



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:53 AM UTC

PDB ID : 6FT6 / pdb_00006ft6
EMDB ID : EMD-4302
Title : Structure of the Nop53 pre-60S particle bound to the exosome nuclear cofactors
Authors : Schuller, J.M.; Falk, S.; Conti, E.
Deposited on : 2018-02-20
Resolution : 3.90 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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

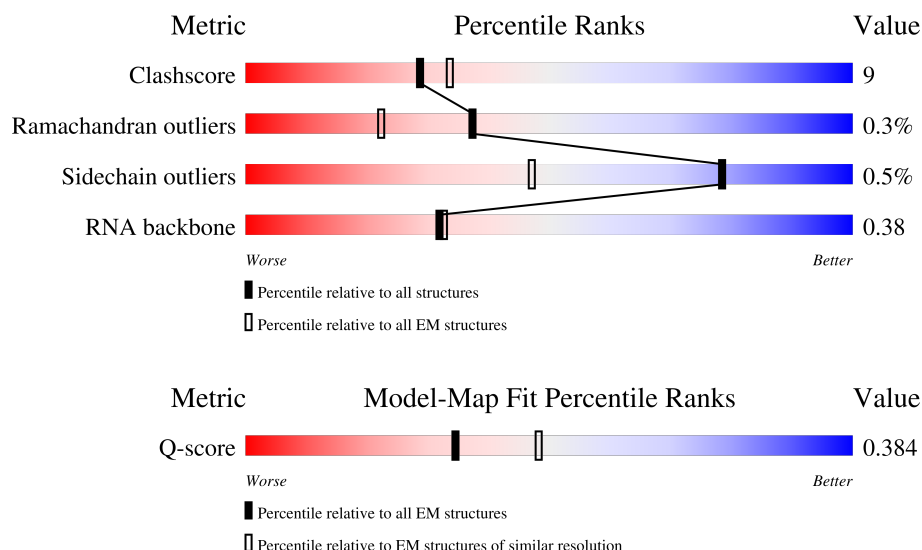
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



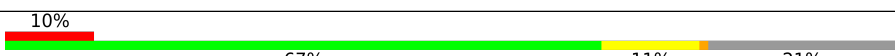
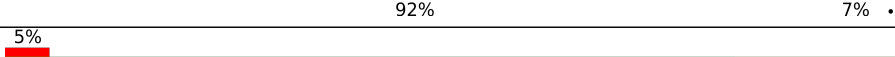
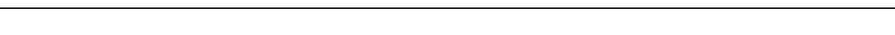
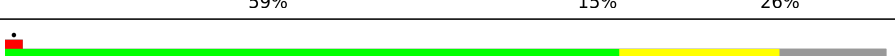
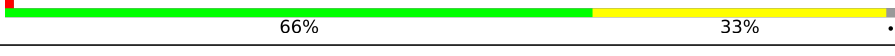
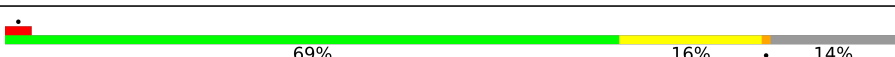
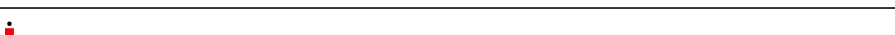
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	2	162	54% 41% 5%
2	A	254	63% 20% 16%
3	B	387	74% 26% .

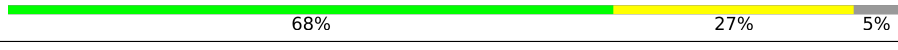
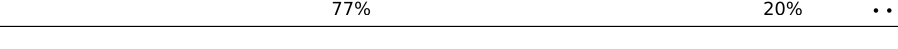
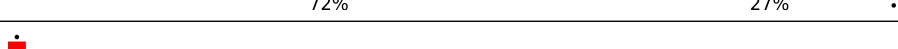
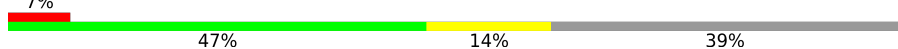
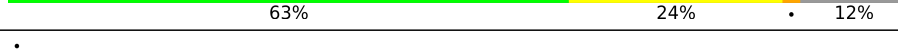
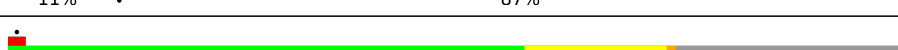
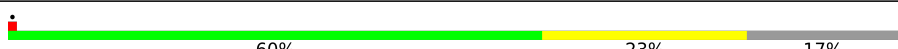
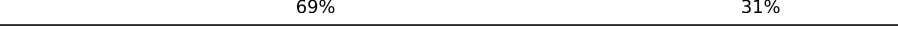
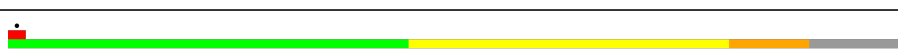
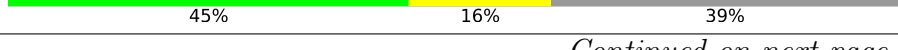
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Mol	Chain	Length	Quality of chain
4	C	362	
5	D	297	
6	E	176	
7	F	244	
8	G	256	
9	H	191	
10	I	166	
11	J	174	
12	L	199	
13	M	138	
14	N	204	
15	O	199	
16	P	184	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	121	
22	V	137	
23	W	236	
24	X	142	
25	Y	127	
26	Z	136	
27	a	149	
28	b	647	

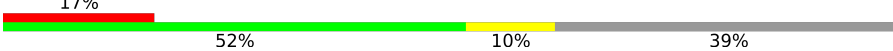
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Mol	Chain	Length	Quality of chain
29	c	105	
30	d	113	
31	e	130	
32	f	107	
33	g	121	
34	h	120	
35	i	100	
36	j	88	
37	k	78	
38	l	51	
39	m	486	
40	n	605	
41	p	92	
42	r	261	
43	s	520	
44	u	199	
45	v	344	
46	w	203	
47	x	515	
48	y	245	
49	z	106	
50	1	3396	
51	3	121	
52	4	593	
53	5	120	

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Mol	Chain	Length	Quality of chain
54	KK	733	 9% 88%
55	LL	184	 17% 52% 10% 39%
56	MM	1011	 23% 71% 26%
57	NN	11	 27% 100%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 157395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 7S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	162	Total	C	N	O	P	0	0
			3441	1540	606	1133	162		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	157	A	-	expression tag	GB 1279395616
2	158	A	-	expression tag	GB 1279395616
2	159	A	-	expression tag	GB 1279395616
2	160	A	-	expression tag	GB 1279395616
2	161	U	-	expression tag	GB 1279395616
2	162	U	-	expression tag	GB 1279395616

- Molecule 2 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 5 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	276	Total	C	N	O	S	0	0
			2211	1397	391	421	2		

- Molecule 6 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 7 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 8 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	233	Total	C	N	O	S	0	0
			1817	1159	326	329	3		

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 10 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 11 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	187	Total	C	N	O	0	0
			1499	934	307	258		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	183	Total	C	N	O	0	0
			1442	896	287	259		

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	119	Total	C	N	O	S	0	0
			943	595	180	165	3		

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	106	Total	C	N	O	S	0	0
			844	545	138	161			

- Molecule 22 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 23 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	122	Total	C	N	O	S	0	0
			977	629	172	174	2		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 26 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	135	Total	C	N	O		
			1092	710	202	180	0	0

- Molecule 27 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	93	Total	C	N	O	S		
			735	479	130	125	1	0	0

- Molecule 28 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	642	Total	C	N	O	S		
			5185	3251	938	970	26	0	0

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	97	Total	C	N	O	S		
			743	479	124	139	1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	107	Total	C	N	O	S		
			873	553	165	154	1	0	0

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	127	Total	C	N	O	S		
			1020	647	205	167	1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	106	Total	C	N	O	S		
			850	540	165	144	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 34 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 36 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 37 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 39 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	469	Total	C	N	O	S	0	0
			3774	2381	685	699	9		

- Molecule 40 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 41 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 42 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 43 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	69	Total	C	N	O	S	0	0
			573	359	113	98	3		

- Molecule 44 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 45 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	287	Total	C	N	O	S	0	0
			2318	1482	408	412	16		

- Molecule 46 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	w	182	Total	C	N	O	S	0	0
			1448	911	261	271	5		

- Molecule 47 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	488	Total	C	N	O	S	0	0
			3807	2398	677	711	21		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 49 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 50 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	3058	Total	C	N	O	P	0	0
			65427	29223	11807	21339	3058		

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 52 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	516	Total	C	N	O	S	0	0
			3999	2530	688	766	15		

- Molecule 53 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			645	395	133	114	3		

- Molecule 54 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	KK	86	Total	C	N	O	S	0	0
			661	411	112	134	4		

- Molecule 55 is a protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LL	113	Total	C	N	O	S	0	0
			894	565	151	174	4		

- Molecule 56 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	MM	977	Total	C	N	O	S	0	0
			7619	4866	1293	1418	42		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MM	1	MET	-	initiating methionine	UNP P47047
MM	2	ASP	-	expression tag	UNP P47047
MM	3	SER	-	expression tag	UNP P47047
MM	4	THR	-	expression tag	UNP P47047
MM	5	ASP	-	expression tag	UNP P47047
MM	6	LEU	-	expression tag	UNP P47047
MM	7	PHE	-	expression tag	UNP P47047
MM	8	ASP	-	expression tag	UNP P47047
MM	9	VAL	-	expression tag	UNP P47047
MM	10	PHE	-	expression tag	UNP P47047
MM	11	GLU	-	expression tag	UNP P47047
MM	12	GLU	-	expression tag	UNP P47047
MM	13	THR	-	expression tag	UNP P47047
MM	14	PRO	-	expression tag	UNP P47047
MM	15	VAL	-	expression tag	UNP P47047
MM	16	GLU	-	expression tag	UNP P47047
MM	17	LEU	-	expression tag	UNP P47047

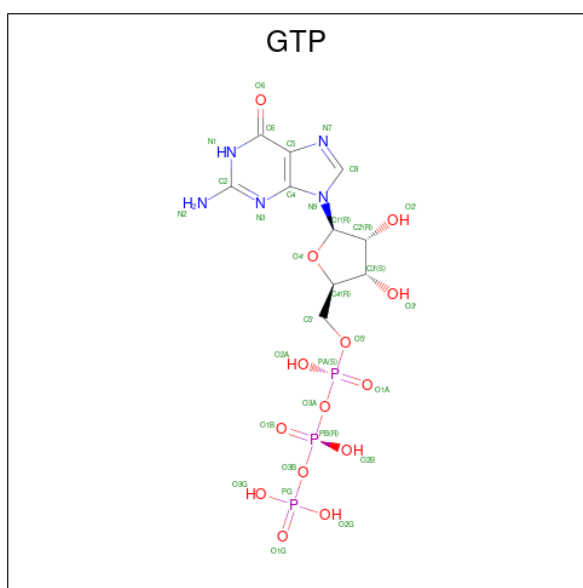
- Molecule 57 is a protein called MPP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	NN	11	Total	C	N	O	0	0
			55	33	11	11		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	I	1	Total	Zn	0
			1	1	
58	j	1	Total	Zn	0
			1	1	
58	p	1	Total	Zn	0
			1	1	
58	u	1	Total	Zn	0
			1	1	

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

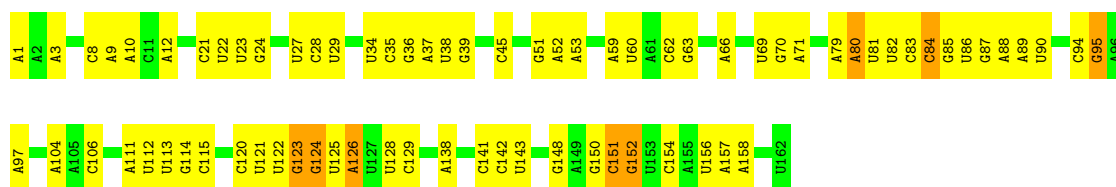


3 Residue-property plots

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.

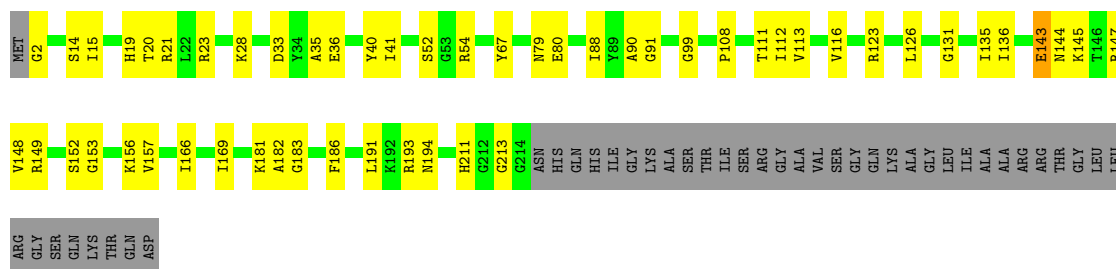
• Molecule 1: 7S ribosomal RNA

Chain 2: 



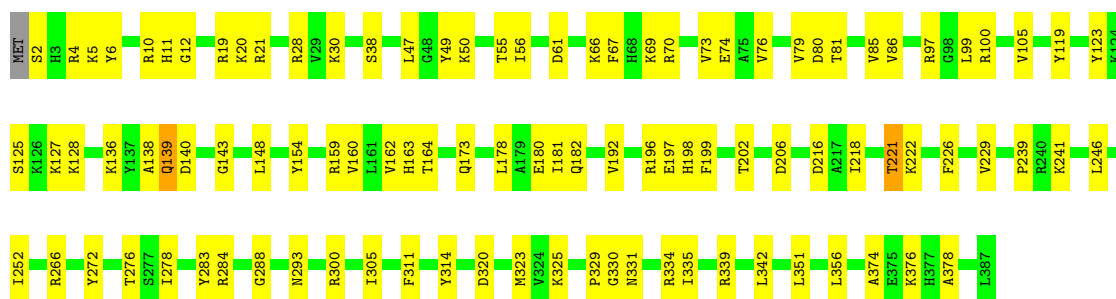
• Molecule 2: 60S ribosomal protein L2-A

Chain A: 



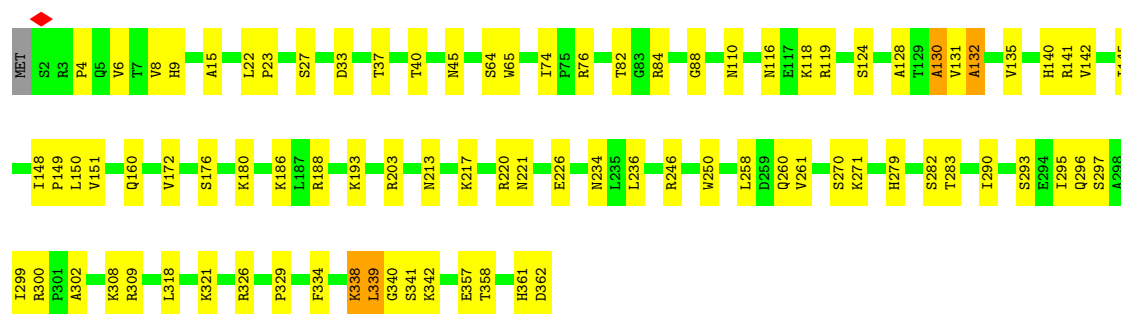
• Molecule 3: 60S ribosomal protein L3

Chain B: 



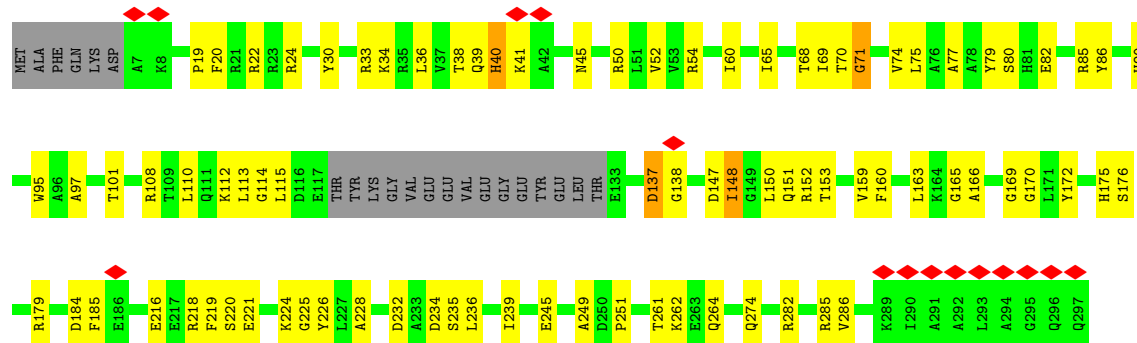
• Molecule 4: 60S ribosomal protein L4-A

Chain C:  76% 23% .



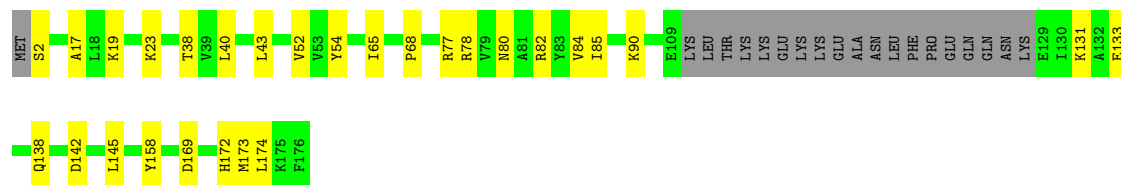
• Molecule 5: 60S ribosomal protein L5

Chain D:  5% 64% 27% 7% .



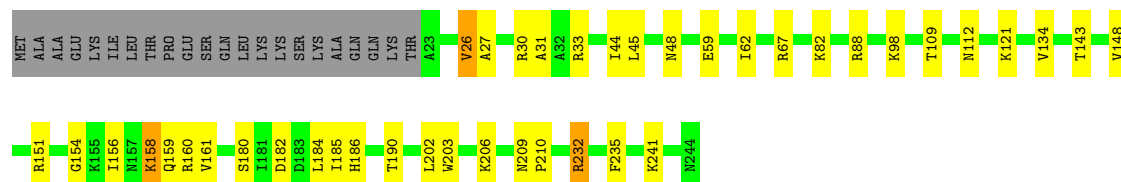
• Molecule 6: 60S ribosomal protein L6-A

Chain E:  73% 16% 11% .



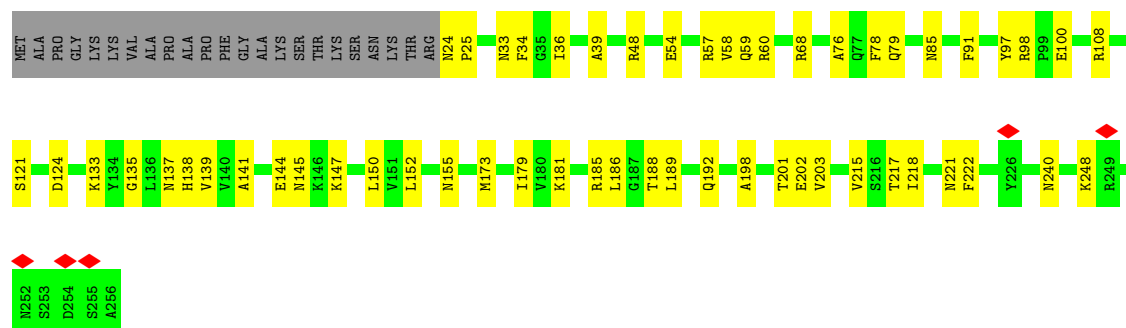
• Molecule 7: 60S ribosomal protein L7-A

Chain F:  74% 16% 9% .

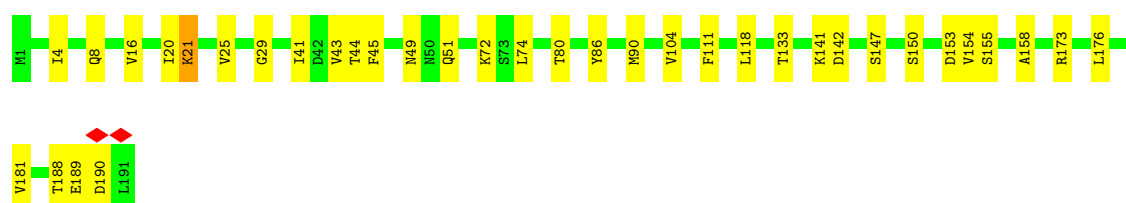
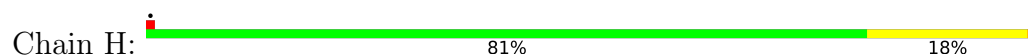


• Molecule 8: 60S ribosomal protein L8-A

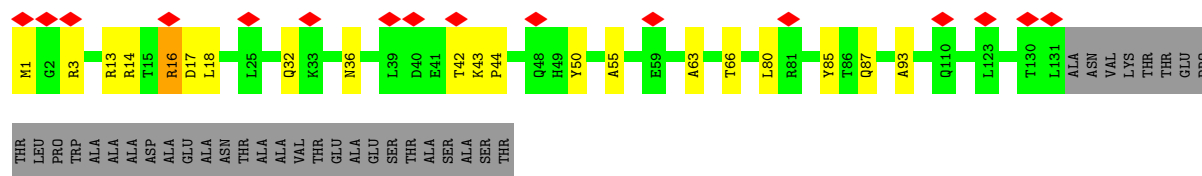
Chain G:  70% 21% 9% .



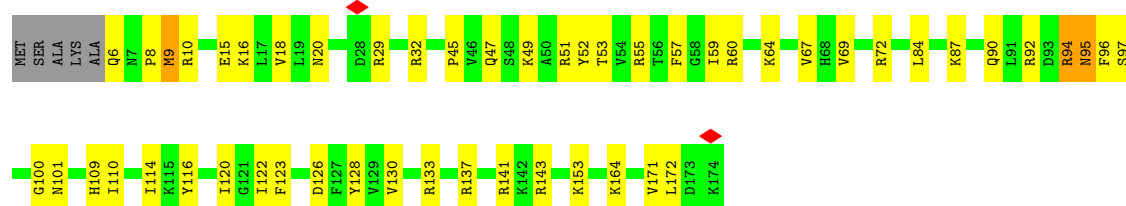
• Molecule 9: 60S ribosomal protein L9-A



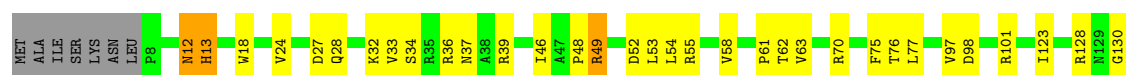
• Molecule 10: Bud site selection protein 20



• Molecule 11: 60S ribosomal protein L11-A



• Molecule 12: 60S ribosomal protein L13-A





- Molecule 13: 60S ribosomal protein L14-A

Chain M: 80% 19%



- Molecule 14: 60S ribosomal protein L15-A

Chain N: 70% 29%



- Molecule 15: 60S ribosomal protein L16-A

Chain O: 92% 7%



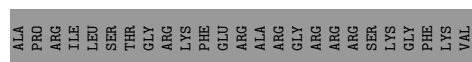
- Molecule 16: 60S ribosomal protein L17-A

Chain P: 5% 82% 18%



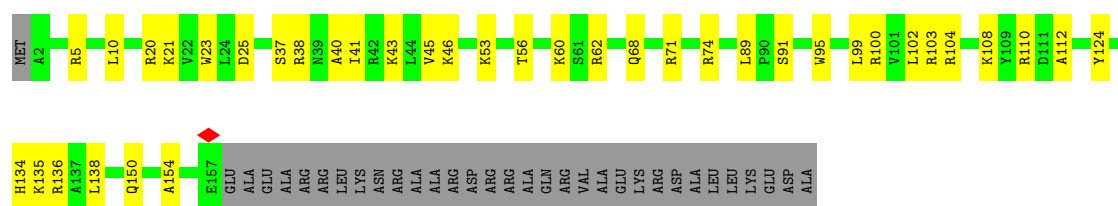
- Molecule 17: 60S ribosomal protein L18-A

Chain Q: 63% 9% 28%



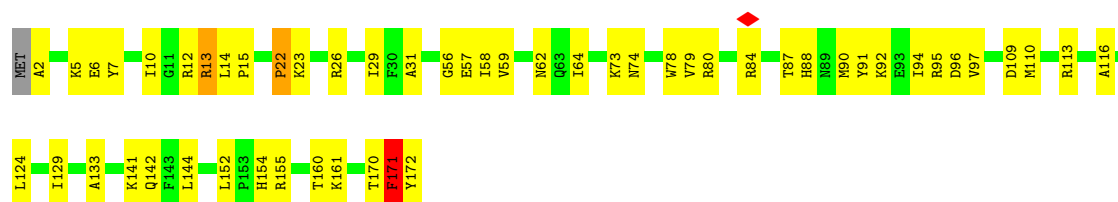
- Molecule 18: 60S ribosomal protein L19-A

Chain R: 



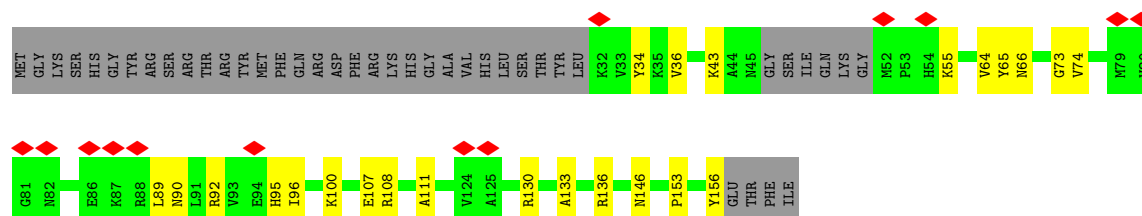
- Molecule 19: 60S ribosomal protein L20-A

Chain S: 



- Molecule 20: 60S ribosomal protein L21-A

Chain T: 



- Molecule 21: 60S ribosomal protein L22-A

Chain U: 



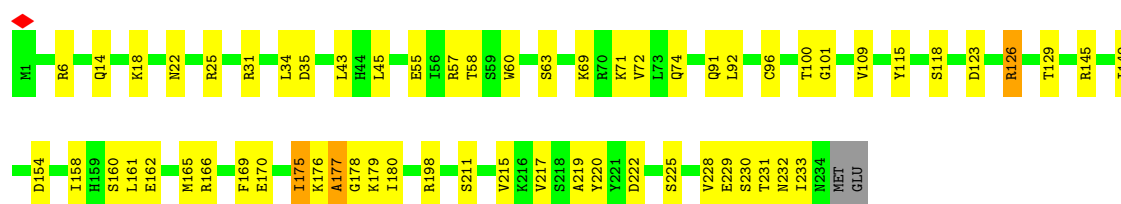
- Molecule 22: 60S ribosomal protein L23-A

Chain V: 



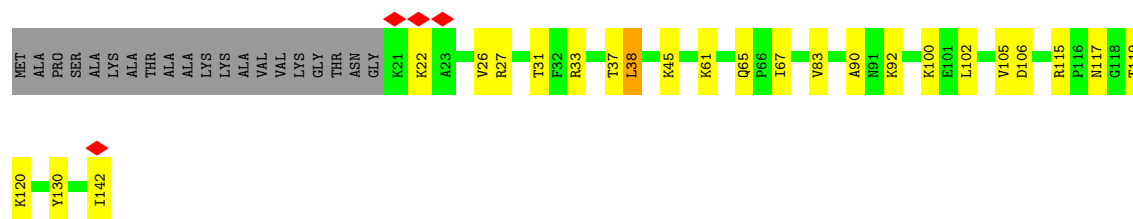
- Molecule 23: Ribosome assembly factor MRT4

Chain W:  73% 25% ..



- Molecule 24: 60S ribosomal protein L25

Chain X:  69% 16% 14%



- Molecule 25: 60S ribosomal protein L26-A

Chain Y:  79% 20%



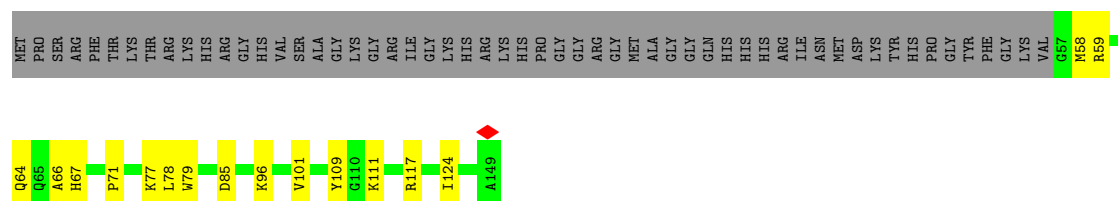
- Molecule 26: 60S ribosomal protein L27-A

Chain Z:  72% 26% ..

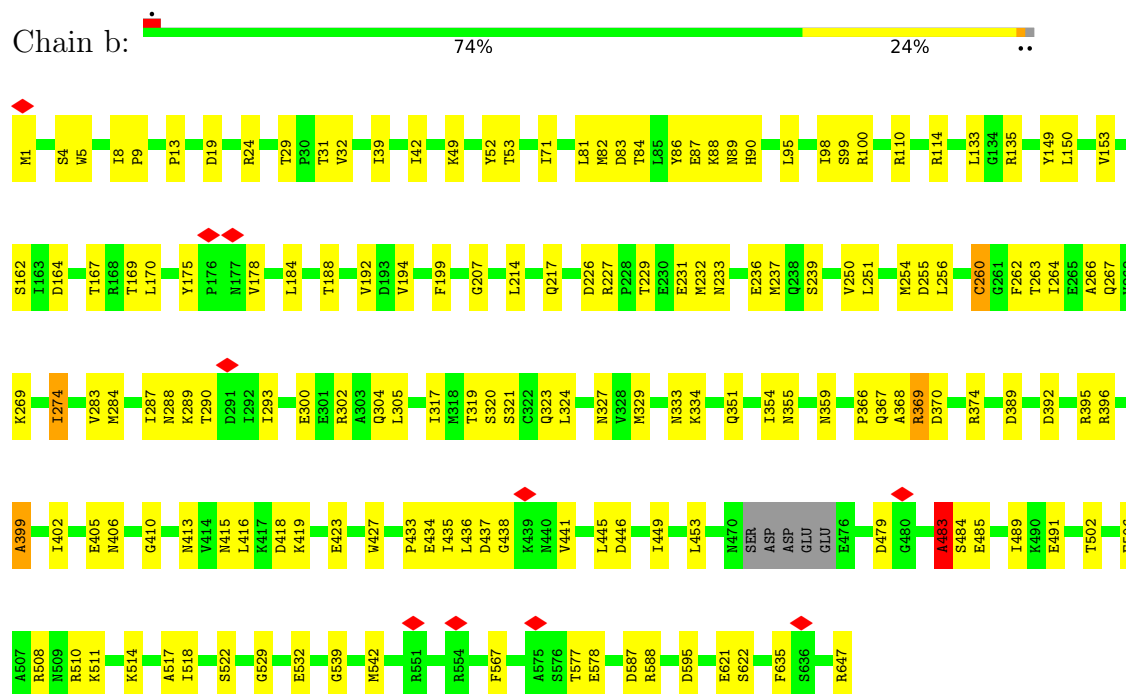


- Molecule 27: 60S ribosomal protein L28

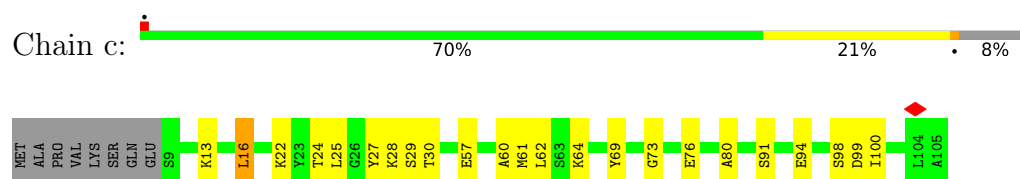
Chain a:  52% 11% 38%



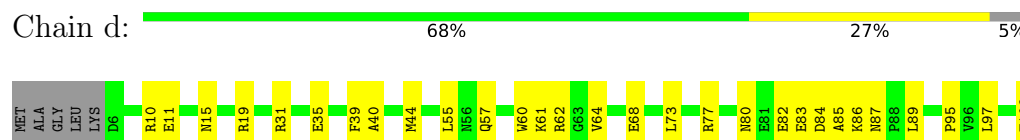
- Molecule 28: Nucleolar GTP-binding protein 1



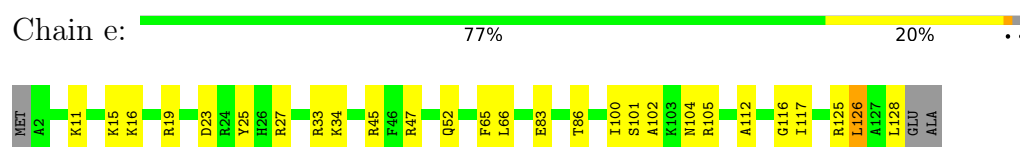
- Molecule 29: 60S ribosomal protein L30



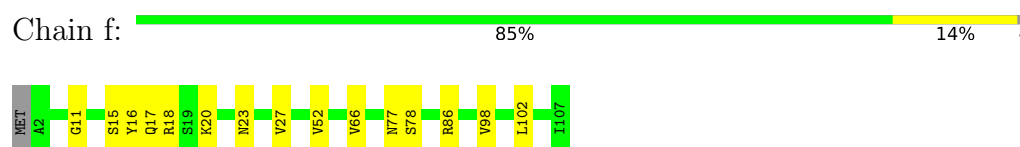
- Molecule 30: 60S ribosomal protein L31-A



- Molecule 31: 60S ribosomal protein L32



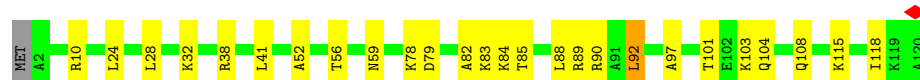
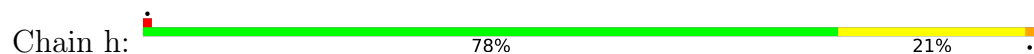
- Molecule 32: 60S ribosomal protein L33-A



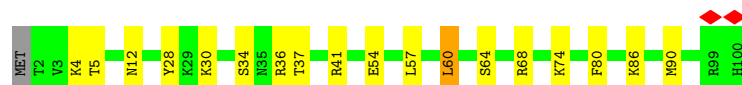
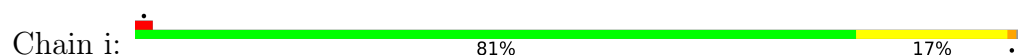
- Molecule 33: 60S ribosomal protein L34-A



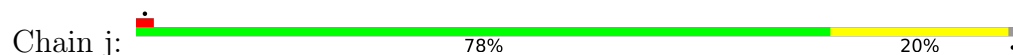
- Molecule 34: 60S ribosomal protein L35-A



- Molecule 35: 60S ribosomal protein L36-A



- Molecule 36: 60S ribosomal protein L37-A



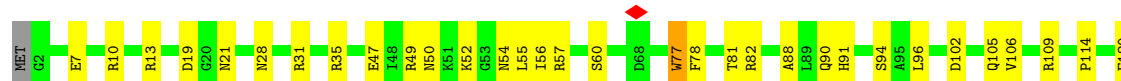
- Molecule 37: 60S ribosomal protein L38

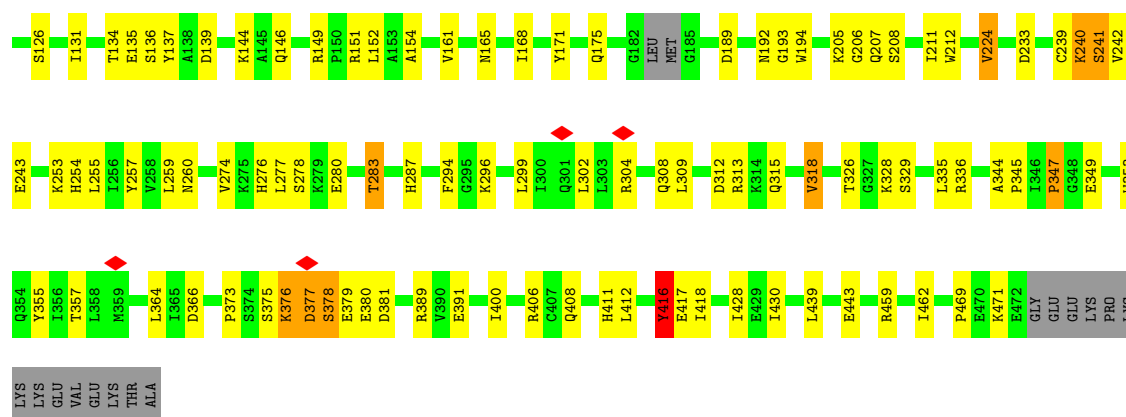


- Molecule 38: 60S ribosomal protein L39

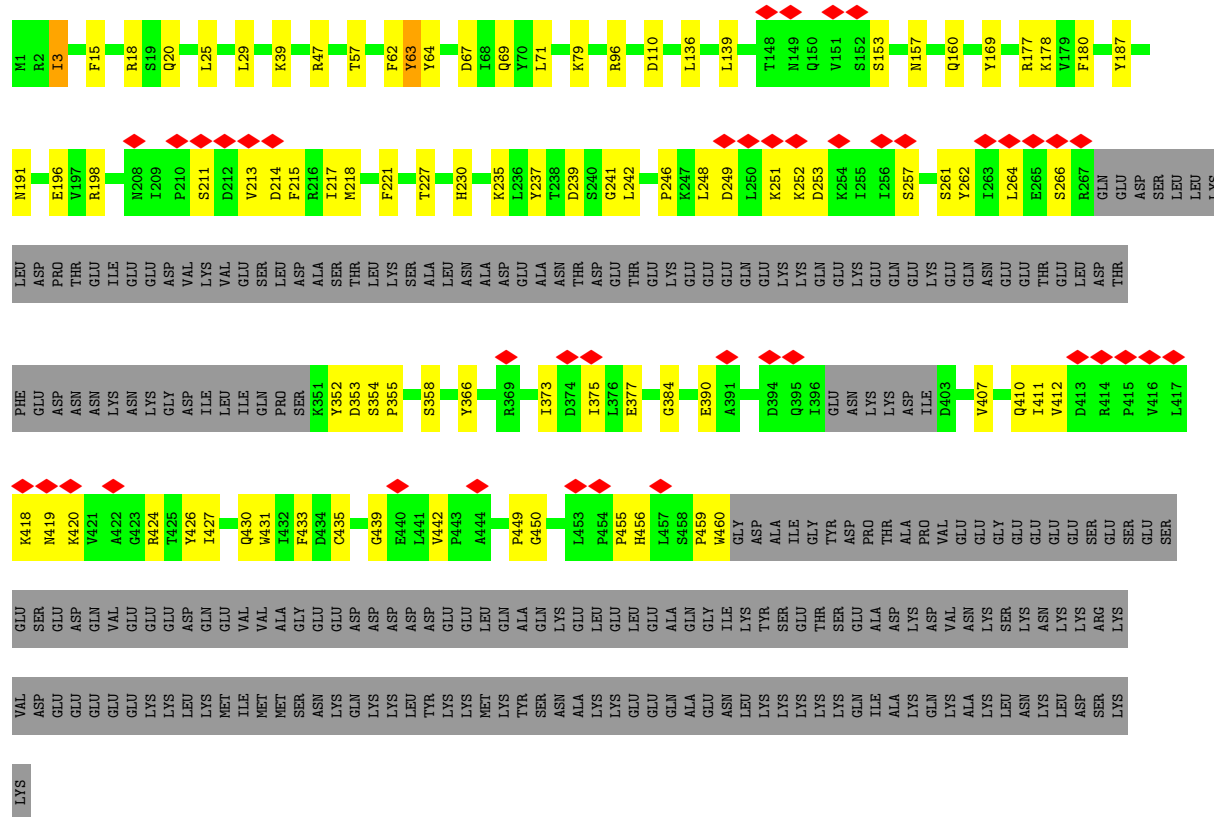


- Molecule 39: Nucleolar GTP-binding protein 2





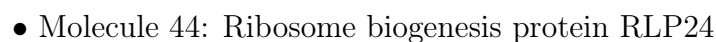
• Molecule 40: Pescadillo homolog



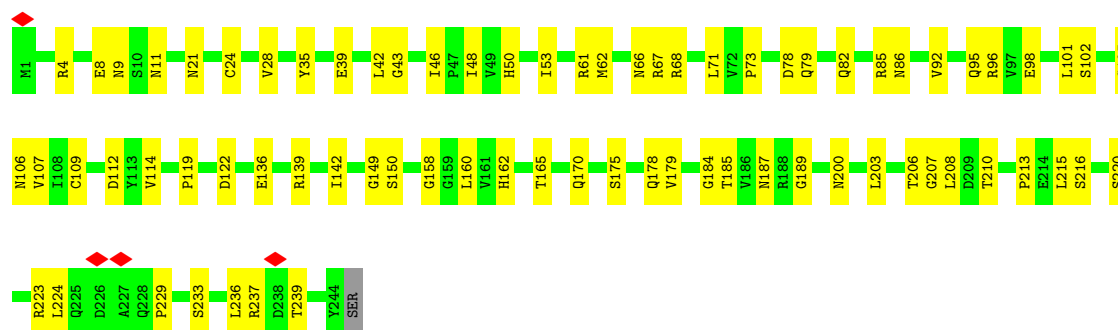
• Molecule 41: 60S ribosomal protein L43-A



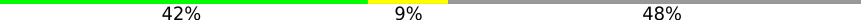
• Molecule 42: Ribosome biogenesis protein NSA2

