



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:19 PM EDT

PDB ID : 8VVQ / pdb_00008vvq
EMDB ID : EMD-43565
Title : Codon sampling state of elongation inhibitor-treated mammalian ribosomes
obtained from merged datasets
Authors : Loerch, S.; Petrossian, E.; Smith, P.R.; Campbell, Z.T.
Deposited on : 2024-01-31
Resolution : 2.70 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:

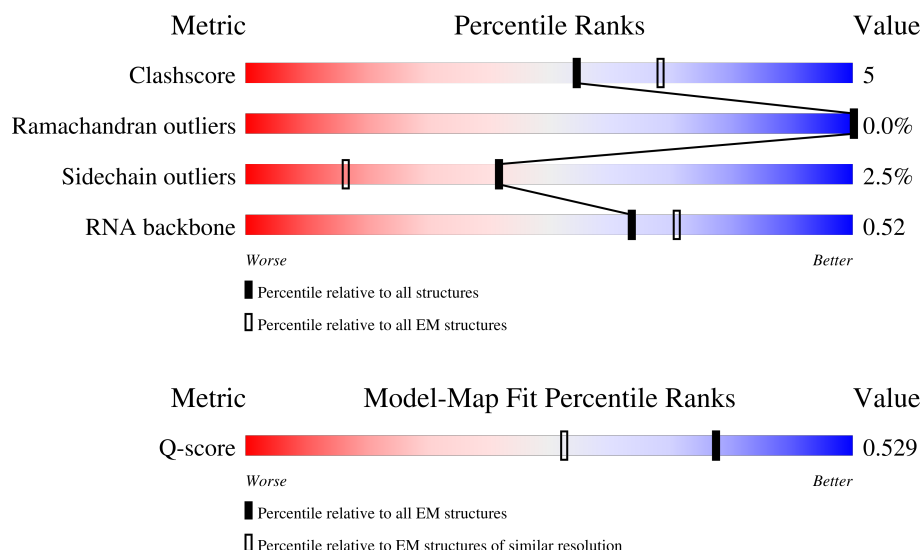
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 2.70 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.



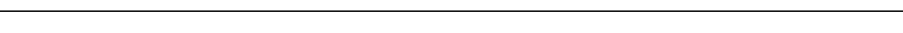
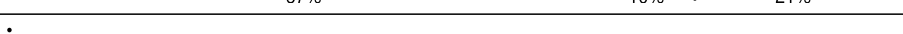
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	A	257	
2	B	403	
3	C	413	

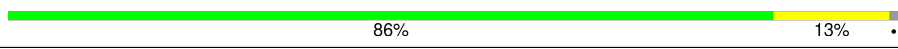
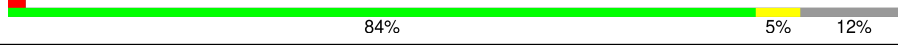
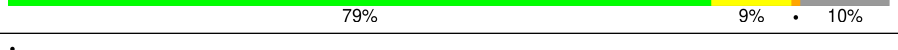
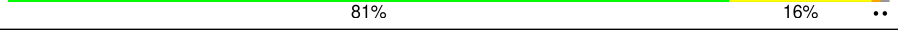
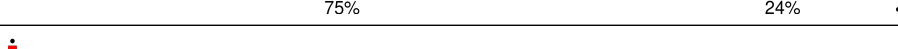
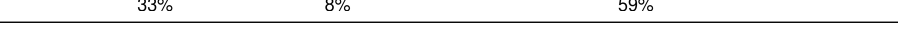
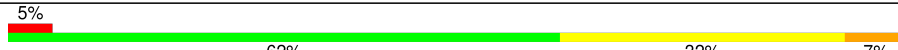
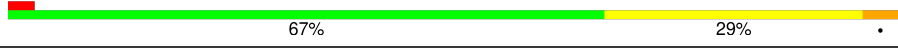
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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	249	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	K	211	
12	L	218	
13	M	204	
14	N	203	
15	O	213	
16	P	188	
17	Q	212	
18	R	224	
19	S	160	
20	T	128	
21	U	140	
22	V	157	
23	W	156	
24	X	145	
25	Y	136	
26	Z	148	
27	AA	245	
28	BA	115	

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Mol	Chain	Length	Quality of chain
29	CA	125	
30	DA	135	
31	EA	110	
32	FA	129	
33	GA	123	
34	HA	105	
35	IA	97	
36	JA	70	
37	KA	51	
38	LA	128	
39	MA	25	
40	NA	106	
41	OA	92	
42	PA	137	
43	RA	165	
44	SA	76	
45	TA	76	
46	UA	75	
47	VA	12	
48	WA	3584	
49	XA	120	
50	YA	156	
51	ZA	1869	
52	AB	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CB	293	
55	DB	281	
56	EB	263	
57	FB	204	
58	GB	249	
59	HB	432	
60	IB	208	
61	JB	194	
62	KB	165	
63	LB	158	
64	MB	132	
65	NB	151	
66	OB	151	
67	PB	145	
68	QB	172	
69	RB	135	
70	SB	152	
71	TB	145	
72	UB	119	
73	VB	83	
74	WB	130	
75	XB	143	
76	YB	131	
77	ZB	124	
78	AC	115	

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Mol	Chain	Length	Quality of chain
79	BC	84	
80	CC	69	
81	DC	56	
82	EC	133	
83	FC	188	
84	GC	317	
85	HC	462	
86	IC	4	
87	b	318	
88	c	14	

2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 222430 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	250	Total	C	N	O	S	0	0
			1914	1199	392	317	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			3196	2035	603	545	13		

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	294	Total	C	N	O	S	0	0
			2395	1514	439	428	14		

- Molecule 5 is a protein called L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	228	Total	C	N	O	S	0	0
			1823	1173	349	298	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	227	Total	C	N	O	S	0	0
			1897	1217	366	305	9		

- Molecule 7 is a protein called L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	229	Total	C	N	O	S	0	0
			1850	1181	356	309	4		

- Molecule 8 is a protein called L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1372	867	256	243	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	46	ILE	-	insertion	UNP G1TPV0
K	47	ALA	-	insertion	UNP G1TPV0
K	48	PRO	-	insertion	UNP G1TPV0
K	49	ARG	-	insertion	UNP G1TPV0
K	50	PRO	-	insertion	UNP G1TPV0
K	51	ALA	-	insertion	UNP G1TPV0
K	52	ALA	-	insertion	UNP G1TPV0
K	53	GLY	-	insertion	UNP G1TPV0
K	54	PRO	-	insertion	UNP G1TPV0

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	156	Total	C	N	O	S	0	0
			1266	793	245	219	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	43	SER	ALA	conflict	UNP G1TVT6

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	4	ASP	ASN	conflict	UNP G1TFE0
P	14	ARG	TRP	conflict	UNP G1TFE0
P	53	MET	LEU	conflict	UNP G1TFE0
P	58	ARG	TRP	conflict	UNP G1TFE0
P	75	ARG	GLN	conflict	UNP G1TFE0
P	80	ALA	PRO	conflict	UNP G1TFE0
P	86	VAL	ILE	conflict	UNP G1TFE0

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Chain	Residue	Modelled	Actual	Comment	Reference
P	104	ARG	HIS	conflict	UNP G1TFE0
P	110	ARG	CYS	conflict	UNP G1TFE0
P	137	VAL	GLY	conflict	UNP G1TFE0
P	157	GLY	ARG	conflict	UNP G1TFE0
P	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	101	Total	C	N	O	S	0	0
			826	530	144	150	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	18	LEU	VAL	conflict	UNP G1TSG1
T	32	GLY	ARG	conflict	UNP G1TSG1
T	36	ALA	GLU	conflict	UNP G1TSG1
T	39	PHE	SER	conflict	UNP G1TSG1
T	54	GLY	ARG	conflict	UNP G1TSG1
T	60	VAL	ALA	conflict	UNP G1TSG1
T	62	SER	THR	conflict	UNP G1TSG1
T	63	LEU	ILE	conflict	UNP G1TSG1

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Chain	Residue	Modelled	Actual	Comment	Reference
T	97	ARG	HIS	conflict	UNP G1TSG1
T	106	THR	SER	conflict	UNP G1TSG1
T	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 21 is a protein called L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	135	Total	C	N	O	S	0	0
			1004	631	191	177	5		

- Molecule 22 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	110	Total	C	N	O	S	0	0
			887	555	179	149	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	78	SER	PHE	conflict	UNP G1SE28

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 24 is a protein called L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called L27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 27 is a protein called L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AA	107	Total	C	N	O	S	0	0
			873	542	195	133	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	99	Total	C	N	O	S	0	0
			769	486	135	141	7		

- Molecule 29 is a protein called L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CA	108	Total	C	N	O	S	0	0
			893	563	172	156	2		

- Molecule 30 is a protein called L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DA	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	EA	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FA	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 33 is a protein called L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	GA	121	Total	C	N	O	S	0	0
			1008	637	203	167	1		

- Molecule 34 is a protein called L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	HA	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	IA	87	Total	C	N	O	S	0	0
			716	440	159	112	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JA	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
JA	24	LYS	ASN	conflict	UNP G1U001

