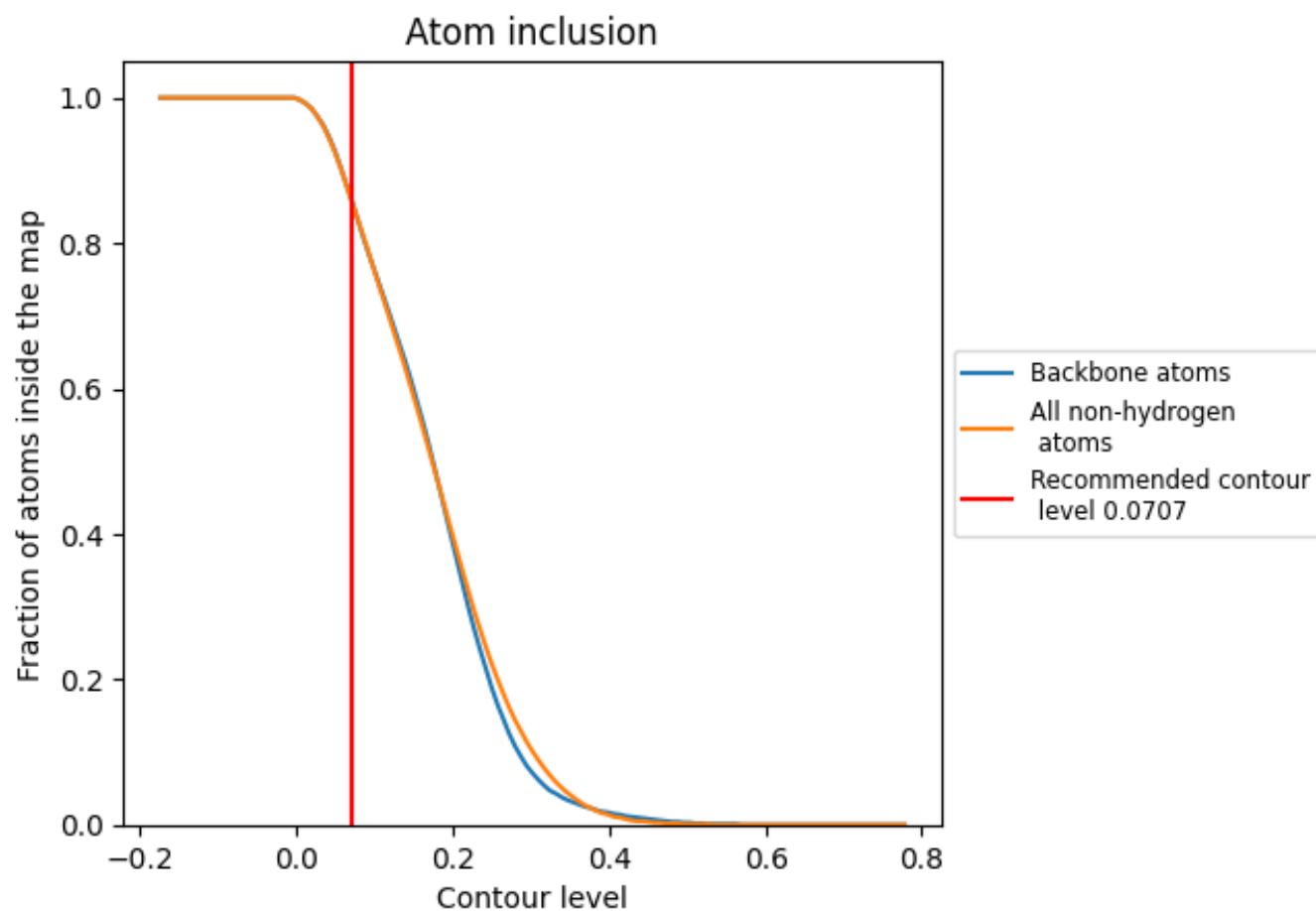
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0707).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.0707) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.5450
0	 0.9280	 0.6230
1	 0.9550	 0.6040
2	 0.9690	 0.5740
3	 0.9110	 0.5200
4	 0.9690	 0.6090
5	 0.9780	 0.6170
6	 0.9080	 0.6070
7	 0.9340	 0.6300
8	 0.9650	 0.6330
9	 0.9400	 0.6230
A	 0.5700	 0.4400
B	 0.9430	 0.6360
C	 0.9250	 0.6210
D	 0.9420	 0.6230
E	 0.6740	 0.4790
F	 0.7930	 0.5490
G	 0.7610	 0.5110
H	 0.1980	 0.2310
I	 0.0790	 0.1530
J	 0.9350	 0.6230
K	 0.9080	 0.6180
L	 0.9000	 0.6010
M	 0.9290	 0.6170
N	 0.9550	 0.6290
O	 0.8520	 0.5570
P	 0.8550	 0.5890
Q	 0.9600	 0.6330
R	 0.9360	 0.6220
S	 0.9100	 0.6180
T	 0.9220	 0.6090
U	 0.8860	 0.6000
V	 0.8710	 0.5780
W	 0.9070	 0.6110
X	 0.8890	 0.5910



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Chain	Atom inclusion	Q-score
Y	 0.6180	 0.3790
Z	 0.9250	 0.6130
a	 0.4100	 0.2630
b	 0.4540	 0.3110
c	 0.5940	 0.3770
d	 0.7000	 0.4560
e	 0.4390	 0.3110
f	 0.8390	 0.5580
g	 0.7280	 0.5010
h	 0.8710	 0.5800
i	 0.6840	 0.4470
j	 0.8030	 0.5300
k	 0.8350	 0.5700
l	 0.9120	 0.5960
m	 0.8550	 0.5450
n	 0.9090	 0.5820
o	 0.8410	 0.5550
p	 0.9210	 0.5850
q	 0.8510	 0.5700
r	 0.9010	 0.5820
s	 0.8760	 0.5600
t	 0.8250	 0.5170
u	 0.7450	 0.5300
v	 0.3990	 0.2730
w	 0.4220	 0.2690
x	 0.8680	 0.5690
xx	 0.7600	 0.5060
y	 0.7690	 0.4680