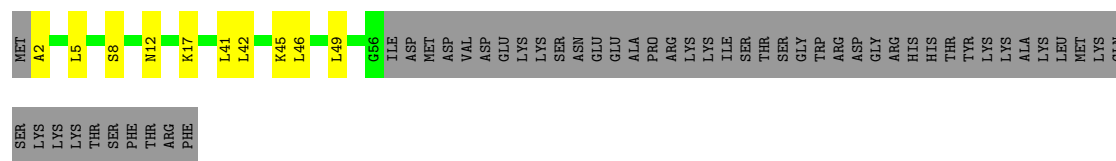


Chain y:  69% 31%

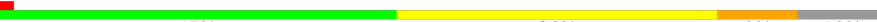


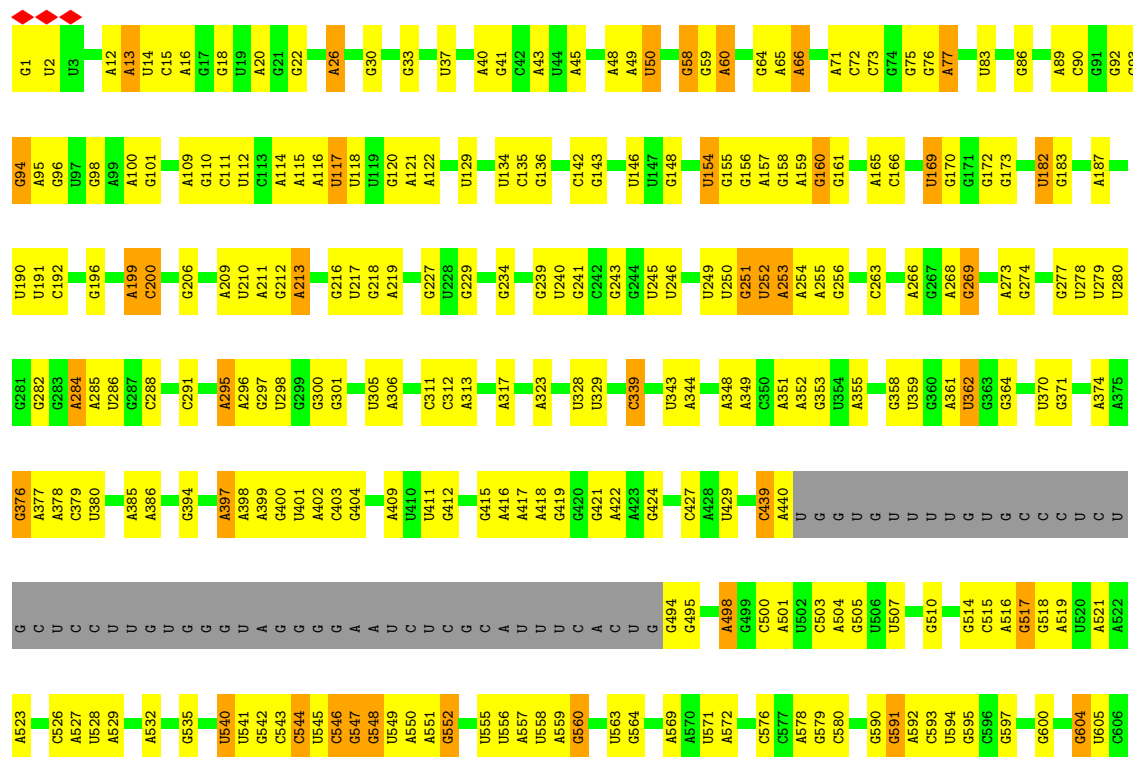
• Molecule 49: UPF0642 protein YBL028C

Chain z:  42% 9% 48%



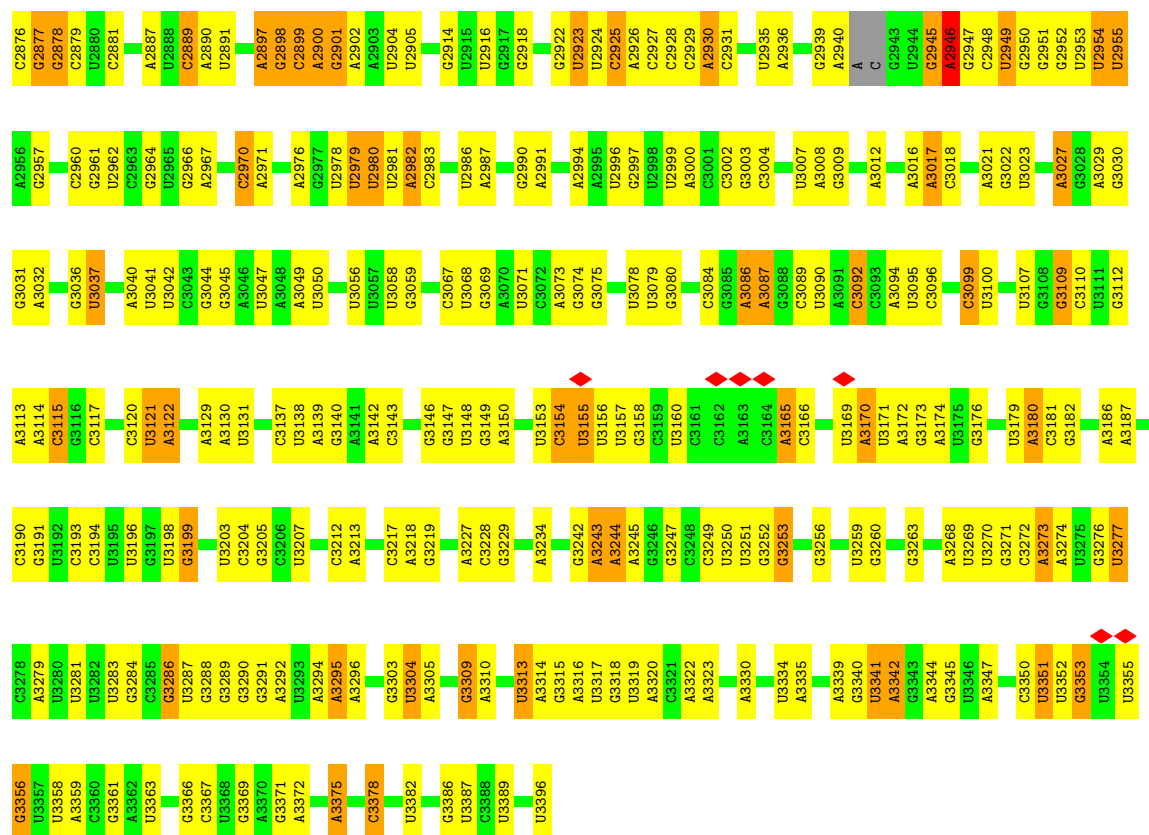
• Molecule 50: 25S ribosomal RNA

Chain 1:  45% 36% 9% 10%

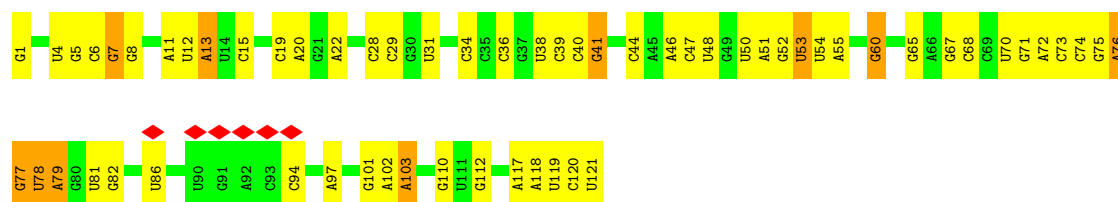


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C1726	U1616	U1523	G1429	U1336	A1263	U1191	U1109	C375	C886	G785	C696	A608
G1727	G1617	U1524	U1430	A1337	G1264	A1192	C1192	U976	G887	A786	C696	G609
A1729	G1618	C1527	C1432	U1340	U1265	A1193	U1111	C977	C890	G787	A705	G610
G1736	U1619	U1536	A1433	U1341	G1266	C1196	G1115	U978	C890	C788	G708	A611
U1737	U1620	G1536	G1434	C1342	A1271	A1197	G1116	A980	A895	U790	G708	U612
G1738	A1621	A1539	A1435	A1343	C1272	A1198	G1117	U981	A896	A791	A709	G613
U1739	U1622	A1539	U1436	G1344	A1273	C1199	G1118	U986	G901	G792	A709	A619
U1740	C1631	G1542	C1437	U1348	C1277	A1200	A1119	U986	A896	C793	A710	U620
A1741	U1627	G1542	U1438	A1349	C1278	C1201	A1120	U986	A896	U797	G714	A622
G1742	U1628	G1547	U1439	A1350	A1278	A1204	U1123	G891	A895	G798	A715	U627
G1743	U1630	C1548	G1440	U1351	C1279	A1205	U1124	A992	A896	C802	A716	A628
G1744	C1631	U1549	G1441	A1352	G1280	G1206	U1125	G993	A896	C803	A717	U629
U1748	G1635	U1553	U1445	U1353	G1282	G1207	U1126	U995	G902	U806	A718	A630
A1749	U1638	U1554	A1446	G1354	A1286	U1211	U1127	U996	G907	A807	A719	U631
U1750	U1638	U1555	G1447	A1355	A1287	A1212	U1128	U997	G908	A808	A720	G632
G1751	C1639	C1556	U1455	U1356	U1288	A1214	A1129	A998	G909	A809	G721	C636
U1760	A1642	A1557	U1455	G1357	U1289	U1214	G1131	G999	A914	G802	G722	C637
C1761	A1643	U1560	A1461	G1362	U1293	A1217	C1132	C1000	A915	C802	A716	U632
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U1763	U1645	C1562	A1468	G1367	G1295	C1219	A1136	A1002	A917	U802	A718	U634
U1764	C1657	U1564	G1469	U1367	C1296	U1220	G1137	A1003	A920	C803	A719	U635
G1766	C1657	G1565	U1470	G1370	C1297	A1221	U1138	U	C923	A806	A720	G632
U1770	C1660	U1566	U1471	U1378	U1298	G1222	U1139	G	G924	A807	G721	C636
C1771	G1661	U1567	A1474	U1379	U1299	C1227	G1142	U	C928	A808	G722	C637
U1772	C1665	U1569	A1475	G1380	A1301	G1230	U1143	G	A929	G815	G727	U642
G1775	C1671	U1570	G1476	A1381	A1302	A1231	U1144	A	U932	G816	G728	U643
U1778	G1675	U1571	U1480	C1385	A1303	G1232	G1145	U	U933	A817	C729	U644
C1779	A1676	C1574	A1481	A1386	A1304	G1233	U1146	C	U934	U829	A741	A645
G1780	C1680	A1575	A1482	G1387	U1305	G1234	G1147	U	A935	A830	G742	A646
U1781	U1681	U1575	U1483	U1388	G1306	U1235	U1148	U	U936	G833	G743	A647
A1782	U1682	U1575	A1484	U1389	A1307	U1236	U1149	C	A936	U825	A744	C648
U1797	A1683	C1582	G1487	G1391	U1308	U1237	U1150	U	A937	G826	G745	A649
G1808	U1687	A1583	A1491	A1393	U1309	C1239	U1151	C	C938	U827	A746	C650
A1809	U1688	U1589	G1492	A1399	G1310	U1240	G1152	G	U939	G845	A751	A650
G1811	U1699	A1593	U1494	G1400	G1313	U1241	A1153	G	G940	A848	G754	A655
A1812	G1700	C1596	C1497	A1404	C1313	G1242	C1155	U	U943	C849	A761	U871
A1813	G1712	G1597	A1498	G1417	A1317	G1243	A1159	C	C944	U850	U762	A672
U1814	U1716	G1598	A1503	A1418	A1318	A1244	C1160	G	C945	U857	G763	U673
A1815	U1717	A1603	C1505	C1420	G1319	G1245	U1167	A	U946	G857	C765	G674
G1817	U1718	U1606	G1506	G1421	C1320	U1247	A1093	A	A951	G860	U766	C675
U1820	G1719	G1607	A1507	G1422	U1321	C1248	U1094	U	A952	C861	C768	G676
U1821	U1720	C1608	G1508	C1423	U1322	G1249	U1095	G	G953	U874	A771	U679
A1828	U1721	G1609	U1425	U1426	U1323	A1250	U1096	C	U956	A875	U776	G680
G1830	U1724	G1610	G1513	U1427	U1324	A1251	G1178	C	C957	G875	U777	G681
					A1325	A1252	A1179	U	U958	C877	U778	G686
					A1326	A1253	A1180	U	C959	G878	G779	U687
					U1329	A1254	A1181	U	G971	U879	A780	A690
					A1330	C1254	A1182	C	A972	G880	G781	A691
					U1331	U1258	G1186	A	A973	C881	A781	A691
					U1334	A1260	C1189	U		U874	A782	A691
						G1261		C		A875	A783	A691
										C877	A784	A691
										G878	A785	A691
										U879	A786	A691
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										C881	A788	A691
										U874	A789	A691
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										U879	A793	A691
										G880	A794	A691
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										U874	A817	A691
										A875	A818	A691
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										C877	A826	A691
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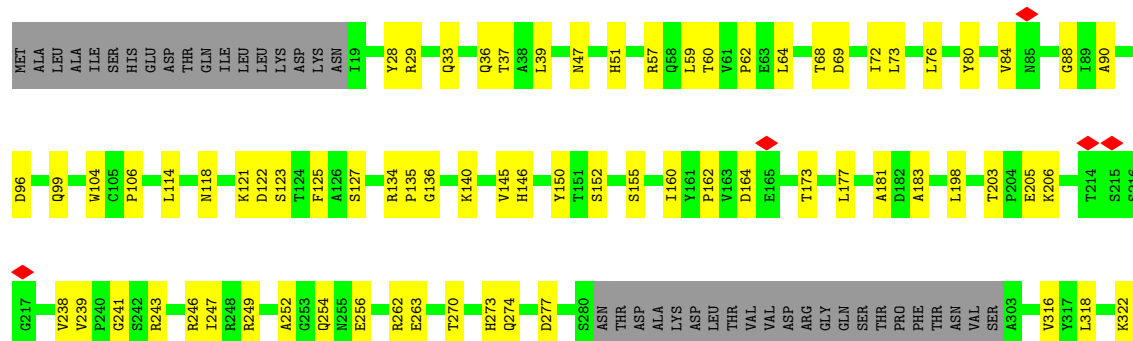




• Molecule 51: 5S ribosomal RNA

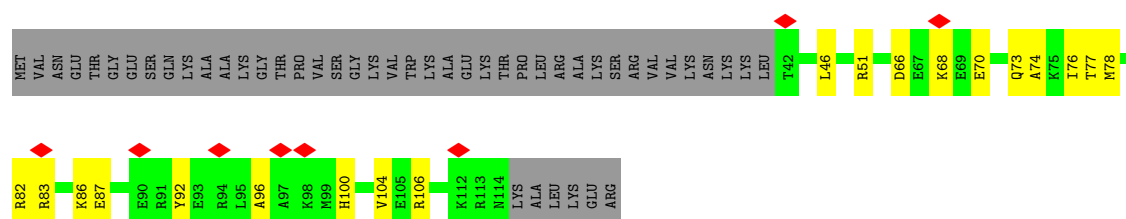
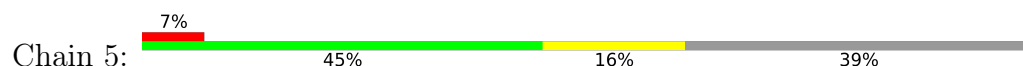


• Molecule 52: Probable metalloprotease ARX1

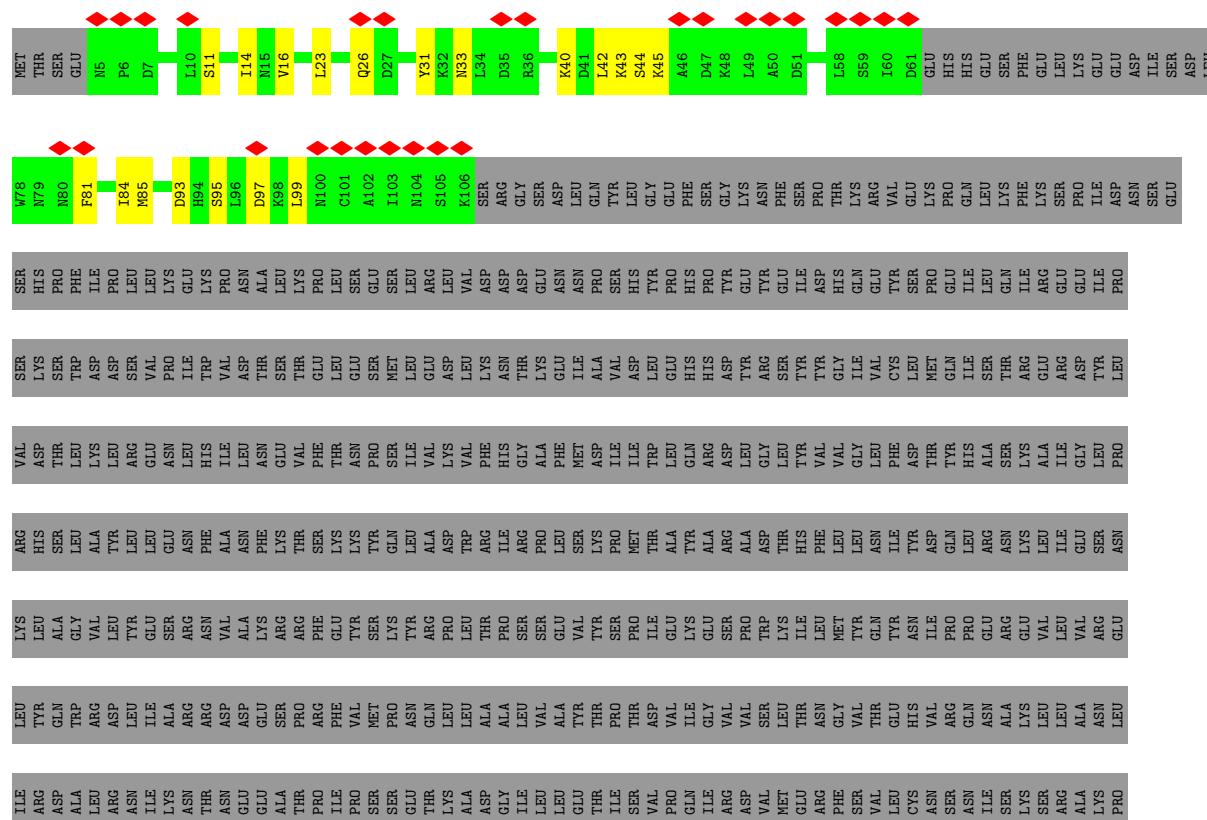


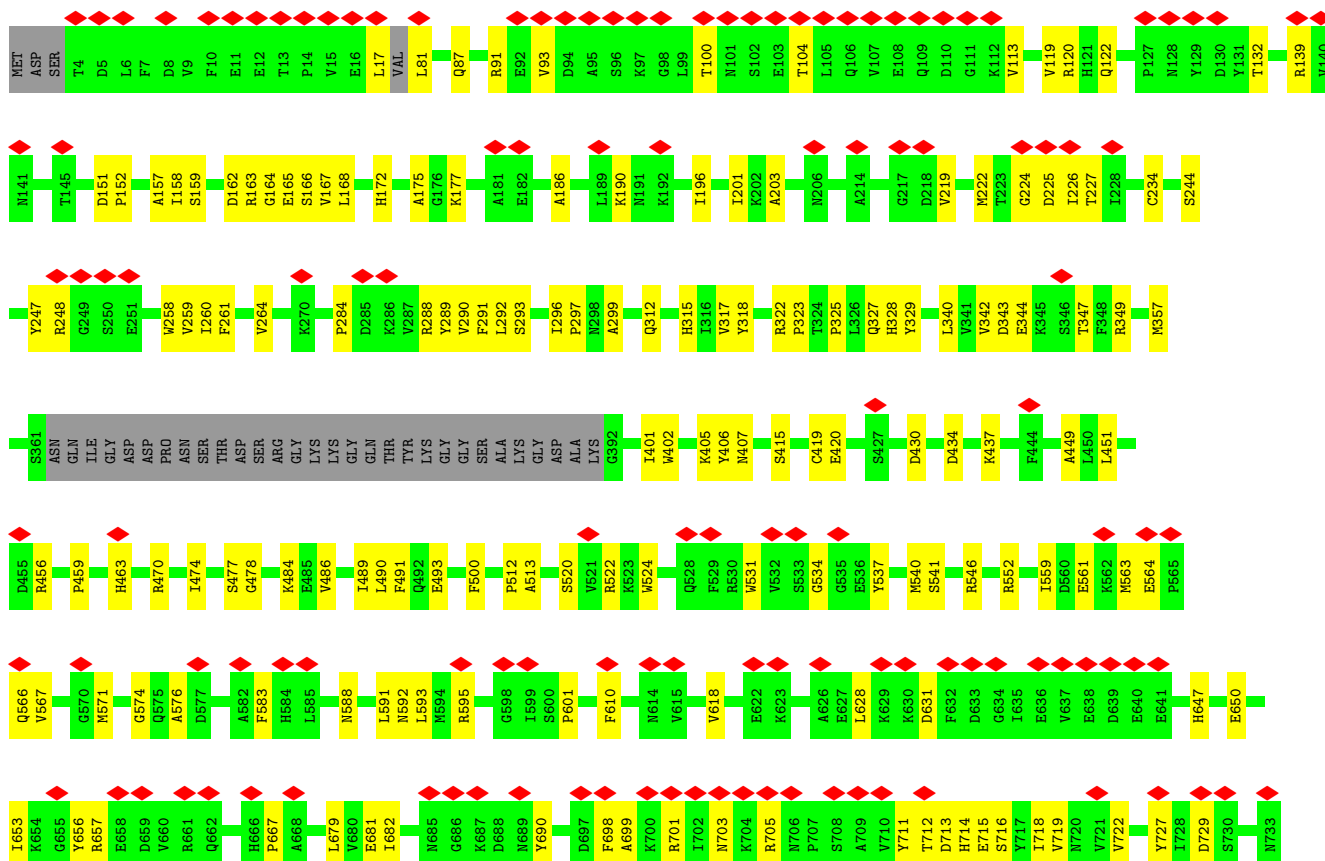


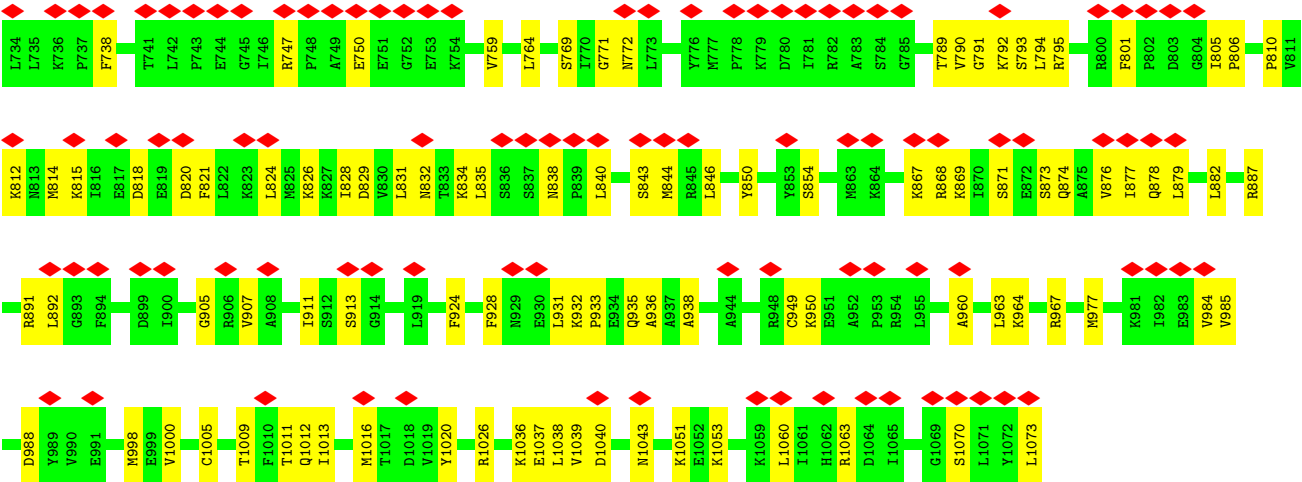
- Molecule 53: rRNA-processing protein CGR1



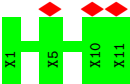
- Molecule 54: Exosome complex exonuclease RRP6







• Molecule 57: MPP6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, GTP

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	2	0.70	0/3846	0.51	0/5988
2	A	0.64	0/1666	0.74	0/2241
3	B	0.70	2/3152 (0.1%)	0.88	3/4239 (0.1%)
4	C	0.63	0/2801	0.83	2/3792 (0.1%)
5	D	0.49	1/2257 (0.0%)	0.75	2/3043 (0.1%)
6	E	0.54	0/1260	0.69	0/1694
7	F	0.63	0/1821	0.79	1/2451 (0.0%)
8	G	0.63	1/1849 (0.1%)	0.81	2/2495 (0.1%)
9	H	0.61	0/1539	0.85	2/2073 (0.1%)
10	I	0.40	0/1075	0.75	2/1443 (0.1%)
11	J	0.37	0/1374	0.82	1/1842 (0.1%)
12	L	0.62	1/1524 (0.1%)	0.85	2/2046 (0.1%)
13	M	0.58	0/1074	0.74	0/1446
14	N	0.70	0/1757	0.82	1/2354 (0.0%)
15	O	0.67	0/1585	0.78	2/2128 (0.1%)
16	P	0.61	0/1465	0.73	0/1968
17	Q	0.61	0/1050	0.73	0/1419
18	R	0.63	0/1275	0.78	0/1702
19	S	0.61	0/1473	0.82	4/1980 (0.2%)
20	T	0.40	0/957	0.82	2/1285 (0.2%)
21	U	0.53	0/861	0.79	3/1167 (0.3%)
22	V	0.70	0/1018	0.82	0/1369
23	W	0.55	0/1918	0.81	3/2586 (0.1%)
24	X	0.63	0/992	0.73	0/1336
25	Y	0.62	0/1004	0.77	0/1341
26	Z	0.58	0/1118	0.79	2/1497 (0.1%)
27	a	0.62	0/751	0.80	1/1013 (0.1%)
28	b	0.56	0/5270	0.81	4/7080 (0.1%)
29	c	0.61	0/751	0.67	0/1008
30	d	0.61	0/887	0.74	0/1191
31	e	0.59	0/1041	0.72	0/1394
32	f	0.73	1/868 (0.1%)	0.73	0/1168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.63	0/891	0.77	0/1191
34	h	0.64	0/978	0.85	1/1301 (0.1%)
35	i	0.56	0/778	0.82	1/1034 (0.1%)
36	j	0.69	0/696	0.85	0/923
37	k	0.56	0/618	0.71	0/826
38	l	0.72	0/443	0.83	0/588
39	m	0.60	0/3848	0.88	10/5181 (0.2%)
40	n	0.50	0/3101	0.84	3/4187 (0.1%)
41	p	0.62	0/701	0.88	0/934
42	r	0.64	0/1892	0.92	5/2528 (0.2%)
43	s	0.51	0/577	0.73	0/752
44	u	0.48	0/1287	0.77	0/1711
45	v	0.50	0/2361	0.70	1/3153 (0.0%)
46	w	0.48	0/1471	0.75	0/1980
47	x	0.54	1/3897 (0.0%)	0.74	4/5282 (0.1%)
48	y	0.59	0/1872	0.75	0/2548
49	z	0.56	0/445	0.62	0/585
50	1	0.66	0/73234	0.56	20/114167 (0.0%)
51	3	0.44	0/2883	0.49	0/4491
52	4	0.49	0/4069	0.76	0/5520
53	5	0.40	0/649	0.66	0/848
54	KK	0.22	0/667	0.53	0/899
55	LL	0.28	0/903	0.55	0/1210
56	MM	0.30	0/7765	0.62	0/10511
All	All	0.61	7/167305 (0.0%)	0.67	84/242129 (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
2	A	0	1
3	B	0	3
4	C	0	3
5	D	0	4
7	F	0	2
8	G	0	2
9	H	0	1
10	I	0	1
11	J	0	1
12	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	2
19	S	0	3
23	W	0	2
26	Z	0	3
27	a	0	1
28	b	0	15
30	d	0	1
34	h	0	1
37	k	0	2
38	l	0	1
39	m	0	8
40	n	0	3
42	r	0	4
43	s	0	1
44	u	0	3
47	x	0	4
48	y	0	1
52	4	0	2
56	MM	0	1
All	All	0	78

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	102	LEU	C-N	-9.45	1.14	1.33
3	B	197	GLU	CA-C	-7.87	1.41	1.52
8	G	33	ASN	CA-CB	-7.12	1.43	1.52
5	D	179	ARG	CA-C	-7.06	1.42	1.52
47	x	129	VAL	C-N	-6.86	1.22	1.33
3	B	123	TYR	CA-C	-5.86	1.44	1.52
12	L	13	HIS	CA-CB	-5.75	1.39	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	m	377	ASP	N-CA-C	9.04	130.05	110.80
20	T	153	PRO	CA-C-N	8.04	125.31	120.24
20	T	153	PRO	C-N-CA	8.04	125.31	120.24
9	H	188	THR	CA-C-N	7.87	135.86	121.70
9	H	188	THR	C-N-CA	7.87	135.86	121.70
35	i	28	TYR	N-CA-C	-7.78	104.94	114.75
3	B	97	ARG	N-CA-C	-7.24	105.62	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	2528	G	O4'-C1'-N9	6.70	118.24	108.20
19	S	13	ARG	CA-C-N	6.63	137.98	121.80
19	S	13	ARG	C-N-CA	6.63	137.98	121.80
39	m	283	THR	N-CA-C	6.58	118.60	110.91
26	Z	102	GLU	CA-C-N	6.50	137.66	121.80
26	Z	102	GLU	C-N-CA	6.50	137.66	121.80
39	m	206	GLY	CA-C-N	6.29	133.03	121.70
39	m	206	GLY	C-N-CA	6.29	133.03	121.70
42	r	16	LYS	CA-C-N	6.27	133.51	121.54
42	r	16	LYS	C-N-CA	6.27	133.51	121.54
42	r	162	THR	CA-C-N	6.25	130.62	121.31
42	r	162	THR	C-N-CA	6.25	130.62	121.31
8	G	145	ASN	CA-C-N	6.22	132.89	121.70
8	G	145	ASN	C-N-CA	6.22	132.89	121.70
50	1	2728	G	P-O3'-C3'	6.03	129.24	120.20
40	n	39	LYS	CA-C-N	5.96	132.43	121.70
40	n	39	LYS	C-N-CA	5.96	132.43	121.70
19	S	171	PHE	CA-C-N	5.93	132.38	121.70
19	S	171	PHE	C-N-CA	5.93	132.38	121.70
14	N	184	LYS	N-CA-C	-5.91	105.32	113.18
50	1	1307	G	C2'-C3'-O3'	5.91	118.36	109.50
39	m	52	LYS	CA-C-N	5.90	132.32	121.70
39	m	52	LYS	C-N-CA	5.90	132.32	121.70
27	a	66	ALA	N-CA-C	-5.86	107.12	114.56
47	x	129	VAL	CA-C-N	5.85	128.79	120.49
47	x	129	VAL	C-N-CA	5.85	128.79	120.49
28	b	436	LEU	N-CA-C	-5.78	101.46	110.42
23	W	176	LYS	CA-C-N	5.75	130.53	121.56
23	W	176	LYS	C-N-CA	5.75	130.53	121.56
50	1	1716	U	C2'-C3'-O3'	5.74	118.11	109.50
21	U	60	GLY	N-CA-C	-5.73	107.66	114.48
3	B	351	LEU	N-CA-C	-5.72	108.10	114.62
50	1	284	A	P-O3'-C3'	5.64	128.67	120.20
10	I	42	THR	CA-C-N	5.56	128.58	120.51
10	I	42	THR	C-N-CA	5.56	128.58	120.51
50	1	2954	U	P-O3'-C3'	5.56	128.53	120.20
12	L	130	GLY	CA-C-N	5.56	128.04	120.54
12	L	130	GLY	C-N-CA	5.56	128.04	120.54
50	1	2866	U	P-O3'-C3'	5.52	128.48	120.20
28	b	406	ASN	CA-C-N	5.49	131.58	121.70
28	b	406	ASN	C-N-CA	5.49	131.58	121.70
50	1	1241	U	C2'-C3'-O3'	5.49	117.73	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	v	285	LEU	CA-CB-CG	5.45	135.36	116.30
50	1	1581	C	P-O3'-C3'	5.40	128.30	120.20
28	b	274	ILE	CB-CA-C	5.39	120.43	111.37
50	1	1307	G	P-O3'-C3'	5.38	128.26	120.20
39	m	77	TRP	CA-C-N	5.37	131.79	121.54
39	m	77	TRP	C-N-CA	5.37	131.79	121.54
50	1	2658	G	P-O3'-C3'	5.36	128.24	120.20
50	1	2861	U	C2-N1-C1'	5.35	133.76	117.70
50	1	649	A	C2'-C3'-O3'	5.33	121.69	113.70
50	1	2946	A	C2'-C3'-O3'	5.32	117.48	109.50
15	O	107	GLY	CA-C-N	-5.30	117.42	123.25
15	O	107	GLY	C-N-CA	-5.30	117.42	123.25
34	h	97	ALA	N-CA-C	-5.30	106.50	113.12
50	1	1568	U	P-O3'-C3'	5.30	128.15	120.20
39	m	416	TYR	CA-C-N	5.29	131.22	121.70
39	m	416	TYR	C-N-CA	5.29	131.22	121.70
40	n	63	TYR	N-CA-C	5.29	120.53	112.54
50	1	2801	A	C2'-C3'-O3'	5.29	117.43	109.50
11	J	9	MET	N-CA-C	-5.27	108.11	114.75
50	1	1570	U	P-O3'-C3'	5.22	128.03	120.20
7	F	26	VAL	N-CA-C	5.21	115.36	110.30
3	B	38	SER	N-CA-C	-5.21	107.95	114.56
50	1	2728	G	O4'-C1'-N9	5.20	116.00	108.20
5	D	40	HIS	CA-C-N	5.18	131.02	121.70
5	D	40	HIS	C-N-CA	5.18	131.02	121.70
50	1	2537	U	P-O3'-C3'	5.17	127.95	120.20
4	C	130	ALA	CA-C-N	5.16	131.25	121.97
4	C	130	ALA	C-N-CA	5.16	131.25	121.97
47	x	27	LYS	CA-C-N	5.15	130.97	121.70
47	x	27	LYS	C-N-CA	5.15	130.97	121.70
23	W	176	LYS	N-CA-C	-5.14	103.75	110.53
50	1	1716	U	P-O3'-C3'	5.06	127.79	120.20
21	U	51	GLY	CA-C-N	5.05	130.49	122.61
21	U	51	GLY	C-N-CA	5.05	130.49	122.61
42	r	162	THR	CA-CB-CG2	5.01	119.01	110.50

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	4	104	TRP	Peptide
52	4	379	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	A	143	GLU	Peptide
3	B	138	ALA	Peptide
3	B	139	GLN	Peptide
3	B	221	THR	Peptide
4	C	132	ALA	Peptide
4	C	318	LEU	Peptide
4	C	338	LYS	Peptide
5	D	137	ASP	Peptide
5	D	251	PRO	Peptide
5	D	40	HIS	Peptide
5	D	71	GLY	Peptide
7	F	158	LYS	Peptide
7	F	232	ARG	Peptide
8	G	76	ALA	Peptide
8	G	79	GLN	Peptide
9	H	21	LYS	Peptide
10	I	16	ARG	Peptide
11	J	94	ARG	Peptide
12	L	49	ARG	Peptide
12	L	76	THR	Peptide
56	MM	1063	ARG	Peptide
16	P	156	ALA	Peptide
16	P	9	THR	Peptide
19	S	12	ARG	Peptide
19	S	171	PHE	Peptide
19	S	22	PRO	Peptide
23	W	175	ILE	Peptide
23	W	177	ALA	Peptide
26	Z	101	PHE	Peptide
26	Z	102	GLU	Peptide
26	Z	58	GLY	Peptide
27	a	96	LYS	Peptide
28	b	13	PRO	Peptide
28	b	226	ASP	Peptide
28	b	260	CYS	Peptide
28	b	367	GLN	Peptide
28	b	368	ALA	Peptide
28	b	369	ARG	Mainchain,Peptide
28	b	399	ALA	Peptide
28	b	435	ILE	Peptide
28	b	437	ASP	Peptide
28	b	438	GLY	Peptide

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Mol	Chain	Res	Type	Group
28	b	446	ASP	Peptide
28	b	483	ALA	Peptide
28	b	635	PHE	Peptide
28	b	8	ILE	Peptide
30	d	86	LYS	Peptide
34	h	83	LYS	Peptide
37	k	33	LYS	Peptide
37	k	34	ALA	Peptide
38	l	4	GLN	Peptide
39	m	154	ALA	Peptide
39	m	240	LYS	Peptide
39	m	253	LYS	Peptide
39	m	376	LYS	Peptide
39	m	377	ASP	Peptide
39	m	378	SER	Peptide
39	m	416	TYR	Peptide
39	m	77	TRP	Peptide
40	n	3	ILE	Peptide
40	n	354	SER	Peptide
40	n	375	ILE	Peptide
42	r	145	LYS	Peptide
42	r	15	GLY	Peptide
42	r	16	LYS	Peptide
42	r	205	GLN	Peptide
43	s	2	ARG	Peptide
44	u	2	ARG	Peptide
44	u	78	PRO	Peptide
44	u	79	VAL	Peptide
47	x	20	ARG	Peptide
47	x	208	ASN	Peptide
47	x	25	ILE	Peptide
47	x	29	LEU	Peptide
48	y	8	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	3441	0	1739	41	0
2	A	1634	0	1685	42	0
3	B	3081	0	3165	68	0
4	C	2749	0	2863	55	0
5	D	2211	0	2175	62	0
6	E	1239	0	1326	19	0
7	F	1784	0	1862	28	0
8	G	1817	0	1908	33	0
9	H	1518	0	1587	23	0
10	I	1059	0	1089	13	0
11	J	1353	0	1383	36	0
12	L	1499	0	1558	31	0
13	M	1059	0	1154	16	0
14	N	1720	0	1779	46	0
15	O	1555	0	1659	11	0
16	P	1442	0	1485	25	0
17	Q	1035	0	1115	14	0
18	R	1258	0	1342	30	0
19	S	1437	0	1475	36	0
20	T	943	0	994	22	0
21	U	844	0	855	13	0
22	V	1003	0	1048	35	0
23	W	1885	0	1921	40	0
24	X	977	0	1049	19	0
25	Y	993	0	1081	19	0
26	Z	1092	0	1155	23	0
27	a	735	0	776	12	0
28	b	5185	0	5250	115	0
29	c	743	0	797	13	0
30	d	873	0	914	19	0
31	e	1020	0	1090	21	0
32	f	850	0	880	9	0
33	g	881	0	945	23	0
34	h	969	0	1078	24	0
35	i	771	0	849	13	0
36	j	681	0	683	15	0
37	k	612	0	682	12	0
38	l	436	0	475	17	0
39	m	3774	0	3835	97	0
40	n	3030	0	3107	55	0
41	p	694	0	735	17	0
42	r	1860	0	1965	53	0
43	s	573	0	643	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	u	1265	0	1314	25	0
45	v	2318	0	2398	54	0
46	w	1448	0	1510	36	0
47	x	3807	0	3790	77	0
48	y	1849	0	1836	54	0
49	z	444	0	478	7	0
50	1	65427	0	32879	760	0
51	3	2579	0	1304	44	0
52	4	3999	0	4088	89	0
53	5	645	0	688	17	0
54	KK	661	0	645	16	0
55	LL	894	0	917	14	0
56	MM	7619	0	7512	157	0
57	NN	55	0	13	0	0
58	I	1	0	0	0	0
58	j	1	0	0	0	0
58	p	1	0	0	0	0
58	u	1	0	0	0	0
59	b	32	0	12	1	0
59	m	32	0	12	2	0
60	b	1	0	0	0	0
60	m	1	0	0	0	0
All	All	157395	0	124552	2172	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 9.