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	KA	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LA	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	MA	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NA	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	OA	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 42 is a protein called L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	PA	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 43 is a protein called L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	RA	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 44 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SA	76	Total	C	N	O	P	0	0
			1622	726	300	521	75		

- Molecule 45 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	TA	76	Total	C	N	O	P	0	0
			1615	722	286	532	75		

- Molecule 46 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	UA	75	Total	C	N	O	P	0	0
			1586	711	279	521	75		

- Molecule 47 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	VA	12	Total	C	N	O	P	0	0
			249	114	42	81	12		

- Molecule 48 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	WA	3578	Total	C	N	O	P	0	0
			76735	34173	14061	24923	3578		

- Molecule 49 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	XA	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XA	2	U	N	conflict	GB X06789.1
XA	36	C	N	conflict	GB X06789.1
XA	102	U	N	conflict	GB X06789.1
XA	112	U	N	conflict	GB X06789.1
XA	114	U	N	conflict	GB X06789.1
XA	119	U	C	conflict	GB X06789.1
XA	120	U	N	conflict	GB X06789.1

- Molecule 50 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	YA	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	ZA	1716	Total	C	N	O	P	0	0
			36623	16347	6572	11989	1715		

- Molecule 52 is a protein called RPSA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AB	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 53 is a protein called S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 54 is a protein called S2-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CB	220	Total	C	N	O	S	0	0
			1707	1105	293	300	9		

- Molecule 55 is a protein called S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DB	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 56 is a protein called S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EB	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EB	25	GLY	SER	conflict	UNP G1TK17
EB	51	ARG	LYS	conflict	UNP G1TK17
EB	78	THR	ALA	conflict	UNP G1TK17
EB	156	VAL	MET	conflict	UNP G1TK17

- Molecule 57 is a protein called S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FB	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 58 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	GB	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HB	185	Total	C	N	O	S	0	0
			1489	952	271	265	1		

- Molecule 60 is a protein called S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	IB	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IB	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 61 is a protein called S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	JB	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 62 is a protein called S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KB	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 63 is a protein called S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LB	144	Total	C	N	O	S	0	0
			1180	752	223	199	6		

- Molecule 64 is a protein called S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MB	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NB	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 66 is a protein called S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	OB	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 67 is a protein called S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PB	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QB	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RB	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 70 is a protein called S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SB	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 71 is a protein called S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TB	142	Total	C	N	O	S	0	0
			1104	693	212	196	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TB	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UB	102	Total	C	N	O	S	0	0
			808	507	154	143	4		

- Molecule 73 is a protein called S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VB	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VB	3	ASN	SER	conflict	UNP G1TM82
VB	4	ASP	ASN	conflict	UNP G1TM82
VB	33	GLN	PRO	conflict	UNP G1TM82
VB	50	PHE	SER	conflict	UNP G1TM82
VB	75	ALA	SER	conflict	UNP G1TM82
VB	76	ASP	HIS	conflict	UNP G1TM82
VB	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 74 is a protein called S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	WB	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 75 is a protein called S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	XB	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 76 is a protein called S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YB	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ZB	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 78 is a protein called S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AC	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	28	ARG	CYS	conflict	UNP G1TFE8
AC	56	ALA	VAL	conflict	UNP G1TFE8
AC	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 79 is a protein called S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	BC	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 80 is a protein called S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	CC	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	DC	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 82 is a protein called S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	EC	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 83 is a protein called S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	FC	69	Total	C	N	O	S	0	0
			564	357	105	95	7		

- Molecule 84 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	GC	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 85 is a protein called eukaryotic elongation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	HC	440	Total	C	N	O	S	0	0
			3371	2143	581	630	17		

- Molecule 86 is a protein called peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	IC	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 87 is a protein called RPLP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	b	167	Total	C	N	O	S	0	0
			1279	813	228	229	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	82	LEU	ILE	conflict	UNP G1SPK4

- Molecule 88 is a protein called RPLP peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	c	11	Total	C	N	O	S	0	0
			86	53	11	21	1		

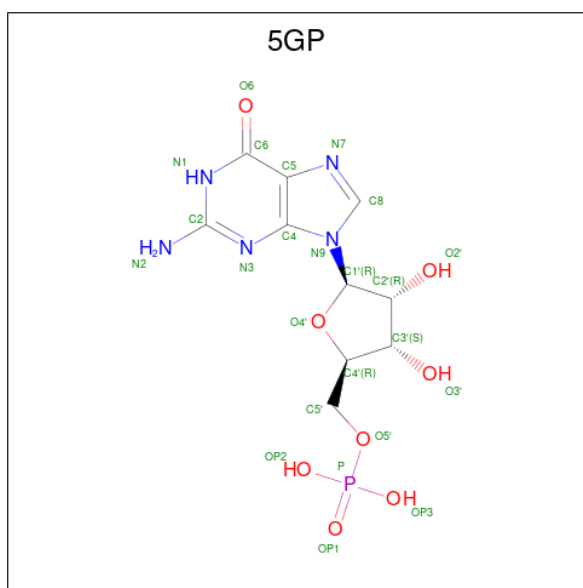
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	A	1	Total	Mg	0
			1	1	
89	B	1	Total	Mg	0
			1	1	
89	I	1	Total	Mg	0
			1	1	
89	O	1	Total	Mg	0
			1	1	
89	U	1	Total	Mg	0
			1	1	
89	Z	1	Total	Mg	0
			1	1	
89	DA	1	Total	Mg	0
			1	1	
89	FA	1	Total	Mg	0
			1	1	
89	IA	1	Total	Mg	0
			1	1	
89	SA	1	Total	Mg	0
			1	1	
89	WA	186	Total	Mg	0
			186	186	
89	XA	6	Total	Mg	0
			6	6	
89	YA	4	Total	Mg	0
			4	4	
89	ZA	80	Total	Mg	0
			80	80	
89	LB	1	Total	Mg	0
			1	1	
89	AC	1	Total	Mg	0
			1	1	
89	HC	1	Total	Mg	0
			1	1	
89	b	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

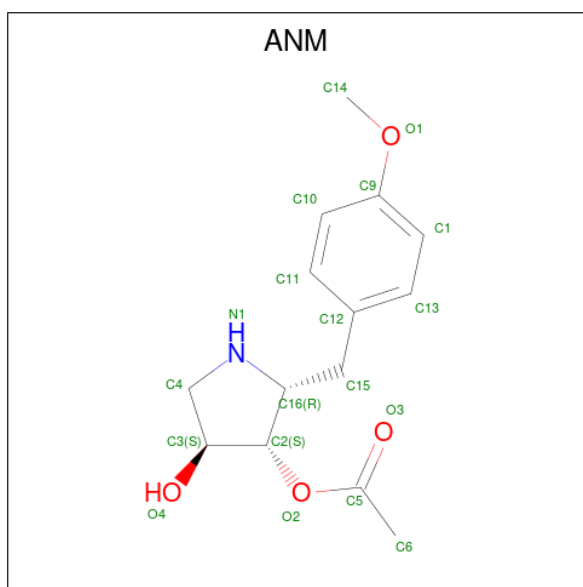
Mol	Chain	Residues	Atoms		AltConf
90	FA	1	Total	Zn	0
			1	1	
90	IA	1	Total	Zn	0
			1	1	
90	LA	1	Total	Zn	0
			1	1	
90	NA	1	Total	Zn	0
			1	1	
90	OA	1	Total	Zn	0
			1	1	
90	AC	1	Total	Zn	0
			1	1	
90	DC	1	Total	Zn	0
			1	1	
90	FC	1	Total	Zn	0
			1	1	

- Molecule 91 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



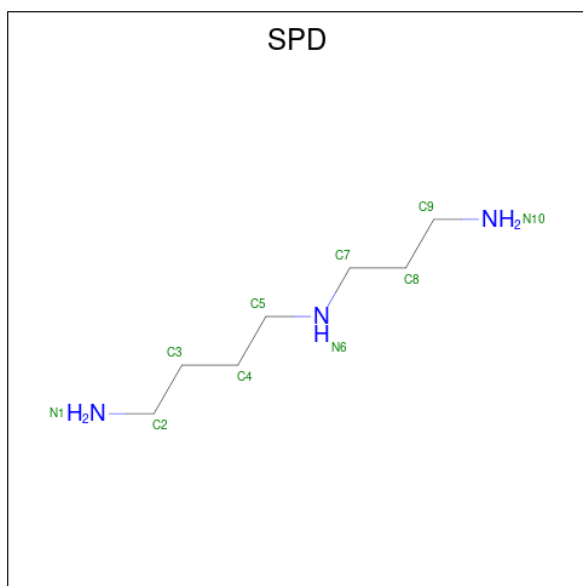
Mol	Chain	Residues	Atoms					AltConf
91	UA	1	Total	C	N	O	P	0
			24	10	5	8	1	

- Molecule 92 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
92	WA	1	Total	C	N	O	0
			19	14	1	4	

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

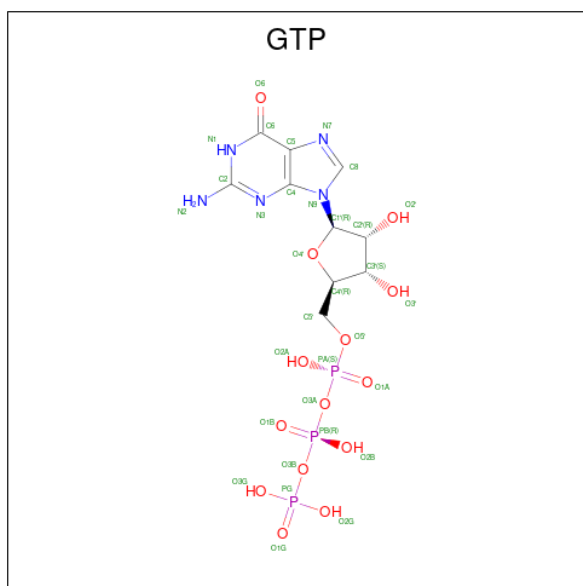


Mol	Chain	Residues	Atoms			AltConf
93	WA	1	Total	C	N	0
			10	7	3	

- Molecule 94 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
94	WA	1	Total	K	0
			1	1	

- Molecule 95 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

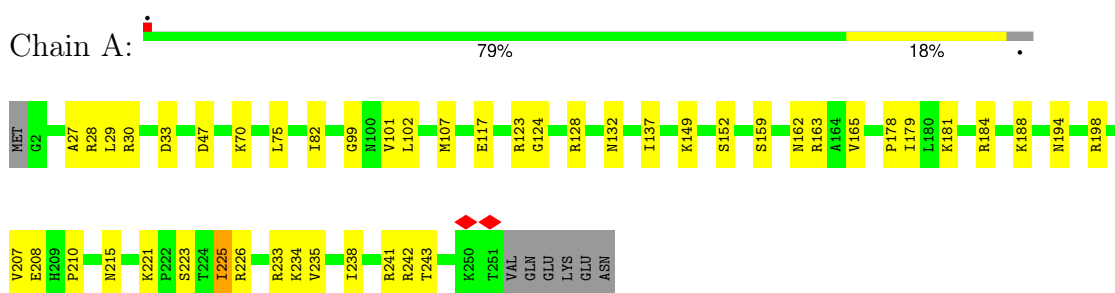


Mol	Chain	Residues	Atoms				AltConf
96	HC	1	Total	C	N	O	0
			6	3	1	2	

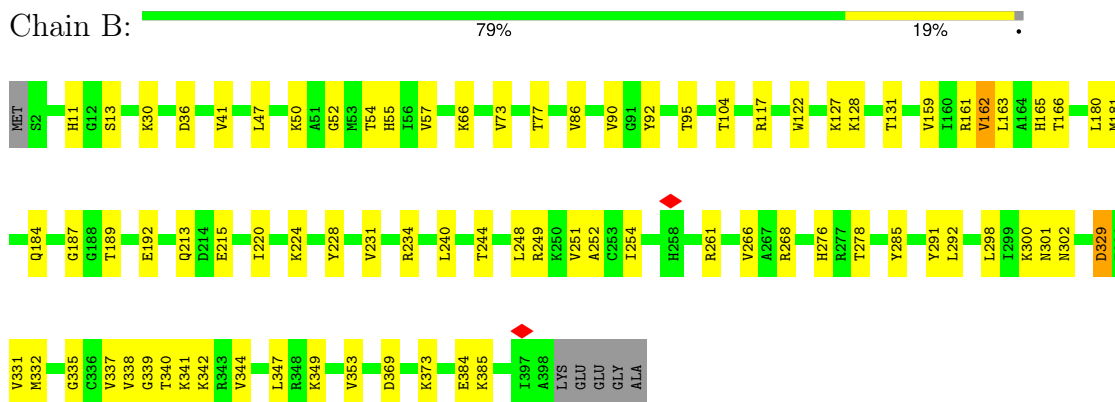
3 Residue-property plots

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.

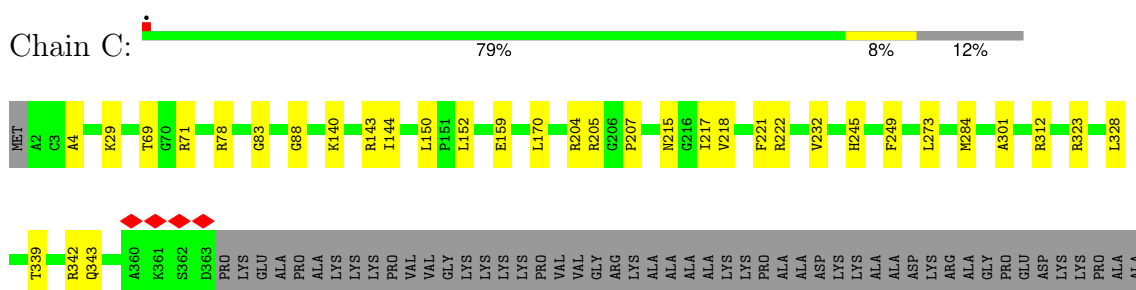
• Molecule 1: uL2



• Molecule 2: uL3



• Molecule 3: uL4



• Molecule 4: uL18

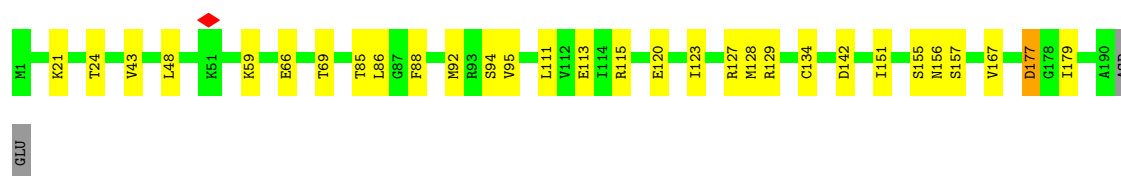
Sequence logo for the 100th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows amino acid positions from 1 to 100. The sequence is: MET, C2, V7, Y16, T28, R33, V37, D40, K43, R50, M51, I52, V53, I60, I64, A65, I74, A80, V88, L105, D116, T126, G127, D128, D136, P139, L146, L150, G156, V159, L163, A166, L171, T181. The G127 position shows a high peak in information content, reaching approximately 0.35 bits.

[illegible]

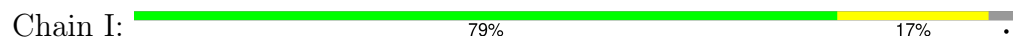
Sequence logo for the 22nd position of the 22-residue protein. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the 22 positions. Position 22 is highlighted with a red diamond and a red arrow. The sequence logo shows that position 22 is highly conserved, with a strong preference for the amino acid 'R' (Arginine). Other positions show varying degrees of conservation, with positions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, and 21 showing lower information content.

MET	SER	SER	SER	TYR	ARG	LEU	GLY	CYS	TYR	MET	LYS	GLU	GLU	ARG	HIS	ASN	LEU	VAL	LEU	CYS	LEU	TRP	SER	GLN	SER	PRO	GLY	ILE	LEU	ASN	SER	LYS	CYS	LEU	TRP	PRO	PHE	THR	ASN	ILE	HIS	LEU	LEU	VAL	GLY	ALA	LEU	PRO	ARG	GLY	GLY	ALA	TRP	GLY	GLY	GLY	ARG
PRO	THR	K184	P187	V193	I210	D213	V214	D215	E218	I236	L237	K238	A241	T253	T254	Q259	L271	V294	K312	E313	L314	A315	THR	LYS	LEU	GLY	K387	K90	Q96	R106	P111	I114	R115	L116	R126	L127	K128	F136	V139	R142	L148	L157	R170	K173	K174	A175	A176	GLY	LYS	ASP							

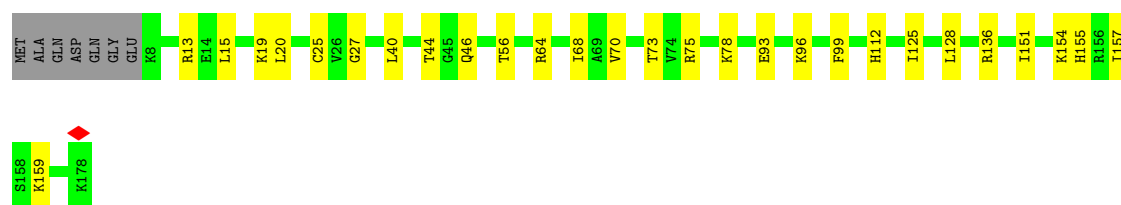
Chain H: 83% 15%



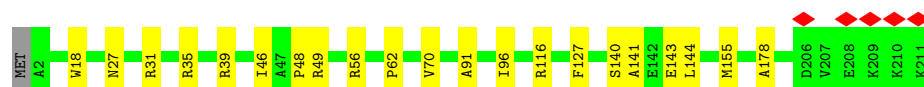
• Molecule 9: L10



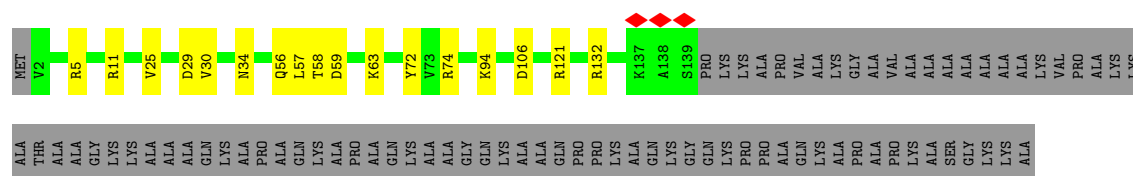
• Molecule 10: uL5



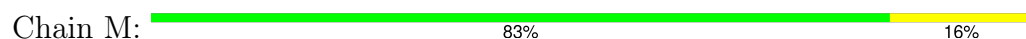
• Molecule 11: eL13



• Molecule 12: eL14



• Molecule 13: L15





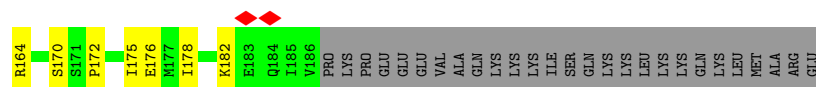
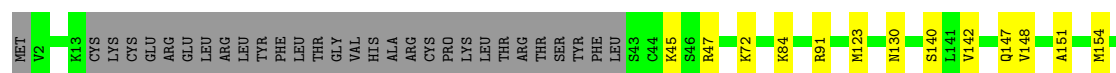
• Molecule 14: uL13