All (2172) 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)
36:j:2:GLY:N	50:1:2138:A:HO2'	1.61	0.96
54:KK:31:TYR:HH	55:LL:5:GLU:N	1.73	0.87
50:1:542:G:H1	50:1:549:U:H3	1.32	0.77
50:1:2253:G:H1	50:1:2264:U:H3	1.32	0.77
28:b:510:ARG:HH12	50:1:1681:U:H5''	1.51	0.76
50:1:2721:A:H61	50:1:2735:U:H3	1.31	0.76
39:m:277:LEU:HB3	39:m:283:THR:HG21	1.70	0.73
17:Q:69:ARG:HH12	50:1:720:A:H5'	1.54	0.73
48:y:21:ASN:HD22	48:y:67:ARG:HD3	1.54	0.72
15:O:68:ARG:HH12	50:1:2987:A:H5''	1.54	0.72
50:1:3165:A:H1'	50:1:3286:G:H22	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:270:THR:H	52:4:273:HIS:HD2	1.38	0.71
50:1:2842:U:OP1	50:1:2844:C:N4	2.22	0.71
12:L:46:ILE:HG22	12:L:49:ARG:HB2	1.73	0.71
14:N:187:ARG:HE	14:N:188:ARG:HD3	1.55	0.70
39:m:257:TYR:HB2	39:m:283:THR:HG22	1.74	0.70
26:Z:64:LYS:NZ	50:1:1812:G:N7	2.40	0.70
23:W:71:LYS:NZ	50:1:1222:G:N7	2.40	0.69
52:4:127:SER:HB2	52:4:134:ARG:HE	1.57	0.69
29:c:22:LYS:H	29:c:94:GLU:HB2	1.56	0.69
56:MM:168:LEU:HA	56:MM:291:PHE:HB2	1.75	0.69
17:Q:141:ARG:NH2	50:1:743:C:N3	2.40	0.69
26:Z:54:THR:HG23	26:Z:56:LYS:H	1.58	0.69
50:1:2767:U:H3	50:1:2791:G:H1	1.39	0.69
47:x:325:HIS:HD2	47:x:408:VAL:H	1.40	0.68
28:b:647:ARG:NH1	50:1:877:C:N3	2.41	0.68
42:r:203:ASN:H	42:r:210:THR:HG22	1.59	0.68
11:J:10:ARG:HB2	11:J:133:ARG:HD3	1.75	0.68
11:J:20:ASN:HB3	11:J:126:ASP:HB2	1.76	0.68
28:b:164:ASP:H	28:b:217:GLN:HE22	1.42	0.68
42:r:164:ARG:HD3	50:1:2727:A:H1'	1.74	0.67
25:Y:112:ASP:H	25:Y:115:ARG:HB3	1.58	0.67
9:H:90:MET:HG2	9:H:181:VAL:HA	1.76	0.67
56:MM:810:PRO:HA	56:MM:814:MET:HB2	1.77	0.67
48:y:223:ARG:HE	48:y:229:PRO:HA	1.60	0.67
14:N:37:HIS:HE1	14:N:63:ARG:HH11	1.41	0.66
50:1:2566:C:O2'	56:MM:1012:GLN:NE2	2.28	0.66
56:MM:401:ILE:HG23	56:MM:406:TYR:HB2	1.78	0.66
9:H:155:SER:HG	50:1:3110:C:HO2'	1.42	0.66
30:d:31:ARG:NH2	50:1:1884:A:OP1	2.28	0.66
52:4:164:ASP:HB2	52:4:173:THR:HB	1.76	0.66
51:3:81:U:H2'	51:3:82:G:H8	1.60	0.66
36:j:52:LYS:NZ	50:1:364:G:OP2	2.29	0.66
46:w:73:THR:HG23	46:w:83:GLN:HE21	1.60	0.66
33:g:58:ARG:HD3	33:g:59:PRO:HD2	1.76	0.65
47:x:263:TRP:HA	47:x:270:CYS:HA	1.76	0.65
50:1:2252:A:H61	50:1:2265:C:H42	1.45	0.65
50:1:2531:C:N3	50:1:2547:A:N6	2.45	0.65
50:1:2687:G:N2	50:1:2689:A:O2'	2.29	0.65
50:1:1117:G:H1	50:1:1142:G:H21	1.43	0.65
23:W:165:MET:HA	23:W:169:PHE:HB2	1.78	0.65
28:b:392:ASP:HB3	28:b:395:ARG:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2795:U:O2	50:1:2798:C:N4	2.30	0.65
15:O:60:LYS:HE3	50:1:1307:G:H5''	1.79	0.65
8:G:100:GLU:OE1	8:G:108:ARG:NH1	2.30	0.64
39:m:439:LEU:HB2	39:m:443:GLU:HB2	1.78	0.64
3:B:266:ARG:NH2	50:1:2392:C:O2'	2.30	0.64
15:O:171:LYS:NZ	50:1:3180:A:OP1	2.30	0.64
38:l:2:ALA:N	50:1:1493:G:O6	2.30	0.64
47:x:39:LEU:HD21	47:x:120:LEU:HB3	1.78	0.64
14:N:14:LYS:HE2	50:1:269:G:H5''	1.80	0.64
50:1:971:G:N1	50:1:1111:U:O2	2.30	0.64
50:1:2655:U:H4'	50:1:2656:A:H5''	1.79	0.64
33:g:79:SER:OG	33:g:80:ARG:NH1	2.30	0.64
6:E:169:ASP:HB3	6:E:174:LEU:HD11	1.78	0.64
28:b:588:ARG:HG3	38:l:21:ARG:HE	1.61	0.64
25:Y:4:GLN:HB2	50:1:229:G:H5''	1.80	0.64
50:1:2687:G:N2	50:1:2691:A:OP1	2.31	0.64
48:y:119:PRO:O	48:y:139:ARG:NH1	2.31	0.64
22:V:15:LEU:HA	22:V:53:SER:HB3	1.81	0.63
45:v:50:SER:HB3	45:v:57:MET:HE2	1.80	0.63
3:B:28:ARG:NH2	50:1:3140:G:N7	2.45	0.63
11:J:47:GLN:HG2	11:J:67:VAL:HG12	1.79	0.63
15:O:59:ARG:NH1	50:1:1307:G:OP1	2.31	0.63
50:1:845:G:N2	50:1:848:A:OP2	2.31	0.63
50:1:3166:C:O2	50:1:3284:G:N2	2.29	0.63
25:Y:16:ARG:NH1	50:1:216:G:OP1	2.31	0.63
26:Z:48:ARG:NH2	50:1:1631:C:OP2	2.32	0.63
27:a:117:ARG:NH2	50:1:718:G:OP1	2.32	0.63
34:h:90:ARG:NH2	50:1:20:A:OP2	2.32	0.63
2:A:54:ARG:NH2	50:1:2176:U:OP1	2.32	0.63
39:m:90:GLN:HE22	47:x:477:LYS:HG3	1.64	0.63
11:J:92:ARG:HA	11:J:172:LEU:HB2	1.80	0.63
50:1:3109:G:OP2	50:1:3120:C:N4	2.31	0.63
28:b:227:ARG:HD3	28:b:232:MET:HA	1.79	0.63
47:x:472:ASP:HB3	47:x:475:THR:HG22	1.81	0.63
56:MM:718:ILE:HG21	56:MM:738:PHE:HA	1.81	0.63
2:A:80:GLU:HG3	41:p:66:GLY:HA2	1.81	0.62
7:F:158:LYS:HB3	7:F:159:GLN:HG3	1.79	0.62
12:L:36:ARG:NH2	50:1:687:U:OP2	2.32	0.62
20:T:156:TYR:OH	53:5:68:LYS:NZ	2.32	0.62
11:J:90:GLN:HB3	11:J:172:LEU:HD11	1.81	0.62
50:1:2627:C:H2'	50:1:2628:A:H8	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:135:PRO:HB3	52:4:162:PRO:HD3	1.81	0.62
2:A:136:ILE:HA	2:A:148:VAL:HG12	1.81	0.62
14:N:85:THR:O	14:N:87:GLN:NE2	2.32	0.62
18:R:74:ARG:NH1	50:1:1942:U:OP2	2.33	0.62
28:b:256:LEU:HG	28:b:293:ILE:HD13	1.82	0.62
29:c:28:LYS:NZ	50:1:1712:G:O6	2.33	0.62
56:MM:177:LYS:HB3	56:MM:292:LEU:HD22	1.82	0.62
3:B:218:ILE:HG22	3:B:276:THR:HA	1.81	0.62
23:W:14:GLN:O	42:r:72:LYS:NZ	2.30	0.62
42:r:40:GLN:NE2	50:1:1207:G:N3	2.47	0.62
48:y:175:SER:O	48:y:178:GLN:NE2	2.33	0.62
50:1:2628:A:N6	50:1:2650:U:O2	2.33	0.62
28:b:263:THR:HG23	28:b:266:ALA:H	1.64	0.62
46:w:128:ARG:HH11	50:1:2754:G:H8	1.47	0.62
11:J:55:ARG:HH12	50:1:2630:C:H5'	1.65	0.62
22:V:74:MET:HE3	22:V:102:ILE:HG21	1.82	0.62
50:1:627:U:H4'	50:1:1399:A:H1'	1.82	0.62
40:n:253:ASP:HA	40:n:257:SER:HA	1.81	0.62
40:n:411:ILE:HG12	40:n:427:ILE:HD11	1.82	0.61
37:k:2:ALA:N	50:1:1613:A:OP1	2.32	0.61
46:w:40:ASP:HB3	46:w:43:ASN:HB2	1.82	0.61
52:4:518:ASP:OD1	52:4:518:ASP:N	2.33	0.61
56:MM:747:ARG:NH1	56:MM:750:GLU:OE1	2.32	0.61
3:B:222:LYS:HD3	3:B:331:ASN:HB3	1.82	0.61
14:N:140:LYS:HB3	14:N:144:ARG:HH12	1.65	0.61
18:R:5:ARG:NH1	50:1:1513:G:OP1	2.33	0.61
25:Y:2:ALA:N	50:1:212:G:OP2	2.33	0.61
5:D:71:GLY:O	51:3:7:G:O2'	2.17	0.61
45:v:103:ILE:HG12	45:v:113:MET:HG2	1.82	0.61
45:v:191:GLN:H	45:v:194:GLU:HB2	1.66	0.61
50:1:1063:G:O2'	50:1:1097:G:N2	2.33	0.61
56:MM:667:PRO:HB2	56:MM:713:ASP:HB2	1.83	0.61
4:C:6:VAL:HG21	4:C:149:PRO:HD2	1.83	0.61
22:V:38:ALA:HB3	22:V:59:MET:HB2	1.82	0.61
35:i:5:THR:HG23	35:i:12:ASN:HB2	1.82	0.61
47:x:383:MET:HB2	47:x:398:MET:HB2	1.83	0.61
50:1:671:U:H2'	50:1:672:A:H8	1.64	0.61
50:1:708:G:N2	50:1:711:A:OP2	2.34	0.61
3:B:66:LYS:O	3:B:70:ARG:NH1	2.33	0.61
8:G:201:THR:HG22	8:G:202:GLU:HG2	1.83	0.61
50:1:1683:A:H61	50:1:3071:U:H3	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:103:ARG:NH1	50:1:1721:U:OP2	2.34	0.61
50:1:655:C:H2'	50:1:656:A:H8	1.66	0.61
50:1:2628:A:N6	50:1:2650:U:O2'	2.29	0.61
52:4:396:SER:OG	52:4:398:ASN:OD1	2.19	0.61
2:A:21:ARG:HD3	50:1:824:C:H5''	1.81	0.61
29:c:13:LYS:HB3	29:c:100:ILE:HG22	1.82	0.61
47:x:261:LYS:NZ	47:x:273:THR:OG1	2.30	0.61
50:1:64:G:O2'	50:1:77:A:N3	2.33	0.61
50:1:733:G:N2	50:1:736:A:OP2	2.34	0.61
56:MM:583:PHE:HB3	56:MM:610:PHE:HB2	1.82	0.61
3:B:241:LYS:NZ	50:1:1891:A:OP2	2.34	0.60
46:w:157:GLN:NE2	46:w:159:LEU:O	2.34	0.60
51:3:70:U:H2'	51:3:71:G:H8	1.66	0.60
54:KK:33:ASN:O	56:MM:834:LYS:NZ	2.34	0.60
1:2:53:A:OP1	38:l:19:GLN:NE2	2.34	0.60
28:b:510:ARG:NH2	50:1:1681:U:OP1	2.32	0.60
39:m:126:SER:HB3	47:x:400:GLY:H	1.66	0.60
47:x:83:ILE:HG12	47:x:89:SER:HA	1.83	0.60
1:2:29:U:H5''	12:L:27:ASP:HB3	1.83	0.60
14:N:176:LYS:NZ	50:1:66:A:N3	2.49	0.60
28:b:135:ARG:NH2	50:1:2858:U:O2	2.32	0.60
50:1:1896:A:H61	50:1:2339:C:H42	1.48	0.60
50:1:2635:A:N6	50:1:2642:A:OP2	2.34	0.60
3:B:216:ASP:OD1	3:B:216:ASP:N	2.31	0.60
16:P:23:ARG:NH1	50:1:1504:A:OP1	2.33	0.60
20:T:92:ARG:HB2	20:T:95:HIS:HD2	1.67	0.60
24:X:100:LYS:NZ	24:X:106:ASP:OD1	2.35	0.60
40:n:242:LEU:HA	40:n:266:SER:HA	1.82	0.60
44:u:111:ARG:NH2	50:1:3367:C:OP1	2.35	0.60
56:MM:512:PRO:HG2	56:MM:546:ARG:HG2	1.83	0.60
23:W:74:GLN:NE2	23:W:96:CYS:SG	2.74	0.60
33:g:74:ARG:NH2	50:1:1639:C:OP2	2.29	0.60
40:n:177:ARG:NH2	40:n:353:ASP:OD2	2.34	0.60
50:1:2842:U:OP1	50:1:2847:A:N6	2.32	0.60
2:A:131:GLY:H	2:A:169:ILE:HB	1.65	0.60
39:m:31:ARG:NH2	50:1:2964:G:O2'	2.35	0.60
3:B:55:THR:OG1	50:1:3049:A:N3	2.34	0.60
18:R:62:ARG:HH12	50:1:3067:C:H3'	1.65	0.60
25:Y:89:LYS:NZ	50:1:376:G:OP2	2.33	0.60
42:r:126:ARG:HB3	50:1:1128:U:H5''	1.84	0.60
50:1:2664:C:N4	50:1:2704:A:OP2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:191:TRP:O	14:N:195:ASN:ND2	2.35	0.60
48:y:21:ASN:ND2	48:y:112:ASP:OD2	2.35	0.60
28:b:396:ARG:NH2	48:y:39:GLU:O	2.34	0.60
42:r:155:THR:HG21	42:r:173:ARG:HD2	1.83	0.60
42:r:209:TYR:HA	42:r:212:LEU:HB2	1.84	0.60
44:u:61:LYS:NZ	50:1:3366:G:OP1	2.34	0.60
47:x:378:SER:OG	47:x:380:ASP:OD1	2.20	0.60
56:MM:87:GLN:HB3	56:MM:119:VAL:HB	1.84	0.60
21:U:99:LYS:H	21:U:102:GLU:HB2	1.66	0.59
45:v:28:LYS:NZ	46:w:100:PRO:O	2.35	0.59
47:x:201:ILE:HB	47:x:213:TRP:HB2	1.84	0.59
50:1:2541:U:H1'	50:1:2542:U:H4'	1.83	0.59
14:N:49:ARG:NH1	50:1:115:A:OP1	2.35	0.59
30:d:82:GLU:HG3	30:d:83:GLU:HG3	1.83	0.59
44:u:74:ARG:NH1	48:y:98:GLU:OE2	2.35	0.59
2:A:149:ARG:HH21	2:A:153:GLY:HA2	1.67	0.59
40:n:79:LYS:NZ	40:n:110:ASP:OD2	2.34	0.59
42:r:173:ARG:N	50:1:2727:A:N1	2.49	0.59
45:v:105:THR:HA	45:v:111:TYR:H	1.66	0.59
50:1:3092:C:O2'	50:1:3094:A:OP2	2.19	0.59
3:B:334:ARG:NH2	50:1:3304:U:O3'	2.35	0.59
21:U:109:GLN:NE2	28:b:522:SER:O	2.35	0.59
23:W:158:ILE:HG22	23:W:160:SER:H	1.66	0.59
23:W:219:ALA:HA	23:W:230:SER:HA	1.83	0.59
50:1:1482:A:N7	50:1:1866:C:O2'	2.33	0.59
50:1:2841:G:H3'	50:1:2844:C:H41	1.67	0.59
56:MM:165:GLU:OE1	56:MM:315:HIS:NE2	2.30	0.59
25:Y:60:ARG:NH1	50:1:200:C:OP1	2.36	0.59
39:m:49:ARG:HG2	39:m:55:LEU:HA	1.85	0.59
50:1:563:U:H2'	50:1:564:G:H8	1.66	0.59
50:1:2745:G:N2	50:1:2748:A:OP2	2.32	0.59
3:B:50:LYS:NZ	3:B:330:GLY:O	2.36	0.59
28:b:232:MET:HE3	28:b:237:MET:HE1	1.84	0.59
45:v:83:ASP:OD1	45:v:108:TYR:OH	2.21	0.59
45:v:144:GLN:HA	46:w:30:ASP:HB3	1.83	0.59
56:MM:657:ARG:NH2	56:MM:832:ASN:OD1	2.35	0.59
8:G:133:LYS:HD2	8:G:138:HIS:HE1	1.67	0.59
31:e:101:SER:HB3	50:1:1389:G:H5''	1.85	0.59
42:r:135:LYS:NZ	50:1:2873:U:OP2	2.33	0.59
52:4:507:ILE:HG22	52:4:524:ARG:HA	1.85	0.59
56:MM:166:SER:OG	56:MM:312:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4:ARG:NH1	3:B:6:TYR:O	2.36	0.58
19:S:22:PRO:O	20:T:146:ASN:ND2	2.34	0.58
26:Z:52:LYS:O	26:Z:65:ARG:NH1	2.36	0.58
3:B:11:HIS:NE2	50:1:2881:C:OP1	2.37	0.58
4:C:188:ARG:NH1	50:1:1382:G:OP2	2.35	0.58
5:D:24:ARG:NH2	51:3:13:A:O2'	2.36	0.58
28:b:514:LYS:NZ	50:1:1477:A:OP2	2.36	0.58
45:v:28:LYS:HE2	46:w:102:GLU:HB2	1.85	0.58
50:1:2393:G:O2'	50:1:2982:A:N6	2.36	0.58
52:4:96:ASP:HB2	52:4:140:LYS:HB2	1.84	0.58
6:E:43:LEU:HD11	6:E:85:ILE:HG13	1.85	0.58
16:P:30:ARG:HA	16:P:119:VAL:HG11	1.86	0.58
27:a:58:MET:SD	50:1:2787:G:O2'	2.62	0.58
47:x:470:VAL:HG13	47:x:479:SER:HB3	1.84	0.58
13:M:108:ARG:NH2	15:O:196:ALA:O	2.34	0.58
41:p:41:PHE:O	50:1:1729:A:N6	2.35	0.58
47:x:260:ILE:HD11	47:x:281:VAL:HG11	1.85	0.58
50:1:2516:U:O2	50:1:2594:C:N4	2.36	0.58
25:Y:55:GLU:HB2	25:Y:108:LYS:HB2	1.84	0.58
39:m:376:LYS:HA	39:m:378:SER:H	1.67	0.58
45:v:22:LYS:O	46:w:101:ARG:NH1	2.35	0.58
50:1:1813:A:O2'	50:1:1816:A:N3	2.35	0.58
50:1:2692:A:C4	50:1:2693:C:H1'	2.38	0.58
1:2:158:A:H4'	56:MM:415:SER:HA	1.85	0.58
50:1:3042:U:OP2	50:1:3092:C:N4	2.36	0.58
50:1:3341:U:H1'	50:1:3342:A:H5'	1.85	0.58
3:B:10:ARG:NH1	3:B:12:GLY:O	2.36	0.58
19:S:78:TRP:HB3	19:S:124:LEU:HD12	1.85	0.58
41:p:17:ARG:NH2	50:1:860:G:OP1	2.36	0.58
5:D:75:LEU:O	5:D:112:LYS:NZ	2.35	0.58
18:R:68:GLN:OE1	18:R:71:ARG:NH1	2.36	0.58
31:e:16:LYS:NZ	50:1:1404:G:O6	2.35	0.58
54:KK:26:GLN:HE21	56:MM:17:LEU:HD13	1.69	0.58
18:R:38:ARG:NH1	50:1:1603:A:OP1	2.36	0.58
28:b:302:ARG:O	28:b:302:ARG:NH2	2.37	0.58
47:x:142:HIS:HD1	47:x:169:ARG:HG3	1.69	0.58
11:J:95:ASN:HA	50:1:2673:A:H5''	1.86	0.57
13:M:128:ARG:NH2	50:1:3213:A:OP2	2.37	0.57
14:N:182:ASN:ND2	50:1:280:U:O2'	2.37	0.57
35:i:34:SER:OG	35:i:37:THR:N	2.30	0.57
4:C:261:VAL:O	4:C:271:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:60:ILE:HB	5:D:80:SER:HB3	1.86	0.57
13:M:8:LYS:HG2	13:M:9:ALA:HB2	1.84	0.57
26:Z:10:VAL:HG22	26:Z:24:VAL:HG12	1.86	0.57
52:4:246:ARG:NH2	52:4:263:GLU:OE2	2.37	0.57
56:MM:701:ARG:HB2	56:MM:718:ILE:HG12	1.87	0.57
56:MM:1009:THR:HG22	56:MM:1011:THR:H	1.69	0.57
28:b:110:ARG:NH2	50:1:2869:U:OP2	2.37	0.57
28:b:389:ASP:HB3	28:b:392:ASP:HB2	1.84	0.57
41:p:23:ARG:HH12	50:1:1927:G:H8	1.53	0.57
51:3:34:C:N3	51:3:46:A:O2'	2.37	0.57
28:b:647:ARG:NH2	50:1:885:U:O4	2.37	0.57
39:m:171:TYR:O	39:m:175:GLN:NE2	2.37	0.57
50:1:516:A:H2'	50:1:517:G:H8	1.69	0.57
52:4:277:ASP:N	52:4:277:ASP:OD1	2.34	0.57
31:e:11:LYS:NZ	50:1:1404:G:OP2	2.37	0.57
32:f:20:LYS:NZ	50:1:1149:G:OP1	2.37	0.57
50:1:2841:G:N1	50:1:2845:A:O2'	2.32	0.57
52:4:528:GLY:H	52:4:531:THR:HB	1.70	0.57
4:C:76:ARG:HA	4:C:88:GLY:HA2	1.87	0.57
11:J:110:ILE:HA	11:J:114:ILE:HB	1.84	0.57
28:b:24:ARG:NH2	28:b:52:TYR:OH	2.37	0.57
30:d:55:LEU:HB2	30:d:95:PRO:HD3	1.87	0.57
39:m:274:VAL:O	39:m:278:SER:N	2.37	0.57
8:G:91:PHE:HE2	8:G:185:ARG:HE	1.51	0.57
21:U:17:VAL:HG22	21:U:103:TYR:HB2	1.85	0.57
22:V:12:ARG:NH1	50:1:3041:U:OP1	2.38	0.57
28:b:491:GLU:OE1	44:u:137:ARG:NH2	2.37	0.57
12:L:53:LEU:HB2	12:L:55:ARG:HH12	1.69	0.57
40:n:227:THR:HA	40:n:230:HIS:HD2	1.70	0.57
42:r:145:LYS:HE3	50:1:2970:C:H5'	1.86	0.57
50:1:2168:A:N6	50:1:2170:U:O2	2.38	0.57
2:A:112:ILE:HG12	2:A:135:ILE:HG12	1.87	0.57
3:B:339:ARG:HH11	3:B:342:LEU:HD11	1.70	0.57
50:1:903:U:H2'	50:1:904:A:H8	1.69	0.57
5:D:65:ILE:HG12	5:D:74:VAL:HG22	1.86	0.57
23:W:57:ARG:NH2	50:1:1258:U:O3'	2.38	0.57
50:1:2865:U:H2'	50:1:2866:U:H2'	1.87	0.57
4:C:23:PRO:HG2	4:C:258:LEU:HD23	1.87	0.56
5:D:33:ARG:NH1	51:3:7:G:O5'	2.38	0.56
5:D:216:GLU:O	5:D:220:SER:N	2.38	0.56
11:J:9:MET:HE2	51:3:29:C:H4'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:38:LEU:O	33:g:58:ARG:NH2	2.38	0.56
39:m:60:SER:OG	42:r:149:ARG:NH1	2.38	0.56
3:B:288:GLY:N	3:B:320:ASP:OD1	2.35	0.56
1:2:37:A:OP1	34:h:89:ARG:NH2	2.36	0.56
15:O:25:LYS:NZ	50:1:1178:G:OP2	2.37	0.56
18:R:150:GLN:O	18:R:154:ALA:N	2.37	0.56
39:m:120:GLU:HG3	47:x:441:ARG:HH21	1.70	0.56
41:p:49:ARG:HH21	41:p:52:ALA:HB2	1.70	0.56
50:1:1189:C:N4	50:1:1316:C:OP2	2.38	0.56
52:4:73:LEU:HD23	52:4:76:LEU:HD12	1.87	0.56
56:MM:711:TYR:HB3	56:MM:715:GLU:HB2	1.87	0.56
3:B:331:ASN:HD21	3:B:334:ARG:HH21	1.53	0.56
5:D:261:THR:OG1	5:D:264:GLN:NE2	2.38	0.56
9:H:16:VAL:HG12	9:H:29:GLY:HA3	1.87	0.56
45:v:205:LYS:HB2	45:v:226:ILE:HD13	1.86	0.56
56:MM:846:LEU:O	56:MM:850:TYR:N	2.36	0.56
1:2:95:G:O2'	36:j:81:GLY:O	2.23	0.56
16:P:131:ARG:NH1	50:1:879:U:O2'	2.39	0.56
45:v:112:ASP:HB3	45:v:240:PRO:HD3	1.88	0.56
49:z:8:SER:O	49:z:12:ASN:ND2	2.38	0.56
1:2:3:A:H4'	16:P:61:ARG:HH11	1.69	0.56
1:2:84:C:N4	25:Y:111:LEU:O	2.37	0.56
2:A:193:ARG:NH2	50:1:2181:C:OP1	2.38	0.56
11:J:109:HIS:CD2	11:J:123:PHE:H	2.23	0.56
22:V:135:VAL:HG22	48:y:101:LEU:HA	1.87	0.56
8:G:218:ILE:O	8:G:222:PHE:N	2.38	0.56
21:U:21:SER:O	21:U:25:ASN:ND2	2.39	0.56
21:U:90:ARG:NH1	50:1:1682:U:O4	2.39	0.56
23:W:22:ASN:HD21	23:W:25:ARG:HH21	1.53	0.56
27:a:117:ARG:NH2	50:1:716:A:O2'	2.38	0.56
35:i:68:ARG:NH2	50:1:2218:G:OP1	2.39	0.56
56:MM:93:VAL:HG11	56:MM:325:PRO:HG2	1.88	0.56
56:MM:420:GLU:HG2	56:MM:474:ILE:HD13	1.87	0.56
6:E:77:ARG:NH2	50:1:3273:A:OP2	2.38	0.56
11:J:164:LYS:HE2	11:J:171:VAL:HB	1.88	0.56
14:N:203:ARG:NH1	50:1:665:A:OP1	2.38	0.56
39:m:400:ILE:HG13	39:m:428:ILE:HD11	1.87	0.56
50:1:1:G:N2	56:MM:949:CYS:O	2.39	0.56
4:C:8:VAL:HG13	4:C:151:VAL:HG12	1.87	0.56
5:D:79:TYR:HB2	5:D:82:GLU:HG3	1.88	0.56
8:G:152:LEU:HB2	8:G:198:ALA:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:39:ARG:NH2	50:1:686:G:OP2	2.39	0.56
13:M:37:GLU:OE2	13:M:74:ARG:NH2	2.39	0.56
45:v:202:ARG:HG3	46:w:50:ILE:HG21	1.88	0.56
48:y:9:ASN:ND2	50:1:3018:C:OP1	2.39	0.56
50:1:951:A:OP2	50:1:1367:G:N2	2.38	0.56
50:1:975:C:O2'	50:1:977:C:OP2	2.23	0.56
56:MM:132:THR:O	56:MM:163:ARG:NH1	2.38	0.56
1:2:36:G:OP2	34:h:85:THR:OG1	2.22	0.56
13:M:20:VAL:O	13:M:66:THR:OG1	2.21	0.56
29:c:24:THR:HG22	29:c:91:SER:HB3	1.87	0.56
39:m:19:ASP:OD1	46:w:120:LYS:NZ	2.39	0.56
40:n:366:TYR:HB2	40:n:407:VAL:HG11	1.88	0.56
42:r:30:ARG:NH2	50:1:3120:C:OP1	2.38	0.56
50:1:677:A:N6	50:1:786:A:O4'	2.39	0.56
16:P:172:GLN:NE2	50:1:3277:U:O4	2.39	0.55
23:W:18:LYS:HE2	50:1:1260:A:H5''	1.87	0.55
28:b:289:LYS:HE2	59:b:701:GTP:C4	2.41	0.55
40:n:435:CYS:O	40:n:439:GLY:N	2.33	0.55
42:r:164:ARG:HB2	50:1:2727:A:H8	1.71	0.55
47:x:297:HIS:HA	47:x:322:TRP:HB2	1.89	0.55
47:x:501:VAL:HB	47:x:513:TRP:HB2	1.88	0.55
50:1:2344:U:H2'	50:1:2345:A:H8	1.70	0.55
3:B:2:SER:N	50:1:2940:A:OP2	2.39	0.55
3:B:196:ARG:HH21	3:B:199:PHE:HD2	1.54	0.55
8:G:240:ASN:ND2	50:1:2584:G:O2'	2.39	0.55
12:L:128:ARG:HH11	50:1:169:U:H5'	1.71	0.55
31:e:112:ALA:O	31:e:116:GLY:N	2.39	0.55
37:k:45:VAL:HG23	37:k:52:TYR:HB2	1.88	0.55
47:x:139:ILE:HB	47:x:510:VAL:HB	1.88	0.55
56:MM:520:SER:OG	56:MM:522:ARG:O	2.23	0.55
7:F:30:ARG:NH1	50:1:595:G:OP2	2.39	0.55
18:R:43:LYS:HA	18:R:46:LYS:HE3	1.86	0.55
22:V:79:VAL:HG22	22:V:100:GLY:HA2	1.89	0.55
33:g:41:ARG:O	33:g:43:LYS:NZ	2.39	0.55
37:k:42:LYS:NZ	50:1:1748:G:OP2	2.39	0.55
56:MM:201:ILE:HG22	56:MM:203:ALA:H	1.70	0.55
7:F:151:ARG:NH1	7:F:206:LYS:O	2.39	0.55
28:b:233:ASN:ND2	50:1:1242:G:OP2	2.39	0.55
34:h:104:GLN:NE2	50:1:112:U:OP1	2.39	0.55
39:m:35:ARG:NH2	50:1:2964:G:OP1	2.40	0.55
42:r:251:ARG:HH22	50:1:1129:A:H5'	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:251:G:H4'	50:1:252:U:H5'	1.87	0.55
18:R:135:LYS:NZ	50:1:1949:G:OP2	2.35	0.55
23:W:45:LEU:HB3	23:W:215:VAL:HG23	1.87	0.55
30:d:62:ARG:NH1	30:d:68:GLU:OE2	2.40	0.55
56:MM:260:ILE:HA	56:MM:290:VAL:HB	1.89	0.55
1:2:38:U:OP2	34:h:78:LYS:NZ	2.37	0.55
20:T:108:ARG:NH1	50:1:1062:A:O2'	2.39	0.55
24:X:115:ARG:NH1	24:X:119:THR:OG1	2.39	0.55
26:Z:22:LYS:NZ	26:Z:129:TRP:O	2.35	0.55
28:b:622:SER:OG	38:l:46:ARG:NH1	2.40	0.55
40:n:366:TYR:OH	40:n:390:GLU:OE1	2.23	0.55
50:1:3353:G:O2'	50:1:3356:G:OP2	2.25	0.55
52:4:198:LEU:HD12	52:4:507:ILE:HD11	1.88	0.55
5:D:85:ARG:NH1	5:D:86:TYR:OH	2.40	0.55
17:Q:16:ARG:NH1	17:Q:53:PHE:O	2.35	0.55
48:y:68:ARG:NH1	48:y:112:ASP:O	2.40	0.55
1:2:8:C:H2'	1:2:9:A:C8	2.42	0.55
4:C:124:SER:O	4:C:128:ALA:N	2.39	0.55
8:G:121:SER:HB2	8:G:124:ASP:H	1.71	0.55
28:b:502:THR:O	28:b:506:GLU:N	2.37	0.55
46:w:55:ARG:NH1	46:w:56:ASP:OD1	2.36	0.55
47:x:403:LYS:H	47:x:423:ASP:HB3	1.72	0.55
47:x:421:SER:OG	47:x:422:PHE:N	2.39	0.55
50:1:3074:G:H2'	50:1:3075:G:H8	1.71	0.55
56:MM:104:THR:O	56:MM:349:ARG:NH2	2.39	0.55
3:B:67:PHE:HA	3:B:70:ARG:HD2	1.89	0.55
11:J:51:ARG:NH1	50:1:2681:U:OP2	2.37	0.55
42:r:7:ILE:H	50:1:2898:G:H22	1.54	0.55
47:x:122:THR:OG1	47:x:415:ARG:NH1	2.40	0.55
50:1:15:C:H2'	50:1:16:A:H8	1.71	0.55
50:1:631:U:H2'	50:1:632:G:H8	1.71	0.55
51:3:41:G:N3	51:3:44:C:N4	2.52	0.55
56:MM:681:GLU:HB3	56:MM:769:SER:H	1.70	0.55
21:U:36:TYR:O	21:U:40:HIS:ND1	2.40	0.55
34:h:38:ARG:HH22	52:4:345:GLY:H	1.55	0.55
45:v:90:MET:HE1	45:v:100:MET:HE3	1.88	0.55
52:4:99:GLN:HB3	52:4:439:ILE:HG23	1.89	0.55
52:4:322:LYS:HD3	52:4:502:ARG:HH11	1.72	0.55
4:C:309:ARG:NH1	50:1:590:G:O2'	2.40	0.54
5:D:50:ARG:NH2	51:3:6:C:O2'	2.39	0.54
6:E:158:TYR:OH	13:M:114:ASP:OD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:8:GLN:HB3	9:H:72:LYS:HD2	1.87	0.54
9:H:141:LYS:HG3	9:H:142:ASP:HB2	1.88	0.54
11:J:8:PRO:HB2	51:3:53:U:H4'	1.88	0.54
36:j:56:ARG:NH2	50:1:364:G:N7	2.55	0.54
40:n:237:TYR:HE2	40:n:246:PRO:HD3	1.72	0.54
50:1:2901:G:H3'	50:1:2902:A:H8	1.72	0.54
56:MM:537:TYR:O	56:MM:541:SER:N	2.40	0.54
5:D:45:ASN:HB2	45:v:173:GLN:HE22	1.72	0.54
6:E:131:LYS:HE2	6:E:133:GLU:HB3	1.88	0.54
25:Y:42:GLN:O	25:Y:125:LYS:NZ	2.37	0.54
33:g:91:ARG:NH2	50:1:2554:A:OP1	2.41	0.54
34:h:85:THR:HG23	34:h:88:LEU:H	1.71	0.54
50:1:1740:U:H4'	50:1:1741:A:H5'	1.87	0.54
3:B:376:LYS:NZ	50:1:3330:A:OP2	2.36	0.54
15:O:18:ARG:NH2	50:1:1318:A:OP1	2.37	0.54
33:g:3:GLN:HE22	33:g:29:ILE:HB	1.72	0.54
45:v:185:THR:HB	45:v:200:LEU:HB2	1.89	0.54
47:x:158:ARG:NH1	47:x:172:ASP:OD1	2.40	0.54
50:1:2416:U:O2	50:1:2966:G:N2	2.39	0.54
50:1:2516:U:O2'	50:1:2595:A:N6	2.40	0.54
23:W:166:ARG:NH1	42:r:18:LEU:O	2.41	0.54
26:Z:17:ARG:H	33:g:74:ARG:HG2	1.72	0.54
47:x:193:SER:OG	47:x:237:TRP:NE1	2.41	0.54
56:MM:91:ARG:NH2	56:MM:322:ARG:O	2.41	0.54
56:MM:139:ARG:NH1	56:MM:159:SER:OG	2.40	0.54
56:MM:701:ARG:HD2	56:MM:718:ILE:HD11	1.90	0.54
5:D:110:LEU:O	5:D:114:GLY:N	2.34	0.54
16:P:69:ARG:HD2	50:1:3309:G:H1'	1.89	0.54
39:m:139:ASP:OD1	39:m:139:ASP:N	2.41	0.54
40:n:18:ARG:NH2	50:1:1565:G:OP2	2.40	0.54
42:r:58:LYS:NZ	50:1:1207:G:OP2	2.41	0.54
54:KK:85:MET:HE2	55:LL:79:GLU:HB3	1.90	0.54
4:C:132:ALA:HA	4:C:135:VAL:H	1.73	0.54
10:I:87:GLN:OE1	44:u:7:HIS:ND1	2.41	0.54
14:N:93:LYS:NZ	50:1:2600:C:OP1	2.39	0.54
16:P:122:ALA:HB3	16:P:143:PRO:HB2	1.90	0.54
31:e:47:ARG:NH1	50:1:1147:G:OP1	2.40	0.54
37:k:32:ASN:OD1	37:k:36:LYS:N	2.34	0.54
48:y:200:ASN:OD1	48:y:203:LEU:N	2.41	0.54
50:1:1322:U:H2'	50:1:1323:G:H8	1.73	0.54
56:MM:288:ARG:NH1	56:MM:312:GLN:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:MM:588:ASN:O	56:MM:592:ASN:ND2	2.41	0.54
6:E:82:ARG:NH2	50:1:501:A:OP1	2.41	0.54
1:2:120:C:OP2	40:n:69:GLN:NE2	2.40	0.54
2:A:79:ASN:ND2	2:A:166:ILE:O	2.41	0.54
5:D:38:THR:HA	5:D:41:LYS:HE2	1.90	0.54
6:E:17:ALA:O	50:1:591:G:O2'	2.25	0.54
30:d:15:ASN:O	30:d:19:ARG:NH1	2.41	0.54
31:e:15:LYS:NZ	50:1:427:C:OP2	2.34	0.54
37:k:26:LYS:NZ	37:k:28:ASN:OD1	2.41	0.54
48:y:4:ARG:HB3	48:y:208:LEU:HD23	1.89	0.54
50:1:1362:G:H2'	50:1:1363:A:C8	2.43	0.54
50:1:3344:A:N6	50:1:3361:G:O2'	2.39	0.54
56:MM:656:TYR:HB2	56:MM:831:LEU:HD11	1.90	0.54
5:D:77:ALA:O	5:D:108:ARG:NH1	2.41	0.54
10:I:1:MET:N	50:1:3084:C:OP2	2.34	0.54
18:R:103:ARG:NH1	18:R:124:TYR:OH	2.39	0.54
20:T:100:LYS:NZ	50:1:991:G:OP2	2.40	0.54
24:X:33:ARG:HH12	50:1:1581:C:H41	1.56	0.54
39:m:57:ARG:NH1	50:1:2619:G:OP1	2.40	0.54
40:n:178:LYS:HD2	40:n:459:PRO:HB2	1.90	0.54
50:1:1301:A:N6	50:1:2827:U:O2'	2.41	0.54
50:1:1863:G:N1	50:1:1866:C:OP2	2.36	0.54
52:4:553:ILE:O	52:4:557:ALA:N	2.38	0.54
56:MM:534:GLY:HA3	56:MM:574:GLY:HA3	1.90	0.54
11:J:137:ARG:O	11:J:141:ARG:N	2.39	0.54
23:W:43:LEU:HD23	23:W:215:VAL:HG21	1.90	0.54
23:W:69:LYS:NZ	50:1:1282:G:OP2	2.41	0.54
26:Z:24:VAL:HG11	26:Z:87:LEU:HD23	1.89	0.54
45:v:29:GLN:HB2	45:v:84:CYS:HA	1.90	0.54
50:1:2413:A:HO2'	50:1:2414:G:H8	1.56	0.54
50:1:3160:U:H3	50:1:3290:G:H1	1.54	0.54
51:3:77:G:N2	51:3:78:U:O4	2.38	0.54
20:T:89:LEU:HD21	46:w:159:LEU:HB2	1.90	0.53
39:m:408:GLN:HB2	39:m:411:HIS:HD2	1.72	0.53
50:1:2443:A:H2'	50:1:2444:C:H4'	1.90	0.53
50:1:2636:A:N1	50:1:2640:A:N6	2.55	0.53
56:MM:264:VAL:HB	56:MM:293:SER:HB2	1.89	0.53
4:C:217:LYS:HG2	4:C:220:ARG:HH21	1.73	0.53
4:C:341:SER:OG	50:1:514:G:N3	2.40	0.53
46:w:181:ARG:NH1	50:1:2649:A:OP1	2.42	0.53
47:x:491:THR:O	47:x:504:GLY:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:4:383:ASP:OD1	52:4:383:ASP:N	2.39	0.53
1:2:12:A:OP1	16:P:3:ARG:NH2	2.41	0.53
1:2:152:G:H5'	8:G:59:GLN:HG3	1.91	0.53
28:b:506:GLU:HA	30:d:97:LEU:HD13	1.90	0.53
28:b:621:GLU:OE2	38:l:38:ASN:N	2.40	0.53
45:v:36:GLN:HA	45:v:63:LYS:HB3	1.88	0.53
3:B:10:ARG:NH1	3:B:11:HIS:O	2.42	0.53
8:G:248:LYS:NZ	50:1:2529:A:OP1	2.39	0.53
11:J:29:ARG:NH2	11:J:122:ILE:O	2.38	0.53
39:m:47:GLU:OE2	39:m:49:ARG:NH2	2.41	0.53
42:r:231:VAL:HG22	42:r:237:VAL:HG12	1.89	0.53
45:v:221:ILE:O	46:w:55:ARG:NH2	2.40	0.53
50:1:1063:G:H21	50:1:1066:G:H1'	1.73	0.53
50:1:1380:G:N2	50:1:1426:C:O2	2.26	0.53
50:1:1381:A:H2'	50:1:1382:G:H8	1.73	0.53
56:MM:244:SER:OG	56:MM:248:ARG:NH1	2.42	0.53
2:A:99:GLY:H	2:A:166:ILE:HB	1.73	0.53
5:D:176:SER:HB2	50:1:2746:A:H4'	1.89	0.53
44:u:76:ASN:HB3	48:y:95:GLN:HG3	1.91	0.53
52:4:243:ARG:NH1	52:4:256:GLU:OE2	2.42	0.53
52:4:247:ILE:HD11	52:4:318:LEU:HB2	1.91	0.53
52:4:396:SER:HB3	52:4:399:PHE:HB2	1.90	0.53
2:A:40:TYR:HA	2:A:91:GLY:HA3	1.90	0.53
3:B:47:LEU:HD12	3:B:335:ILE:HD11	1.89	0.53
7:F:30:ARG:HG3	7:F:33:ARG:HH21	1.72	0.53
44:u:2:ARG:NH2	48:y:78:ASP:OD2	2.42	0.53
50:1:439:C:O2'	50:1:494:G:N2	2.42	0.53
56:MM:402:TRP:O	56:MM:405:LYS:NZ	2.37	0.53
11:J:109:HIS:HD2	11:J:123:PHE:H	1.54	0.53
12:L:32:LYS:NZ	50:1:686:G:O6	2.41	0.53
12:L:171:ARG:NH2	50:1:713:U:OP1	2.38	0.53
28:b:300:GLU:O	28:b:304:GLN:N	2.42	0.53
39:m:345:PRO:O	39:m:459:ARG:NH2	2.42	0.53
50:1:348:A:N3	50:1:352:A:O2'	2.42	0.53
50:1:1761:C:O2'	50:1:1763:U:OP2	2.25	0.53
52:4:33:GLN:HB2	52:4:574:PRO:HA	1.91	0.53
52:4:239:VAL:HG12	52:4:241:GLY:H	1.73	0.53
54:KK:42:LEU:HA	54:KK:45:LYS:HB2	1.91	0.53
56:MM:224:GLY:O	56:MM:1036:LYS:NZ	2.42	0.53
4:C:361:HIS:ND1	4:C:362:ASP:O	2.42	0.53
16:P:27:LYS:NZ	50:1:1446:A:O2'	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:28:ASN:ND2	22:V:112:SER:OG	2.39	0.53
42:r:7:ILE:H	50:1:2898:G:N2	2.06	0.53
44:u:32:CYS:SG	44:u:33:ARG:NH2	2.82	0.53
45:v:219:PRO:O	46:w:59:GLN:NE2	2.42	0.53
4:C:9:HIS:HA	4:C:15:ALA:HA	1.90	0.53
22:V:80:ARG:NH1	22:V:117:PRO:O	2.40	0.53
35:i:34:SER:HG	35:i:37:THR:H	1.54	0.53
36:j:24:ARG:NH1	50:1:361:A:OP1	2.41	0.53
40:n:261:SER:OG	40:n:262:TYR:N	2.41	0.53
41:p:84:ARG:HG2	41:p:87:ARG:HH22	1.72	0.53
45:v:138:LYS:NZ	45:v:166:ARG:O	2.39	0.53
50:1:655:C:H2'	50:1:656:A:C8	2.44	0.53
56:MM:284:PRO:O	56:MM:289:TYR:OH	2.27	0.53
3:B:56:ILE:HG21	3:B:356:LEU:HD22	1.91	0.53
3:B:226:PHE:O	50:1:1886:A:O2'	2.27	0.53
5:D:172:TYR:CZ	47:x:134:ARG:HB2	2.44	0.53
5:D:274:GLN:NE2	51:3:20:A:O2'	2.41	0.53
8:G:135:GLY:O	8:G:139:VAL:N	2.37	0.53
22:V:133:SER:O	48:y:106:ASN:ND2	2.41	0.53
28:b:89:ASN:ND2	50:1:2862:U:O4	2.41	0.53
28:b:164:ASP:OD2	28:b:167:THR:N	2.41	0.53
33:g:81:CYS:HB2	33:g:84:CYS:H	1.74	0.53
37:k:58:ASP:OD2	37:k:61:LYS:N	2.35	0.53
39:m:233:ASP:N	39:m:233:ASP:OD1	2.42	0.53
39:m:313:ARG:NE	50:1:2729:U:OP2	2.42	0.53
47:x:173:CYS:O	47:x:176:GLN:NE2	2.42	0.53
47:x:438:SER:OG	47:x:439:THR:N	2.41	0.53
48:y:206:THR:OG1	48:y:207:GLY:N	2.42	0.53
56:MM:167:VAL:HG23	56:MM:315:HIS:HB2	1.91	0.53
8:G:144:GLU:HA	8:G:173:MET:HE2	1.91	0.52
18:R:60:LYS:NZ	50:1:1671:C:OP1	2.42	0.52
22:V:59:MET:HE1	22:V:75:PRO:HG3	1.91	0.52
28:b:483:ALA:O	28:b:485:GLU:N	2.42	0.52
39:m:161:VAL:O	39:m:165:ASN:ND2	2.42	0.52
50:1:546:C:H5''	50:1:547:G:C6	2.44	0.52
50:1:797:U:H2'	50:1:798:G:H8	1.74	0.52
50:1:3334:U:H4'	50:1:3335:A:H5'	1.90	0.52
52:4:57:ARG:HH21	52:4:59:LEU:HD21	1.74	0.52
55:LL:114:ILE:HA	55:LL:117:ASN:HB2	1.91	0.52
7:F:186:HIS:O	7:F:190:THR:OG1	2.21	0.52
9:H:133:THR:OG1	9:H:147:SER:OG	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:126:LEU:HD13	31:e:128:LEU:HD23	1.91	0.52
35:i:30:LYS:NZ	50:1:317:A:OP2	2.41	0.52
41:p:46:THR:HB	41:p:58:SER:HB3	1.92	0.52
56:MM:932:LYS:H	56:MM:935:GLN:HB2	1.74	0.52
3:B:216:ASP:HB3	3:B:278:ILE:HA	1.92	0.52
14:N:182:ASN:ND2	50:1:282:G:O6	2.42	0.52
24:X:142:ILE:HG21	52:4:420:ARG:HB3	1.91	0.52
34:h:79:ASP:OD1	34:h:79:ASP:N	2.43	0.52
45:v:199:VAL:HB	45:v:232:PHE:HB2	1.91	0.52
46:w:30:ASP:OD1	46:w:32:ASN:ND2	2.42	0.52
50:1:2760:C:N4	50:1:2761:G:O6	2.42	0.52
51:3:39:C:H5''	53:5:100:HIS:HE1	1.75	0.52
56:MM:172:HIS:HB2	56:MM:175:ALA:HB2	1.90	0.52
56:MM:327:GLN:HE21	56:MM:552:ARG:HH11	1.55	0.52
5:D:282:ARG:O	5:D:286:VAL:N	2.40	0.52
6:E:138:GLN:NE2	6:E:142:ASP:OD2	2.43	0.52
14:N:105:ARG:NE	50:1:1547:G:OP1	2.38	0.52
24:X:67:ILE:HD12	24:X:83:VAL:HG12	1.92	0.52
38:l:42:ARG:NH2	50:1:1494:U:OP2	2.40	0.52
39:m:347:PRO:HD2	39:m:389:ARG:HG2	1.92	0.52
50:1:939:U:H2'	50:1:940:G:H8	1.74	0.52
50:1:2660:G:O3'	50:1:2749:G:N2	2.42	0.52
51:3:11:A:O2'	51:3:13:A:OP2	2.28	0.52
56:MM:1005:CYS:HA	56:MM:1060:LEU:HB3	1.90	0.52
18:R:37:SER:HG	18:R:40:ALA:H	1.56	0.52
28:b:266:ALA:HA	28:b:269:LYS:HB2	1.90	0.52
2:A:193:ARG:NH1	50:1:2174:G:OP2	2.41	0.52
3:B:86:VAL:HA	3:B:162:VAL:HG12	1.90	0.52
3:B:325:LYS:NZ	50:1:3096:C:O3'	2.38	0.52
8:G:85:ASN:HD22	56:MM:524:TRP:HZ2	1.57	0.52
10:I:16:ARG:NH1	10:I:50:TYR:OH	2.42	0.52
12:L:98:ASP:OD2	12:L:101:ARG:N	2.41	0.52
12:L:188:ARG:NH1	12:L:192:GLU:OE1	2.43	0.52
26:Z:9:LYS:HB3	26:Z:25:ILE:HD12	1.90	0.52
26:Z:121:ARG:NH2	26:Z:127:ASN:OD1	2.42	0.52
39:m:260:ASN:ND2	39:m:326:THR:O	2.40	0.52
45:v:280:GLN:O	50:1:2271:A:N6	2.43	0.52
50:1:114:A:N1	50:1:266:A:O2'	2.42	0.52
50:1:1947:G:H1	50:1:2101:C:H42	1.57	0.52
22:V:104:ASN:OD1	22:V:108:GLU:N	2.43	0.52
39:m:10:ARG:HA	39:m:13:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:v:220:ARG:NH1	46:w:10:PRO:O	2.42	0.52
50:1:665:A:H61	50:1:797:U:H3	1.57	0.52
50:1:2405:C:N3	50:1:2817:A:N6	2.57	0.52
51:3:38:U:N3	51:3:41:G:OP2	2.42	0.52
52:4:247:ILE:HG23	52:4:252:ALA:HA	1.92	0.52
3:B:76:VAL:HA	3:B:325:LYS:HA	1.91	0.52
4:C:329:PRO:HB2	7:F:45:LEU:HD12	1.91	0.52
7:F:154:GLY:N	7:F:161:VAL:O	2.42	0.52
9:H:80:THR:OG1	9:H:86:TYR:OH	2.26	0.52
14:N:122:ASN:HB3	14:N:129:TYR:HD2	1.74	0.52
31:e:101:SER:OG	31:e:104:ASN:OD1	2.28	0.52
39:m:189:ASP:OD1	39:m:194:TRP:NE1	2.43	0.52
46:w:59:GLN:O	46:w:63:ASN:ND2	2.43	0.52
50:1:545:U:H5'	50:1:546:C:H5'	1.92	0.52
52:4:29:ARG:NH2	52:4:572:THR:OG1	2.43	0.52
52:4:80:TYR:HB3	52:4:84:VAL:HG12	1.91	0.52
56:MM:93:VAL:O	56:MM:113:VAL:N	2.38	0.52
1:2:141:C:O2	14:N:112:ASN:ND2	2.42	0.52
9:H:44:THR:OG1	50:1:3186:A:N3	2.33	0.52
9:H:173:ARG:NH2	50:1:2898:G:OP2	2.42	0.52
28:b:81:LEU:O	28:b:84:THR:OG1	2.27	0.52
35:i:86:LYS:NZ	50:1:296:A:OP1	2.43	0.52
40:n:136:LEU:HA	40:n:139:LEU:HD12	1.92	0.52
40:n:235:LYS:O	40:n:239:ASP:N	2.38	0.52
48:y:85:ARG:NH2	48:y:92:VAL:O	2.32	0.52
54:KK:95:SER:HB3	55:LL:47:LEU:HD13	1.90	0.52
56:MM:490:LEU:HA	56:MM:493:GLU:HB2	1.90	0.52
8:G:217:THR:O	8:G:221:ASN:ND2	2.42	0.52
39:m:102:ASP:HB2	39:m:105:GLN:HB2	1.91	0.52
47:x:61:GLU:OE2	47:x:124:ARG:NH2	2.42	0.52
47:x:156:SER:O	47:x:500:ARG:NH1	2.43	0.52
50:1:3154:C:O2'	50:1:3155:U:O2	2.18	0.52
52:4:274:GLN:HE22	52:4:335:VAL:HB	1.74	0.52
56:MM:588:ASN:ND2	56:MM:911:ILE:O	2.42	0.52
56:MM:928:PHE:HA	56:MM:931:LEU:HD12	1.92	0.52
2:A:156:LYS:NZ	50:1:2158:A:OP2	2.36	0.51
7:F:232:ARG:O	7:F:235:PHE:N	2.41	0.51
24:X:65:GLN:HE21	34:h:32:LYS:HD2	1.74	0.51
35:i:41:ARG:HH12	50:1:297:G:H2'	1.76	0.51
50:1:2124:G:H2'	50:1:2125:A:H8	1.75	0.51
50:1:2213:A:H2'	50:1:2214:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:3375:A:O2'	50:1:3378:C:OP2	2.26	0.51
3:B:284:ARG:HB3	3:B:323:MET:HB3	1.91	0.51
6:E:19:LYS:NZ	50:1:593:C:OP2	2.35	0.51
24:X:90:ALA:O	24:X:120:LYS:NZ	2.43	0.51
47:x:76:PRO:HB2	47:x:124:ARG:HD2	1.92	0.51
47:x:426:ILE:HB	47:x:440:PHE:HB2	1.92	0.51
47:x:463:SER:OG	47:x:464:LYS:N	2.41	0.51
50:1:277:G:H1	50:1:288:C:H42	1.57	0.51
52:4:114:LEU:O	52:4:118:ASN:ND2	2.43	0.51
5:D:151:GLN:HG2	5:D:159:VAL:HG21	1.92	0.51
7:F:241:LYS:NZ	50:1:576:C:OP1	2.37	0.51
21:U:81:LYS:NZ	50:1:1680:G:N7	2.57	0.51
28:b:236:GLU:O	28:b:239:SER:OG	2.25	0.51
39:m:366:ASP:OD1	39:m:366:ASP:N	2.42	0.51
50:1:2546:C:H2'	50:1:2547:A:H4'	1.92	0.51
51:3:81:U:H2'	51:3:82:G:C8	2.41	0.51
8:G:48:ARG:NH2	50:1:2588:U:OP1	2.40	0.51
18:R:134:HIS:HE1	18:R:136:ARG:HE	1.58	0.51
50:1:2742:C:H2'	50:1:2743:A:H8	1.75	0.51
56:MM:876:VAL:HG12	56:MM:878:GLN:H	1.75	0.51
3:B:85:VAL:HA	3:B:202:THR:HA	1.92	0.51
18:R:25:ASP:N	18:R:25:ASP:OD1	2.40	0.51
39:m:312:ASP:N	39:m:312:ASP:OD1	2.44	0.51
39:m:329:SER:N	59:m:501:GTP:O2B	2.35	0.51
39:m:357:THR:HG23	50:1:2962:U:H5''	1.92	0.51
50:1:2945:G:H4'	50:1:2946:A:H5''	1.93	0.51
50:1:3295:A:H2'	50:1:3296:A:H8	1.75	0.51
51:3:76:A:N6	51:3:103:A:OP2	2.38	0.51
52:4:546:GLN:H	52:4:551:GLN:HE22	1.59	0.51
14:N:46:ASP:N	14:N:46:ASP:OD1	2.41	0.51
22:V:68:GLU:O	22:V:72:LYS:NZ	2.44	0.51
28:b:359:ASN:OD1	48:y:170:GLN:NE2	2.43	0.51
46:w:102:GLU:HG2	46:w:103:LYS:HG3	1.92	0.51
47:x:258:GLY:HA2	47:x:281:VAL:HG23	1.92	0.51
1:2:128:U:O4	40:n:47:ARG:NH2	2.44	0.51
7:F:27:ALA:O	7:F:31:ALA:N	2.43	0.51
8:G:98:ARG:NH2	8:G:188:THR:O	2.44	0.51
8:G:147:LYS:NZ	56:MM:705:ARG:O	2.39	0.51
9:H:176:LEU:HD22	42:r:17:ARG:HA	1.93	0.51
13:M:90:VAL:O	13:M:94:TRP:N	2.44	0.51
16:P:62:ARG:NH1	50:1:412:G:OP1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:91:SER:O	18:R:95:TRP:N	2.43	0.51
39:m:328:LYS:NZ	59:m:501:GTP:O1B	2.43	0.51
56:MM:843:SER:OG	56:MM:844:MET:SD	2.68	0.51
20:T:64:VAL:HG22	20:T:74:VAL:HG22	1.93	0.51
34:h:103:LYS:NZ	50:1:154:U:OP2	2.44	0.51
52:4:155:SER:HB3	52:4:504:CYS:HB3	1.92	0.51
54:KK:97:ASP:OD2	56:MM:891:ARG:NH2	2.44	0.51
17:Q:74:GLU:HB2	50:1:741:U:H4'	1.93	0.51
28:b:359:ASN:ND2	48:y:165:THR:O	2.38	0.51
28:b:415:ASN:ND2	28:b:418:ASP:OD2	2.43	0.51
31:e:100:ILE:O	31:e:125:ARG:NH1	2.43	0.51
42:r:46:LYS:O	42:r:50:PHE:N	2.43	0.51
43:s:19:ILE:O	43:s:23:ALA:N	2.41	0.51
50:1:409:A:O2'	50:1:654:C:O2'	2.28	0.51
50:1:2534:G:H21	50:1:2548:C:H42	1.59	0.51
56:MM:790:VAL:O	56:MM:794:LEU:N	2.41	0.51
5:D:236:LEU:HA	5:D:239:ILE:HD12	1.92	0.51
12:L:18:TRP:NE1	50:1:799:G:O2'	2.38	0.51
20:T:130:ARG:NH1	50:1:1062:A:N3	2.57	0.51
23:W:123:ASP:N	23:W:211:SER:O	2.44	0.51
40:n:15:PHE:HB3	40:n:62:PHE:HB3	1.94	0.51
44:u:85:LEU:O	44:u:88:THR:OG1	2.28	0.51
47:x:194:TRP:HE1	47:x:198:GLY:HA2	1.75	0.51
50:1:675:C:O2'	50:1:679:U:OP1	2.29	0.51
50:1:829:U:H3	50:1:895:A:H62	1.57	0.51
50:1:3204:C:H2'	50:1:3205:G:C8	2.46	0.51
2:A:52:SER:HB3	2:A:191:LEU:HD13	1.93	0.50
7:F:88:ARG:HA	7:F:134:VAL:HG12	1.93	0.50
12:L:49:ARG:HD3	34:h:115:LYS:HA	1.93	0.50
14:N:94:TYR:OH	14:N:96:ARG:NH2	2.43	0.50
50:1:544:C:H2'	50:1:547:G:N1	2.27	0.50
50:1:2922:G:H5''	50:1:2923:U:H5''	1.93	0.50
50:1:2960:C:H2'	50:1:2961:G:H8	1.75	0.50
56:MM:531:TRP:NE1	56:MM:561:GLU:OE2	2.31	0.50
5:D:218:ARG:HH12	51:3:31:U:H4'	1.75	0.50
19:S:133:ALA:HB1	53:5:46:LEU:HD21	1.93	0.50
28:b:95:LEU:HD23	28:b:98:ILE:HD12	1.94	0.50
28:b:302:ARG:HH22	28:b:305:LEU:HB2	1.76	0.50
31:e:45:ARG:O	50:1:1145:G:O2'	2.29	0.50
45:v:220:ARG:NE	45:v:222:GLU:OE2	2.45	0.50
47:x:176:GLN:HG3	47:x:512:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2728:G:H1'	50:1:2729:U:H5''	1.92	0.50
51:3:12:U:OP2	51:3:68:C:O2'	2.28	0.50
53:5:92:TYR:O	53:5:96:ALA:N	2.43	0.50
56:MM:537:TYR:HA	56:MM:540:MET:HB2	1.93	0.50
4:C:141:ARG:HH11	4:C:180:LYS:HD2	1.75	0.50
4:C:326:ARG:NH1	50:1:608:A:O2'	2.45	0.50
17:Q:38:ARG:NH2	50:1:1348:U:OP2	2.37	0.50
26:Z:90:GLU:HA	26:Z:93:LYS:HG2	1.94	0.50
28:b:100:ARG:NH2	50:1:2860:U:OP1	2.44	0.50
28:b:419:LYS:NZ	48:y:35:TYR:OH	2.36	0.50
29:c:57:GLU:OE2	29:c:69:TYR:OH	2.28	0.50
29:c:73:GLY:N	29:c:76:GLU:OE2	2.43	0.50
48:y:106:ASN:OD1	48:y:150:SER:OG	2.28	0.50
50:1:1240:A:H2	50:1:1248:C:H41	1.59	0.50
56:MM:593:LEU:HD13	56:MM:601:PRO:HA	1.93	0.50
28:b:227:ARG:O	28:b:229:THR:N	2.38	0.50
31:e:112:ALA:HB1	31:e:117:ILE:HB	1.93	0.50
39:m:373:PRO:HG2	50:1:2867:C:H2'	1.94	0.50
43:s:32:LYS:NZ	50:1:1126:G:O6	2.44	0.50
49:z:17:LYS:NZ	50:1:3037:U:OP2	2.36	0.50
51:3:36:C:H5	53:5:106:ARG:HH22	1.60	0.50
52:4:545:PRO:HA	52:4:550:VAL:HG11	1.93	0.50
56:MM:247:TYR:O	56:MM:595:ARG:NH2	2.44	0.50
56:MM:297:PRO:HD3	56:MM:576:ALA:HB3	1.94	0.50
56:MM:891:ARG:HB2	56:MM:892:LEU:HD22	1.94	0.50
56:MM:1039:VAL:HG13	56:MM:1051:LYS:HE3	1.93	0.50
4:C:37:THR:O	4:C:40:THR:OG1	2.28	0.50
4:C:141:ARG:NH1	50:1:1385:C:OP1	2.44	0.50
14:N:136:ASP:OD1	14:N:138:GLN:NE2	2.44	0.50
16:P:70:THR:OG1	16:P:71:ALA:N	2.45	0.50
28:b:184:LEU:HD23	28:b:192:VAL:HG21	1.92	0.50
28:b:321:SER:HB3	28:b:324:LEU:HG	1.94	0.50
50:1:1343:A:H2'	50:1:1344:G:H8	1.77	0.50
4:C:4:PRO:HD2	4:C:22:LEU:HD12	1.92	0.50
4:C:302:ALA:HB2	17:Q:39:ARG:HH22	1.76	0.50
28:b:39:ILE:HA	28:b:42:ILE:HD12	1.93	0.50
31:e:83:GLU:O	31:e:86:THR:OG1	2.29	0.50
39:m:224:VAL:HG13	39:m:318:VAL:HB	1.93	0.50
39:m:353:TRP:HH2	42:r:166:VAL:HG21	1.76	0.50
50:1:2830:G:H2'	50:1:2831:G:C8	2.47	0.50
1:2:126:A:O2'	1:2:129:C:N4	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:PHE:HB2	3:B:314:TYR:HB3	1.92	0.50
4:C:119:ARG:NH2	50:1:696:C:OP2	2.38	0.50
5:D:150:LEU:HD12	11:J:143:ARG:HG3	1.94	0.50
5:D:218:ARG:HH22	51:3:31:U:H4'	1.76	0.50
18:R:20:ARG:NH2	50:1:1873:U:OP2	2.45	0.50
26:Z:33:SER:OG	26:Z:34:LYS:N	2.45	0.50
31:e:25:TYR:HB3	31:e:27:ARG:HD3	1.92	0.50
50:1:928:C:H2'	50:1:929:A:C8	2.47	0.50
52:4:122:ASP:N	52:4:122:ASP:OD1	2.43	0.50
22:V:127:PRO:O	22:V:131:SER:N	2.42	0.50
23:W:31:ARG:HA	23:W:34:LEU:HD12	1.94	0.50
34:h:82:ALA:HB1	34:h:84:LYS:HG3	1.92	0.50
39:m:240:LYS:O	39:m:242:VAL:N	2.33	0.50
39:m:381:ASP:OD1	39:m:406:ARG:NH2	2.45	0.50
50:1:268:A:H61	50:1:295:A:H3'	1.76	0.50
50:1:2218:G:H2'	50:1:2219:A:H8	1.76	0.50
53:5:96:ALA:HA	53:5:104:VAL:HG21	1.94	0.50
2:A:36:GLU:HG3	2:A:91:GLY:HA2	1.94	0.50
8:G:137:ASN:HD22	14:N:2:GLY:HA3	1.77	0.50
26:Z:5:LEU:HD21	26:Z:82:PRO:HB3	1.94	0.50
40:n:237:TYR:O	40:n:241:GLY:N	2.45	0.50
50:1:1468:A:N6	50:1:1508:C:O2	2.44	0.50
52:4:145:VAL:O	52:4:152:SER:N	2.44	0.50
53:5:83:ARG:O	53:5:87:GLU:N	2.41	0.50
8:G:54:GLU:O	8:G:58:VAL:N	2.38	0.49
12:L:28:GLN:HB3	14:N:201:ARG:HE	1.77	0.49
45:v:298:ASP:OD1	45:v:298:ASP:N	2.42	0.49
46:w:111:MET:N	46:w:111:MET:SD	2.85	0.49
47:x:79:PHE:HB3	47:x:119:LEU:HD11	1.93	0.49
50:1:544:C:O2	50:1:548:G:N1	2.45	0.49
50:1:551:A:O2'	50:1:552:G:O5'	2.30	0.49
50:1:3169:U:H2'	50:1:3170:A:H8	1.77	0.49
50:1:3283:U:H2'	50:1:3284:G:C8	2.46	0.49
52:4:121:LYS:HG2	52:4:350:ALA:HA	1.94	0.49
56:MM:100:THR:HG23	56:MM:329:TYR:HE1	1.77	0.49
56:MM:491:PHE:HZ	56:MM:513:ALA:HB2	1.77	0.49
2:A:67:TYR:OH	50:1:2525:G:N7	2.42	0.49
22:V:66:LYS:HB2	22:V:69:LEU:HD13	1.93	0.49
28:b:321:SER:OG	28:b:323:GLN:OE1	2.30	0.49
45:v:209:TYR:HB2	45:v:220:ARG:HB3	1.94	0.49
48:y:66:ASN:HD22	48:y:112:ASP:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2137:U:OP2	50:1:2142:A:N6	2.40	0.49
51:3:36:C:OP2	53:5:106:ARG:NH2	2.45	0.49
52:4:441:ARG:NH1	52:4:495:SER:O	2.45	0.49
1:2:80:A:H3'	1:2:81:U:H2'	1.95	0.49
4:C:33:ASP:N	4:C:33:ASP:OD1	2.46	0.49
5:D:68:THR:HG22	5:D:70:THR:H	1.77	0.49
13:M:23:ILE:O	13:M:30:GLY:N	2.37	0.49
19:S:14:LEU:HD21	20:T:136:ARG:HH22	1.77	0.49
32:f:86:ARG:NH2	50:1:498:A:O5'	2.44	0.49
45:v:99:ASN:OD1	45:v:116:LEU:N	2.45	0.49
47:x:163:ALA:H	47:x:189:VAL:HG23	1.77	0.49
47:x:305:ASP:OD2	47:x:308:SER:N	2.44	0.49
52:4:485:LEU:HA	52:4:488:LEU:HD12	1.95	0.49
56:MM:564:GLU:OE1	56:MM:566:GLN:NE2	2.45	0.49
56:MM:877:ILE:HG13	56:MM:878:GLN:HG3	1.93	0.49
25:Y:119:ILE:O	25:Y:124:GLY:N	2.37	0.49
27:a:64:GLN:HE21	27:a:67:HIS:HE1	1.59	0.49
27:a:71:PRO:HG2	27:a:109:TYR:HA	1.94	0.49
28:b:150:LEU:HA	28:b:153:VAL:HG22	1.94	0.49
28:b:250:VAL:HG13	28:b:283:VAL:HG13	1.94	0.49
48:y:114:VAL:HG22	48:y:136:GLU:HB2	1.94	0.49
50:1:358:G:N2	50:1:361:A:OP2	2.38	0.49
50:1:627:U:H2'	50:1:628:A:C8	2.48	0.49
50:1:2767:U:H2'	50:1:2768:U:H6	1.77	0.49
50:1:3295:A:H2'	50:1:3296:A:C8	2.47	0.49
4:C:186:LYS:NZ	50:1:1389:G:O6	2.39	0.49
5:D:36:LEU:O	5:D:39:GLN:NE2	2.46	0.49
14:N:54:LYS:NZ	50:1:114:A:OP1	2.46	0.49
23:W:161:LEU:HD23	50:1:1273:A:H2	1.78	0.49
25:Y:103:LYS:NZ	50:1:217:U:O2	2.39	0.49
50:1:86:G:O2'	50:1:98:G:O6	2.31	0.49
50:1:1073:U:O4	50:1:1084:A:N6	2.44	0.49
50:1:1261:G:O2'	50:1:1278:A:N1	2.45	0.49
56:MM:344:GLU:OE2	56:MM:552:ARG:NH1	2.44	0.49
4:C:338:LYS:O	4:C:340:GLY:N	2.36	0.49
7:F:98:LYS:NZ	50:1:985:U:OP1	2.38	0.49
11:J:18:VAL:HB	11:J:128:TYR:HB3	1.95	0.49
13:M:124:ARG:NH2	50:1:3212:C:OP2	2.45	0.49
15:O:161:LYS:NZ	50:1:3182:G:O3'	2.44	0.49
29:c:98:SER:OG	29:c:99:ASP:N	2.45	0.49
30:d:60:TRP:HZ3	30:d:64:VAL:HG12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:8:ARG:HH22	33:g:31:ARG:HD3	1.77	0.49
45:v:81:LYS:NZ	50:1:2697:A:N3	2.61	0.49
52:4:247:ILE:HD12	52:4:316:VAL:HG12	1.95	0.49
56:MM:835:LEU:HA	56:MM:838:ASN:HD22	1.77	0.49
56:MM:1013:ILE:HA	56:MM:1016:MET:HE2	1.94	0.49
1:2:150:G:OP1	24:X:27:ARG:NH2	2.46	0.49
3:B:100:ARG:NE	50:1:3244:A:OP2	2.45	0.49
4:C:151:VAL:HG22	4:C:250:TRP:HB2	1.95	0.49
9:H:20:ILE:HG21	9:H:45:PHE:HD2	1.77	0.49
56:MM:477:SER:HA	56:MM:484:LYS:HE2	1.94	0.49
56:MM:653:ILE:HA	56:MM:831:LEU:HD13	1.95	0.49
1:2:97:A:O2'	34:h:59:ASN:ND2	2.45	0.49
5:D:216:GLU:HA	5:D:219:PHE:HB3	1.94	0.49
5:D:232:ASP:O	5:D:235:SER:OG	2.31	0.49
14:N:68:ARG:NE	14:N:124:ASP:O	2.43	0.49
17:Q:69:ARG:NE	50:1:784:A:N7	2.61	0.49
38:l:9:ILE:HG22	38:l:13:MET:HE3	1.94	0.49
50:1:3303:G:O2'	50:1:3305:A:N7	2.39	0.49
52:4:69:ASP:HA	52:4:72:ILE:HD12	1.95	0.49
7:F:184:LEU:HD21	7:F:202:LEU:HD11	1.94	0.49
11:J:97:SER:OG	11:J:100:GLY:N	2.46	0.49
19:S:73:LYS:NZ	19:S:97:VAL:O	2.39	0.49
20:T:43:LYS:HG3	50:1:992:A:H5''	1.95	0.49
36:j:14:LYS:HE2	50:1:1491:A:H5''	1.94	0.49
40:n:237:TYR:O	40:n:242:LEU:N	2.38	0.49
40:n:410:GLN:HE21	40:n:424:ARG:HH21	1.60	0.49
48:y:122:ASP:OD1	48:y:122:ASP:N	2.43	0.49
50:1:1:G:H21	56:MM:950:LYS:HA	1.77	0.49
50:1:26:A:N3	50:1:328:U:O2'	2.41	0.49
50:1:371:G:N1	50:1:374:A:OP2	2.27	0.49
56:MM:703:ASN:ND2	56:MM:711:TYR:OH	2.45	0.49
11:J:52:TYR:OH	50:1:2679:A:O2'	2.30	0.49
21:U:39:ASP:N	21:U:39:ASP:OD1	2.45	0.49
21:U:89:LEU:HB3	21:U:93:ILE:HD12	1.95	0.49
28:b:577:THR:OG1	28:b:578:GLU:N	2.44	0.49
41:p:39:CYS:HB3	41:p:43:GLY:H	1.78	0.49
47:x:331:ASP:OD1	47:x:331:ASP:N	2.46	0.49
50:1:377:A:N6	50:1:400:G:O2'	2.46	0.49
50:1:629:U:H2'	50:1:630:A:C8	2.47	0.49
50:1:1894:U:H2'	50:1:1895:A:C8	2.48	0.49
50:1:2615:G:N2	50:1:2619:G:OP2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2655:U:H2'	50:1:2657:A:C5	2.48	0.49
2:A:181:LYS:HB2	50:1:860:G:C5	2.48	0.48
18:R:41:ILE:O	18:R:45:VAL:N	2.46	0.48
19:S:79:VAL:O	19:S:90:MET:N	2.45	0.48
23:W:177:ALA:O	23:W:179:LYS:N	2.46	0.48
30:d:80:ASN:ND2	30:d:84:ASP:OD1	2.46	0.48
33:g:92:ALA:HB2	50:1:2555:G:H1'	1.94	0.48
37:k:40:GLN:HE21	37:k:55:VAL:HG13	1.78	0.48
53:5:82:ARG:HG2	53:5:86:LYS:HE2	1.95	0.48
56:MM:701:ARG:N	56:MM:716:SER:O	2.37	0.48
56:MM:834:LYS:O	56:MM:838:ASN:N	2.46	0.48
1:2:27:U:H2'	1:2:28:C:H6	1.78	0.48
4:C:118:LYS:NZ	50:1:681:U:O4	2.41	0.48
5:D:274:GLN:OE1	51:3:60:G:N2	2.32	0.48
19:S:87:THR:OG1	19:S:88:HIS:N	2.45	0.48
24:X:92:LYS:NZ	50:1:1831:U:OP2	2.38	0.48
28:b:31:THR:HG23	28:b:32:VAL:HG23	1.94	0.48
28:b:254:MET:O	28:b:288:ASN:N	2.38	0.48
28:b:423:GLU:HB2	28:b:427:TRP:HZ2	1.78	0.48
42:r:5:ASP:N	42:r:5:ASP:OD1	2.44	0.48
48:y:28:VAL:HG12	48:y:50:HIS:HB3	1.93	0.48
48:y:82:GLN:HG3	48:y:86:ASN:HD21	1.77	0.48
50:1:353:G:O2'	50:1:364:G:O6	2.28	0.48
50:1:878:G:O2'	50:1:2980:U:O2	2.31	0.48
3:B:276:THR:HG21	50:1:3137:C:H5''	1.94	0.48
4:C:221:ASN:ND2	50:1:209:A:N3	2.62	0.48
8:G:192:GLN:O	40:n:96:ARG:NH1	2.40	0.48
11:J:15:GLU:HB3	11:J:130:VAL:HG23	1.95	0.48
47:x:35:LYS:O	47:x:119:LEU:N	2.34	0.48
50:1:516:A:H2'	50:1:517:G:C8	2.48	0.48
50:1:1740:U:H1'	50:1:1741:A:H2	1.79	0.48
50:1:3121:U:H1'	50:1:3122:A:H5''	1.94	0.48
2:A:54:ARG:HH22	50:1:2176:U:H5''	1.79	0.48
5:D:113:LEU:HG	5:D:115:LEU:HD23	1.95	0.48
6:E:52:VAL:HG11	6:E:65:ILE:HD12	1.95	0.48
13:M:38:ILE:HG13	13:M:44:VAL:HG12	1.94	0.48
19:S:2:ALA:N	50:1:1323:G:O3'	2.46	0.48
22:V:89:ASP:OD1	22:V:89:ASP:N	2.39	0.48
29:c:60:ALA:O	29:c:64:LYS:N	2.45	0.48
39:m:82:ARG:O	42:r:239:TRP:NE1	2.47	0.48
40:n:246:PRO:HB3	40:n:264:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:209:TYR:O	42:r:213:GLY:N	2.46	0.48
49:z:2:ALA:N	50:1:2891:U:HO2'	2.11	0.48
50:1:1065:A:H5''	50:1:1066:G:C8	2.49	0.48
56:MM:81:LEU:HB3	56:MM:122:GLN:HE21	1.79	0.48
5:D:30:TYR:O	5:D:34:LYS:N	2.46	0.48
9:H:21:LYS:NZ	50:1:3199:G:OP1	2.44	0.48
17:Q:66:ARG:NH1	50:1:744:A:OP1	2.40	0.48
24:X:31:THR:OG1	50:1:2523:A:OP1	2.28	0.48
28:b:114:ARG:NH2	50:1:2870:C:OP2	2.42	0.48
34:h:24:LEU:O	34:h:28:LEU:N	2.46	0.48
39:m:375:SER:OG	39:m:376:LYS:N	2.46	0.48
48:y:216:SER:O	48:y:220:SER:OG	2.27	0.48
50:1:1423:C:H2'	50:1:1424:C:H6	1.77	0.48
3:B:125:SER:O	3:B:127:LYS:NZ	2.46	0.48
28:b:178:VAL:HG13	28:b:255:ASP:HB2	1.96	0.48
30:d:57:GLN:NE2	50:1:1474:A:O3'	2.47	0.48
47:x:78:THR:HB	47:x:122:THR:HG23	1.96	0.48
50:1:998:A:H2'	50:1:999:G:C8	2.49	0.48
50:1:1340:G:H2'	50:1:1341:U:H6	1.79	0.48
56:MM:459:PRO:O	56:MM:463:HIS:ND1	2.39	0.48
56:MM:591:LEU:HD13	56:MM:905:GLY:HA2	1.95	0.48
2:A:40:TYR:N	50:1:2550:U:O4	2.41	0.48
6:E:40:LEU:HD13	6:E:84:VAL:HG11	1.95	0.48
11:J:133:ARG:NH1	11:J:153:LYS:O	2.39	0.48
14:N:99:ARG:NH2	14:N:118:SER:O	2.41	0.48
28:b:319:THR:O	28:b:327:ASN:ND2	2.47	0.48
47:x:139:ILE:N	47:x:510:VAL:O	2.44	0.48
50:1:544:C:H2'	50:1:547:G:H1	1.78	0.48
50:1:1378:U:N3	50:1:1430:U:O2	2.47	0.48
1:2:115:C:OP1	50:1:1830:G:N2	2.46	0.48
2:A:19:HIS:O	2:A:23:ARG:NH1	2.47	0.48
2:A:20:THR:O	2:A:20:THR:OG1	2.31	0.48
3:B:192:VAL:O	3:B:196:ARG:N	2.43	0.48
4:C:82:THR:OG1	50:1:355:A:N1	2.41	0.48
4:C:160:GLN:NE2	4:C:213:ASN:O	2.47	0.48
7:F:148:VAL:HG21	7:F:185:ILE:HG12	1.96	0.48
11:J:94:ARG:O	11:J:96:PHE:N	2.47	0.48
16:P:118:GLN:NE2	50:1:412:G:H21	2.12	0.48
28:b:366:PRO:HB3	48:y:178:GLN:HA	1.95	0.48
28:b:508:ARG:NH1	50:1:3073:A:O2'	2.46	0.48
48:y:187:ASN:OD1	48:y:210:THR:OG1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:LL:44:ARG:NH1	55:LL:44:ARG:O	2.42	0.48
4:C:203:ARG:NH1	4:C:226:GLU:OE2	2.47	0.48
6:E:78:ARG:NH2	50:1:3272:C:OP1	2.47	0.48
26:Z:15:ARG:HG3	26:Z:79:HIS:HD2	1.77	0.48
39:m:82:ARG:HB3	42:r:240:GLY:HA3	1.95	0.48
39:m:109:ARG:NE	50:1:2731:U:OP1	2.41	0.48
46:w:70:MET:N	46:w:70:MET:SD	2.86	0.48
50:1:659:G:H2'	50:1:1432:C:H42	1.78	0.48
50:1:1675:G:H2'	50:1:1676:A:H8	1.79	0.48
56:MM:91:ARG:NH1	56:MM:323:PRO:O	2.39	0.48
56:MM:1000:VAL:HG22	56:MM:1016:MET:HE3	1.96	0.48
4:C:45:ASN:HA	4:C:110:ASN:HD22	1.79	0.48
5:D:218:ARG:NH2	51:3:31:U:O2'	2.47	0.48
20:T:55:LYS:HB2	46:w:159:LEU:HD21	1.94	0.48
23:W:220:TYR:HD2	23:W:229:GLU:HB3	1.78	0.48
28:b:479:ASP:OD1	28:b:479:ASP:N	2.45	0.48
36:j:19:CYS:HB3	36:j:23:GLY:H	1.78	0.48
39:m:189:ASP:HA	39:m:192:ASN:HB2	1.96	0.48
39:m:336:ARG:NH1	39:m:357:THR:O	2.47	0.48
48:y:42:LEU:HD13	48:y:46:ILE:HD11	1.95	0.48
50:1:312:C:H2'	50:1:313:A:H8	1.79	0.48
50:1:994:G:N2	50:1:1056:U:O4	2.47	0.48
50:1:2396:G:H2'	50:1:2398:A:H5'	1.94	0.48
50:1:2439:A:H2'	50:1:2440:G:H8	1.79	0.48
3:B:173:GLN:HE21	50:1:3313:U:H4'	1.79	0.47
27:a:111:LYS:NZ	50:1:714:G:N7	2.45	0.47
38:l:28:ARG:HA	38:l:33:ASN:HD22	1.79	0.47
45:v:106:PHE:N	45:v:109:LYS:O	2.44	0.47
50:1:411:U:H2'	50:1:412:G:C8	2.49	0.47
50:1:710:A:H2'	50:1:711:A:C8	2.49	0.47
50:1:1236:G:N2	50:1:1244:A:OP1	2.46	0.47
56:MM:430:ASP:HA	56:MM:470:ARG:HG2	1.95	0.47
56:MM:868:ARG:HA	56:MM:871:SER:HB3	1.94	0.47
2:A:20:THR:HA	2:A:23:ARG:HH11	1.80	0.47
11:J:29:ARG:HH11	11:J:32:ARG:HH12	1.61	0.47
28:b:622:SER:HG	38:l:46:ARG:HH11	1.60	0.47
33:g:82:ALA:HA	33:g:85:VAL:HB	1.95	0.47
39:m:165:ASN:HA	39:m:168:ILE:HD12	1.95	0.47
41:p:46:THR:OG1	41:p:57:CYS:SG	2.66	0.47
42:r:186:HIS:ND1	42:r:188:GLU:O	2.46	0.47
47:x:325:HIS:CD2	47:x:408:VAL:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:791:A:H2'	50:1:792:G:H8	1.79	0.47
56:MM:789:THR:O	56:MM:793:SER:N	2.41	0.47
3:B:206:ASP:OD1	3:B:206:ASP:N	2.47	0.47
4:C:260:GLN:O	4:C:270:SER:OG	2.27	0.47
31:e:125:ARG:NH2	50:1:1393:A:OP1	2.38	0.47
40:n:20:GLN:NE2	50:1:1563:C:OP1	2.43	0.47
45:v:201:PHE:HD2	45:v:230:LEU:HB2	1.79	0.47
50:1:100:A:H3'	50:1:101:G:H21	1.78	0.47
50:1:297:G:OP2	50:1:297:G:N2	2.35	0.47
50:1:542:G:N2	50:1:549:U:O2	2.44	0.47
50:1:1230:G:H1	50:1:1279:C:N4	2.13	0.47
52:4:206:LYS:HD3	52:4:559:LEU:HD21	1.94	0.47
54:KK:93:ASP:OD2	56:MM:887:ARG:NH2	2.48	0.47
2:A:33:ASP:OD1	2:A:33:ASP:N	2.47	0.47
5:D:137:ASP:HA	5:D:138:GLY:HA3	1.69	0.47
7:F:159:GLN:HG2	50:1:1362:G:H1'	1.95	0.47
9:H:20:ILE:HG12	9:H:25:VAL:HG22	1.97	0.47
12:L:53:LEU:HB2	12:L:55:ARG:NH1	2.28	0.47
14:N:47:LYS:HD2	14:N:50:ARG:HD2	1.95	0.47
22:V:88:ARG:NH1	50:1:3095:U:OP1	2.47	0.47
47:x:410:PHE:O	47:x:452:TRP:NE1	2.48	0.47
50:1:563:U:H2'	50:1:564:G:C8	2.49	0.47
50:1:1481:A:O2'	50:1:1858:A:N3	2.39	0.47
52:4:203:THR:HG22	52:4:205:GLU:HB3	1.95	0.47
56:MM:261:PHE:N	56:MM:290:VAL:O	2.40	0.47
28:b:396:ARG:CZ	48:y:43:GLY:HA2	2.43	0.47
32:f:18:ARG:HA	32:f:23:ASN:HA	1.96	0.47
39:m:205:LYS:NZ	50:1:2923:U:OP1	2.37	0.47
46:w:132:MET:HG2	46:w:143:PRO:HB3	1.95	0.47
48:y:109:CYS:HB3	48:y:149:GLY:HA2	1.97	0.47
50:1:394:G:N1	50:1:397:A:OP2	2.48	0.47
3:B:61:ASP:OD2	28:b:413:ASN:ND2	2.48	0.47
10:I:14:ARG:NH2	10:I:17:ASP:OD1	2.48	0.47
18:R:23:TRP:CH2	18:R:25:ASP:HB3	2.49	0.47
19:S:14:LEU:HG	19:S:56:GLY:HA2	1.95	0.47
32:f:77:ASN:ND2	50:1:1326:A:O2'	2.47	0.47
40:n:418:LYS:HA	40:n:419:ASN:HA	1.64	0.47
41:p:37:TYR:HB2	41:p:47:VAL:HB	1.96	0.47
41:p:88:GLU:HA	41:p:91:GLU:HB2	1.96	0.47
44:u:61:LYS:HB3	44:u:62:GLU:H	1.60	0.47
52:4:453:ASN:HB3	52:4:484:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:5:96:ALA:HB2	53:5:104:VAL:HG11	1.95	0.47
56:MM:196:ILE:HB	56:MM:259:VAL:HG22	1.96	0.47
3:B:61:ASP:OD1	3:B:69:LYS:NZ	2.43	0.47
4:C:82:THR:HG23	4:C:84:ARG:H	1.80	0.47
7:F:160:ARG:HG3	7:F:203:TRP:CG	2.49	0.47
22:V:18:PRO:HA	22:V:51:ALA:HA	1.96	0.47
23:W:115:TYR:O	23:W:118:SER:OG	2.28	0.47
36:j:3:LYS:N	50:1:2138:A:O2'	2.44	0.47
37:k:3:ARG:HD3	37:k:52:TYR:HE1	1.79	0.47
39:m:136:SER:OG	39:m:137:TYR:N	2.43	0.47
42:r:181:LYS:HA	42:r:196:PRO:HA	1.95	0.47
50:1:58:G:H21	50:1:60:A:H1'	1.80	0.47
50:1:1281:G:H2'	50:1:1282:G:H8	1.80	0.47
50:1:1717:U:H2'	50:1:1718:G:C8	2.49	0.47
50:1:1778:G:O2'	50:1:1780:G:OP2	2.33	0.47
50:1:2108:C:H1'	50:1:3344:A:H8	1.80	0.47
50:1:2519:A:H2'	50:1:2520:A:H8	1.80	0.47
50:1:2657:A:H2'	50:1:2658:G:C8	2.50	0.47
50:1:2738:A:H2'	50:1:2739:A:H8	1.79	0.47
50:1:3086:A:H3'	50:1:3087:A:H8	1.78	0.47
51:3:19:C:H2'	51:3:20:A:H8	1.79	0.47
52:4:347:SER:HB3	52:4:349:LYS:HG2	1.97	0.47
56:MM:933:PRO:HG3	56:MM:1053:LYS:HG3	1.96	0.47
3:B:69:LYS:NZ	28:b:413:ASN:OD1	2.47	0.47
3:B:284:ARG:NH2	3:B:293:ASN:O	2.47	0.47
6:E:40:LEU:HD11	6:E:54:TYR:HB2	1.97	0.47
11:J:92:ARG:HB2	11:J:95:ASN:HD22	1.80	0.47
19:S:57:GLU:OE1	20:T:136:ARG:NH2	2.47	0.47
19:S:129:ILE:HA	43:s:56:TYR:HE2	1.79	0.47
25:Y:59:VAL:HG13	25:Y:60:ARG:HG2	1.97	0.47
32:f:17:GLN:N	32:f:27:VAL:O	2.48	0.47
42:r:209:TYR:HB3	42:r:214:VAL:HB	1.95	0.47
44:u:45:ASN:HD22	44:u:46:PRO:HD2	1.80	0.47
50:1:526:C:H2'	50:1:527:A:H8	1.80	0.47
50:1:1288:U:H2'	50:1:1289:G:H8	1.79	0.47
50:1:2662:G:H2'	50:1:2663:G:C8	2.50	0.47
56:MM:1070:SER:HB2	56:MM:1073:LEU:HG	1.97	0.47
2:A:14:SER:OG	2:A:15:ILE:N	2.46	0.47
15:O:91:LYS:NZ	50:1:2382:G:N7	2.55	0.47
23:W:175:ILE:HG22	23:W:180:ILE:HA	1.97	0.47
25:Y:54:ASP:OD1	25:Y:54:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:208:SER:HB2	39:m:211:ILE:HB	1.96	0.47
39:m:355:TYR:HE2	42:r:166:VAL:H	1.62	0.47
42:r:164:ARG:HB2	50:1:2727:A:C8	2.49	0.47
50:1:727:G:OP2	50:1:742:G:N2	2.40	0.47
50:1:901:G:H2'	50:1:902:G:H8	1.79	0.47
50:1:1200:A:H2	50:1:2824:G:H22	1.63	0.47
50:1:1718:G:H2'	50:1:1719:G:H8	1.80	0.47
50:1:2146:C:H2'	50:1:2147:A:C8	2.50	0.47
1:2:66:A:H5'	34:h:10:ARG:HH22	1.78	0.47
2:A:116:VAL:HG13	2:A:126:LEU:HB2	1.97	0.47
7:F:112:ASN:ND2	7:F:209:ASN:OD1	2.48	0.47
26:Z:76:ASN:HB3	26:Z:79:HIS:ND1	2.30	0.47
28:b:529:GLY:HA2	28:b:532:GLU:HB2	1.95	0.47
30:d:40:ALA:O	30:d:44:MET:N	2.37	0.47
40:n:3:ILE:H	40:n:3:ILE:HG13	1.52	0.47
46:w:17:ILE:HD12	46:w:32:ASN:HA	1.97	0.47
50:1:504:A:H2'	50:1:505:G:H8	1.80	0.47
50:1:528:U:H2'	50:1:529:A:C8	2.50	0.47
50:1:1322:U:H2'	50:1:1323:G:C8	2.50	0.47
50:1:1699:A:H2'	50:1:1700:G:H8	1.80	0.47
50:1:1922:A:H62	50:1:1929:G:H21	1.62	0.47
52:4:60:THR:HG22	52:4:62:PRO:HD2	1.97	0.47
56:MM:647:HIS:HA	56:MM:850:TYR:HE1	1.80	0.47
56:MM:840:LEU:HA	56:MM:843:SER:HB3	1.97	0.47
12:L:141:ALA:O	12:L:145:PHE:N	2.42	0.46
23:W:57:ARG:NH1	50:1:1259:A:OP1	2.40	0.46
23:W:126:ARG:NH2	50:1:1230:G:OP1	2.44	0.46
26:Z:46:ILE:HA	26:Z:70:PRO:HA	1.96	0.46
40:n:430:GLN:HA	40:n:433:PHE:HD2	1.80	0.46
50:1:628:A:H5'	50:1:1399:A:N1	2.30	0.46
50:1:1635:G:N2	50:1:1638:A:OP2	2.38	0.46
50:1:2738:A:H2'	50:1:2739:A:C8	2.50	0.46
1:2:151:C:C2	24:X:22:LYS:HG3	2.51	0.46
5:D:148:ILE:HD13	50:1:2746:A:H61	1.80	0.46
14:N:188:ARG:HH21	50:1:30:G:H5''	1.81	0.46
23:W:96:CYS:HB2	23:W:100:THR:HG21	1.96	0.46
39:m:13:ARG:NH2	50:1:2418:G:N7	2.63	0.46
47:x:514:THR:OG1	47:x:515:HIS:N	2.49	0.46
50:1:2949:U:H2'	50:1:2950:G:C8	2.50	0.46
4:C:150:LEU:HD21	4:C:172:VAL:HG11	1.98	0.46
12:L:75:PHE:H	12:L:97:VAL:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:27:VAL:HG23	14:N:129:TYR:HE2	1.80	0.46
17:Q:123:THR:OG1	17:Q:125:ASP:OD1	2.30	0.46
22:V:104:ASN:HD21	22:V:108:GLU:HB2	1.79	0.46
23:W:170:GLU:HB3	23:W:198:ARG:HH11	1.79	0.46
34:h:38:ARG:CZ	52:4:343:TYR:HB3	2.46	0.46
36:j:28:HIS:N	36:j:33:THR:O	2.45	0.46
44:u:106:ALA:HA	44:u:109:LYS:HD3	1.98	0.46
49:z:5:LEU:HD21	50:1:3099:C:H2'	1.97	0.46
50:1:1445:U:H3'	50:1:1446:A:H8	1.80	0.46
2:A:2:GLY:N	50:1:2415:C:OP1	2.49	0.46
4:C:203:ARG:HB3	4:C:246:ARG:HH21	1.81	0.46
16:P:78:VAL:HG12	16:P:80:LYS:H	1.79	0.46
19:S:74:ASN:HD21	19:S:95:ARG:HH11	1.63	0.46
27:a:59:ARG:NH2	50:1:90:C:OP2	2.48	0.46
28:b:284:MET:HE1	28:b:334:LYS:HB3	1.98	0.46
28:b:508:ARG:O	30:d:61:LYS:NZ	2.35	0.46
37:k:29:LYS:HE2	37:k:37:PRO:HB3	1.97	0.46
39:m:131:ILE:N	50:1:2861:U:O4	2.48	0.46
39:m:280:GLU:OE1	39:m:280:GLU:N	2.48	0.46
44:u:115:ASN:O	44:u:119:ASP:N	2.42	0.46
50:1:541:U:H2'	50:1:542:G:C8	2.50	0.46
50:1:1390:A:H4'	50:1:1391:C:H5''	1.97	0.46
50:1:2261:G:O2'	50:1:2263:C:N4	2.46	0.46
52:4:410:GLN:HA	52:4:413:LYS:HB2	1.97	0.46
4:C:342:LYS:O	50:1:515:C:O2'	2.31	0.46
19:S:155:ARG:N	19:S:170:THR:OG1	2.49	0.46
24:X:37:THR:OG1	24:X:38:LEU:N	2.48	0.46
39:m:276:HIS:NE2	39:m:469:PRO:O	2.48	0.46
45:v:151:HIS:HB3	45:v:154:TYR:HD2	1.81	0.46
50:1:2568:C:O2'	50:1:2569:A:O4'	2.32	0.46
54:KK:16:VAL:HG21	55:LL:21:LEU:HD22	1.98	0.46
56:MM:222:MET:HG2	56:MM:227:THR:HG23	1.97	0.46
56:MM:963:LEU:HD21	56:MM:967:ARG:HH21	1.81	0.46
56:MM:1040:ASP:HA	56:MM:1043:ASN:HD22	1.81	0.46
10:I:3:ARG:NH2	50:1:1894:U:OP1	2.45	0.46
13:M:127:LYS:O	13:M:130:THR:OG1	2.27	0.46
22:V:12:ARG:HB2	50:1:3040:A:H5''	1.97	0.46
23:W:35:ASP:N	23:W:35:ASP:OD1	2.39	0.46
26:Z:23:VAL:HG12	26:Z:45:GLY:HA3	1.97	0.46
27:a:117:ARG:HG3	50:1:716:A:N7	2.30	0.46
28:b:99:SER:OG	50:1:2865:U:O4	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:434:GLU:OE2	48:y:79:GLN:NE2	2.49	0.46
40:n:169:TYR:HB2	40:n:237:TYR:HE1	1.81	0.46
40:n:431:TRP:NE1	40:n:442:VAL:O	2.44	0.46
46:w:11:VAL:HG23	46:w:12:THR:HG23	1.96	0.46
47:x:282:SER:H	47:x:296:SER:HA	1.79	0.46
47:x:500:ARG:HD3	47:x:512:LEU:HD13	1.96	0.46
50:1:409:A:HO2'	50:1:654:C:HO2'	1.56	0.46
50:1:1232:C:H2'	50:1:1233:G:H8	1.80	0.46
50:1:1597:C:H2'	50:1:1598:G:H8	1.81	0.46
50:1:1687:U:H5''	50:1:1688:U:H5'	1.97	0.46
50:1:2752:U:H2'	50:1:2753:G:C8	2.50	0.46
50:1:2999:U:H3	50:1:3149:G:H1	1.64	0.46
50:1:3138:U:H2'	50:1:3139:A:C8	2.49	0.46
50:1:3234:A:H2	50:1:3253:G:H22	1.62	0.46
52:4:270:THR:H	52:4:273:HIS:CD2	2.27	0.46
56:MM:559:ILE:HG12	56:MM:561:GLU:H	1.81	0.46
2:A:211:HIS:ND1	50:1:2185:G:OP1	2.39	0.46
5:D:165:GLY:O	5:D:169:GLY:N	2.44	0.46
12:L:131:LYS:HG3	12:L:133:PRO:HD3	1.96	0.46
26:Z:51:LEU:HB2	26:Z:65:ARG:HD2	1.97	0.46
30:d:77:ARG:HG2	30:d:89:LEU:HD23	1.98	0.46
45:v:202:ARG:CZ	45:v:229:ARG:HG3	2.46	0.46
50:1:571:U:H2'	50:1:572:A:H8	1.80	0.46
54:KK:40:LYS:O	54:KK:44:SER:N	2.46	0.46
56:MM:449:ALA:O	56:MM:456:ARG:NH2	2.40	0.46
4:C:334:PHE:HA	4:C:339:LEU:HD12	1.97	0.46
11:J:49:LYS:HA	11:J:64:LYS:HA	1.98	0.46
11:J:57:PHE:HB2	11:J:59:ILE:HG12	1.98	0.46
12:L:52:ASP:OD2	12:L:141:ALA:N	2.46	0.46
31:e:102:ALA:HA	31:e:105:ARG:HD3	1.98	0.46
40:n:211:SER:HA	40:n:215:PHE:HE2	1.80	0.46
48:y:160:LEU:HD11	48:y:184:GLY:HA3	1.97	0.46
50:1:1119:C:H2'	50:1:1120:A:H8	1.79	0.46
50:1:2810:C:OP2	50:1:2955:U:O2'	2.33	0.46
1:2:71:A:OP2	25:Y:51:ARG:NH1	2.48	0.46
9:H:41:ILE:HG23	9:H:43:VAL:HG13	1.98	0.46
9:H:49:ASN:O	9:H:51:GLN:N	2.48	0.46
9:H:189:GLU:HA	9:H:190:ASP:HA	1.69	0.46
12:L:123:ILE:HG22	34:h:118:ILE:HG12	1.97	0.46
18:R:20:ARG:NH1	50:1:1874:A:N7	2.64	0.46
27:a:85:ASP:OD1	27:a:85:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:587:ASP:OD1	28:b:587:ASP:N	2.45	0.46
40:n:248:LEU:HA	40:n:262:TYR:HA	1.98	0.46
45:v:66:ILE:HG21	45:v:75:LEU:HD21	1.97	0.46
52:4:409:LEU:O	52:4:413:LYS:N	2.41	0.46
53:5:73:GLN:HA	53:5:76:ILE:HD12	1.97	0.46
56:MM:567:VAL:O	56:MM:571:MET:N	2.44	0.46
56:MM:679:LEU:O	56:MM:771:GLY:N	2.42	0.46
3:B:160:VAL:N	3:B:181:ILE:O	2.47	0.46
11:J:84:LEU:HA	11:J:87:LYS:HB3	1.97	0.46
22:V:86:ARG:NH1	22:V:88:ARG:HH11	2.14	0.46
29:c:76:GLU:O	29:c:80:ALA:N	2.49	0.46
37:k:12:LEU:O	37:k:15:THR:OG1	2.30	0.46
38:l:27:ILE:O	38:l:33:ASN:ND2	2.49	0.46
47:x:468:LEU:HD12	47:x:482:LEU:HD11	1.98	0.46
50:1:33:G:N1	50:1:50:U:OP2	2.38	0.46
50:1:541:U:H2'	50:1:542:G:H8	1.79	0.46
50:1:1497:C:H2'	50:1:1498:A:H8	1.81	0.46
50:1:2389:C:H2'	50:1:2390:A:H8	1.81	0.46
50:1:3008:A:H2'	50:1:3009:G:H8	1.81	0.46
52:4:362:ARG:HH22	52:4:431:LEU:HD22	1.81	0.46
56:MM:87:GLN:HE22	56:MM:152:PRO:HB2	1.81	0.46
56:MM:869:LYS:O	56:MM:873:SER:OG	2.26	0.46
2:A:147:ARG:HA	2:A:157:VAL:HA	1.98	0.45
3:B:20:LYS:NZ	3:B:21:ARG:O	2.49	0.45
10:I:18:LEU:HD22	10:I:80:LEU:HD21	1.98	0.45
10:I:32:GLN:HG2	10:I:36:ASN:HD21	1.81	0.45
38:l:6:SER:HB2	38:l:9:ILE:HG12	1.98	0.45
40:n:420:LYS:HB2	40:n:426:TYR:CZ	2.51	0.45
42:r:66:LYS:HE2	42:r:70:GLN:HE21	1.80	0.45
46:w:53:LEU:HG	46:w:57:ASN:HD21	1.81	0.45
50:1:671:U:H2'	50:1:672:A:C8	2.49	0.45
50:1:1200:A:O2'	50:1:1201:C:O2	2.29	0.45
50:1:1597:C:H2'	50:1:1598:G:C8	2.51	0.45
50:1:2108:C:H1'	50:1:3344:A:C8	2.50	0.45
50:1:2444:C:H5'	50:1:2445:A:C5	2.51	0.45
52:4:361:VAL:HG22	52:4:389:PRO:HB3	1.98	0.45
54:KK:23:LEU:HD23	55:LL:67:VAL:HG22	1.98	0.45
54:KK:40:LYS:HA	54:KK:43:LYS:HB3	1.98	0.45
5:D:262:LYS:NZ	51:3:1:G:O6	2.43	0.45
14:N:152:CYS:HB2	34:h:92:LEU:HD11	1.97	0.45
19:S:141:LYS:HA	19:S:144:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:x:383:MET:O	47:x:398:MET:N	2.48	0.45
2:A:152:SER:OG	50:1:2157:G:N7	2.47	0.45
5:D:52:VAL:HA	5:D:147:ASP:HB3	1.98	0.45
8:G:155:ASN:HD21	8:G:181:LYS:HG3	1.82	0.45
18:R:21:LYS:HA	18:R:53:LYS:HD2	1.98	0.45
19:S:2:ALA:HA	50:1:1324:U:H5'	1.98	0.45
28:b:288:ASN:HD22	28:b:289:LYS:N	2.13	0.45
28:b:489:ILE:HG23	44:u:127:VAL:HG21	1.98	0.45
30:d:84:ASP:OD2	30:d:87:ASN:N	2.30	0.45
35:i:60:LEU:HD13	35:i:64:SER:HB3	1.98	0.45
38:l:10:LYS:NZ	50:1:1834:U:OP2	2.39	0.45
47:x:144:SER:OG	47:x:165:ASP:N	2.50	0.45
47:x:295:GLY:HA2	47:x:301:VAL:HG22	1.99	0.45
50:1:273:A:H2'	50:1:274:G:H8	1.81	0.45
50:1:1343:A:H2'	50:1:1344:G:C8	2.51	0.45
50:1:2535:A:H3'	50:1:2536:A:H8	1.81	0.45
50:1:2821:C:OP2	50:1:2825:C:N4	2.43	0.45
56:MM:357:MET:SD	56:MM:563:MET:N	2.88	0.45
1:2:24:G:OP2	25:Y:13:ARG:NH2	2.39	0.45
2:A:15:ILE:HD12	2:A:194:ASN:HD22	1.81	0.45
3:B:105:VAL:HG11	3:B:148:LEU:HD11	1.99	0.45
6:E:38:THR:OG1	6:E:90:LYS:NZ	2.46	0.45
6:E:68:PRO:HG3	6:E:145:LEU:HD23	1.98	0.45
22:V:73:VAL:O	39:m:194:TRP:HB2	2.16	0.45
28:b:82:MET:O	28:b:86:TYR:N	2.44	0.45
35:i:4:LYS:HA	35:i:12:ASN:HB3	1.98	0.45
42:r:43:THR:HG22	50:1:1299:U:H4'	1.97	0.45
43:s:10:ARG:NH2	50:1:1308:A:O2'	2.50	0.45
46:w:147:TYR:HA	50:1:2656:A:N7	2.32	0.45
50:1:1062:A:H5''	50:1:1063:G:H5''	1.97	0.45
50:1:1440:G:H2'	50:1:1441:G:H8	1.81	0.45
50:1:2667:A:N6	50:1:2668:U:O2	2.49	0.45
52:4:509:LEU:HD23	52:4:522:LEU:HD13	1.98	0.45
5:D:176:SER:N	50:1:2746:A:O2'	2.36	0.45
10:I:13:ARG:NH2	50:1:2333:C:OP1	2.40	0.45
10:I:85:TYR:OH	44:u:7:HIS:O	2.30	0.45
12:L:48:PRO:HG2	34:h:115:LYS:HD3	1.98	0.45
30:d:10:ARG:HG2	30:d:108:VAL:HG22	1.99	0.45
31:e:34:LYS:NZ	31:e:52:GLN:OE1	2.44	0.45
39:m:418:ILE:HD12	39:m:430:ILE:HG22	1.99	0.45
47:x:37:GLN:HB3	47:x:120:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:y:185:THR:HB	48:y:189:GLY:HA2	1.99	0.45
50:1:628:A:H4'	50:1:1399:A:N6	2.32	0.45
50:1:720:A:O2'	50:1:784:A:OP2	2.29	0.45
50:1:1506:A:H5''	50:1:1507:G:H5''	1.98	0.45
50:1:2689:A:H2'	50:1:2691:A:C8	2.51	0.45
50:1:3314:A:H2'	50:1:3315:G:H8	1.81	0.45
51:3:38:U:H3	51:3:40:C:H3'	1.81	0.45
52:4:343:TYR:H	52:4:354:ILE:HD11	1.82	0.45
53:5:74:ALA:O	53:5:77:THR:OG1	2.28	0.45
56:MM:343:ASP:OD1	56:MM:347:THR:N	2.37	0.45
4:C:299:ILE:HG22	4:C:300:ARG:O	2.16	0.45
6:E:80:ASN:HD21	50:1:500:C:H4'	1.81	0.45
12:L:33:VAL:HG12	12:L:37:ASN:HD21	1.81	0.45
23:W:92:LEU:HD23	23:W:228:VAL:HG22	1.98	0.45
28:b:53:THR:HG21	28:b:133:LEU:HD22	1.98	0.45
39:m:144:LYS:NZ	50:1:1249:G:OP1	2.41	0.45
40:n:18:ARG:HG2	40:n:63:TYR:HE2	1.80	0.45
41:p:44:LYS:NZ	50:1:1727:G:OP1	2.42	0.45
42:r:23:ARG:NH1	50:1:3109:G:OP1	2.50	0.45
47:x:411:SER:N	47:x:416:TYR:O	2.49	0.45
50:1:1743:G:H2'	50:1:1744:G:H8	1.82	0.45
50:1:3146:G:H2'	50:1:3147:G:C8	2.51	0.45
1:2:1:A:N1	50:1:2994:A:O2'	2.45	0.45
1:2:94:C:OP1	36:j:75:LYS:NZ	2.41	0.45
5:D:54:ARG:NE	51:3:6:C:OP1	2.43	0.45
17:Q:92:ARG:NH1	50:1:784:A:O2'	2.50	0.45
28:b:90:HIS:NE2	39:m:135:GLU:O	2.48	0.45
34:h:38:ARG:CZ	34:h:41:LEU:HD13	2.47	0.45
39:m:109:ARG:NH1	50:1:2720:G:OP1	2.45	0.45
39:m:207:GLN:H	39:m:212:TRP:HE1	1.63	0.45
45:v:121:ASN:ND2	45:v:231:ASP:OD2	2.48	0.45
50:1:415:G:H2'	50:1:416:A:H8	1.82	0.45
50:1:532:A:H2	50:1:560:G:H22	1.64	0.45
50:1:1094:U:O2'	50:1:1096:U:O5'	2.34	0.45
50:1:1660:C:H2'	50:1:1661:G:H8	1.80	0.45
50:1:2586:G:O2'	50:1:2588:U:OP2	2.32	0.45
50:1:2766:U:H2'	50:1:2767:U:C6	2.52	0.45
52:4:140:LYS:HD2	52:4:502:ARG:HB3	1.99	0.45
3:B:331:ASN:OD1	3:B:334:ARG:NE	2.29	0.45
3:B:374:ALA:O	3:B:378:ALA:N	2.50	0.45
4:C:293:SER:O	4:C:297:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:82:LYS:H	7:F:82:LYS:HG2	1.60	0.45
10:I:63:ALA:O	10:I:66:THR:OG1	2.32	0.45
14:N:175:ASN:HB2	14:N:180:PHE:CE2	2.52	0.45
20:T:130:ARG:NE	50:1:1098:A:OP1	2.35	0.45
22:V:135:VAL:HA	48:y:102:SER:HB3	1.98	0.45
28:b:287:ILE:HD11	28:b:317:ILE:HB	1.98	0.45
42:r:243:ALA:HB2	42:r:259:LEU:HD23	1.97	0.45
49:z:46:LEU:HD23	49:z:49:LEU:HD12	1.99	0.45
50:1:1472:U:H2'	50:1:1473:G:H8	1.82	0.45
50:1:2251:G:H1	50:1:2266:U:H3	1.63	0.45
50:1:3044:G:H2'	50:1:3045:G:C8	2.52	0.45
50:1:3351:U:H2'	50:1:3353:G:H21	1.81	0.45
4:C:116:ASN:HD21	50:1:675:C:H5'	1.81	0.45
4:C:308:LYS:NZ	50:1:594:U:O2'	2.49	0.45
6:E:23:LYS:NZ	50:1:611:A:O4'	2.50	0.45
18:R:108:LYS:O	18:R:112:ALA:N	2.46	0.45
20:T:136:ARG:HD3	20:T:136:ARG:H	1.82	0.45
28:b:329:MET:O	28:b:333:ASN:ND2	2.50	0.45
47:x:39:LEU:HD12	47:x:122:THR:HB	1.98	0.45
50:1:1563:C:H2'	50:1:1564:U:H6	1.82	0.45
50:1:2568:C:H2'	50:1:2569:A:C4	2.52	0.45
50:1:2872:A:H61	50:1:2925:C:H2'	1.82	0.45
14:N:24:ARG:HH12	50:1:2435:G:H4'	1.81	0.45
33:g:60:ARG:HG2	50:1:1593:A:H4'	1.98	0.45
40:n:47:ARG:HE	50:1:1620:U:H5'	1.81	0.45
45:v:144:GLN:OE1	45:v:185:THR:OG1	2.30	0.45
47:x:366:LYS:NZ	47:x:414:GLY:O	2.49	0.45
50:1:972:A:H2'	50:1:973:A:C8	2.53	0.45
50:1:1193:A:O2'	50:1:1298:C:OP1	2.32	0.45
50:1:2768:U:H2'	50:1:2769:A:H8	1.82	0.45
52:4:62:PRO:HB3	52:4:106:PRO:HG2	1.99	0.45
52:4:316:VAL:HG22	52:4:508:VAL:HG22	1.99	0.45
56:MM:913:SER:N	56:MM:1037:GLU:OE2	2.50	0.45
56:MM:1039:VAL:O	56:MM:1043:ASN:ND2	2.50	0.45
3:B:252:ILE:HG22	50:1:2394:G:H5'	1.99	0.44
5:D:19:PRO:HD2	5:D:24:ARG:HD3	1.99	0.44
12:L:24:VAL:HG12	14:N:199:LEU:HB2	1.99	0.44
14:N:112:ASN:OD1	14:N:112:ASN:N	2.48	0.44
25:Y:35:LEU:HD11	25:Y:48:LEU:HG	1.99	0.44
28:b:410:GLY:HA3	50:1:3037:U:H1'	1.99	0.44
40:n:249:ASP:HB3	40:n:252:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:u:77:VAL:HA	44:u:78:PRO:HD3	1.74	0.44
50:1:182:U:H2'	50:1:183:G:H8	1.82	0.44
50:1:1220:U:OP2	53:5:51:ARG:NH2	2.45	0.44
50:1:1427:U:H2'	50:1:1428:A:C8	2.52	0.44
56:MM:296:ILE:HG13	56:MM:299:ALA:HB2	2.00	0.44
56:MM:703:ASN:HB2	56:MM:711:TYR:HE2	1.83	0.44
56:MM:879:LEU:HD23	56:MM:882:LEU:HD23	2.00	0.44
5:D:95:TRP:N	51:3:47:C:OP1	2.50	0.44
5:D:152:ARG:HG3	51:3:44:C:H4'	1.98	0.44
8:G:137:ASN:O	8:G:141:ALA:N	2.41	0.44
14:N:192:LYS:O	14:N:196:THR:OG1	2.27	0.44
19:S:6:GLU:HG2	19:S:64:ILE:HD12	1.98	0.44
28:b:83:ASP:HB2	28:b:88:LYS:HB2	1.99	0.44
33:g:6:THR:HG22	50:1:1486:G:H21	1.82	0.44
39:m:7:GLU:OE1	39:m:10:ARG:NH1	2.49	0.44
41:p:49:ARG:HB2	41:p:55:TRP:CZ3	2.52	0.44
50:1:952:A:OP2	50:1:1143:A:N6	2.42	0.44
50:1:2438:A:H2'	50:1:2439:A:C8	2.52	0.44
51:3:71:G:H2'	51:3:72:A:C8	2.53	0.44
52:4:183:ALA:HB2	52:4:325:SER:HB3	1.98	0.44
52:4:391:LYS:H	52:4:394:HIS:CD2	2.35	0.44
53:5:66:ASP:O	53:5:70:GLU:N	2.42	0.44
56:MM:489:ILE:O	56:MM:493:GLU:N	2.48	0.44
56:MM:682:ILE:O	56:MM:690:TYR:N	2.42	0.44
3:B:198:HIS:CE1	49:z:41:LEU:HD11	2.53	0.44
8:G:34:PHE:HA	8:G:39:ALA:HB3	1.99	0.44
9:H:49:ASN:OD1	9:H:49:ASN:N	2.50	0.44
9:H:104:VAL:O	9:H:111:PHE:N	2.50	0.44
11:J:137:ARG:HG2	11:J:141:ARG:HB3	1.98	0.44
12:L:34:SER:HA	12:L:37:ASN:HD22	1.82	0.44
14:N:155:VAL:HG12	50:1:58:G:H4'	1.98	0.44
16:P:74:LYS:NZ	50:1:3310:A:OP1	2.34	0.44
19:S:5:LYS:N	19:S:31:ALA:O	2.43	0.44
40:n:57:THR:O	50:1:1810:A:O2'	2.27	0.44
40:n:412:VAL:HG13	40:n:449:PRO:HG3	2.00	0.44
42:r:161:PHE:O	42:r:164:ARG:NH1	2.48	0.44
50:1:3291:G:H2'	50:1:3292:A:C8	2.52	0.44
51:3:4:U:H2'	51:3:5:G:C8	2.52	0.44
4:C:234:ASN:HD21	4:C:236:LEU:HB2	1.81	0.44
8:G:186:LEU:HD23	8:G:189:LEU:HD21	2.00	0.44
18:R:62:ARG:NH1	50:1:3067:C:O5'	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:16:LEU:HB3	29:c:98:SER:HB2	1.98	0.44
32:f:15:SER:OG	32:f:16:TYR:N	2.49	0.44
39:m:50:ASN:OD1	39:m:54:ASN:N	2.33	0.44
41:p:83:ILE:O	41:p:87:ARG:N	2.46	0.44
42:r:88:PRO:HD2	42:r:91:LEU:HD12	1.98	0.44
50:1:155:G:H5'	50:1:156:G:C8	2.53	0.44
50:1:253:A:H2'	50:1:254:A:C8	2.52	0.44
50:1:1211:U:H2'	50:1:1212:A:C8	2.51	0.44
50:1:2627:C:H2'	50:1:2628:A:C8	2.48	0.44
56:MM:478:GLY:HA3	56:MM:1020:TYR:HD2	1.82	0.44
8:G:68:ARG:NH1	50:1:2514:U:OP2	2.47	0.44
20:T:90:ASN:HB2	46:w:160:VAL:HG21	1.98	0.44
39:m:149:ARG:HG3	39:m:151:ARG:HH21	1.82	0.44
45:v:277:MET:HE2	45:v:277:MET:HB2	1.81	0.44
50:1:717:C:OP1	50:1:751:A:O2'	2.34	0.44
50:1:3044:G:H2'	50:1:3045:G:H8	1.82	0.44
50:1:3146:G:H2'	50:1:3147:G:H8	1.82	0.44
56:MM:157:ALA:HB2	56:MM:317:VAL:HG21	1.99	0.44
56:MM:225:ASP:HB3	56:MM:226:ILE:HD12	2.00	0.44
56:MM:401:ILE:O	56:MM:405:LYS:N	2.50	0.44
56:MM:931:LEU:HD13	56:MM:936:ALA:HA	1.99	0.44
56:MM:977:MET:HE2	56:MM:984:VAL:HG21	1.99	0.44
2:A:41:ILE:HG22	2:A:90:ALA:HB3	1.99	0.44
3:B:246:LEU:N	50:1:1889:G:OP1	2.41	0.44
11:J:97:SER:OG	11:J:101:ASN:N	2.39	0.44
23:W:6:ARG:HB2	50:1:3115:C:C2	2.53	0.44
28:b:170:LEU:HD12	28:b:251:LEU:HD13	1.98	0.44
28:b:188:THR:HG21	28:b:207:GLY:HA3	1.98	0.44
39:m:239:CYS:O	39:m:241:SER:OG	2.33	0.44
39:m:378:SER:OG	39:m:379:GLU:N	2.49	0.44
39:m:416:TYR:H	39:m:417:GLU:HA	1.83	0.44
42:r:125:VAL:HG21	42:r:218:GLY:HA3	1.99	0.44
46:w:22:ASP:HB3	46:w:27:ALA:HB3	1.99	0.44
47:x:257:ASP:N	47:x:257:ASP:OD1	2.45	0.44
47:x:321:HIS:ND1	47:x:379:ASP:HB2	2.33	0.44
50:1:1138:U:H2'	50:1:1139:G:H8	1.81	0.44
50:1:1186:G:H1	50:1:1320:C:H42	1.66	0.44
50:1:1616:U:H2'	50:1:1617:G:C8	2.52	0.44
50:1:2104:A:H2'	50:1:2105:G:H8	1.83	0.44
50:1:3190:C:H2'	50:1:3191:G:H8	1.83	0.44
52:4:507:ILE:HB	52:4:522:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:67:ARG:HH21	50:1:518:G:P	2.41	0.44