Chain N: 84% 13%



• Molecule 15: uL22

Chain O: 64% 9% 27%



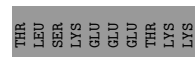
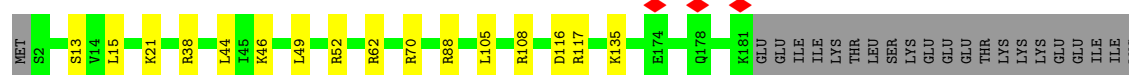
• Molecule 16: eL18

Chain P: 84% 15%



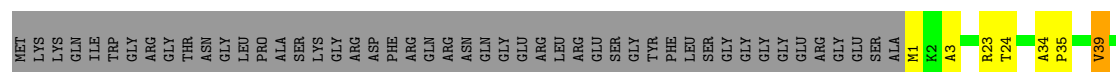
• Molecule 17: eL19

Chain Q: 77% 8% 15%



• Molecule 18: L18A

Chain R: 67% 10% 21%



• Molecule 19: eL21

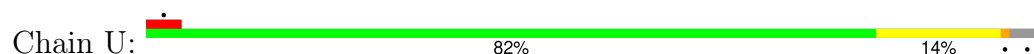
Chain S: 84% 15%



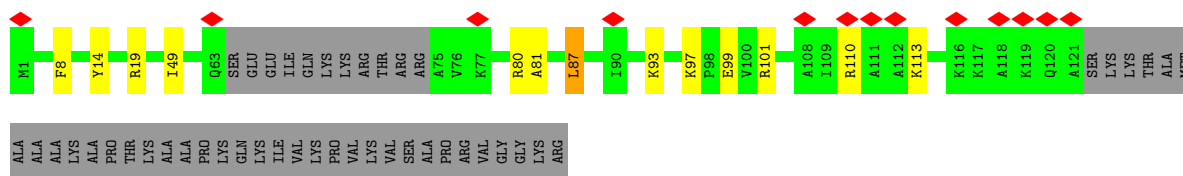
• Molecule 20: eL22



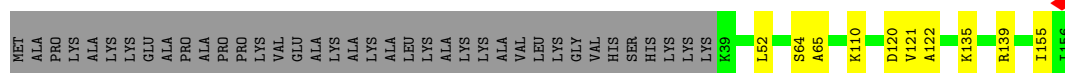
• Molecule 21: L23



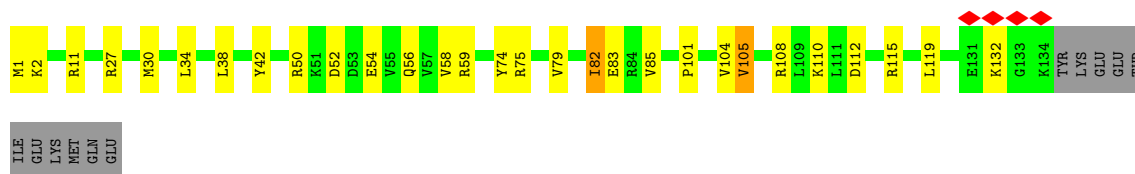
• Molecule 22: uL24



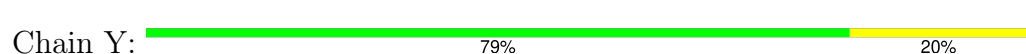
• Molecule 23: uL23

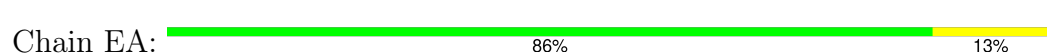


• Molecule 24: L26



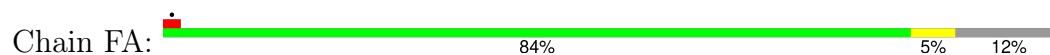
• Molecule 25: L27



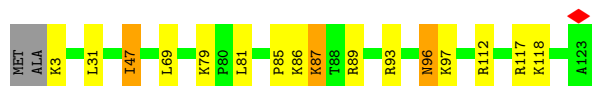
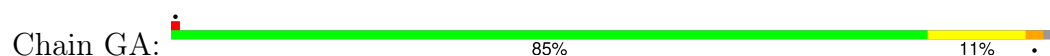




- Molecule 32: L34



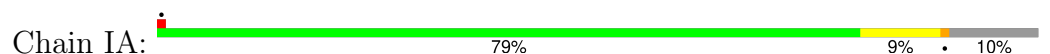
- Molecule 33: L35



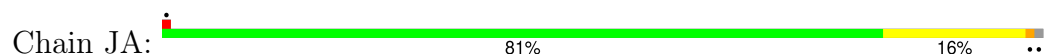
- Molecule 34: L36



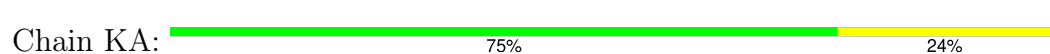
- Molecule 35: L37



- Molecule 36: eL38



- Molecule 37: eL39



- Molecule 38: eL40



MET GLN ILE PHE VAL SER THR THR THR GLY THR LYS THR ILE THR LEU GLY VAL GLU VAL GLU PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLY GLY PRO ILE PRO ASP GLN GLN ARG LEU PHE ALA LYS GLN LEU GLU ASP GLY THR LEU SER TYR ASN

ILE GLN LYS SER THR LEU HIS VAL LEU ARG ILE HIS GLY I51 Q58 L59 A60 N64 Y74 R85 K86 K87 K88 T92 N93 N94 K99 K102

• Molecule 39: eL41

Chain MA: 84% 16%

M1 R2 W5 R9 K25

• Molecule 40: eL42

Chain NA: 88% 10%

MET V2 N3 V4 C15 Q19 Y26 T63 K64 V67 C72 R81 R87 G94 Q105 PHE

• Molecule 41: eL43

Chain OA: 90% 8%

MET A2 K3 R4 K13 Y14 V26 E30 Q33 V52 I83 D91 Q92

• Molecule 42: L28

Chain PA: 72% 18% 9%

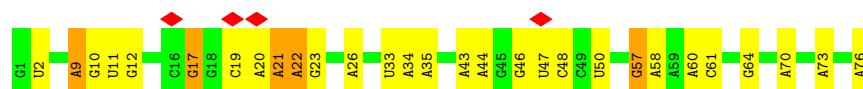
MET S2 Q6 L17 I18 K19 Y25 N31 R35 F38 R39 I44 H45 V49 K65 R66 R67 R87 T25 L90 I97 Y102 H103 P104 D105 L106 R107 I111 R112 V124 M125 VAL LYS ARG LYS THR ARG PRO LYS SER

• Molecule 43: L12

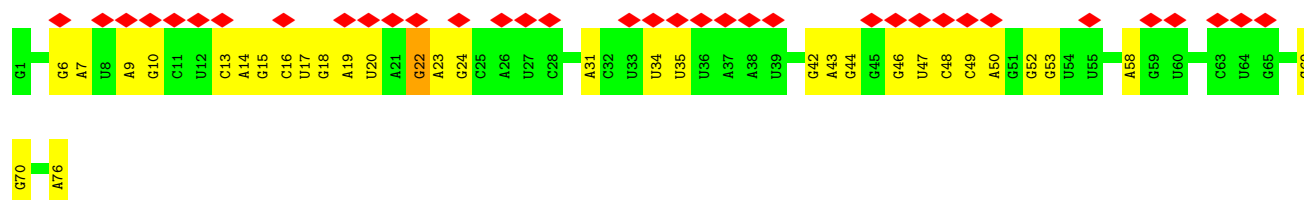
Chain RA: 67% 68% 24% 7%

MET PRO PRO LYS PHE ASP PRO ASN E9 I10 K11 V12 V13 Y14 L15 R16 C17 T18 G19 G20 E21 V22 G23 A24 T25 S26 A27 K31 I32 G33 P34 L35 G36 L37 S38 P39 K40 K41 V42 G43 D44 D45 I46 A47 K48 A49 T50 G51 D52 W53 K54 G55 L56 R57 I58 T59 V60 K61 L62 T63 I64 Q65 N66 R67 Q68 A69 Q70 I71 E72 V73 V74 P75 S76 A77 A78 A79 L80 I81 I82 K83 A84 L85 K86 E87 P88 P89 R90 D91 R92 K93 K94 Q95 Q96 N97 I98 K99 H100 S101 G102 N103 I104 T105 F106 D107 E108 I109 V110 N111 R114 Q115 M116 R117 H118 R119 V120 S120 A122 R123 E124 L125 S126 G127 K130 L133 G134 T135 A136 Q137 S138 V139 G140 C141 S142 N143 D144 G145 R146 H147 P148 H149 D150 I151 I152 P153 D154 I155 N156 S157 V160 E161 CYS PRO ALA SER