20:T:36:VAL:HG13	20:T:65:TYR:HA	1.99	0.44
39:m:257:TYR:HD2	39:m:277:LEU:HD23	1.83	0.44
50:1:12:A:H2'	50:1:13:A:C8	2.52	0.44
50:1:1439:U:H2'	50:1:1440:G:H8	1.81	0.44
50:1:1845:G:N2	50:1:1849:C:O2'	2.44	0.44
50:1:2156:C:H2'	50:1:2178:A:H61	1.83	0.44
3:B:74:GLU:OE2	3:B:283:TYR:OH	2.25	0.44
3:B:119:TYR:OH	3:B:128:LYS:N	2.51	0.44
5:D:166:ALA:O	5:D:170:GLY:N	2.51	0.44
9:H:154:VAL:O	9:H:158:ALA:N	2.46	0.44
14:N:7:LEU:O	14:N:11:GLN:N	2.49	0.44
20:T:66:ASN:HB3	20:T:73:GLY:HA3	2.00	0.44
24:X:33:ARG:NH1	50:1:1581:C:H41	2.16	0.44
26:Z:54:THR:OG1	26:Z:55:LYS:N	2.49	0.44
28:b:588:ARG:HE	50:1:1518:U:P	2.40	0.44
47:x:407:HIS:CD2	47:x:450:VAL:H	2.36	0.44
48:y:158:GLY:HA2	48:y:179:VAL:HB	2.00	0.44
50:1:815:G:N2	50:1:920:A:OP2	2.43	0.44
1:2:60:U:OP2	24:X:61:LYS:NZ	2.40	0.44
3:B:69:LYS:HE2	28:b:416:LEU:HG	2.00	0.44
11:J:45:PRO:HB3	11:J:69:VAL:HB	2.00	0.44
12:L:12:ASN:HD22	12:L:13:HIS:H	1.66	0.44
19:S:92:LYS:NZ	50:1:1212:A:O3'	2.51	0.44
28:b:29:THR:OG1	28:b:49:LYS:NZ	2.47	0.44
28:b:595:ASP:OD1	28:b:595:ASP:N	2.45	0.44
45:v:117:MET:HB2	45:v:233:LYS:HB3	2.00	0.44
46:w:75:GLU:O	46:w:85:SER:OG	2.32	0.44
50:1:1204:A:H2'	50:1:1205:A:O4'	2.18	0.44
50:1:1204:A:H62	50:1:1300:G:H21	1.66	0.44
1:2:21:C:N4	1:2:22:U:O4	2.51	0.43
3:B:99:LEU:O	50:1:3004:C:O2'	2.34	0.43
7:F:121:LYS:HB2	20:T:133:ALA:HB3	1.98	0.43
7:F:156:ILE:C	7:F:158:LYS:H	2.26	0.43
28:b:588:ARG:HB2	38:l:21:ARG:HH21	1.82	0.43
36:j:27:PHE:HA	36:j:34:CYS:HA	2.00	0.43
38:l:42:ARG:HH22	50:1:1494:U:P	2.40	0.43
39:m:151:ARG:HA	39:m:152:LEU:HA	1.74	0.43
40:n:180:PHE:HA	40:n:456:HIS:CE1	2.53	0.43
45:v:42:LEU:HA	45:v:45:ILE:HD12	1.99	0.43
47:x:214:ASP:OD2	47:x:217:SER:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:x:360:TYR:O	47:x:364:CYS:N	2.50	0.43
47:x:501:VAL:N	47:x:513:TRP:O	2.50	0.43
50:1:155:G:H4'	50:1:156:G:H2'	1.99	0.43
50:1:300:G:H2'	50:1:301:G:H8	1.83	0.43
50:1:1100:U:H2'	50:1:1101:G:H8	1.82	0.43
50:1:1470:U:H2'	50:1:1471:U:H6	1.83	0.43
51:3:71:G:H2'	51:3:72:A:H8	1.83	0.43
3:B:180:GLU:OE2	50:1:3002:C:O2'	2.33	0.43
4:C:64:SER:OG	4:C:65:TRP:N	2.50	0.43
4:C:176:SER:O	4:C:180:LYS:N	2.51	0.43
5:D:163:LEU:HD21	5:D:175:HIS:CG	2.53	0.43
8:G:141:ALA:HB1	50:1:117:U:C2	2.52	0.43
18:R:56:THR:HA	28:b:517:ALA:HB2	1.99	0.43
21:U:57:THR:OG1	21:U:64:THR:O	2.30	0.43
22:V:14:SER:O	22:V:81:GLN:NE2	2.43	0.43
28:b:169:THR:HG22	28:b:217:GLN:HE21	1.83	0.43
28:b:539:GLY:HA2	44:u:139:VAL:HG21	1.99	0.43
39:m:91:HIS:O	39:m:94:SER:OG	2.35	0.43
45:v:31:LEU:O	45:v:88:VAL:N	2.47	0.43
47:x:391:SER:OG	47:x:392:THR:N	2.51	0.43
50:1:385:A:H2'	50:1:386:A:C8	2.54	0.43
50:1:1100:U:H2'	50:1:1101:G:C8	2.53	0.43
50:1:1293:U:H2'	50:1:1294:A:H8	1.82	0.43
50:1:1764:U:H1'	52:4:376:ARG:HD2	2.01	0.43
50:1:1909:A:H2'	50:1:1910:A:C8	2.52	0.43
4:C:27:SER:O	4:C:279:HIS:NE2	2.42	0.43
5:D:153:THR:HG23	5:D:160:PHE:HZ	1.84	0.43
11:J:32:ARG:NH1	11:J:120:ILE:O	2.46	0.43
28:b:19:ASP:OD1	50:1:2828:G:N1	2.32	0.43
39:m:114:PRO:HD3	42:r:239:TRP:CZ2	2.53	0.43
44:u:45:ASN:HB3	44:u:48:LYS:HB2	2.00	0.43
48:y:142:ILE:HG22	48:y:162:HIS:HE1	1.83	0.43
50:1:159:A:H2'	50:1:160:G:H8	1.83	0.43
50:1:417:A:H2'	50:1:418:A:C8	2.53	0.43
50:1:1146:C:H4'	50:1:1331:U:C4	2.53	0.43
50:1:3016:A:O2'	50:1:3017:A:H8	2.02	0.43
3:B:178:LEU:HD13	3:B:178:LEU:HA	1.90	0.43
23:W:91:GLN:HB2	23:W:228:VAL:HG21	2.01	0.43
42:r:137:ILE:HD11	42:r:150:MET:HE3	2.01	0.43
48:y:101:LEU:HD13	48:y:107:VAL:HG21	2.01	0.43
50:1:2502:A:OP2	50:1:2503:G:N1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2732:G:H2'	50:1:2733:A:C8	2.52	0.43
50:1:2889:C:H2'	50:1:2890:A:H8	1.84	0.43
50:1:2966:G:H2'	50:1:2967:A:C8	2.54	0.43
50:1:3112:G:N2	50:1:3113:A:N7	2.66	0.43
52:4:122:ASP:HA	52:4:123:SER:HA	1.72	0.43
1:2:79:A:H4'	52:4:348:HIS:CD2	2.54	0.43
2:A:143:GLU:O	2:A:145:LYS:HG2	2.19	0.43
2:A:182:ALA:O	2:A:186:PHE:N	2.49	0.43
8:G:54:GLU:HG2	8:G:57:ARG:HH21	1.83	0.43
10:I:93:ALA:HA	44:u:57:LYS:HG3	2.01	0.43
14:N:77:LYS:NZ	50:1:909:G:OP2	2.41	0.43
15:O:126:VAL:HG22	19:S:154:HIS:HE1	1.83	0.43
20:T:34:TYR:OH	20:T:96:ILE:O	2.34	0.43
28:b:260:CYS:O	28:b:262:PHE:N	2.46	0.43
28:b:567:PHE:CG	52:4:364:PHE:HB2	2.53	0.43
31:e:19:ARG:HH21	31:e:33:ARG:HG3	1.83	0.43
33:g:4:ARG:NH2	50:1:1485:G:N3	2.66	0.43
33:g:20:ILE:HD12	33:g:32:ALA:HB1	2.00	0.43
35:i:54:GLU:HA	35:i:57:LEU:HB2	1.99	0.43
40:n:67:ASP:O	40:n:71:LEU:N	2.51	0.43
45:v:47:VAL:HA	45:v:59:ARG:HH21	1.83	0.43
48:y:4:ARG:HE	48:y:215:LEU:HD11	1.84	0.43
48:y:24:CYS:HB3	48:y:48:ILE:HG23	2.01	0.43
48:y:233:SER:OG	48:y:237:ARG:NH1	2.50	0.43
50:1:571:U:H2'	50:1:572:A:C8	2.52	0.43
50:1:1724:U:H1'	50:1:1725:C:C6	2.54	0.43
50:1:2668:U:H2'	50:1:2669:G:C8	2.53	0.43
56:MM:419:CYS:HB3	56:MM:500:PHE:HB3	2.00	0.43
2:A:28:LYS:HB3	2:A:123:ARG:HB3	2.01	0.43
3:B:221:THR:O	3:B:272:TYR:N	2.37	0.43
5:D:20:PHE:O	5:D:24:ARG:N	2.42	0.43
14:N:199:LEU:HD23	14:N:199:LEU:HA	1.84	0.43
18:R:110:ARG:HH12	50:1:1720:U:P	2.42	0.43
36:j:28:HIS:HE1	36:j:30:GLN:HB2	1.84	0.43
42:r:201:LYS:NZ	50:1:2717:U:OP1	2.41	0.43
44:u:76:ASN:HD22	48:y:96:ARG:HB2	1.82	0.43
47:x:331:ASP:O	47:x:335:ARG:N	2.51	0.43
50:1:936:A:O2'	50:1:938:C:N4	2.50	0.43
50:1:1219:C:H2'	53:5:51:ARG:HH12	1.83	0.43
50:1:2171:G:H2'	50:1:2172:A:H8	1.84	0.43
50:1:2842:U:H3'	50:1:2844:C:N4	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:3314:A:H2'	50:1:3315:G:C8	2.54	0.43
56:MM:120:ARG:HB2	56:MM:318:TYR:HB3	2.00	0.43
56:MM:650:GLU:HA	56:MM:653:ILE:HD12	2.01	0.43
5:D:90:HIS:HB2	5:D:226:TYR:CZ	2.54	0.43
5:D:245:GLU:O	5:D:249:ALA:N	2.50	0.43
12:L:27:ASP:N	12:L:27:ASP:OD1	2.38	0.43
22:V:15:LEU:HD23	22:V:53:SER:HB3	2.01	0.43
39:m:21:ASN:OD1	39:m:21:ASN:N	2.52	0.43
39:m:304:ARG:O	39:m:308:GLN:N	2.47	0.43
40:n:180:PHE:O	40:n:187:TYR:N	2.47	0.43
46:w:115:GLU:O	46:w:119:ALA:N	2.51	0.43
50:1:94:G:H2'	50:1:95:A:C8	2.53	0.43
50:1:1621:A:H2'	50:1:1622:U:C6	2.54	0.43
50:1:1718:G:H2'	50:1:1719:G:C8	2.54	0.43
50:1:2901:G:H3'	50:1:2902:A:C8	2.54	0.43
52:4:29:ARG:HH11	52:4:523:LEU:HD22	1.84	0.43
56:MM:328:HIS:HB2	56:MM:342:VAL:HB	2.01	0.43
56:MM:434:ASP:HA	56:MM:437:LYS:HD3	2.00	0.43
3:B:19:ARG:N	50:1:2990:G:OP1	2.52	0.43
8:G:24:ASN:HA	8:G:25:PRO:HD3	1.88	0.43
28:b:351:GLN:HA	28:b:354:ILE:HG22	2.01	0.43
50:1:604:G:H2'	50:1:605:U:C6	2.54	0.43
50:1:2846:U:H5'	50:1:2847:A:H3'	1.99	0.43
54:KK:11:SER:HA	54:KK:14:ILE:HD12	2.01	0.43
55:LL:109:GLU:O	55:LL:113:ASN:ND2	2.52	0.43
56:MM:186:ALA:O	56:MM:190:LYS:N	2.49	0.43
56:MM:867:LYS:O	56:MM:871:SER:N	2.43	0.43
2:A:113:VAL:HG12	2:A:166:ILE:HA	2.00	0.43
4:C:357:GLU:O	4:C:361:HIS:N	2.51	0.43
6:E:172:HIS:CD2	6:E:173:MET:HG3	2.53	0.43
15:O:156:LEU:HD13	50:1:3243:A:C5	2.53	0.43
16:P:171:ARG:NH2	50:1:3274:A:N7	2.67	0.43
19:S:80:ARG:NH2	43:s:48:PRO:HD2	2.33	0.43
19:S:91:TYR:N	50:1:1214:U:OP1	2.45	0.43
24:X:115:ARG:HH11	24:X:117:ASN:HD21	1.65	0.43
28:b:87:GLU:HB3	28:b:90:HIS:HB2	2.01	0.43
39:m:88:ALA:HA	39:m:91:HIS:HB3	2.00	0.43
39:m:287:HIS:HB3	39:m:294:PHE:HB3	2.01	0.43
42:r:247:ASN:ND2	42:r:254:CYS:O	2.51	0.43
50:1:339:C:OP1	50:1:1380:G:O2'	2.36	0.43
50:1:788:C:H2'	50:1:789:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2221:G:N2	50:1:2224:A:OP2	2.41	0.43
50:1:2412:G:H2'	50:1:2413:A:C8	2.54	0.43
50:1:2568:C:OP2	50:1:2569:A:N6	2.52	0.43
50:1:2620:G:H21	50:1:2621:G:H1'	1.84	0.43
52:4:391:LYS:H	52:4:394:HIS:HD2	1.67	0.43
56:MM:960:ALA:O	56:MM:964:LYS:N	2.49	0.43
2:A:35:ALA:HA	8:G:36:ILE:HD11	2.00	0.43
5:D:69:ILE:HG23	45:v:135:VAL:HG22	2.01	0.43
14:N:56:LYS:NZ	14:N:145:ASP:OD2	2.50	0.43
16:P:31:GLU:HG2	16:P:60:PHE:CD1	2.54	0.43
20:T:92:ARG:HB2	20:T:95:HIS:CD2	2.52	0.43
22:V:101:VAL:HB	22:V:109:MET:HE1	2.00	0.43
23:W:43:LEU:N	23:W:101:GLY:O	2.51	0.43
23:W:100:THR:HA	23:W:101:GLY:HA3	1.73	0.43
28:b:4:SER:HB3	28:b:162:SER:HB3	2.01	0.43
28:b:87:GLU:HG2	28:b:90:HIS:ND1	2.33	0.43
28:b:95:LEU:HD23	28:b:95:LEU:HA	1.84	0.43
28:b:511:LYS:HA	28:b:518:ILE:HD11	2.00	0.43
30:d:61:LYS:HA	30:d:61:LYS:HD2	1.87	0.43
32:f:52:VAL:HG22	32:f:66:VAL:HG22	2.01	0.43
40:n:211:SER:HA	40:n:215:PHE:CE2	2.54	0.43
43:s:13:THR:HG22	43:s:16:LYS:HD2	2.01	0.43
50:1:788:C:H2'	50:1:789:A:C8	2.54	0.43
50:1:2314:U:H2'	50:1:2315:G:C8	2.54	0.43
50:1:2357:A:H2'	50:1:2358:A:C8	2.54	0.43
50:1:2636:A:N6	50:1:2641:U:O2	2.52	0.43
52:4:76:LEU:HD13	52:4:88:GLY:HA2	2.00	0.43
1:2:21:C:OP1	4:C:193:LYS:NZ	2.44	0.42
3:B:21:ARG:NH2	50:1:2991:A:O3'	2.52	0.42
5:D:110:LEU:HD11	5:D:115:LEU:HB2	2.00	0.42
7:F:109:THR:O	50:1:1159:A:N6	2.52	0.42
17:Q:79:LYS:NZ	50:1:729:C:O2'	2.36	0.42
19:S:10:ILE:O	19:S:59:VAL:N	2.46	0.42
28:b:1:MET:O	28:b:5:TRP:NE1	2.50	0.42
30:d:85:ALA:O	30:d:87:ASN:ND2	2.51	0.42
35:i:74:LYS:HE2	35:i:80:PHE:HB2	2.00	0.42
36:j:45:ARG:HH11	36:j:47:TYR:HE2	1.66	0.42
42:r:171:ILE:HG22	50:1:2727:A:H5'	2.00	0.42
42:r:248:GLU:HG2	42:r:251:ARG:HE	1.84	0.42
48:y:11:ASN:OD1	48:y:208:LEU:N	2.51	0.42
50:1:1392:G:O2'	50:1:1417:G:N2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1660:C:H2'	50:1:1661:G:C8	2.53	0.42
50:1:1737:U:H2'	50:1:1738:C:C6	2.54	0.42
50:1:2897:A:H5''	50:1:2899:C:H42	1.84	0.42
56:MM:850:TYR:O	56:MM:854:SER:N	2.48	0.42
3:B:30:LYS:NZ	50:1:3138:U:OP2	2.37	0.42
11:J:6:GLN:HG3	11:J:8:PRO:HD3	2.01	0.42
16:P:94:LEU:O	16:P:98:ALA:N	2.52	0.42
28:b:86:TYR:O	28:b:149:TYR:OH	2.36	0.42
32:f:78:SER:N	50:1:1180:A:OP1	2.48	0.42
33:g:44:CYS:HB3	33:g:47:CYS:HB2	1.43	0.42
33:g:74:ARG:CZ	33:g:82:ALA:HB2	2.50	0.42
39:m:81:THR:OG1	39:m:82:ARG:N	2.52	0.42
50:1:547:G:H1'	50:1:548:G:C8	2.54	0.42
50:1:1190:A:C8	50:1:1193:A:H1'	2.55	0.42
50:1:1334:U:H2'	50:1:1335:C:H6	1.84	0.42
50:1:1553:U:H4'	50:1:1554:U:H5'	2.01	0.42
50:1:1814:A:H1'	50:1:1815:U:C2	2.54	0.42
51:3:19:C:H2'	51:3:20:A:C8	2.53	0.42
51:3:79:A:H62	51:3:101:G:H21	1.67	0.42
52:4:33:GLN:HA	52:4:36:GLN:HB3	1.99	0.42
52:4:125:PHE:CG	52:4:353:LEU:HD12	2.54	0.42
56:MM:628:LEU:HA	56:MM:631:ASP:HB2	2.01	0.42
56:MM:772:ASN:N	56:MM:806:PRO:O	2.51	0.42
4:C:22:LEU:HD23	4:C:22:LEU:HA	1.87	0.42
10:I:43:LYS:HA	10:I:44:PRO:HD3	1.90	0.42
11:J:110:ILE:HG21	11:J:116:TYR:HA	2.02	0.42
16:P:167:ARG:NH2	50:1:620:U:OP1	2.53	0.42
18:R:100:ARG:HB3	18:R:104:ARG:HH11	1.84	0.42
39:m:106:VAL:HG11	39:m:254:HIS:ND1	2.34	0.42
40:n:214:ASP:HB3	40:n:217:ILE:HD12	2.01	0.42
47:x:407:HIS:HD2	47:x:450:VAL:HG22	1.83	0.42
50:1:385:A:H2'	50:1:386:A:H8	1.84	0.42
50:1:1440:G:H2'	50:1:1441:G:C8	2.55	0.42
53:5:70:GLU:O	53:5:74:ALA:N	2.43	0.42
54:KK:99:LEU:HB3	55:LL:93:TYR:CZ	2.54	0.42
56:MM:801:PHE:HB2	56:MM:805:ILE:HD13	2.02	0.42
16:P:31:GLU:OE2	16:P:61:ARG:N	2.47	0.42
19:S:23:LYS:HA	20:T:146:ASN:HD21	1.84	0.42
21:U:9:GLN:HG2	21:U:10:LYS:HG3	2.00	0.42
22:V:120:LYS:HB2	22:V:137:VAL:HG22	2.00	0.42
23:W:126:ARG:O	23:W:129:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:101:VAL:HG22	27:a:124:ILE:HB	2.00	0.42
28:b:288:ASN:HD22	28:b:289:LYS:H	1.67	0.42
29:c:25:LEU:O	29:c:29:SER:OG	2.26	0.42
47:x:338:ALA:HB2	47:x:356:ALA:HB2	2.01	0.42
48:y:61:ARG:HA	48:y:105:GLY:HA3	2.01	0.42
48:y:213:PRO:O	48:y:216:SER:OG	2.33	0.42
50:1:255:A:H2'	50:1:256:G:H8	1.84	0.42
50:1:637:C:OP1	50:1:2377:G:N2	2.53	0.42
51:3:117:A:H2'	51:3:118:A:C8	2.54	0.42
51:3:118:A:H2'	51:3:119:U:C6	2.55	0.42
52:4:118:ASN:O	52:4:121:LYS:N	2.52	0.42
52:4:262:ARG:HA	52:4:263:GLU:HA	1.81	0.42
55:LL:80:LEU:O	55:LL:84:LYS:N	2.49	0.42
56:MM:699:ALA:HB3	56:MM:738:PHE:HE1	1.84	0.42
7:F:154:GLY:O	7:F:161:VAL:N	2.52	0.42
16:P:27:LYS:NZ	50:1:1447:G:OP2	2.35	0.42
18:R:10:LEU:HD11	18:R:38:ARG:HG2	2.01	0.42
23:W:55:GLU:HA	23:W:58:THR:HG22	2.01	0.42
23:W:222:ASP:HB3	23:W:225:SER:HB3	2.02	0.42
39:m:391:GLU:OE2	50:1:2329:C:O2'	2.26	0.42
40:n:157:ASN:HA	40:n:160:GLN:CD	2.44	0.42
43:s:6:ARG:HB2	50:1:1192:C:C4	2.55	0.42
45:v:91:THR:O	45:v:99:ASN:N	2.48	0.42
45:v:222:GLU:OE2	46:w:55:ARG:NH2	2.52	0.42
50:1:429:U:H3	50:1:630:A:H61	1.68	0.42
50:1:1241:U:O2'	50:1:1242:G:O5'	2.34	0.42
56:MM:486:VAL:HA	56:MM:489:ILE:HD12	2.01	0.42
56:MM:828:ILE:HA	56:MM:831:LEU:HD12	2.01	0.42
3:B:329:PRO:HA	50:1:3047:U:H5'	2.02	0.42
4:C:295:ILE:O	4:C:299:ILE:HG12	2.19	0.42
7:F:180:SER:OG	7:F:182:ASP:N	2.53	0.42
8:G:150:LEU:HD21	8:G:215:VAL:HG22	2.01	0.42
12:L:157:ARG:HH21	27:a:124:ILE:HG21	1.83	0.42
22:V:76:ALA:HB2	22:V:102:ILE:HG22	2.01	0.42
24:X:45:LYS:NZ	50:1:129:U:OP1	2.36	0.42
28:b:290:THR:OG1	28:b:320:SER:O	2.33	0.42
33:g:44:CYS:SG	33:g:81:CYS:N	2.92	0.42
39:m:82:ARG:HG3	42:r:239:TRP:CE2	2.55	0.42
39:m:309:LEU:HA	39:m:309:LEU:HD23	1.82	0.42
40:n:218:MET:HA	40:n:221:PHE:HD2	1.84	0.42
42:r:3:GLN:HB3	50:1:3027:A:C2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:160:GLY:HA3	50:1:2730:G:C8	2.54	0.42
48:y:101:LEU:H	48:y:101:LEU:HG	1.73	0.42
50:1:312:C:H2'	50:1:313:A:C8	2.54	0.42
50:1:778:U:H2'	50:1:779:G:C8	2.55	0.42
50:1:792:G:H2'	50:1:793:C:C6	2.55	0.42
50:1:939:U:H2'	50:1:940:G:C8	2.55	0.42
50:1:1921:A:H2'	50:1:1922:A:C8	2.55	0.42
50:1:2668:U:H3	50:1:2686:A:H2	1.66	0.42
50:1:3155:U:H3	50:1:3158:G:H1'	1.84	0.42
50:1:3322:A:H2'	50:1:3323:A:C8	2.53	0.42
50:1:3322:A:H2'	50:1:3323:A:H8	1.84	0.42
56:MM:789:THR:HA	56:MM:792:LYS:HB3	2.01	0.42
56:MM:938:ALA:HB1	56:MM:998:MET:HB3	2.02	0.42
3:B:136:LYS:HD3	3:B:143:GLY:HA3	2.02	0.42
16:P:107:LEU:HD23	16:P:152:GLU:HG3	2.01	0.42
23:W:60:TRP:HD1	23:W:63:SER:H	1.66	0.42
28:b:264:ILE:C	28:b:302:ARG:HH11	2.26	0.42
28:b:302:ARG:HA	28:b:302:ARG:HD2	1.82	0.42
32:f:11:GLY:O	32:f:98:VAL:N	2.42	0.42
40:n:29:LEU:HD22	50:1:1565:G:C4	2.54	0.42
41:p:18:TYR:HA	50:1:2131:A:H61	1.84	0.42
45:v:173:GLN:NE2	45:v:174:ASP:O	2.41	0.42
50:1:2429:G:H2'	50:1:2430:A:H8	1.85	0.42
52:4:334:LEU:N	52:4:443:VAL:O	2.41	0.42
56:MM:618:VAL:HG21	56:MM:874:GLN:HG2	2.02	0.42
56:MM:714:HIS:HD2	56:MM:764:LEU:HB2	1.85	0.42
2:A:111:THR:HB	2:A:136:ILE:HD13	2.01	0.42
2:A:213:GLY:HA3	50:1:2967:A:H5''	2.01	0.42
3:B:159:ARG:HA	3:B:182:GLN:HA	2.00	0.42
6:E:2:SER:OG	50:1:1385:C:O2	2.36	0.42
7:F:59:GLU:HA	7:F:62:ILE:HB	2.01	0.42
7:F:210:PRO:O	50:1:1167:U:O2'	2.37	0.42
11:J:53:THR:HG23	11:J:60:ARG:HA	2.00	0.42
14:N:4:TYR:CE2	14:N:5:LYS:HB2	2.54	0.42
23:W:162:GLU:OE1	23:W:166:ARG:NH2	2.52	0.42
24:X:102:LEU:HD23	24:X:102:LEU:HA	1.86	0.42
24:X:105:VAL:HG13	24:X:130:TYR:HD2	1.85	0.42
26:Z:14:VAL:HG11	33:g:86:LYS:HG2	2.00	0.42
35:i:54:GLU:HG2	35:i:90:MET:HE3	2.01	0.42
38:l:43:ASN:HB3	38:l:46:ARG:HD3	2.02	0.42
39:m:134:THR:OG1	39:m:135:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:318:VAL:HG13	39:m:364:LEU:HD23	2.02	0.42
40:n:352:TYR:HD2	40:n:358:SER:HB3	1.85	0.42
50:1:1246:G:O2'	50:1:1264:G:OP2	2.31	0.42
50:1:2098:C:H2'	50:1:2099:A:C8	2.54	0.42
50:1:2400:G:H2'	50:1:2401:A:C8	2.54	0.42
51:3:28:C:H1'	51:3:55:A:H61	1.85	0.42
52:4:64:LEU:O	52:4:68:THR:N	2.47	0.42
56:MM:340:LEU:HD21	56:MM:343:ASP:HA	2.02	0.42
1:2:123:G:H2'	1:2:124:G:C8	2.55	0.42
5:D:184:ASP:OD1	5:D:185:PHE:N	2.52	0.42
9:H:4:ILE:HG22	19:S:142:GLN:HE21	1.84	0.42
10:I:16:ARG:HD3	10:I:55:ALA:HB1	2.02	0.42
12:L:58:VAL:O	12:L:70:ARG:N	2.51	0.42
18:R:102:LEU:HD22	18:R:138:LEU:HD13	2.00	0.42
34:h:52:ALA:O	34:h:56:THR:OG1	2.37	0.42
40:n:449:PRO:HA	40:n:450:GLY:HA2	1.62	0.42
45:v:74:PRO:HA	45:v:77:PHE:HB3	2.00	0.42
49:z:42:LEU:HD23	49:z:45:LYS:HD2	2.01	0.42
50:1:833:G:H1	50:1:861:C:H42	1.67	0.42
50:1:886:C:H2'	50:1:887:G:H8	1.84	0.42
50:1:2141:U:O2'	50:1:2976:A:O2'	2.34	0.42
52:4:136:GLY:N	52:4:160:ILE:O	2.43	0.42
52:4:206:LYS:HD2	52:4:567:LEU:HD12	2.02	0.42
52:4:238:VAL:HG22	52:4:323:MET:HE1	2.02	0.42
56:MM:451:LEU:O	56:MM:456:ARG:NH2	2.52	0.42
2:A:144:ASN:OD1	2:A:144:ASN:N	2.53	0.42
4:C:282:SER:OG	4:C:283:THR:N	2.53	0.42
4:C:358:THR:O	19:S:26:ARG:NH2	2.53	0.42
5:D:221:GLU:O	51:3:50:U:O2'	2.35	0.42
5:D:234:ASP:N	5:D:234:ASP:OD1	2.52	0.42
9:H:21:LYS:N	50:1:3198:U:O2	2.53	0.42
19:S:7:TYR:N	19:S:29:ILE:O	2.53	0.42
19:S:160:THR:OG1	19:S:161:LYS:N	2.51	0.42
26:Z:89:VAL:HG13	26:Z:93:LYS:HD3	2.02	0.42
39:m:299:LEU:HD22	39:m:335:LEU:HD11	2.02	0.42
39:m:344:ALA:HB3	39:m:349:GLU:HB2	2.02	0.42
45:v:89:LEU:HB3	45:v:101:THR:HB	2.02	0.42
45:v:151:HIS:HA	45:v:152:PRO:HD3	1.90	0.42
45:v:166:ARG:NH1	46:w:25:ASN:OD1	2.48	0.42
50:1:1243:G:O6	50:1:1244:A:N6	2.52	0.42
50:1:2415:C:H2'	50:1:2416:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2677:G:H1	50:1:2680:A:H62	1.67	0.42
51:3:70:U:H2'	51:3:71:G:C8	2.52	0.42
56:MM:907:VAL:HG21	56:MM:924:PHE:HZ	1.84	0.42
19:S:62:ASN:ND2	50:1:519:A:OP1	2.52	0.41
19:S:84:ARG:HD2	19:S:84:ARG:HA	1.92	0.41
20:T:107:GLU:O	20:T:111:ALA:N	2.47	0.41
22:V:26:ALA:HB2	22:V:99:ALA:HB1	2.01	0.41
28:b:175:TYR:CE2	28:b:267:GLN:HG2	2.55	0.41
28:b:449:ILE:O	28:b:453:LEU:N	2.46	0.41
33:g:8:ARG:HD2	50:1:1606:U:C4	2.55	0.41
39:m:10:ARG:NH2	39:m:28:ASN:O	2.40	0.41
40:n:373:ILE:HG13	40:n:377:GLU:HB2	2.01	0.41
42:r:150:MET:HA	42:r:172:ILE:HB	2.02	0.41
43:s:26:HIS:CG	50:1:1200:A:H4'	2.55	0.41
46:w:54:THR:HA	46:w:57:ASN:HD22	1.85	0.41
47:x:228:HIS:ND1	47:x:259:THR:OG1	2.46	0.41
48:y:62:MET:HE3	48:y:73:PRO:HG3	2.01	0.41
50:1:546:C:H5''	50:1:547:G:C5	2.55	0.41
50:1:2426:U:H2'	50:1:2427:U:C6	2.55	0.41
50:1:2655:U:O2'	50:1:2713:U:O4	2.30	0.41
50:1:2986:U:H2'	50:1:2987:A:C8	2.55	0.41
52:4:360:TYR:HE1	52:4:434:GLU:HB3	1.83	0.41
56:MM:158:ILE:O	56:MM:162:ASP:N	2.49	0.41
56:MM:722:VAL:HG22	56:MM:759:VAL:HG22	2.02	0.41
56:MM:820:ASP:O	56:MM:824:LEU:N	2.51	0.41
56:MM:985:VAL:HB	56:MM:988:ASP:HB2	2.02	0.41
1:2:94:C:H5''	36:j:76:ASN:HD21	1.84	0.41
1:2:152:G:OP1	8:G:60:ARG:NE	2.51	0.41
3:B:49:TYR:O	3:B:80:ASP:N	2.50	0.41
5:D:97:ALA:O	5:D:101:THR:N	2.44	0.41
8:G:97:TYR:HE2	8:G:203:VAL:HG23	1.85	0.41
16:P:10:ASN:HD21	16:P:12:ALA:HB3	1.85	0.41
21:U:39:ASP:OD1	21:U:40:HIS:ND1	2.51	0.41
23:W:217:VAL:HG12	23:W:233:ILE:HD11	2.02	0.41
25:Y:85:VAL:HG12	25:Y:97:ILE:HD13	2.02	0.41
28:b:87:GLU:HG3	28:b:90:HIS:H	1.85	0.41
28:b:256:LEU:HD12	28:b:256:LEU:HA	1.92	0.41
39:m:50:ASN:HB3	39:m:56:ILE:HD11	2.01	0.41
39:m:412:LEU:HA	39:m:462:ILE:HD11	2.02	0.41
45:v:140:MET:HB2	45:v:181:VAL:HG23	2.02	0.41
47:x:443:HIS:HA	47:x:469:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:158:G:H2'	50:1:159:A:H8	1.84	0.41
50:1:196:G:N1	50:1:199:A:OP2	2.53	0.41
50:1:643:U:H5''	50:1:644:G:C6	2.55	0.41
50:1:1816:A:H2'	50:1:1817:G:O4'	2.20	0.41
50:1:2211:U:H3	50:1:2234:G:H1	1.67	0.41
50:1:2662:G:H2'	50:1:2663:G:H8	1.85	0.41
52:4:47:ASN:HA	52:4:51:HIS:H	1.85	0.41
55:LL:79:GLU:OE1	55:LL:82:ARG:NH1	2.53	0.41
56:MM:667:PRO:HB3	56:MM:712:THR:HG22	2.02	0.41
5:D:30:TYR:OH	51:3:8:G:OP2	2.26	0.41
5:D:115:LEU:HB3	47:x:130:LYS:NZ	2.34	0.41
12:L:161:ASP:OD1	12:L:162:ASN:N	2.52	0.41
22:V:109:MET:HG3	22:V:132:ASN:HD22	1.85	0.41
28:b:441:VAL:HG22	44:u:93:MET:HE1	2.02	0.41
28:b:532:GLU:HA	28:b:542:MET:HE2	2.01	0.41
38:l:43:ASN:HD22	38:l:44:TRP:H	1.67	0.41
39:m:378:SER:HG	39:m:381:ASP:H	1.67	0.41
39:m:380:GLU:H	39:m:380:GLU:HG3	1.62	0.41
50:1:540:U:H2'	50:1:541:U:C6	2.56	0.41
50:1:1609:C:H2'	50:1:1610:G:H8	1.85	0.41
50:1:1627:U:H2'	50:1:1814:A:N6	2.35	0.41
50:1:2146:C:H2'	50:1:2147:A:H8	1.85	0.41
50:1:2525:G:O2'	50:1:2526:C:OP2	2.33	0.41
50:1:2742:C:H2'	50:1:2743:A:C8	2.54	0.41
50:1:2768:U:H2'	50:1:2769:A:C8	2.55	0.41
56:MM:698:PHE:HA	56:MM:719:VAL:HA	2.02	0.41
56:MM:826:LYS:HA	56:MM:829:ASP:HB2	2.02	0.41
1:2:45:C:OP1	38:l:12:LYS:NZ	2.47	0.41
5:D:22:ARG:HH12	51:3:6:C:H3'	1.85	0.41
7:F:44:ILE:HG22	7:F:48:ASN:HD21	1.85	0.41
8:G:78:PHE:HD1	8:G:179:ILE:HD13	1.85	0.41
12:L:70:ARG:NH1	50:1:76:G:OP1	2.44	0.41
14:N:140:LYS:HB3	14:N:144:ARG:NH1	2.33	0.41
39:m:296:LYS:HE3	39:m:335:LEU:HA	2.03	0.41
39:m:315:GLN:HE21	42:r:165:PRO:HG2	1.84	0.41
40:n:25:LEU:HA	40:n:25:LEU:HD23	1.87	0.41
41:p:11:THR:HG21	41:p:23:ARG:HB3	2.03	0.41
45:v:30:ALA:HA	45:v:86:LEU:HB2	2.02	0.41
50:1:802:C:H2'	50:1:803:C:C6	2.55	0.41
50:1:1439:U:H2'	50:1:1440:G:C8	2.56	0.41
50:1:2727:A:N6	50:1:2871:G:O6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2948:C:H2'	50:1:2949:U:O4'	2.20	0.41
50:1:3007:U:H2'	50:1:3008:A:C8	2.55	0.41
52:4:150:TYR:CZ	52:4:249:ARG:HD3	2.55	0.41
52:4:359:ALA:HB3	52:4:435:SER:HB3	2.02	0.41
52:4:519:ARG:HD3	52:4:519:ARG:HA	1.83	0.41
1:2:79:A:H4'	52:4:348:HIS:HD2	1.85	0.41
2:A:19:HIS:NE2	50:1:822:G:O2'	2.49	0.41
2:A:183:GLY:HA2	50:1:896:A:H5'	2.03	0.41
13:M:102:LYS:HE3	13:M:102:LYS:HB2	1.85	0.41
14:N:140:LYS:HD3	14:N:143:ARG:HD3	2.01	0.41
17:Q:21:SER:OG	50:1:673:U:OP1	2.29	0.41
28:b:214:LEU:HD23	28:b:214:LEU:HA	1.86	0.41
39:m:96:LEU:HD23	39:m:96:LEU:HA	1.81	0.41
45:v:67:HIS:HA	45:v:68:PRO:HD3	1.90	0.41
48:y:236:LEU:O	48:y:239:THR:OG1	2.34	0.41
50:1:677:A:N6	50:1:785:G:O2'	2.53	0.41
50:1:1103:A:H3'	50:1:1104:G:C2	2.55	0.41
50:1:1828:A:H2'	50:1:1829:G:C8	2.55	0.41
50:1:2979:U:H1'	50:1:2980:U:C5	2.56	0.41
50:1:3017:A:H2'	50:1:3018:C:H6	1.85	0.41
52:4:33:GLN:O	52:4:37:THR:N	2.45	0.41
53:5:77:THR:OG1	53:5:78:MET:N	2.54	0.41
56:MM:727:TYR:CE2	56:MM:729:ASP:HB2	2.56	0.41
5:D:38:THR:O	5:D:38:THR:OG1	2.33	0.41
9:H:74:LEU:HD23	9:H:74:LEU:HA	1.89	0.41
18:R:62:ARG:NH1	50:1:3068:U:OP2	2.45	0.41
23:W:145:ARG:N	23:W:154:ASP:OD2	2.33	0.41
28:b:71:ILE:HG13	28:b:82:MET:HE3	2.02	0.41
28:b:355:ASN:OD1	28:b:355:ASN:N	2.53	0.41
42:r:173:ARG:HG3	50:1:2727:A:H2	1.85	0.41
44:u:142:ALA:HA	44:u:145:LEU:HD12	2.03	0.41
50:1:745:C:H2'	50:1:746:A:H8	1.85	0.41
50:1:2697:A:H2'	50:1:2698:G:C8	2.56	0.41
50:1:2775:U:H2'	50:1:2776:C:C6	2.56	0.41
54:KK:81:PHE:HA	54:KK:84:ILE:HD12	2.02	0.41
3:B:300:ARG:HD3	28:b:433:PRO:HB3	2.03	0.41
4:C:290:ILE:O	4:C:296:GLN:NE2	2.43	0.41
22:V:86:ARG:HD2	22:V:88:ARG:NH1	2.35	0.41
26:Z:9:LYS:HD3	26:Z:9:LYS:HA	1.84	0.41
28:b:402:ILE:HA	28:b:405:GLU:HG2	2.02	0.41
29:c:61:MET:HE3	29:c:62:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:38:ARG:HD2	34:h:41:LEU:HB2	2.02	0.41
47:x:490:TYR:H	47:x:505:GLY:HA2	1.85	0.41
50:1:551:A:O2'	50:1:552:G:O4'	2.39	0.41
50:1:877:C:N4	50:1:878:G:O6	2.54	0.41
50:1:901:G:H2'	50:1:902:G:C8	2.55	0.41
50:1:1107:C:N4	50:1:1108:U:O4	2.53	0.41
50:1:1460:A:H2'	50:1:1461:A:C8	2.56	0.41
50:1:1564:U:H2'	50:1:1565:G:C8	2.55	0.41
50:1:2767:U:H2'	50:1:2768:U:C6	2.55	0.41
56:MM:679:LEU:HD13	56:MM:805:ILE:HG23	2.03	0.41
3:B:154:TYR:OH	50:1:3242:G:OP2	2.33	0.41
4:C:145:ILE:HD11	4:C:148:ILE:HD11	2.03	0.41
5:D:90:HIS:CE1	5:D:225:GLY:HA3	2.55	0.41
12:L:165:SER:O	12:L:167:PHE:N	2.54	0.41
14:N:62:TYR:HD1	14:N:62:TYR:HA	1.69	0.41
17:Q:147:ARG:H	17:Q:147:ARG:HG3	1.60	0.41
22:V:84:SER:HA	22:V:94:TYR:HB3	2.01	0.41
25:Y:119:ILE:HG22	25:Y:124:GLY:HA3	2.02	0.41
30:d:11:GLU:O	30:d:106:THR:OG1	2.34	0.41
30:d:35:GLU:O	30:d:39:PHE:N	2.53	0.41
37:k:19:ASP:OD1	37:k:19:ASP:N	2.52	0.41
40:n:251:LYS:HZ3	55:LL:107:GLU:HG2	1.84	0.41
44:u:16:GLY:O	50:1:3050:U:O2'	2.30	0.41
45:v:28:LYS:NZ	45:v:163:ASP:OD2	2.48	0.41
46:w:144:LYS:HB3	46:w:145:TRP:HD1	1.86	0.41
47:x:264:ASP:OD1	47:x:265:THR:N	2.54	0.41
50:1:994:G:H1'	50:1:995:U:C2	2.55	0.41
50:1:1421:G:H2'	50:1:1422:G:H8	1.86	0.41
50:1:1664:G:H2'	50:1:1665:C:C6	2.56	0.41
50:1:1913:A:N3	50:1:2120:A:H2'	2.36	0.41
50:1:2661:G:H2'	50:1:2662:G:H8	1.85	0.41
52:4:140:LYS:HD3	52:4:501:ALA:HA	2.02	0.41
56:MM:164:GLY:HA2	56:MM:258:TRP:HZ2	1.85	0.41
56:MM:477:SER:O	56:MM:1026:ARG:NH1	2.33	0.41
56:MM:818:ASP:HB2	56:MM:821:PHE:HB3	2.03	0.41
1:2:121:U:H2'	1:2:122:U:C6	2.56	0.41
3:B:73:VAL:HG13	22:V:86:ARG:HH21	1.86	0.41
3:B:173:GLN:NE2	50:1:3313:U:O5'	2.54	0.41
5:D:224:LYS:O	5:D:228:ALA:N	2.52	0.41
5:D:282:ARG:HA	5:D:285:ARG:HB2	2.02	0.41
7:F:143:THR:HG22	7:F:241:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:36:VAL:HG11	13:M:55:ARG:HH12	1.86	0.41
14:N:120:TRP:HE1	14:N:123:GLN:HB3	1.85	0.41
14:N:178:HIS:O	14:N:181:ASN:ND2	2.54	0.41
16:P:141:SER:OG	50:1:2355:G:OP1	2.27	0.41
18:R:89:LEU:HD12	18:R:89:LEU:HA	1.88	0.41
19:S:14:LEU:HA	19:S:15:PRO:HD3	1.95	0.41
19:S:80:ARG:NH2	43:s:47:ASP:OD1	2.54	0.41
22:V:117:PRO:HA	22:V:135:VAL:HB	2.03	0.41
25:Y:71:SER:OG	25:Y:72:SER:N	2.54	0.41
27:a:77:LYS:O	27:a:79:TRP:N	2.53	0.41
28:b:199:PHE:CD2	50:1:1242:G:H1'	2.56	0.41
28:b:227:ARG:NH1	28:b:231:GLU:OE1	2.53	0.41
30:d:55:LEU:HD11	30:d:73:LEU:HD22	2.02	0.41
31:e:126:LEU:HD22	31:e:126:LEU:HA	1.80	0.41
37:k:26:LYS:HA	37:k:78:LEU:HD13	2.03	0.41
39:m:211:ILE:HD12	39:m:211:ILE:HA	1.92	0.41
39:m:259:LEU:HD13	39:m:259:LEU:HA	1.85	0.41
40:n:198:ARG:HH21	40:n:460:TRP:CD1	2.39	0.41
44:u:6:CYS:HB3	44:u:9:CYS:HB2	1.85	0.41
47:x:57:GLU:H	47:x:57:GLU:HG3	1.69	0.41
47:x:411:SER:HB3	47:x:416:TYR:HB2	2.02	0.41
48:y:53:ILE:HD13	48:y:53:ILE:HA	1.87	0.41
48:y:71:LEU:HD23	48:y:71:LEU:HA	1.89	0.41
50:1:277:G:H2'	50:1:278:U:C6	2.56	0.41
50:1:754:G:H2'	50:1:755:A:C8	2.56	0.41
50:1:1124:U:H2'	50:1:1125:U:C6	2.56	0.41
50:1:1627:U:O2'	50:1:1630:U:O2	2.34	0.41
50:1:2622:C:N4	50:1:2756:C:H42	2.19	0.41
50:1:2670:G:H2'	50:1:2671:A:C8	2.55	0.41
50:1:2939:G:H2'	50:1:2940:A:C8	2.56	0.41
50:1:3358:U:H2'	50:1:3359:A:H8	1.85	0.41
56:MM:1038:LEU:HD23	56:MM:1038:LEU:HA	1.92	0.41
16:P:118:GLN:HE22	50:1:412:G:H21	1.69	0.41
19:S:94:ILE:HG22	19:S:96:ASP:HB2	2.03	0.41
21:U:43:VAL:HB	21:U:49:ASN:HB3	2.02	0.41
39:m:146:GLN:NE2	50:1:1248:C:O2	2.43	0.41
50:1:2537:U:O2'	50:1:2538:U:O5'	2.35	0.41
54:KK:16:VAL:HG22	55:LL:17:ALA:HB1	2.02	0.41
55:LL:10:TYR:O	55:LL:14:PHE:N	2.52	0.41
56:MM:151:ASP:HA	56:MM:152:PRO:HD3	1.91	0.41
56:MM:791:GLY:O	56:MM:795:ARG:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:27:U:H2'	1:2:28:C:C6	2.55	0.40
1:2:69:U:H3	1:2:89:A:H61	1.67	0.40
18:R:62:ARG:HH11	50:1:3067:C:P	2.43	0.40
19:S:109:ASP:OD1	19:S:113:ARG:NH1	2.54	0.40
23:W:69:LYS:HB2	23:W:72:VAL:HG23	2.02	0.40
24:X:142:ILE:HG12	52:4:421:LEU:HA	2.03	0.40
31:e:23:ASP:OD2	50:1:424:G:O2'	2.31	0.40
40:n:213:VAL:H	40:n:213:VAL:HG22	1.68	0.40
47:x:385:LEU:HB3	47:x:396:ALA:H	1.85	0.40
50:1:417:A:H2'	50:1:418:A:H8	1.85	0.40
50:1:1089:G:H2'	50:1:1090:G:C8	2.56	0.40
50:1:1119:C:H2'	50:1:1120:A:C8	2.55	0.40
50:1:1307:G:H1'	50:1:1308:A:C8	2.56	0.40
50:1:1340:G:H2'	50:1:1341:U:C6	2.54	0.40
50:1:1699:A:H2'	50:1:1700:G:C8	2.56	0.40
50:1:2877:G:H1'	50:1:2878:G:H5'	2.03	0.40
50:1:2900:A:H2'	50:1:2901:G:O4'	2.21	0.40
50:1:3169:U:H2'	50:1:3170:A:C8	2.56	0.40
50:1:3371:G:H2'	50:1:3372:A:C8	2.55	0.40
56:MM:219:VAL:HG22	56:MM:234:CYS:HB3	2.01	0.40
11:J:16:LYS:HB3	11:J:72:ARG:HG2	2.02	0.40
16:P:139:TYR:CZ	50:1:1507:G:H8	2.39	0.40
22:V:39:VAL:HG22	22:V:58:VAL:HG12	2.02	0.40
31:e:65:PHE:N	50:1:1404:G:OP1	2.52	0.40
34:h:104:GLN:O	34:h:108:GLN:N	2.45	0.40
45:v:184:MET:HG2	45:v:201:PHE:HD1	1.87	0.40
46:w:112:THR:O	46:w:198:ASN:ND2	2.54	0.40
47:x:157:SER:HA	47:x:173:CYS:HB2	2.02	0.40
50:1:213:A:H62	50:1:227:G:H21	1.69	0.40
50:1:278:U:H2'	50:1:279:U:H6	1.85	0.40
50:1:1764:U:O2'	52:4:376:ARG:O	2.34	0.40
50:1:1896:A:H61	50:1:2339:C:N4	2.18	0.40
50:1:3203:U:H2'	50:1:3204:C:C6	2.56	0.40
50:1:3249:C:H2'	50:1:3250:U:H6	1.87	0.40
52:4:28:TYR:CZ	52:4:150:TYR:HB3	2.57	0.40
56:MM:407:ASN:OD1	56:MM:407:ASN:N	2.51	0.40
3:B:163:HIS:ND1	3:B:164:THR:O	2.54	0.40
4:C:140:HIS:O	4:C:142:VAL:N	2.54	0.40
5:D:22:ARG:NH1	51:3:6:C:O5'	2.54	0.40
9:H:150:SER:HB3	9:H:153:ASP:HB2	2.02	0.40
14:N:47:LYS:NZ	50:1:268:A:H5''	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:102:ILE:HD12	22:V:110:LYS:HB3	2.02	0.40
23:W:220:TYR:N	23:W:229:GLU:O	2.55	0.40
23:W:232:ASN:ND2	23:W:233:ILE:O	2.55	0.40
28:b:374:ARG:NH2	48:y:178:GLN:HG3	2.37	0.40
33:g:16:ARG:HH11	33:g:16:ARG:HD2	1.75	0.40
33:g:42:PRO:HB2	33:g:51:LEU:HD21	2.02	0.40
39:m:189:ASP:O	39:m:193:GLY:N	2.54	0.40
39:m:243:GLU:OE2	39:m:257:TYR:OH	2.36	0.40
39:m:471:LYS:HD2	50:1:2272:G:N7	2.36	0.40
40:n:3:ILE:HD11	50:1:1593:A:N9	2.36	0.40
42:r:5:ASP:OD1	42:r:9:ARG:NH2	2.54	0.40
43:s:45:LYS:HB3	43:s:46:LYS:H	1.76	0.40
44:u:37:HIS:CE1	44:u:41:LYS:HE3	2.56	0.40
45:v:133:PHE:HE1	45:v:180:HIS:CG	2.39	0.40
47:x:57:GLU:HA	47:x:60:LEU:HB2	2.02	0.40
47:x:445:ALA:HB1	47:x:464:LYS:HB3	2.03	0.40
50:1:418:A:H2'	50:1:419:G:C8	2.56	0.40
50:1:651:G:O2'	50:1:1435:A:OP1	2.40	0.40
50:1:2429:G:H2'	50:1:2430:A:C8	2.56	0.40
50:1:2548:C:H4'	50:1:2549:G:H5'	2.04	0.40
50:1:2930:A:H2'	50:1:2931:C:C6	2.56	0.40
50:1:3193:C:H2'	50:1:3194:C:C6	2.56	0.40
50:1:3251:U:H2'	50:1:3252:G:C8	2.56	0.40
52:4:254:GLN:OE1	52:4:254:GLN:N	2.53	0.40
1:2:142:C:H2'	1:2:143:U:C6	2.57	0.40
2:A:108:PRO:O	2:A:111:THR:OG1	2.30	0.40
4:C:321:LYS:NZ	50:1:580:C:OP1	2.54	0.40
12:L:61:PRO:HB2	12:L:62:THR:HG23	2.02	0.40
13:M:42:LYS:O	13:M:60:LEU:N	2.49	0.40
14:N:72:LYS:NZ	50:1:2166:A:O3'	2.53	0.40
14:N:110:ALA:HB1	14:N:113:LEU:HD23	2.03	0.40
19:S:110:MET:HB3	19:S:116:ALA:HB3	2.03	0.40
29:c:27:TYR:O	29:c:30:THR:OG1	2.39	0.40
40:n:64:TYR:HD1	40:n:64:TYR:HA	1.78	0.40
40:n:191:ASN:HA	40:n:196:GLU:HG2	2.02	0.40
41:p:9:GLY:O	50:1:836:A:O2'	2.33	0.40
42:r:182:ALA:N	42:r:195:LEU:O	2.55	0.40
48:y:142:ILE:HG22	48:y:162:HIS:CE1	2.57	0.40
50:1:612:U:H2'	50:1:613:G:H8	1.86	0.40
50:1:612:U:H2'	50:1:613:G:C8	2.56	0.40
50:1:791:A:H2'	50:1:792:G:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1336:U:H2'	50:1:1337:A:H8	1.87	0.40
50:1:1609:C:H2'	50:1:1610:G:C8	2.57	0.40
50:1:1725:C:H2'	50:1:1726:C:C6	2.57	0.40
50:1:2235:C:H2'	50:1:2236:G:O4'	2.22	0.40
50:1:2698:G:C6	50:1:2699:G:H1'	2.57	0.40
50:1:2904:U:H2'	50:1:2905:U:H6	1.87	0.40
50:1:2999:U:H2'	50:1:3000:A:C8	2.57	0.40
52:4:177:LEU:HA	52:4:181:ALA:HB2	2.03	0.40
1:2:9:A:H2'	1:2:10:A:C8	2.57	0.40
13:M:12:TRP:NE1	19:S:152:LEU:H	2.20	0.40
13:M:23:ILE:HA	13:M:63:VAL:HG23	2.04	0.40
17:Q:89:ASP:OD1	17:Q:90:ASP:N	2.54	0.40
19:S:171:PHE:HA	19:S:172:TYR:O	2.22	0.40
26:Z:80:LEU:HA	26:Z:80:LEU:HD23	1.90	0.40
31:e:66:LEU:HD23	31:e:66:LEU:HA	1.88	0.40
34:h:101:THR:HG23	34:h:104:GLN:H	1.86	0.40
35:i:34:SER:OG	35:i:36:ARG:N	2.55	0.40
36:j:45:ARG:HH22	50:1:362:U:P	2.44	0.40
39:m:106:VAL:HG11	39:m:254:HIS:CE1	2.57	0.40
42:r:185:THR:HA	42:r:192:THR:HA	2.03	0.40
47:x:212:LEU:HD23	47:x:212:LEU:HA	1.89	0.40
48:y:224:LEU:HD13	48:y:224:LEU:HA	1.94	0.40
50:1:379:C:H2'	50:1:380:U:H6	1.87	0.40
50:1:2361:A:H61	50:1:2377:G:H1	1.69	0.40
50:1:3339:A:H2'	50:1:3340:G:C8	2.56	0.40
50:1:3386:G:H2'	50:1:3387:U:C6	2.56	0.40
51:3:75:G:H2'	51:3:76:A:H8	1.86	0.40
52:4:90:ALA:HB2	52:4:146:HIS:HB3	2.03	0.40
56:MM:812:LYS:O	56:MM:815:LYS:NZ	2.37	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	
2	A	211/254 (83%)	194 (92%)	17 (8%)	0	100	100
3	B	384/387 (99%)	327 (85%)	53 (14%)	4 (1%)	12	45
4	C	359/362 (99%)	317 (88%)	39 (11%)	3 (1%)	16	50
5	D	272/297 (92%)	251 (92%)	21 (8%)	0	100	100
6	E	152/176 (86%)	140 (92%)	12 (8%)	0	100	100
7	F	220/244 (90%)	204 (93%)	16 (7%)	0	100	100
8	G	231/256 (90%)	210 (91%)	21 (9%)	0	100	100
9	H	189/191 (99%)	171 (90%)	18 (10%)	0	100	100
10	I	129/166 (78%)	113 (88%)	16 (12%)	0	100	100
11	J	167/174 (96%)	146 (87%)	20 (12%)	1 (1%)	21	55
12	L	185/199 (93%)	162 (88%)	21 (11%)	2 (1%)	11	43
13	M	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
14	N	201/204 (98%)	182 (90%)	19 (10%)	0	100	100
15	O	195/199 (98%)	188 (96%)	7 (4%)	0	100	100
16	P	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
17	Q	132/186 (71%)	124 (94%)	7 (5%)	1 (1%)	16	50
18	R	154/189 (82%)	150 (97%)	4 (3%)	0	100	100
19	S	169/172 (98%)	154 (91%)	14 (8%)	1 (1%)	21	55
20	T	115/160 (72%)	104 (90%)	11 (10%)	0	100	100
21	U	104/121 (86%)	92 (88%)	12 (12%)	0	100	100
22	V	134/137 (98%)	125 (93%)	9 (7%)	0	100	100
23	W	232/236 (98%)	215 (93%)	15 (6%)	2 (1%)	14	47
24	X	120/142 (84%)	112 (93%)	8 (7%)	0	100	100
25	Y	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
26	Z	133/136 (98%)	114 (86%)	18 (14%)	1 (1%)	16	50
27	a	91/149 (61%)	83 (91%)	8 (9%)	0	100	100
28	b	638/647 (99%)	562 (88%)	70 (11%)	6 (1%)	14	47
29	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
30	d	105/113 (93%)	96 (91%)	9 (9%)	0	100	100
31	e	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
32	f	104/107 (97%)	96 (92%)	8 (8%)	0	100	100
33	g	110/121 (91%)	101 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	14	47
35	i	97/100 (97%)	86 (89%)	11 (11%)	0	100	100
36	j	85/88 (97%)	78 (92%)	7 (8%)	0	100	100
37	k	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
38	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
39	m	465/486 (96%)	404 (87%)	58 (12%)	3 (1%)	21	55
40	n	365/605 (60%)	310 (85%)	51 (14%)	4 (1%)	11	43
41	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
42	r	224/261 (86%)	189 (84%)	32 (14%)	3 (1%)	9	40
43	s	65/520 (12%)	59 (91%)	6 (9%)	0	100	100
44	u	148/199 (74%)	138 (93%)	9 (6%)	1 (1%)	18	53
45	v	283/344 (82%)	262 (93%)	21 (7%)	0	100	100
46	w	178/203 (88%)	152 (85%)	26 (15%)	0	100	100
47	x	476/515 (92%)	432 (91%)	44 (9%)	0	100	100
48	y	242/245 (99%)	225 (93%)	17 (7%)	0	100	100
49	z	53/106 (50%)	50 (94%)	3 (6%)	0	100	100
52	4	508/593 (86%)	454 (89%)	54 (11%)	0	100	100
53	5	71/120 (59%)	69 (97%)	2 (3%)	0	100	100
54	KK	82/733 (11%)	80 (98%)	2 (2%)	0	100	100
55	LL	111/184 (60%)	111 (100%)	0	0	100	100
56	MM	971/1011 (96%)	926 (95%)	45 (5%)	0	100	100
All	All	10649/13063 (82%)	9689 (91%)	927 (9%)	33 (0%)	37	69

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	339	LEU
11	J	95	ASN
28	b	484	SER
39	m	241	SER
42	r	17	ARG
3	B	139	GLN
3	B	140	ASP
4	C	131	VAL
23	W	178	GLY

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Mol	Chain	Res	Type
28	b	370	ASP
39	m	78	PHE
40	n	153	SER
40	n	384	GLY
4	C	130	ALA
12	L	63	VAL
12	L	77	LEU
19	S	13	ARG
28	b	369	ARG
28	b	399	ALA
28	b	483	ALA
34	h	92	LEU
40	n	355	PRO
42	r	147	TRP
42	r	162	THR
3	B	5	LYS
3	B	239	PRO
17	Q	41	ASP
26	Z	102	GLU
28	b	9	PRO
44	u	3	ILE
23	W	126	ARG
39	m	347	PRO
40	n	455	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	166/196 (85%)	165 (99%)	1 (1%)	78	80
3	B	322/323 (100%)	318 (99%)	4 (1%)	63	72
4	C	288/289 (100%)	287 (100%)	1 (0%)	86	85
5	D	227/245 (93%)	226 (100%)	1 (0%)	84	83
6	E	134/153 (88%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	186/205 (91%)	185 (100%)	1 (0%)	81	82
8	G	191/208 (92%)	191 (100%)	0	100	100
9	H	171/171 (100%)	170 (99%)	1 (1%)	78	80
10	I	117/141 (83%)	117 (100%)	0	100	100
11	J	147/150 (98%)	147 (100%)	0	100	100
12	L	149/159 (94%)	147 (99%)	2 (1%)	61	71
13	M	108/109 (99%)	107 (99%)	1 (1%)	70	75
14	N	175/176 (99%)	175 (100%)	0	100	100
15	O	160/162 (99%)	159 (99%)	1 (1%)	78	80
16	P	145/146 (99%)	144 (99%)	1 (1%)	76	78
17	Q	110/151 (73%)	109 (99%)	1 (1%)	70	75
18	R	129/154 (84%)	128 (99%)	1 (1%)	73	77
19	S	155/156 (99%)	154 (99%)	1 (1%)	78	80
20	T	102/137 (74%)	102 (100%)	0	100	100
21	U	93/107 (87%)	93 (100%)	0	100	100
22	V	104/105 (99%)	104 (100%)	0	100	100
23	W	211/213 (99%)	208 (99%)	3 (1%)	59	71
24	X	106/118 (90%)	104 (98%)	2 (2%)	50	66
25	Y	109/110 (99%)	108 (99%)	1 (1%)	70	75
26	Z	115/116 (99%)	115 (100%)	0	100	100
27	a	76/119 (64%)	75 (99%)	1 (1%)	61	71
28	b	568/573 (99%)	565 (100%)	3 (0%)	81	82
29	c	81/88 (92%)	80 (99%)	1 (1%)	63	72
30	d	94/97 (97%)	94 (100%)	0	100	100
31	e	109/111 (98%)	108 (99%)	1 (1%)	70	75
32	f	90/91 (99%)	90 (100%)	0	100	100
33	g	95/103 (92%)	94 (99%)	1 (1%)	65	74
34	h	104/105 (99%)	104 (100%)	0	100	100
35	i	81/82 (99%)	80 (99%)	1 (1%)	63	72
36	j	70/71 (99%)	70 (100%)	0	100	100
37	k	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	l	45/46 (98%)	45 (100%)	0	100	100
39	m	413/428 (96%)	409 (99%)	4 (1%)	68	75
40	n	334/548 (61%)	334 (100%)	0	100	100
41	p	71/72 (99%)	71 (100%)	0	100	100
42	r	203/229 (89%)	202 (100%)	1 (0%)	81	82
43	s	62/445 (14%)	62 (100%)	0	100	100
44	u	133/180 (74%)	133 (100%)	0	100	100
45	v	258/309 (84%)	258 (100%)	0	100	100
46	w	161/179 (90%)	159 (99%)	2 (1%)	63	72
47	x	428/451 (95%)	427 (100%)	1 (0%)	87	87
48	y	210/211 (100%)	210 (100%)	0	100	100
49	z	48/95 (50%)	48 (100%)	0	100	100
52	4	453/520 (87%)	448 (99%)	5 (1%)	65	74
53	5	67/106 (63%)	67 (100%)	0	100	100
54	KK	75/671 (11%)	75 (100%)	0	100	100
55	LL	99/168 (59%)	99 (100%)	0	100	100
56	MM	809/895 (90%)	809 (100%)	0	100	100
All	All	9225/11262 (82%)	9181 (100%)	44 (0%)	78	82