• Molecule 44: P-site tRNA



- Molecule 45: E-site tRNA



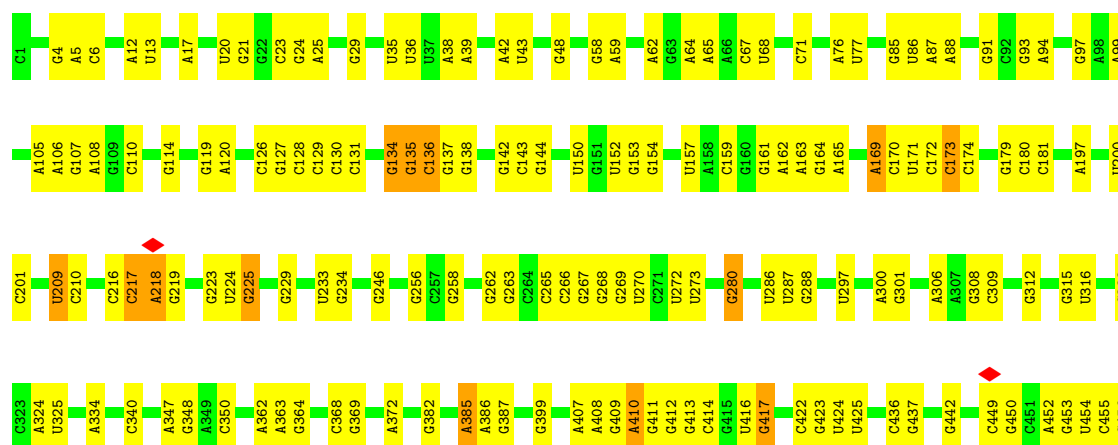
- Molecule 46: A-site tRNA

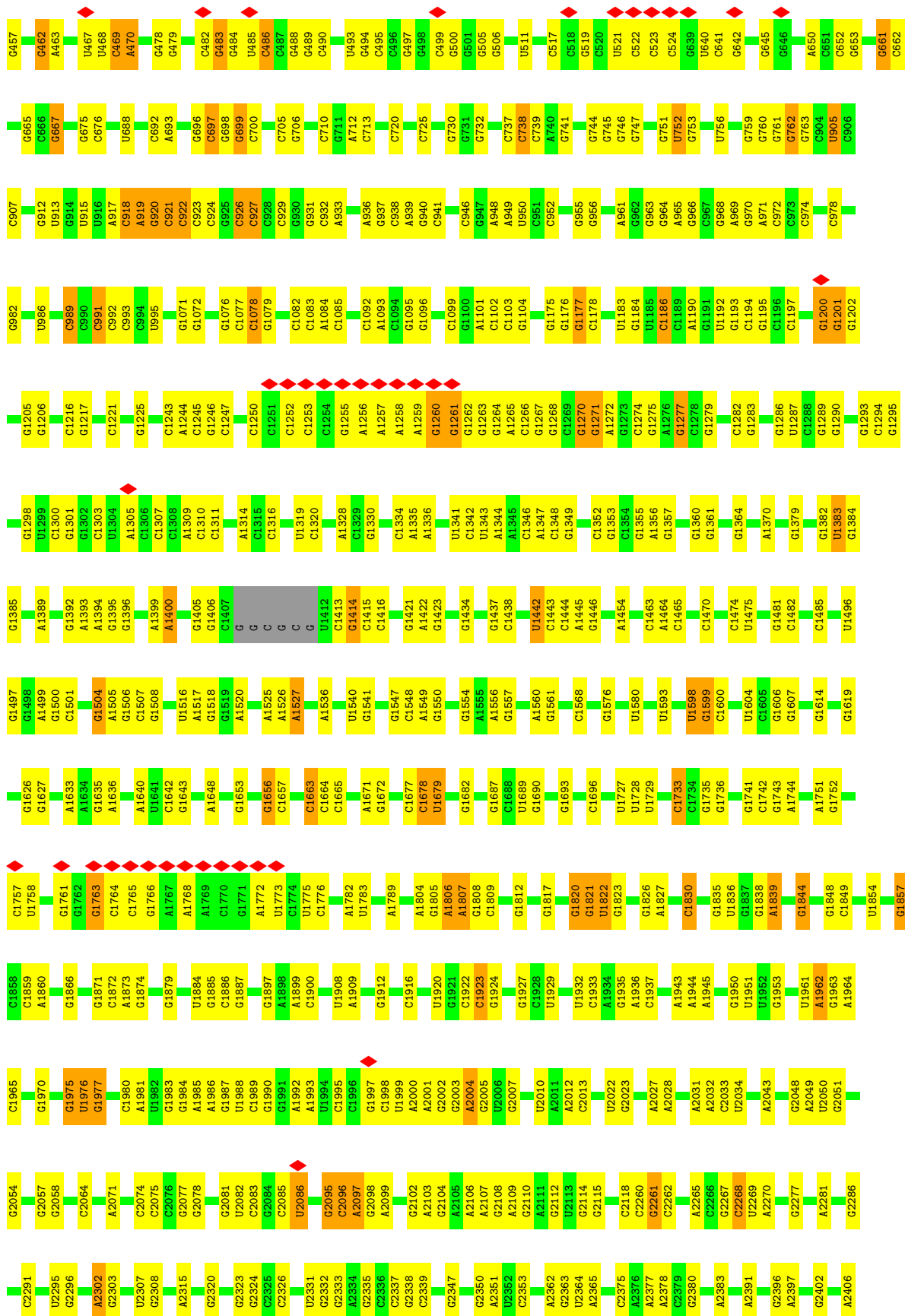


- Molecule 47: mRNA

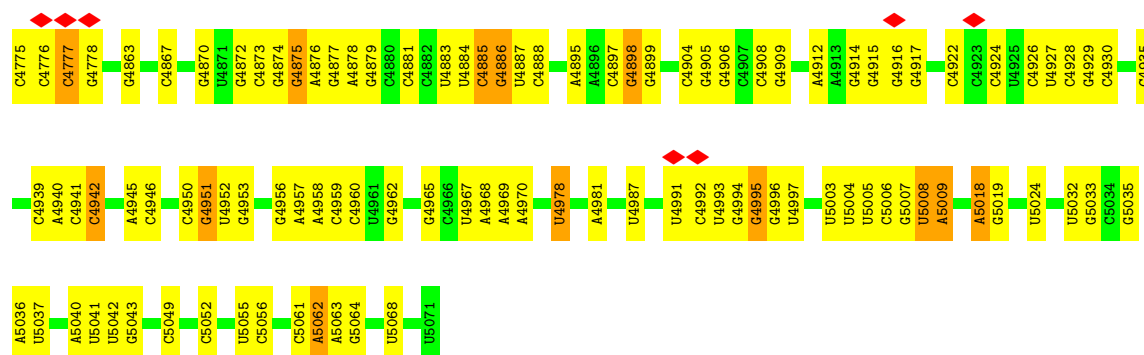


- Molecule 48: 28S rRNA





A4548	A4650	G4654	U4553	U4554	C4562	U4565	U4566	A4567	U4568	G4569	A4682	A4683	C4690	U4701	A4702	C4706	A4707	U4711	C4718	A4725	A4726	U4729	U4730	A4731	C4737	C4738	G4739	C4740	A4601	G4602	A4603	A4604	A4613	G4620	U4754	U4755	G4756	C4759	U4760	C4761	C4762	C4763	A4764	U4765	A4766	C4767	U4772	C4773	C4774																																									
C4436	U4440	C4446	C4450	A4451	U4454	U4459	U4460	U4461	U4462	C4463	U4466	U4467	C4468	A4469	G4474	A4475	A4476	G4477	A4478	A4479	G4480	C4487	G4501	A4502	A4509	A4510	A4511	A4512	A4513	A4514	A4515	C4521	G4522	U4523	A4524	A4525	U4526	C4527	G4531	C4532	A4533	U4534	C4539	U4540	U4541																																													
G4193	A4306	C4307	U4308	C4316	C4321	G4322	U4323	G4324	A4327	G4328	C4329	G4330	C4331	G4332	G4333	C4334	A4338	A4350	C4351	C4352	U4355	U4356	C4372	G4375	C4379	A4380	A4381	C4389	A4392	G4395	U4397	A4398	G4403	C4407	A4417	U4421	U4422	C4423	A4424	C4431	U4433	C4436	U4440	C4446	G4450	A4451	U4454	U4459	U4460	U4461	C4463	U4466	U4467	C4468	A4469	G4474	A4475	A4476	G4477	A4478	A4479	G4480	C4487	G4501	A4502	A4509	A4510	A4511	A4512	A4513	A4514	A4515	C4521	G4522	U4523	A4524	A4525	U4526	C4527	G4531	C4532	A4533	U4534	C4539	U4540	U4541				
C4098	G4099	A4100	G4101	C4102	C4103	G4109	G4110	G4111	C4112	U4113	C4114	G4117	C4118	U4119	U4120	C4121	U4122	G4123	A4124	C4125	G4126	C4127	A4128	A4129	A4130	C4135	C4140	C4141	C4142	C4143	C4144	C4145	G4146	C4147	G4148	G4154	U4165	G4168	C4169	G4170	A4171	C4173	U4176	G4177	G4185	G4186	U4190	U4191	U4192																																									
A3910	C3911	C3912	C3913	U3914	C3915	U3916	U3917	C3918	A3919	A3925	C3926	A3930	U3934	C3935	C3939	G3940	G3941	A3945	G3946	A3947	G3948	A3949	C3950	A3951	U3952	C3953	A3954	C4063	A4064	U4065	C4066	U4069	U4070	U4071	U4072	C4073	A4074	A4075	G4078	G4086	A4087	G4088	C4089	C4090	A4091	G4092	A4093	G4094	A4095	G4096	G4097																																							
G3813	C3814	A3815	U3816	C3817	A3818	A3819	U3820	C3821	G3825	U3840	C3841	U3842	C3845	U3846	A3847	U3850	A3851	C3857	A3858	G3861	A3862	A3863	A3864	C3870	C3871	C3872	A3873	A3879	C3880	G3881	C3882	G3883	U3886	C3891	A3892	A3893	U3894	C3895	A3896	C3897	C3898	C3899	G3900	C3901	G3902	A3903	A3908	C3909																																										
C3675	G3676	G3683	A3684	C3685	U3690	U3691	A3694	U3695	U3699	G3700	U3709	C3710	A3713	A3714	U3715	G3716	A3719	A3720	G3724	A3725	A3734	A3735	G3738	A3739	A3750	G3755	A3762	C3763	U3775	A3776	A3777	G3778	G3779	A3786	A3787	U3788	U3800	A3801	U3804	G3811	C3812																																																	
A2846	A2847	G2850	G2857	G2864	U2865	U2867	U2871	A2876	U2877	A2878	G2760	G2761	G2762	A2767	C2771	C2772	G2775	G2779	G2780	A2789	U2790	A2791	U2792	G2795	C2796	A2800	G2811	U2812	G2813	A2814	C2815	C2816	U2821	U2822	U2823	U2828	U2829	U2830	A2837	U2838	U2844	U2845																																																
C2591	A2603	C2609	C2610	C2615	G2624	U2627	U2628	C2629	G2640	U2641	G2642	A2643	A2649	C2650	G2651	C2655	A2662	U2663	G2664	C2671	C2672	A2678	C2688	U2689	G2695	G2696	A2697	A2698	A2699	U2703	C2704	G2705	C2706	G2707	G2708	U2709	U2710	C2711	C2712	G2713	C2723	G2726	A2727																																															
G2498	C2499	C2500	G2505	C2506	G2508	A2514	A2515	A2518	A2519	C2522	G2523	G2524	A2529	C2530	U2531	C2533	C2534	C2535	A2539	U2540	C2541	C2542	G2543	A2544	A2545	G2546	U2547	G2548	G2549	A2555	U2556	G2559	C2560	G2561	C2565	A2567	G2568	U2572	U2577	C2585	G2588	C2589	C2590																																															
C2407	G2408	C2409	U2410	U2411	C2412	C2413	C2414	U2415	G2416	U2417	C2424	U2427	A2430	G2435	C2436	U2437	U2438	C2443	C2444	G2445	U2446	A2450	A2451	A2455	C2467	G2468	U2469	U2470	G2473	C2477	C2480	G2481	G2482	G2483	C2484	C2485	A2486	U2487	G2488	C2489	C2490	C2491	U2492	C2493	C2494	G2495	U2496	U2497																																										