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	88	ILE
3	B	79	VAL
3	B	81	THR
3	B	229	VAL
3	B	305	ILE
4	C	74	ILE
5	D	148	ILE
7	F	26	VAL
9	H	118	LEU
12	L	12	ASN
12	L	54	LEU
13	M	53	VAL
15	O	124	LEU
16	P	168	LEU

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Mol	Chain	Res	Type
17	Q	147	ARG
18	R	99	LEU
19	S	58	ILE
23	W	109	VAL
23	W	149	ILE
23	W	231	THR
24	X	26	VAL
24	X	38	LEU
25	Y	76	LEU
27	a	78	LEU
28	b	194	VAL
28	b	274	ILE
28	b	445	LEU
29	c	16	LEU
31	e	126	LEU
33	g	95	ILE
35	i	60	LEU
39	m	224	VAL
39	m	255	LEU
39	m	302	LEU
39	m	318	VAL
42	r	225	VAL
46	w	55	ARG
46	w	162	VAL
47	x	480	VAL
52	4	39	LEU
52	4	369	ILE
52	4	475	LEU
52	4	518	ASP
52	4	568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	38	HIS
2	A	139	HIS
3	B	231	HIS
3	B	243	HIS
3	B	269	GLN
4	C	58	HIS
4	C	110	ASN
4	C	116	ASN

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Mol	Chain	Res	Type
4	C	260	GLN
5	D	90	HIS
5	D	264	GLN
7	F	37	ASN
7	F	48	ASN
7	F	186	HIS
8	G	38	GLN
8	G	41	GLN
8	G	85	ASN
8	G	137	ASN
8	G	138	HIS
8	G	221	ASN
8	G	243	GLN
10	I	36	ASN
10	I	48	GLN
10	I	106	GLN
11	J	68	HIS
11	J	95	ASN
12	L	12	ASN
12	L	25	HIS
12	L	37	ASN
13	M	41	GLN
14	N	37	HIS
14	N	156	HIS
14	N	158	HIS
14	N	182	ASN
16	P	34	GLN
16	P	54	HIS
16	P	116	HIS
16	P	118	GLN
18	R	66	HIS
18	R	130	ASN
19	S	74	ASN
19	S	89	ASN
19	S	142	GLN
19	S	154	HIS
20	T	58	GLN
20	T	90	ASN
20	T	95	HIS
20	T	122	GLN
20	T	131	GLN
20	T	149	GLN

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Mol	Chain	Res	Type
21	U	49	ASN
21	U	109	GLN
22	V	132	ASN
23	W	22	ASN
23	W	74	GLN
23	W	88	ASN
23	W	128	ASN
23	W	148	GLN
23	W	167	ASN
23	W	205	GLN
23	W	232	ASN
24	X	65	GLN
25	Y	4	GLN
25	Y	42	GLN
26	Z	29	HIS
26	Z	78	ASN
27	a	62	HIS
27	a	67	HIS
27	a	120	ASN
28	b	26	GLN
28	b	70	ASN
28	b	78	HIS
28	b	107	GLN
28	b	152	GLN
28	b	177	ASN
28	b	217	GLN
28	b	234	ASN
28	b	288	ASN
28	b	333	ASN
28	b	351	GLN
28	b	384	ASN
28	b	429	ASN
28	b	546	GLN
28	b	616	HIS
28	b	619	GLN
28	b	633	HIS
30	d	21	HIS
30	d	57	GLN
31	e	104	ASN
32	f	42	GLN
32	f	77	ASN
32	f	106	ASN

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Mol	Chain	Res	Type
34	h	59	ASN
34	h	113	GLN
35	i	35	ASN
35	i	91	ASN
38	l	43	ASN
39	m	90	GLN
39	m	186	ASN
39	m	227	HIS
39	m	254	HIS
39	m	310	HIS
39	m	411	HIS
40	n	11	ASN
40	n	137	ASN
40	n	157	ASN
40	n	165	GLN
40	n	230	HIS
42	r	70	GLN
44	u	17	HIS
44	u	45	ASN
44	u	76	ASN
44	u	82	ASN
45	v	64	ASN
45	v	173	GLN
45	v	280	GLN
46	w	57	ASN
46	w	83	GLN
47	x	166	ASN
47	x	324	ASN
47	x	325	HIS
47	x	341	HIS
47	x	353	GLN
47	x	359	ASN
47	x	369	ASN
47	x	401	HIS
47	x	407	HIS
47	x	424	ASN
47	x	449	GLN
48	y	21	ASN
48	y	86	ASN
48	y	162	HIS
49	z	12	ASN
52	4	112	GLN

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Mol	Chain	Res	Type
52	4	156	HIS
52	4	273	HIS
52	4	348	HIS
52	4	403	HIS
52	4	428	ASN
52	4	438	GLN
53	5	100	HIS
54	KK	26	GLN
55	LL	64	ASN
55	LL	95	ASN
55	LL	113	ASN
56	MM	87	GLN
56	MM	117	HIS
56	MM	229	ASN
56	MM	445	ASN
56	MM	446	ASN
56	MM	475	HIS
56	MM	528	GLN
56	MM	642	ASN
56	MM	651	GLN
56	MM	662	GLN
56	MM	703	ASN
56	MM	720	ASN
56	MM	838	ASN
56	MM	1012	GLN
56	MM	1062	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	161/162 (99%)	36 (22%)	2 (1%)
50	1	3048/3396 (89%)	902 (29%)	80 (2%)
51	3	120/121 (99%)	28 (23%)	1 (0%)
All	All	3329/3679 (90%)	966 (29%)	83 (2%)

All (966) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	23	U
1	2	34	U
1	2	35	C

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Mol	Chain	Res	Type
1	2	39	G
1	2	51	G
1	2	52	A
1	2	59	A
1	2	62	C
1	2	63	G
1	2	70	G
1	2	80	A
1	2	82	U
1	2	83	C
1	2	84	C
1	2	85	G
1	2	86	U
1	2	87	G
1	2	88	A
1	2	90	U
1	2	95	G
1	2	104	A
1	2	106	C
1	2	111	A
1	2	112	U
1	2	113	U
1	2	114	G
1	2	124	G
1	2	125	U
1	2	126	A
1	2	138	A
1	2	148	G
1	2	151	C
1	2	152	G
1	2	154	C
1	2	156	U
1	2	157	A
50	1	2	U
50	1	13	A
50	1	14	U
50	1	18	G
50	1	22	G
50	1	26	A
50	1	37	U
50	1	40	A
50	1	41	G

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Mol	Chain	Res	Type
50	1	43	A
50	1	45	A
50	1	48	A
50	1	49	A
50	1	50	U
50	1	58	G
50	1	59	G
50	1	60	A
50	1	65	A
50	1	66	A
50	1	71	A
50	1	72	C
50	1	73	C
50	1	75	G
50	1	77	A
50	1	83	U
50	1	89	A
50	1	92	G
50	1	93	C
50	1	94	G
50	1	96	G
50	1	109	A
50	1	110	G
50	1	111	C
50	1	116	A
50	1	117	U
50	1	118	U
50	1	120	G
50	1	121	A
50	1	122	A
50	1	134	U
50	1	135	C
50	1	136	G
50	1	142	C
50	1	143	G
50	1	146	U
50	1	148	G
50	1	154	U
50	1	157	A
50	1	161	G
50	1	165	A
50	1	166	C

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Mol	Chain	Res	Type
50	1	169	U
50	1	170	G
50	1	172	G
50	1	173	G
50	1	182	U
50	1	187	A
50	1	190	U
50	1	191	U
50	1	192	C
50	1	199	A
50	1	200	C
50	1	206	G
50	1	210	U
50	1	211	A
50	1	213	A
50	1	218	G
50	1	219	A
50	1	234	G
50	1	240	U
50	1	241	G
50	1	243	G
50	1	245	U
50	1	246	U
50	1	249	U
50	1	250	U
50	1	251	G
50	1	252	U
50	1	253	A
50	1	263	C
50	1	269	G
50	1	284	A
50	1	285	A
50	1	286	U
50	1	291	C
50	1	295	A
50	1	298	U
50	1	305	U
50	1	306	A
50	1	311	C
50	1	323	A
50	1	329	U
50	1	339	C

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Mol	Chain	Res	Type
50	1	343	U
50	1	344	A
50	1	349	A
50	1	351	A
50	1	359	U
50	1	362	U
50	1	370	U
50	1	376	G
50	1	378	A
50	1	397	A
50	1	398	A
50	1	399	A
50	1	401	U
50	1	402	A
50	1	403	C
50	1	404	G
50	1	421	G
50	1	422	A
50	1	439	C
50	1	440	A
50	1	495	G
50	1	498	A
50	1	503	C
50	1	507	U
50	1	510	G
50	1	517	G
50	1	521	A
50	1	523	A
50	1	535	G
50	1	540	U
50	1	543	C
50	1	544	C
50	1	546	C
50	1	547	G
50	1	548	G
50	1	550	A
50	1	552	G
50	1	555	U
50	1	556	U
50	1	557	A
50	1	558	U
50	1	559	A

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Mol	Chain	Res	Type
50	1	560	G
50	1	569	A
50	1	578	A
50	1	579	G
50	1	591	G
50	1	592	A
50	1	597	G
50	1	600	G
50	1	604	G
50	1	607	A
50	1	609	G
50	1	611	A
50	1	620	U
50	1	621	A
50	1	622	A
50	1	628	A
50	1	636	C
50	1	642	U
50	1	643	U
50	1	644	G
50	1	645	A
50	1	646	A
50	1	647	A
50	1	650	C
50	1	660	A
50	1	677	A
50	1	681	U
50	1	690	A
50	1	691	A
50	1	692	A
50	1	705	A
50	1	708	G
50	1	712	G
50	1	715	A
50	1	717	C
50	1	719	U
50	1	720	A
50	1	721	G
50	1	722	G
50	1	728	G
50	1	761	A
50	1	762	U

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Mol	Chain	Res	Type
50	1	763	G
50	1	764	U
50	1	765	C
50	1	766	U
50	1	767	U
50	1	768	C
50	1	771	A
50	1	776	U
50	1	777	U
50	1	779	G
50	1	780	A
50	1	781	G
50	1	785	G
50	1	786	A
50	1	799	G
50	1	806	A
50	1	808	A
50	1	817	A
50	1	826	G
50	1	830	A
50	1	837	A
50	1	849	C
50	1	850	U
50	1	857	G
50	1	861	C
50	1	874	U
50	1	875	G
50	1	879	U
50	1	880	G
50	1	884	A
50	1	890	C
50	1	896	A
50	1	907	G
50	1	908	G
50	1	911	C
50	1	914	A
50	1	916	G
50	1	917	A
50	1	923	C
50	1	924	G
50	1	932	U
50	1	934	G

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Mol	Chain	Res	Type
50	1	936	A
50	1	938	C
50	1	943	U
50	1	944	C
50	1	946	U
50	1	953	G
50	1	956	U
50	1	957	C
50	1	958	C
50	1	959	C
50	1	974	G
50	1	976	U
50	1	978	G
50	1	980	A
50	1	981	U
50	1	986	U
50	1	991	G
50	1	992	A
50	1	994	G
50	1	996	A
50	1	997	A
50	1	998	A
50	1	999	G
50	1	1000	C
50	1	1001	G
50	1	1048	A
50	1	1049	C
50	1	1050	U
50	1	1051	U
50	1	1054	A
50	1	1057	A
50	1	1058	U
50	1	1063	G
50	1	1064	A
50	1	1065	A
50	1	1066	G
50	1	1093	A
50	1	1094	U
50	1	1095	U
50	1	1097	G
50	1	1098	A
50	1	1102	A

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Mol	Chain	Res	Type
50	1	1103	A
50	1	1104	G
50	1	1106	G
50	1	1107	C
50	1	1110	U
50	1	1111	U
50	1	1115	G
50	1	1116	G
50	1	1117	G
50	1	1118	C
50	1	1123	U
50	1	1127	G
50	1	1128	U
50	1	1129	A
50	1	1130	A
50	1	1132	C
50	1	1135	A
50	1	1136	A
50	1	1151	U
50	1	1153	A
50	1	1155	C
50	1	1160	C
50	1	1176	C
50	1	1178	G
50	1	1180	A
50	1	1181	U
50	1	1182	A
50	1	1190	A
50	1	1191	U
50	1	1192	C
50	1	1193	A
50	1	1196	C
50	1	1197	A
50	1	1198	C
50	1	1199	C
50	1	1200	A
50	1	1201	C
50	1	1204	A
50	1	1206	G
50	1	1217	A
50	1	1220	U
50	1	1221	A

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Mol	Chain	Res	Type
50	1	1227	C
50	1	1235	U
50	1	1239	C
50	1	1240	A
50	1	1241	U
50	1	1242	G
50	1	1244	A
50	1	1245	A
50	1	1248	C
50	1	1251	A
50	1	1252	A
50	1	1253	U
50	1	1254	C
50	1	1258	U
50	1	1262	G
50	1	1263	A
50	1	1264	G
50	1	1265	U
50	1	1266	G
50	1	1271	A
50	1	1272	C
50	1	1277	C
50	1	1278	A
50	1	1286	A
50	1	1287	A
50	1	1296	C
50	1	1299	U
50	1	1301	A
50	1	1302	A
50	1	1303	A
50	1	1304	A
50	1	1305	U
50	1	1306	G
50	1	1307	G
50	1	1308	A
50	1	1310	G
50	1	1313	G
50	1	1316	C
50	1	1317	A
50	1	1325	U
50	1	1330	A
50	1	1331	U

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Mol	Chain	Res	Type
50	1	1348	U
50	1	1349	G
50	1	1351	U
50	1	1352	A
50	1	1353	U
50	1	1354	G
50	1	1355	A
50	1	1356	U
50	1	1357	G
50	1	1370	G
50	1	1386	A
50	1	1387	G
50	1	1392	G
50	1	1399	A
50	1	1400	G
50	1	1404	G
50	1	1419	A
50	1	1434	G
50	1	1437	C
50	1	1446	A
50	1	1455	U
50	1	1475	A
50	1	1480	G
50	1	1481	A
50	1	1487	G
50	1	1494	U
50	1	1497	C
50	1	1503	A
50	1	1508	C
50	1	1523	U
50	1	1527	C
50	1	1536	G
50	1	1539	A
50	1	1542	G
50	1	1549	U
50	1	1554	U
50	1	1555	U
50	1	1556	C
50	1	1557	A
50	1	1560	G
50	1	1561	G
50	1	1562	C

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Mol	Chain	Res	Type
50	1	1566	A
50	1	1567	U
50	1	1568	U
50	1	1569	U
50	1	1570	U
50	1	1571	A
50	1	1572	U
50	1	1573	G
50	1	1575	A
50	1	1580	A
50	1	1581	C
50	1	1582	C
50	1	1583	A
50	1	1589	A
50	1	1593	A
50	1	1596	C
50	1	1606	U
50	1	1607	U
50	1	1613	A
50	1	1619	A
50	1	1620	U
50	1	1629	U
50	1	1639	C
50	1	1642	A
50	1	1643	A
50	1	1645	U
50	1	1657	C
50	1	1680	G
50	1	1683	A
50	1	1687	U
50	1	1716	U
50	1	1717	U
50	1	1724	U
50	1	1736	G
50	1	1741	A
50	1	1742	U
50	1	1750	A
50	1	1751	G
50	1	1760	A
50	1	1762	C
50	1	1763	U
50	1	1764	U

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Mol	Chain	Res	Type
50	1	1765	U
50	1	1766	G
50	1	1770	G
50	1	1772	U
50	1	1775	G
50	1	1780	G
50	1	1782	U
50	1	1797	A
50	1	1808	G
50	1	1810	A
50	1	1812	G
50	1	1814	A
50	1	1815	U
50	1	1816	A
50	1	1817	G
50	1	1820	U
50	1	1821	U
50	1	1830	G
50	1	1834	U
50	1	1839	A
50	1	1840	U
50	1	1841	A
50	1	1842	A
50	1	1846	C
50	1	1848	G
50	1	1849	C
50	1	1851	G
50	1	1858	A
50	1	1871	U
50	1	1880	U
50	1	1886	A
50	1	1898	G
50	1	1901	A
50	1	1906	G
50	1	1909	A
50	1	1926	C
50	1	1930	A
50	1	1935	G
50	1	1937	U
50	1	1941	C
50	1	1952	G
50	1	1953	G

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Mol	Chain	Res	Type
50	1	2094	C
50	1	2102	U
50	1	2107	A
50	1	2108	C
50	1	2110	G
50	1	2113	A
50	1	2120	A
50	1	2121	G
50	1	2122	G
50	1	2126	A
50	1	2131	A
50	1	2134	G
50	1	2141	U
50	1	2144	A
50	1	2158	A
50	1	2162	U
50	1	2163	C
50	1	2169	G
50	1	2170	U
50	1	2176	U
50	1	2184	U
50	1	2188	A
50	1	2193	U
50	1	2194	G
50	1	2195	C
50	1	2196	C
50	1	2198	A
50	1	2200	U
50	1	2205	U
50	1	2207	A
50	1	2208	A
50	1	2210	G
50	1	2212	C
50	1	2213	A
50	1	2225	U
50	1	2237	C
50	1	2242	A
50	1	2243	A
50	1	2244	A
50	1	2245	C
50	1	2247	G
50	1	2248	C

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Mol	Chain	Res	Type
50	1	2249	G
50	1	2250	G
50	1	2252	A
50	1	2253	G
50	1	2255	A
50	1	2256	A
50	1	2257	C
50	1	2264	U
50	1	2268	U
50	1	2269	U
50	1	2270	A
50	1	2271	A
50	1	2274	U
50	1	2275	A
50	1	2276	G
50	1	2277	C
50	1	2278	C
50	1	2279	A
50	1	2280	A
50	1	2316	G
50	1	2317	A
50	1	2318	U
50	1	2334	U
50	1	2335	G
50	1	2336	U
50	1	2347	U
50	1	2365	C
50	1	2369	G
50	1	2371	G
50	1	2378	C
50	1	2385	G
50	1	2386	A
50	1	2388	U
50	1	2393	G
50	1	2397	A
50	1	2398	A
50	1	2401	A
50	1	2402	A
50	1	2405	C
50	1	2409	G
50	1	2410	U
50	1	2411	U

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Mol	Chain	Res	Type
50	1	2412	G
50	1	2414	G
50	1	2418	G
50	1	2419	A
50	1	2435	G
50	1	2437	G
50	1	2443	A
50	1	2444	C
50	1	2445	A
50	1	2502	A
50	1	2503	G
50	1	2504	U
50	1	2514	U
50	1	2515	A
50	1	2522	G
50	1	2523	A
50	1	2525	G
50	1	2526	C
50	1	2527	G
50	1	2528	G
50	1	2529	A
50	1	2531	C
50	1	2532	U
50	1	2533	G
50	1	2534	G
50	1	2537	U
50	1	2538	U
50	1	2539	C
50	1	2540	A
50	1	2541	U
50	1	2542	U
50	1	2543	U
50	1	2544	U
50	1	2547	A
50	1	2548	C
50	1	2549	G
50	1	2550	U
50	1	2551	U
50	1	2552	C
50	1	2554	A
50	1	2555	G
50	1	2560	C

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Mol	Chain	Res	Type
50	1	2561	A
50	1	2566	C
50	1	2567	C
50	1	2568	C
50	1	2569	A
50	1	2570	U
50	1	2571	U
50	1	2572	C
50	1	2573	G
50	1	2576	G
50	1	2578	U
50	1	2585	G
50	1	2586	G
50	1	2593	A
50	1	2594	C
50	1	2595	A
50	1	2596	U
50	1	2606	G
50	1	2607	G
50	1	2614	G
50	1	2621	G
50	1	2623	G
50	1	2625	C
50	1	2626	A
50	1	2628	A
50	1	2635	A
50	1	2638	C
50	1	2644	C
50	1	2645	G
50	1	2648	G
50	1	2649	A
50	1	2650	U
50	1	2651	G
50	1	2652	U
50	1	2653	C
50	1	2654	C
50	1	2655	U
50	1	2656	A
50	1	2657	A
50	1	2659	G
50	1	2668	U
50	1	2670	G

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Mol	Chain	Res	Type
50	1	2672	G
50	1	2674	A
50	1	2677	G
50	1	2681	U
50	1	2686	A
50	1	2687	G
50	1	2688	U
50	1	2689	A
50	1	2690	G
50	1	2691	A
50	1	2692	A
50	1	2693	C
50	1	2694	A
50	1	2695	A
50	1	2696	A
50	1	2698	G
50	1	2699	G
50	1	2700	G
50	1	2702	A
50	1	2704	A
50	1	2706	G
50	1	2713	U
50	1	2714	G
50	1	2715	A
50	1	2719	U
50	1	2720	G
50	1	2721	A
50	1	2722	U
50	1	2724	U
50	1	2725	U
50	1	2726	C
50	1	2727	A
50	1	2728	G
50	1	2729	U
50	1	2730	G
50	1	2731	U
50	1	2732	G
50	1	2740	A
50	1	2749	G
50	1	2752	U
50	1	2754	G
50	1	2756	C

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Mol	Chain	Res	Type
50	1	2758	A
50	1	2759	U
50	1	2761	G
50	1	2762	A
50	1	2763	U
50	1	2764	C
50	1	2765	C
50	1	2766	U
50	1	2767	U
50	1	2768	U
50	1	2770	G
50	1	2771	U
50	1	2772	C
50	1	2773	C
50	1	2777	G
50	1	2778	G
50	1	2789	U
50	1	2790	A
50	1	2791	G
50	1	2793	G
50	1	2794	G
50	1	2795	U
50	1	2796	G
50	1	2798	C
50	1	2799	A
50	1	2800	G
50	1	2801	A
50	1	2802	A
50	1	2803	A
50	1	2804	A
50	1	2805	G
50	1	2810	C
50	1	2814	G
50	1	2816	G
50	1	2817	A
50	1	2818	U
50	1	2820	A
50	1	2821	C
50	1	2822	U
50	1	2824	G
50	1	2825	C
50	1	2826	U

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Mol	Chain	Res	Type
50	1	2827	U
50	1	2842	U
50	1	2844	C
50	1	2845	A
50	1	2846	U
50	1	2847	A
50	1	2857	C
50	1	2858	U
50	1	2859	U
50	1	2860	U
50	1	2861	U
50	1	2862	U
50	1	2863	G
50	1	2864	A
50	1	2865	U
50	1	2866	U
50	1	2867	C
50	1	2868	U
50	1	2869	U
50	1	2870	C
50	1	2871	G
50	1	2872	A
50	1	2873	U
50	1	2874	G
50	1	2875	U
50	1	2876	C
50	1	2877	G
50	1	2878	G
50	1	2879	C
50	1	2887	A
50	1	2889	C
50	1	2897	A
50	1	2898	G
50	1	2899	C
50	1	2901	G
50	1	2914	G
50	1	2916	U
50	1	2918	G
50	1	2923	U
50	1	2924	U
50	1	2925	C
50	1	2926	A

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Mol	Chain	Res	Type
50	1	2927	C
50	1	2928	C
50	1	2929	C
50	1	2930	A
50	1	2935	U
50	1	2936	A
50	1	2945	G
50	1	2946	A
50	1	2947	G
50	1	2949	U
50	1	2951	G
50	1	2952	G
50	1	2953	U
50	1	2954	U
50	1	2955	U
50	1	2957	G
50	1	2970	C
50	1	2971	A
50	1	2978	U
50	1	2979	U
50	1	2980	U
50	1	2981	U
50	1	2982	A
50	1	2983	C
50	1	2996	U
50	1	2997	G
50	1	3003	G
50	1	3012	A
50	1	3017	A
50	1	3021	A
50	1	3022	G
50	1	3023	U
50	1	3027	A
50	1	3029	A
50	1	3030	G
50	1	3031	G
50	1	3032	A
50	1	3036	G
50	1	3037	U
50	1	3056	U
50	1	3058	U
50	1	3059	G

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Mol	Chain	Res	Type
50	1	3069	G
50	1	3078	U
50	1	3079	U
50	1	3080	G
50	1	3086	A
50	1	3087	A
50	1	3089	C
50	1	3090	U
50	1	3092	C
50	1	3099	C
50	1	3100	U
50	1	3107	U
50	1	3109	G
50	1	3114	A
50	1	3115	C
50	1	3117	C
50	1	3122	A
50	1	3129	A
50	1	3130	A
50	1	3131	U
50	1	3142	A
50	1	3143	C
50	1	3148	U
50	1	3150	A
50	1	3153	U
50	1	3154	C
50	1	3155	U
50	1	3156	U
50	1	3157	U
50	1	3165	A
50	1	3170	A
50	1	3172	A
50	1	3173	G
50	1	3174	A
50	1	3176	G
50	1	3179	U
50	1	3180	A
50	1	3181	C
50	1	3187	A
50	1	3196	U
50	1	3199	G
50	1	3207	U

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Mol	Chain	Res	Type
50	1	3217	C
50	1	3218	A
50	1	3219	G
50	1	3227	A
50	1	3228	C
50	1	3229	G
50	1	3243	A
50	1	3244	A
50	1	3245	A
50	1	3247	G
50	1	3253	G
50	1	3256	G
50	1	3259	U
50	1	3260	G
50	1	3263	G
50	1	3268	A
50	1	3270	U
50	1	3271	G
50	1	3273	A
50	1	3276	G
50	1	3277	U
50	1	3279	A
50	1	3281	U
50	1	3286	G
50	1	3287	U
50	1	3288	G
50	1	3289	G
50	1	3294	A
50	1	3295	A
50	1	3304	U
50	1	3309	G
50	1	3313	U
50	1	3316	A
50	1	3317	U
50	1	3318	G
50	1	3319	U
50	1	3320	A
50	1	3341	U
50	1	3342	A
50	1	3345	G
50	1	3347	A
50	1	3351	U

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Mol	Chain	Res	Type
50	1	3352	U
50	1	3353	G
50	1	3355	U
50	1	3356	G
50	1	3363	U
50	1	3369	G
50	1	3375	A
50	1	3378	C
50	1	3382	U
50	1	3389	U
50	1	3396	U
51	3	7	G
51	3	13	A
51	3	15	C
51	3	22	A
51	3	41	G
51	3	48	U
51	3	51	A
51	3	52	G
51	3	53	U
51	3	54	U
51	3	60	G
51	3	65	G
51	3	67	G
51	3	73	C
51	3	74	C
51	3	76	A
51	3	77	G
51	3	78	U
51	3	79	A
51	3	86	U
51	3	94	C
51	3	97	A
51	3	102	A
51	3	103	A
51	3	110	G
51	3	112	G
51	3	120	C
51	3	121	U

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	88	A
1	2	123	G
50	1	13	A
50	1	40	A
50	1	160	G
50	1	169	U
50	1	239	G
50	1	284	A
50	1	619	A
50	1	645	A
50	1	649	A
50	1	720	A
50	1	761	A
50	1	765	C
50	1	849	C
50	1	916	G
50	1	1057	A
50	1	1064	A
50	1	1097	G
50	1	1102	A
50	1	1103	A
50	1	1128	U
50	1	1192	C
50	1	1205	A
50	1	1241	U
50	1	1302	A
50	1	1307	G
50	1	1329	U
50	1	1355	A
50	1	1554	U
50	1	1567	U
50	1	1568	U
50	1	1570	U
50	1	1574	C
50	1	1581	C
50	1	1716	U
50	1	2101	C
50	1	2209	U
50	1	2263	C
50	1	2269	U
50	1	2317	A
50	1	2418	G
50	1	2513	U

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Mol	Chain	Res	Type
50	1	2525	G
50	1	2537	U
50	1	2547	A
50	1	2593	A
50	1	2624	G
50	1	2625	C
50	1	2651	G
50	1	2652	U
50	1	2654	C
50	1	2655	U
50	1	2658	G
50	1	2728	G
50	1	2731	U
50	1	2753	G
50	1	2761	G
50	1	2770	G
50	1	2795	U
50	1	2801	A
50	1	2817	A
50	1	2819	A
50	1	2828	G
50	1	2857	C
50	1	2865	U
50	1	2866	U
50	1	2875	U
50	1	2900	A
50	1	2946	A
50	1	2954	U
50	1	3030	G
50	1	3078	U
50	1	3121	U
50	1	3171	U
50	1	3218	A
50	1	3228	C
50	1	3269	U
50	1	3276	G
50	1	3316	A
50	1	3350	C
50	1	3351	U
51	3	52	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
59	GTP	m	501	60	33,34,34	1.12	2 (6%)	50,54,54	1.61	9 (18%)
59	GTP	b	701	60	33,34,34	1.00	0	50,54,54	1.56	9 (18%)

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
59	GTP	m	501	60	-	3/22/38/38	0/3/3/3
59	GTP	b	701	60	-	7/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	m	501	GTP	C5-N7	-2.46	1.34	1.39
59	m	501	GTP	O4'-C4'	-2.19	1.40	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	m	501	GTP	C5-C4-N3	-4.73	120.87	128.39
59	b	701	GTP	C5-C4-N3	-4.44	121.33	128.39
59	b	701	GTP	C2-N3-C4	4.33	119.76	112.30
59	m	501	GTP	C2-N3-C4	4.10	119.37	112.30
59	m	501	GTP	C2-N1-C6	-3.15	119.40	125.11
59	m	501	GTP	N9-C8-N7	-3.15	107.56	113.40
59	b	701	GTP	C2-N1-C6	-2.98	119.71	125.11
59	b	701	GTP	N9-C8-N7	-2.95	107.94	113.40
59	m	501	GTP	N9-C4-N3	2.81	131.57	125.95
59	m	501	GTP	C8-N7-C5	2.65	108.99	104.26
59	b	701	GTP	C8-N7-C5	2.60	108.89	104.26
59	b	701	GTP	C5-C6-N1	2.54	119.71	113.25
59	b	701	GTP	N9-C4-N3	2.53	131.00	125.95
59	b	701	GTP	O6-C6-C5	-2.41	120.16	126.53
59	m	501	GTP	C5-C6-N1	2.26	119.02	113.25
59	m	501	GTP	C3'-C2'-C1'	2.19	105.61	101.46
59	m	501	GTP	O6-C6-C5	-2.16	120.84	126.53
59	b	701	GTP	C4-C5-N7	-2.03	107.45	110.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	b	701	GTP	C5'-O5'-PA-O3A
59	b	701	GTP	C5'-O5'-PA-O1A
59	b	701	GTP	C5'-O5'-PA-O2A
59	m	501	GTP	C5'-O5'-PA-O1A
59	m	501	GTP	C3'-C4'-C5'-O5'
59	b	701	GTP	C4'-C5'-O5'-PA
59	b	701	GTP	PA-O3A-PB-O1B
59	b	701	GTP	O4'-C4'-C5'-O5'
59	m	501	GTP	O4'-C4'-C5'-O5'
59	b	701	GTP	C3'-C4'-C5'-O5'

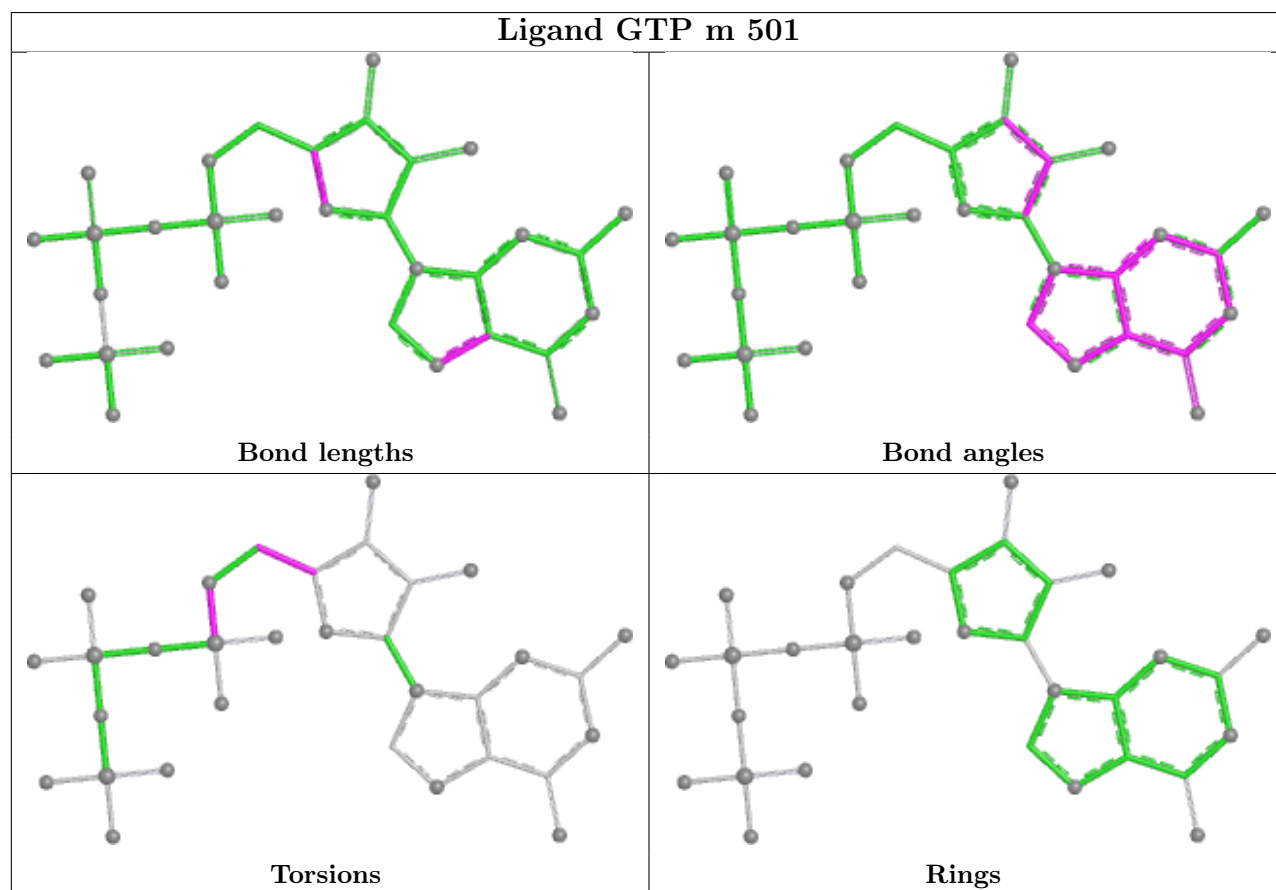
There are no ring outliers.

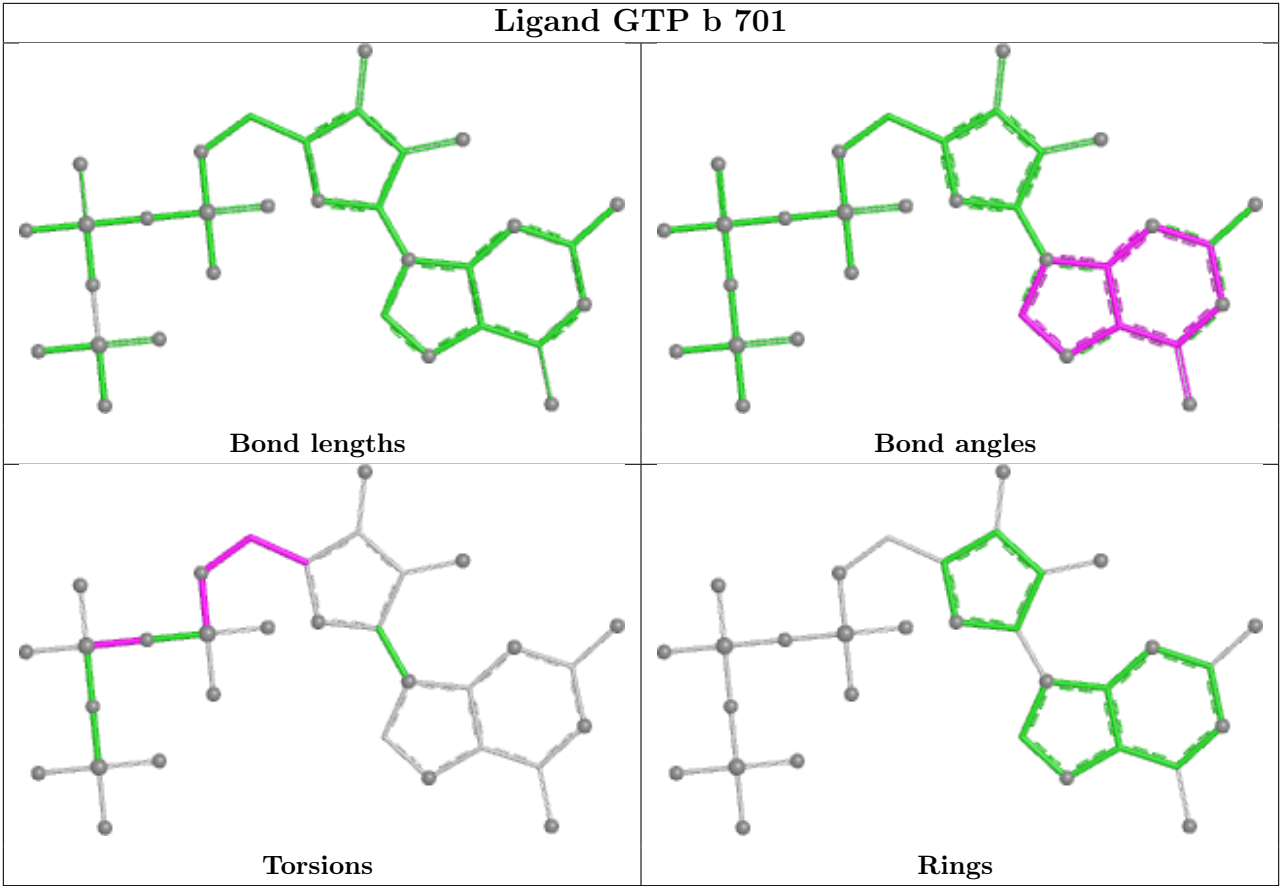
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	m	501	GTP	2	0
59	b	701	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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
43	s	1
32	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	s	53:ASN	C	54:PHE	N	1.17
1	f	102:LEU	C	103:TYR	N	1.14

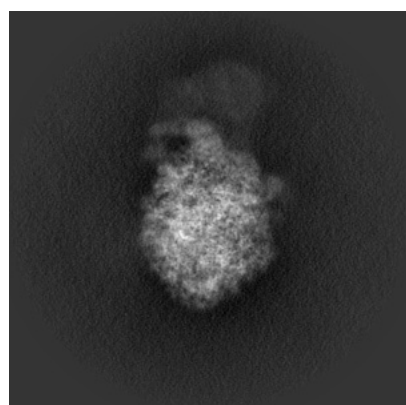
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4302. These allow visual inspection of the internal detail of the map and identification of artifacts.

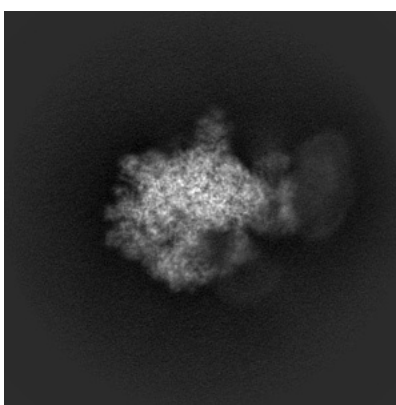
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

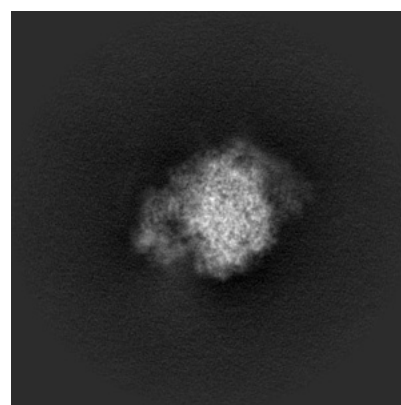
6.1.1 Primary map



X



Y

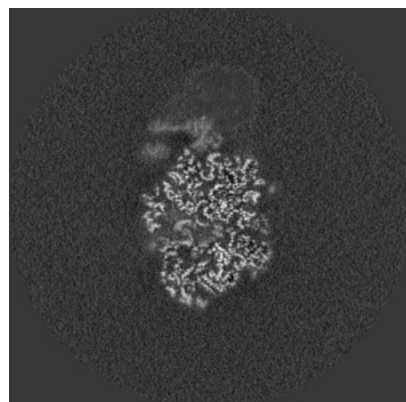


Z

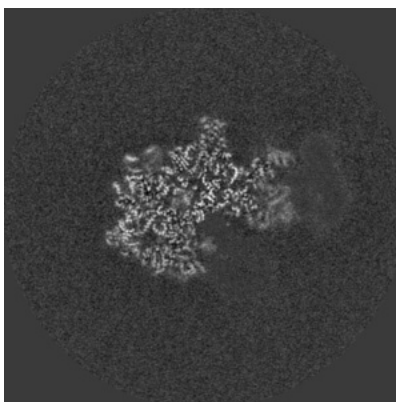
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

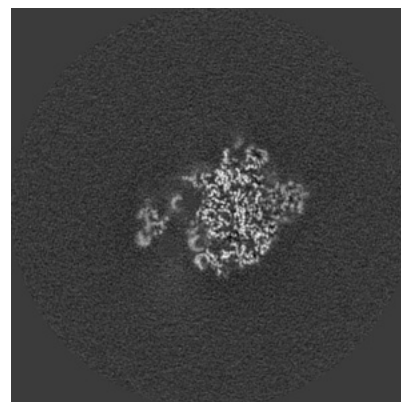
6.2.1 Primary map



X Index: 220



Y Index: 220

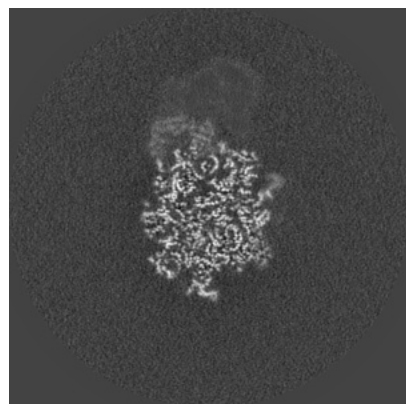


Z Index: 220

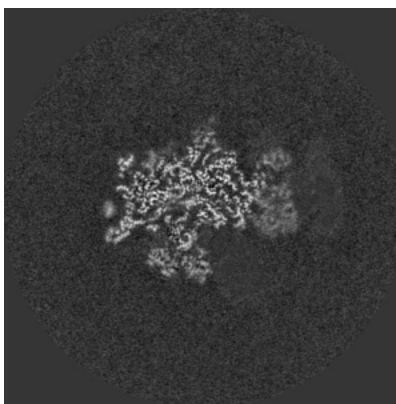
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

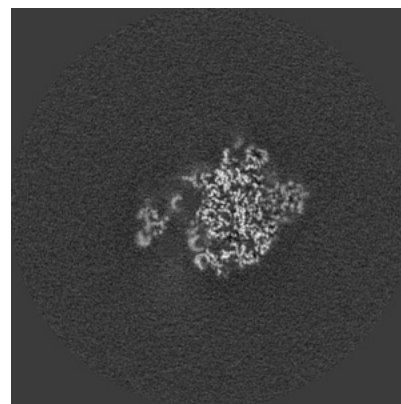
6.3.1 Primary map



X Index: 241



Y Index: 210

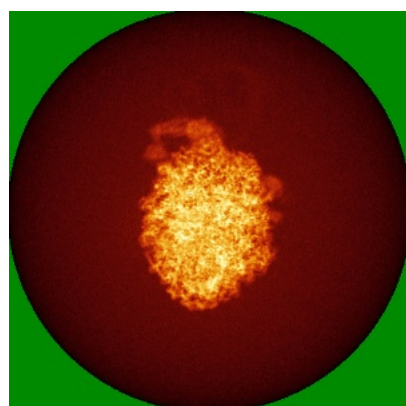


Z Index: 220

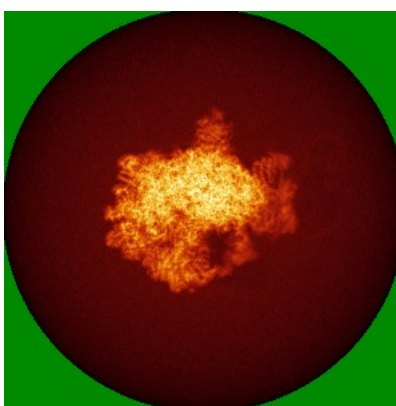
The images above show the largest variance slices of the map in three orthogonal directions.

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

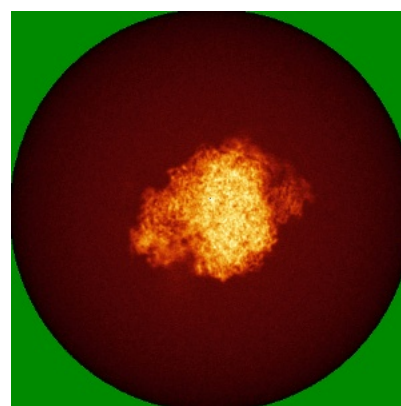
6.4.1 Primary map



X



Y



Z

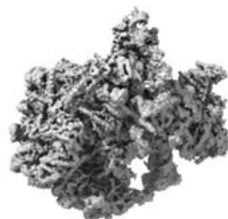
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

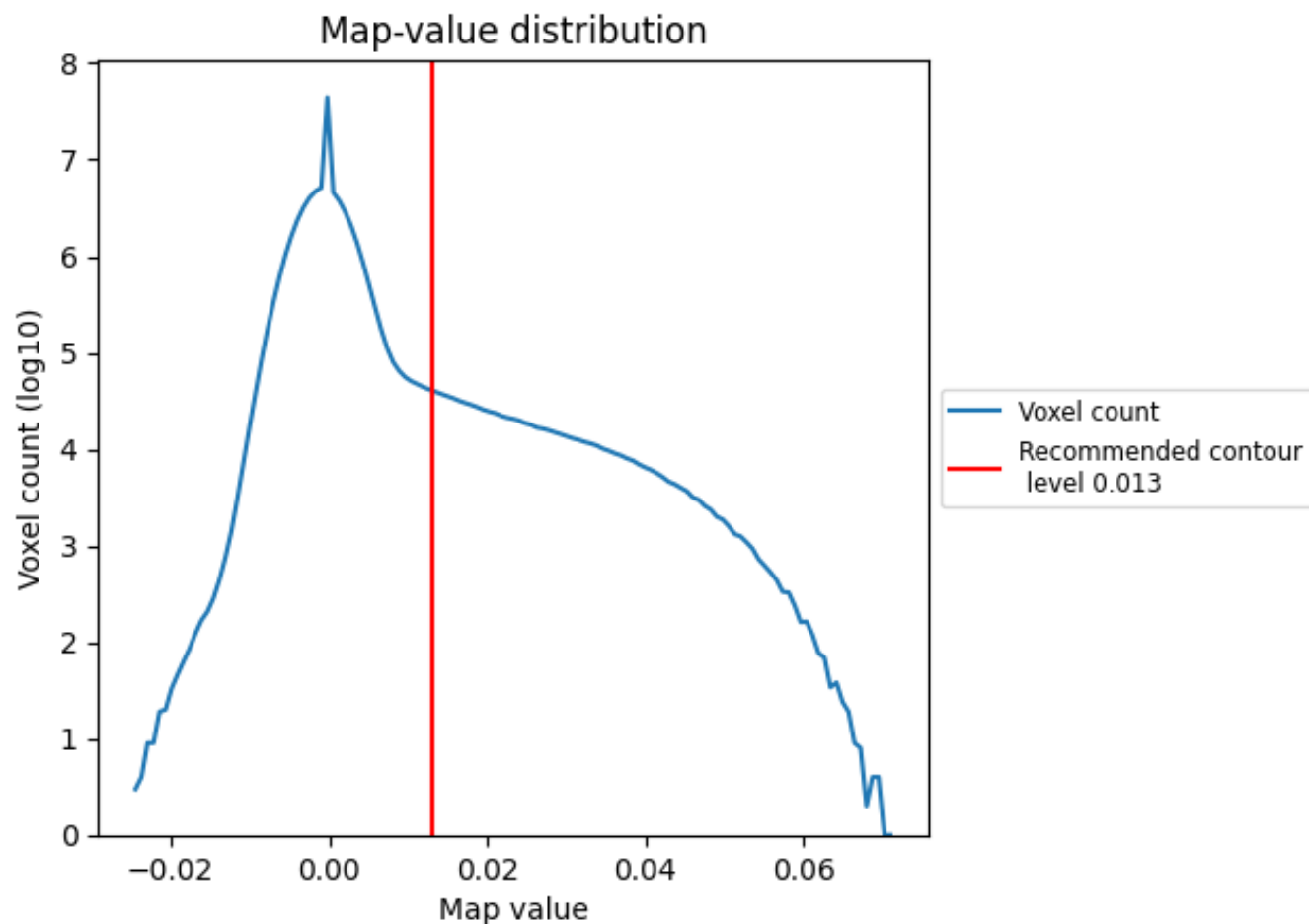
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

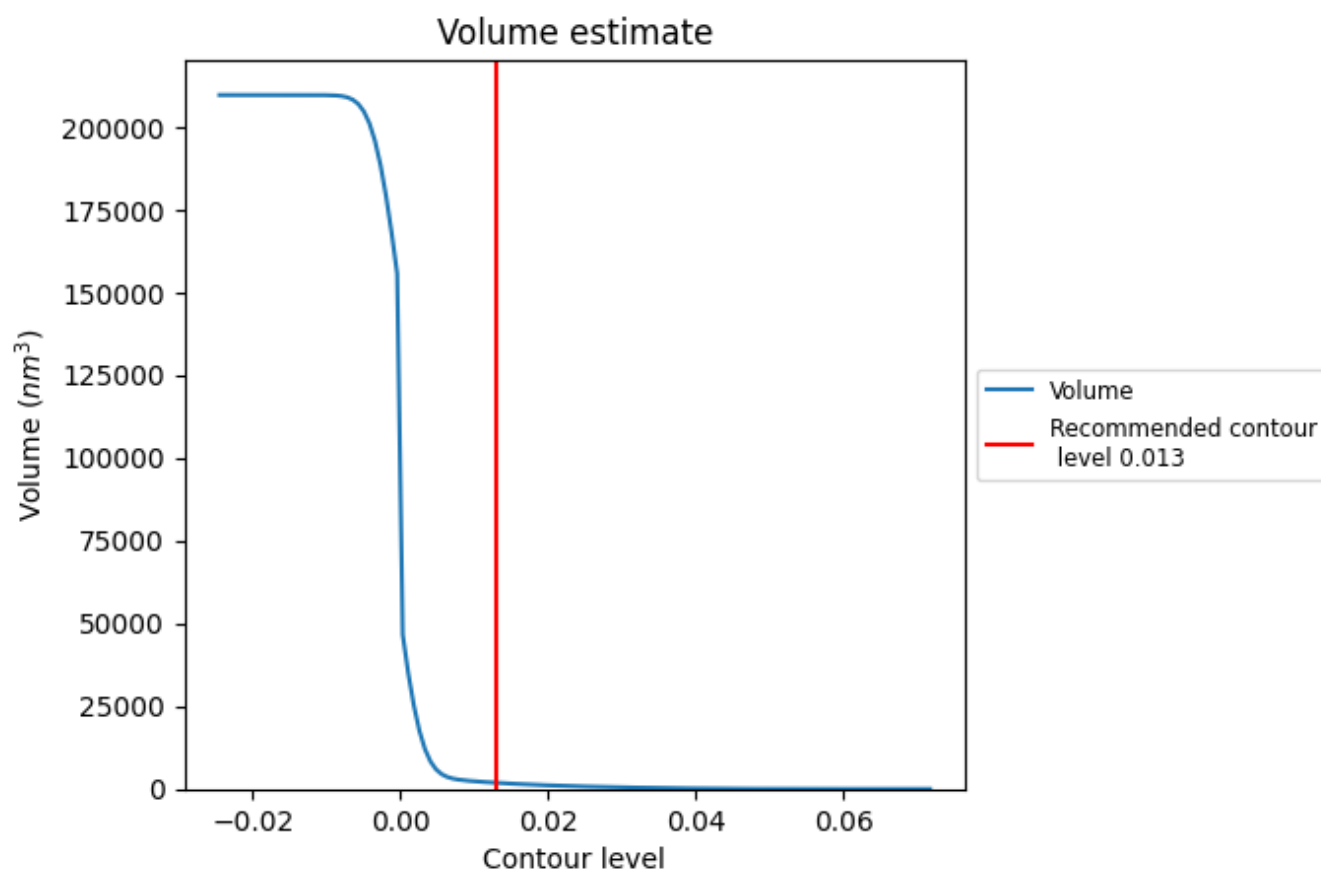
This section contains the results of statistical analysis of the map.

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.

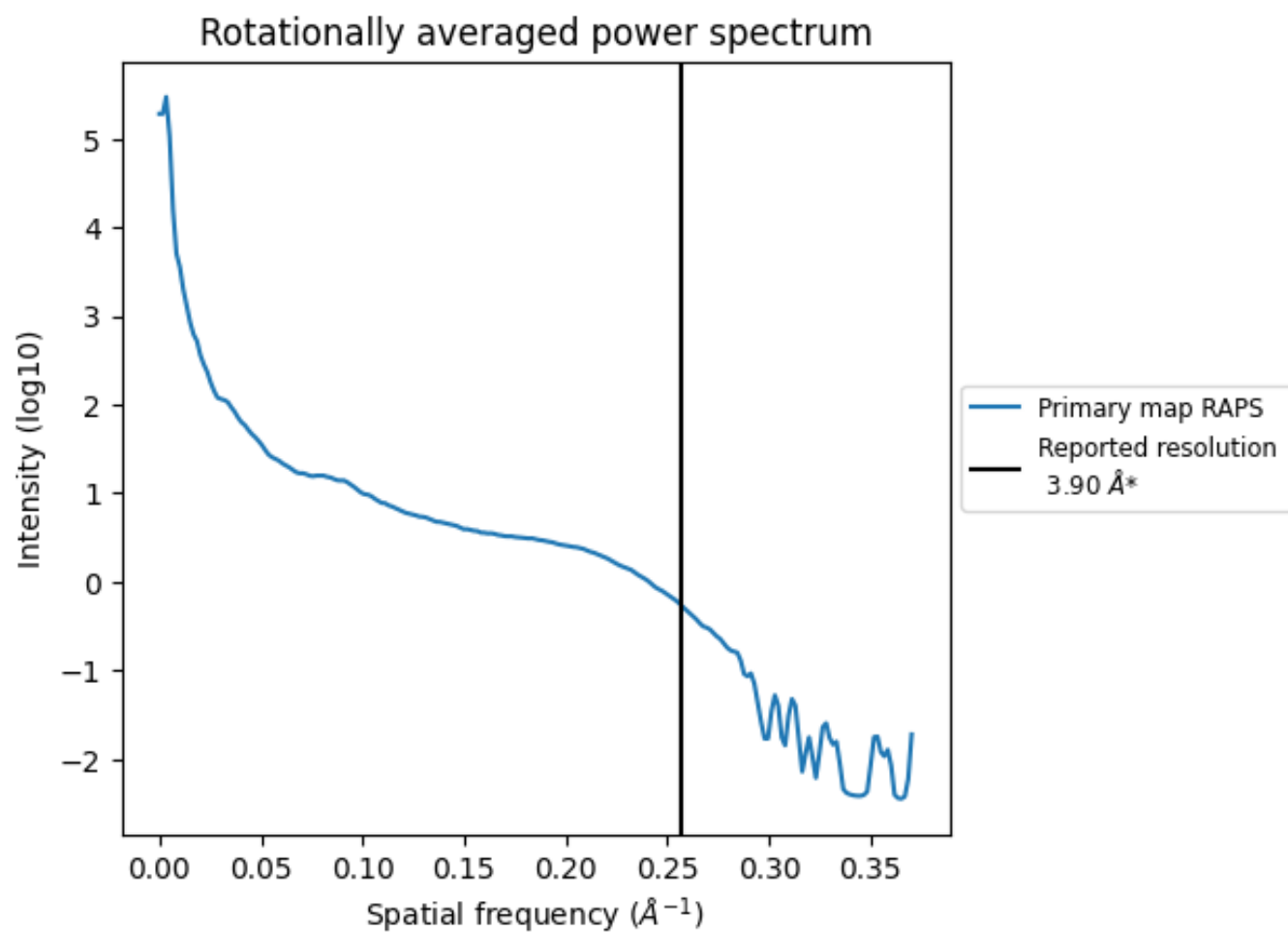
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1864 nm^3 ; this corresponds to an approximate mass of 1683 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 0.256 $\text{\AA}^{-1}$

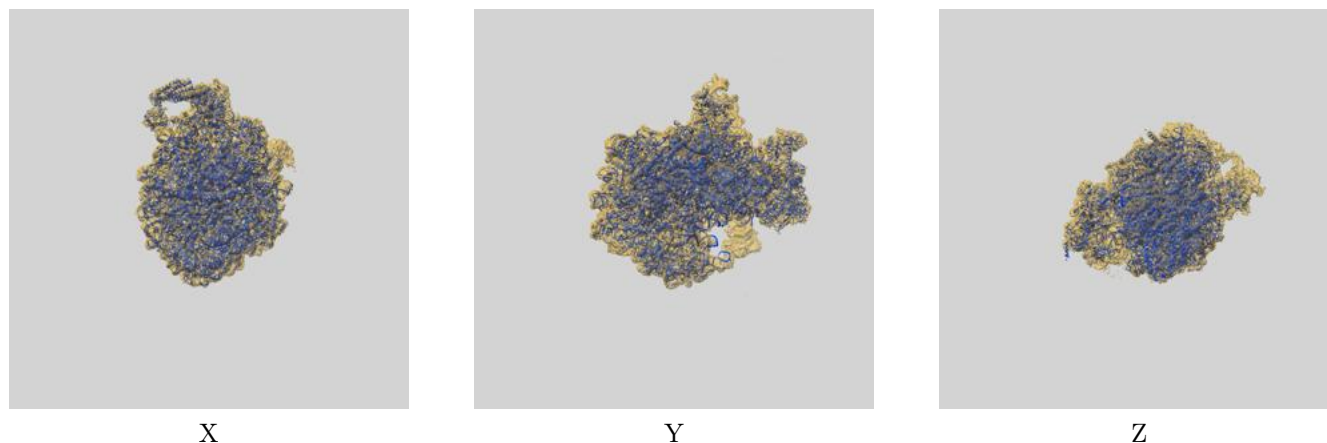
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

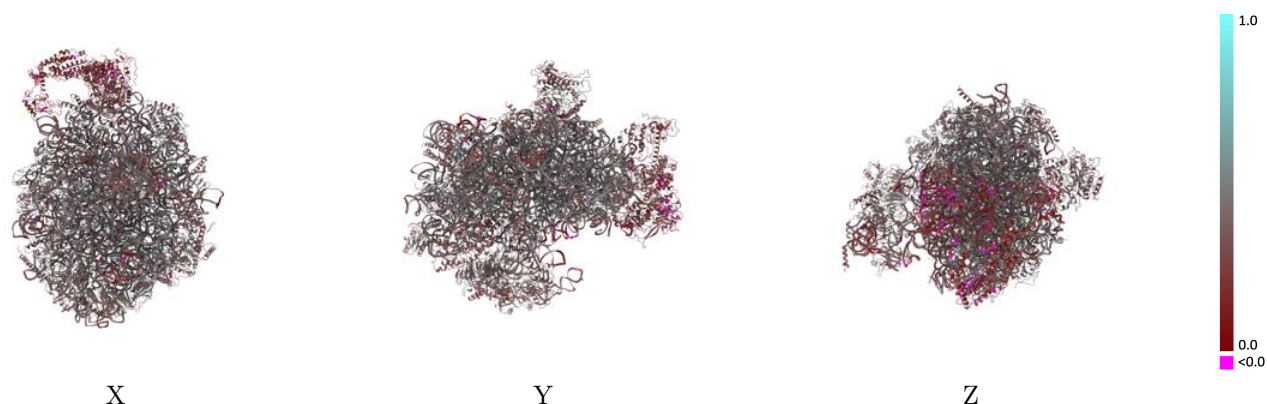
This section contains information regarding the fit between EMDB map EMD-4302 and PDB model 6FT6. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



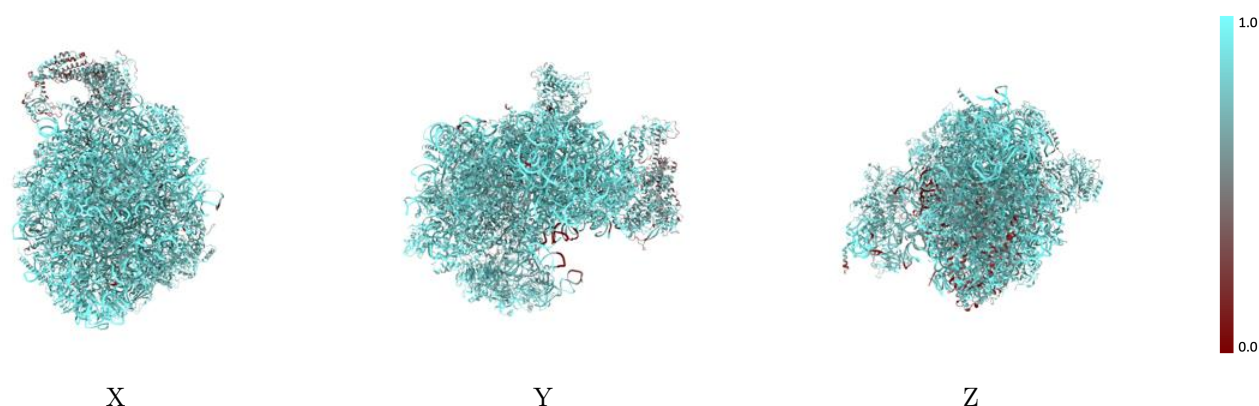
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



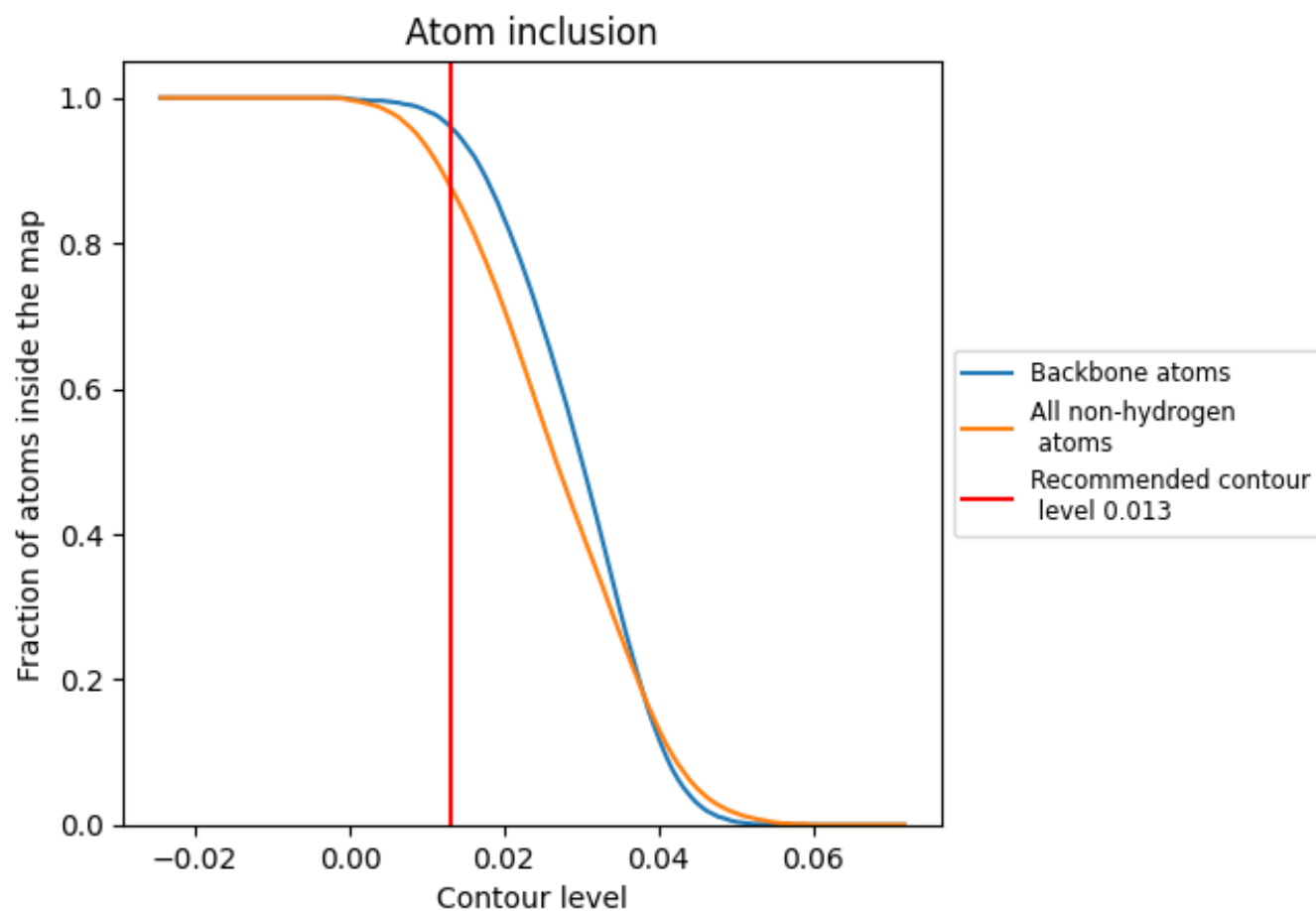
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.3840
1	 0.9610	 0.4040
2	 0.9850	 0.4290
3	 0.9270	 0.3110
4	 0.7890	 0.3690
5	 0.6530	 0.2690
A	 0.8750	 0.4450
B	 0.8890	 0.4320
C	 0.8890	 0.4260
D	 0.8090	 0.3340
E	 0.8760	 0.4010
F	 0.8770	 0.4060
G	 0.8090	 0.3820
H	 0.8650	 0.4280
I	 0.6190	 0.3690
J	 0.8180	 0.2740
KK	 0.5330	 0.1900
L	 0.8790	 0.4100
LL	 0.5380	 0.2130
M	 0.8790	 0.3930
MM	 0.6080	 0.2120
N	 0.8800	 0.4290
NN	 0.6540	 0.3030
O	 0.8910	 0.4230
P	 0.8520	 0.4070
Q	 0.8790	 0.4130
R	 0.8710	 0.4120
S	 0.8450	 0.3950
T	 0.7190	 0.3480
U	 0.8630	 0.3780
V	 0.8510	 0.4410
W	 0.8680	 0.3620
X	 0.8340	 0.4200
Y	 0.8820	 0.4180
Z	 0.8840	 0.4090



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Chain	Atom inclusion	Q-score
a	 0.8670	 0.4060
b	 0.7960	 0.3710
c	 0.8890	 0.3980
d	 0.8650	 0.4290
e	 0.8710	 0.4390
f	 0.9040	 0.4430
g	 0.8730	 0.4260
h	 0.8440	 0.3950
i	 0.8400	 0.3870
j	 0.9040	 0.4460
k	 0.8560	 0.3920
l	 0.8770	 0.4360
m	 0.8280	 0.3940
n	 0.7420	 0.2940
p	 0.8670	 0.4120
r	 0.8400	 0.4140
s	 0.7150	 0.3550
u	 0.8020	 0.3860
v	 0.8100	 0.3590
w	 0.7800	 0.3560
x	 0.8570	 0.3760
y	 0.8470	 0.3890
z	 0.8460	 0.3680