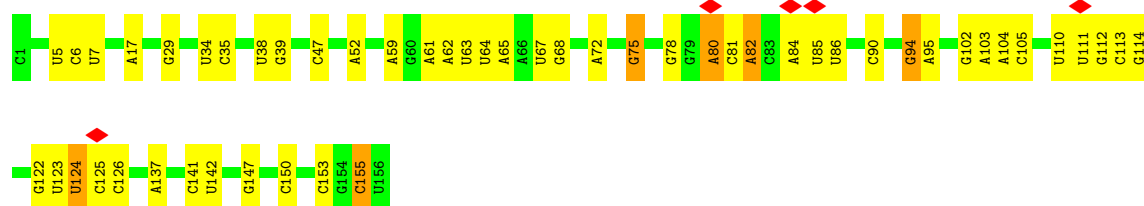
• Molecule 49: 5S rRNA

Chain XA: 72% 23%



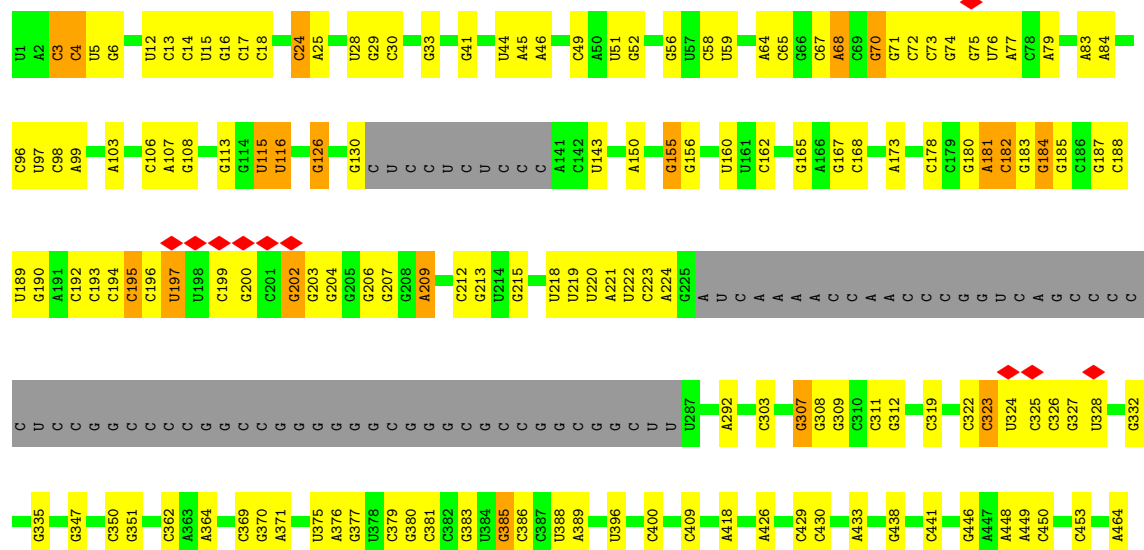
• Molecule 50: 5.8S rRNA

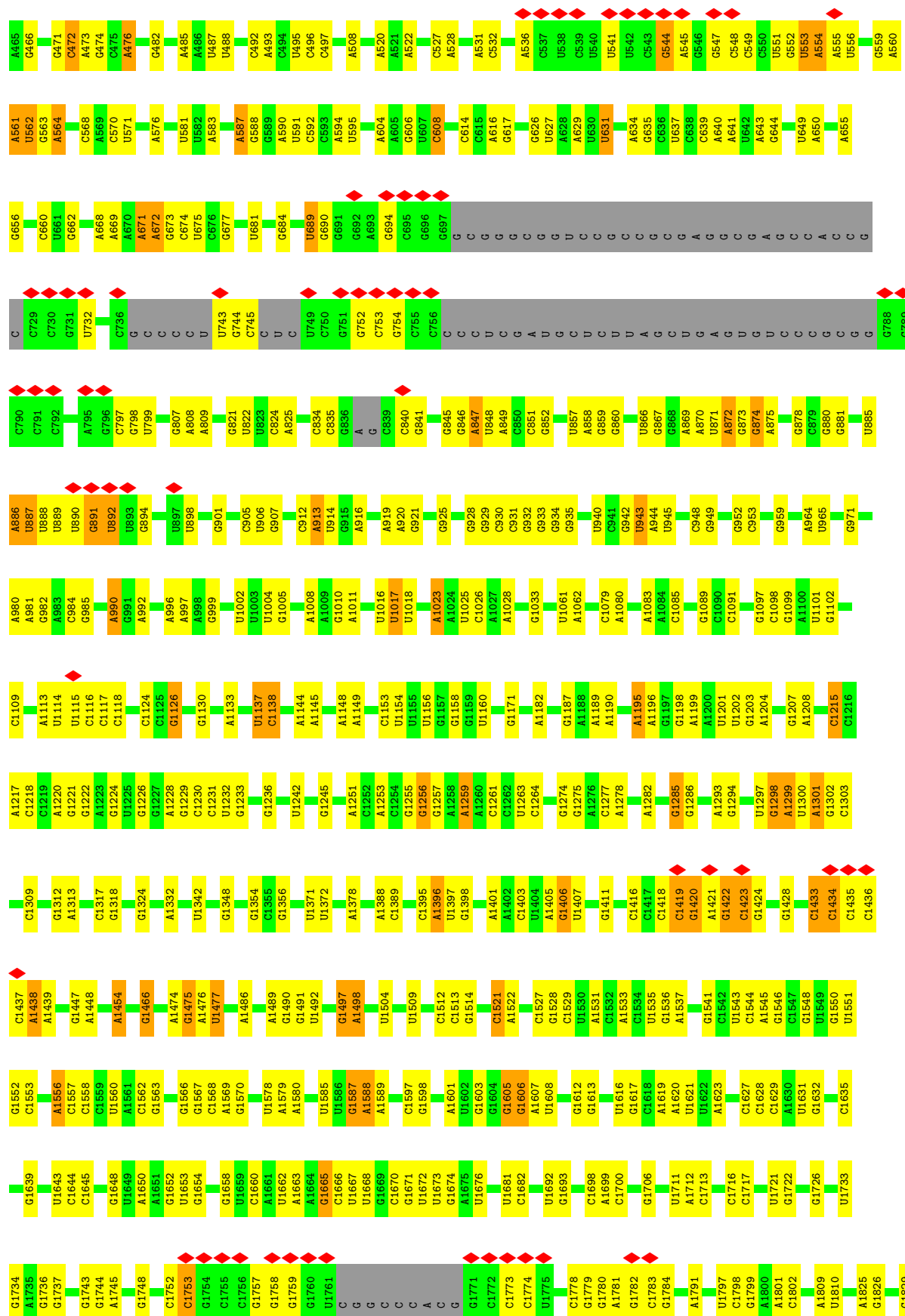
Chain YA: 67% 29%



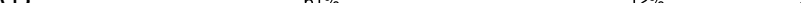
• Molecule 51: 18S rRNA

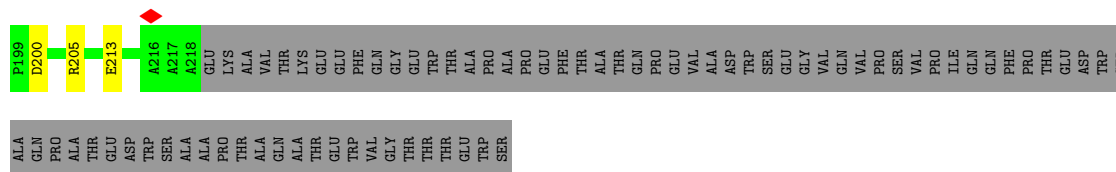
Chain ZA: 57% 31% 8%



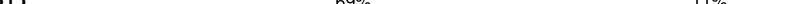


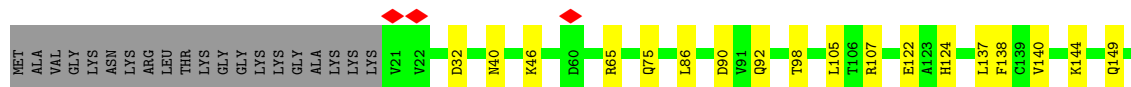
- Molecule 52: RPSA

Chain AB: 

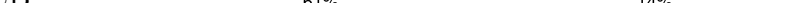


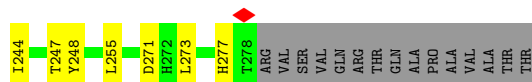
- Molecule 53: S3A

Chain BB:  69% 11% 19%



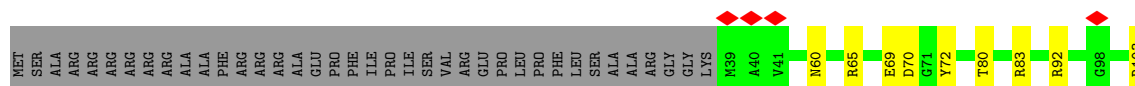
- Molecule 54: S2-like

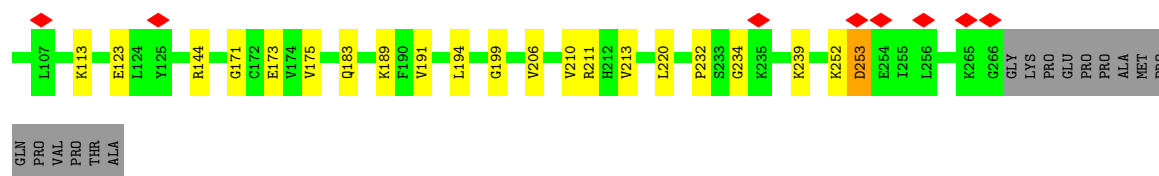
Chain CB: 



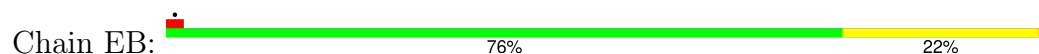
- Molecule 55: S3

Chain DB:

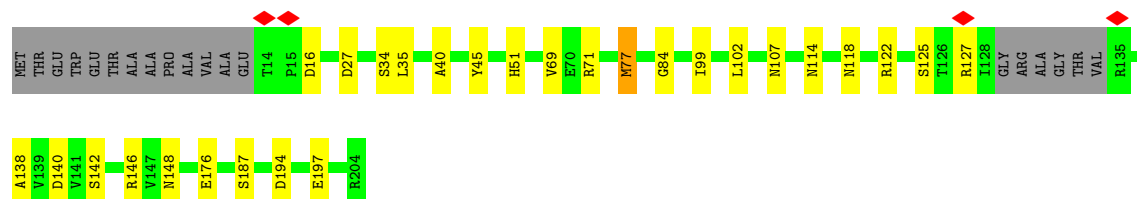
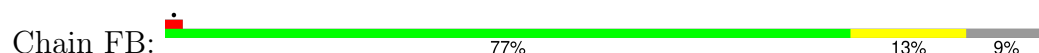




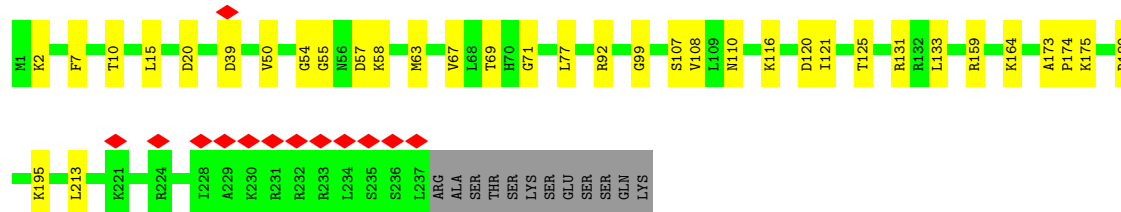
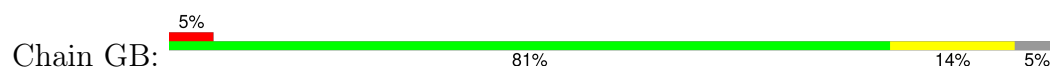
• Molecule 56: S4



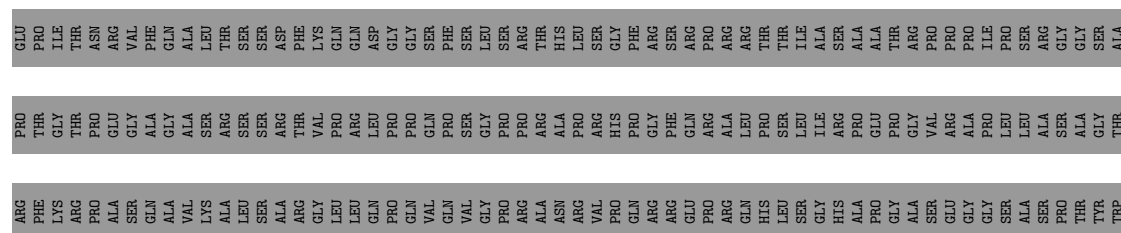
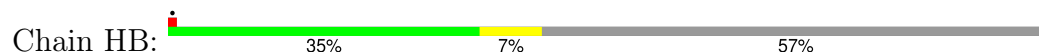
• Molecule 57: S5

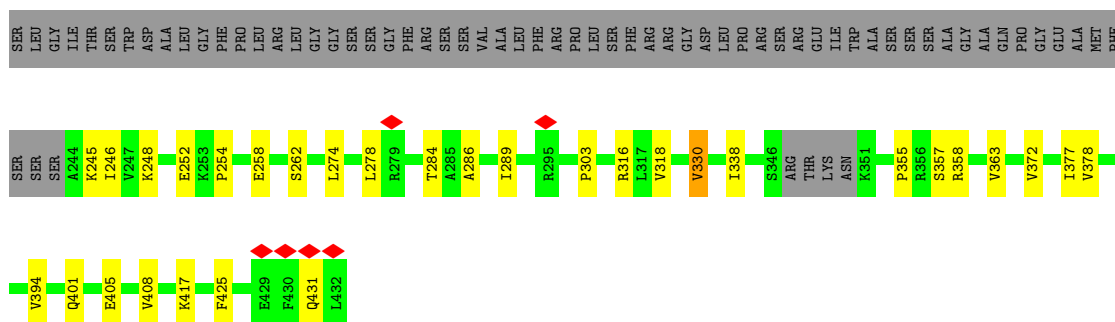


• Molecule 58: eS6

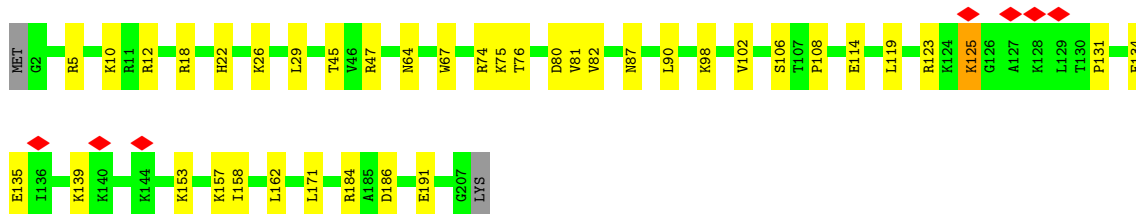
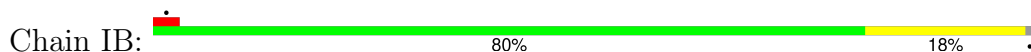


• Molecule 59: eS7

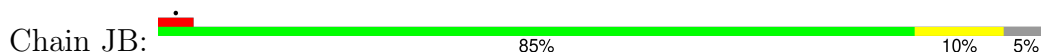




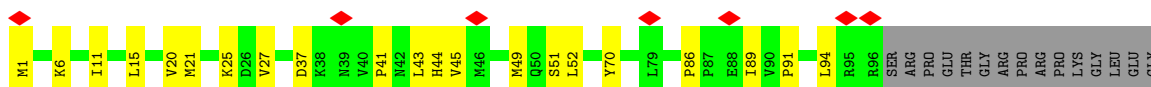
• Molecule 60: S8



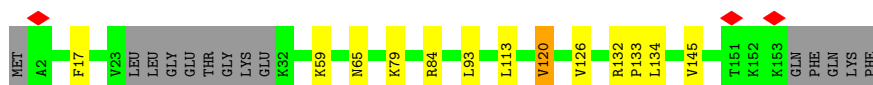
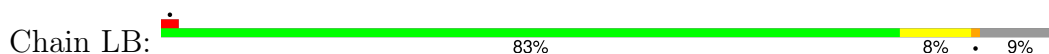
• Molecule 61: S9



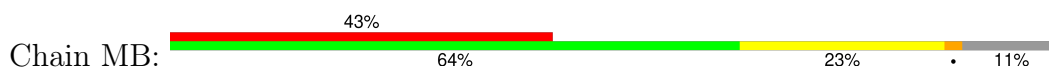
• Molecule 62: S10

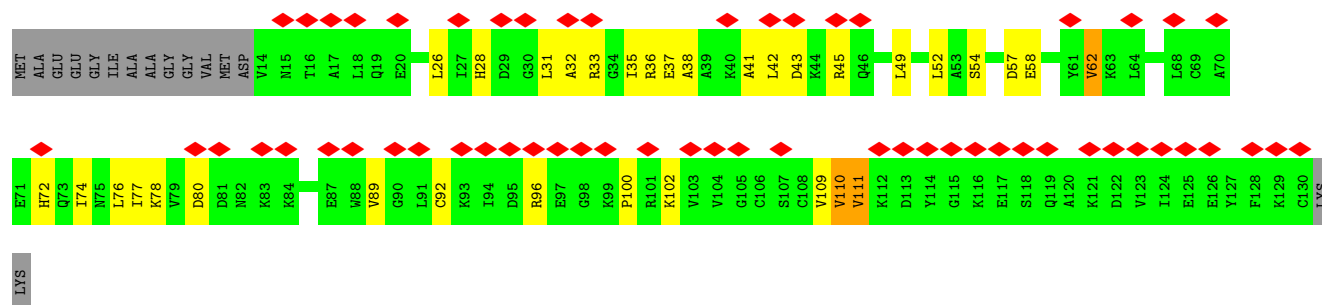


• Molecule 63: S11

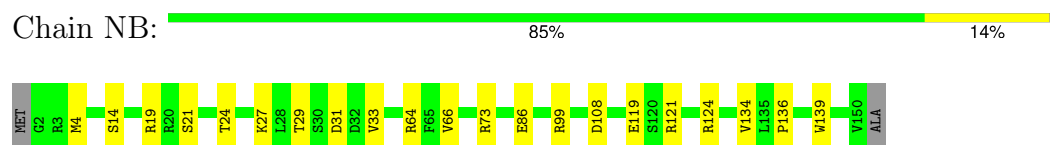


• Molecule 64: S12

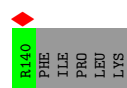
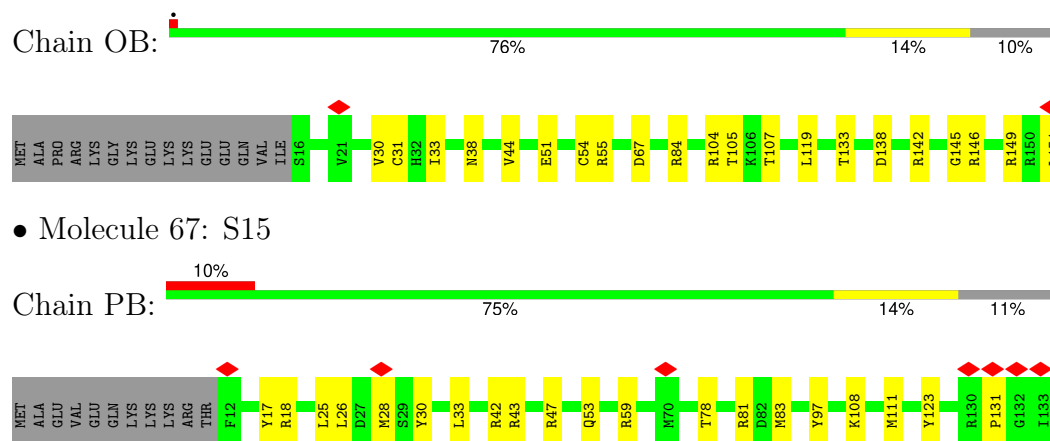




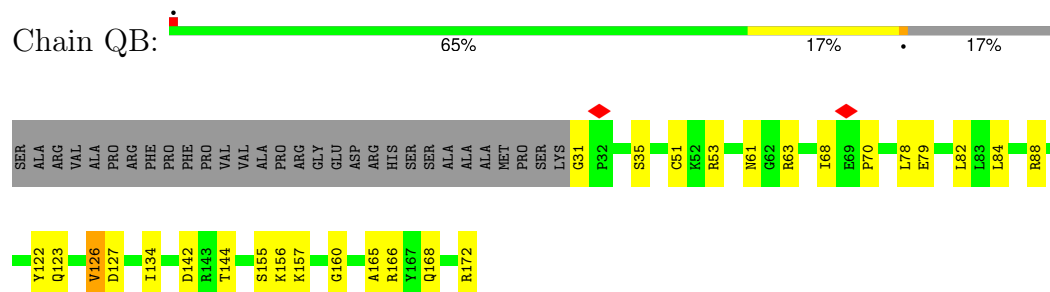
• Molecule 65: uS15



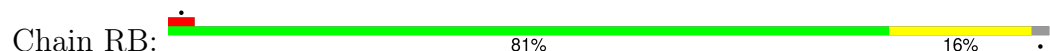
• Molecule 66: S14

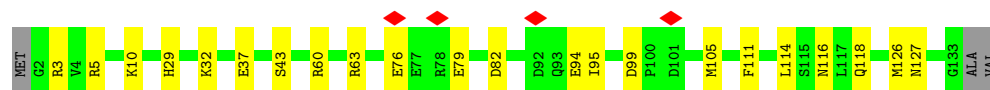


• Molecule 68: uS9

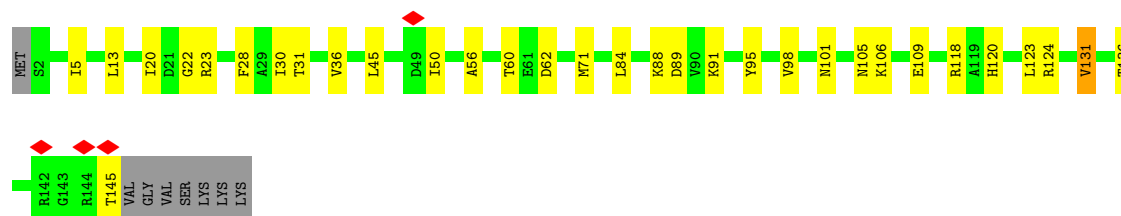
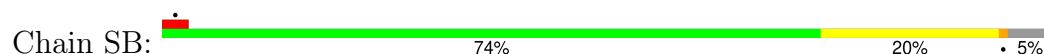


• Molecule 69: eS17

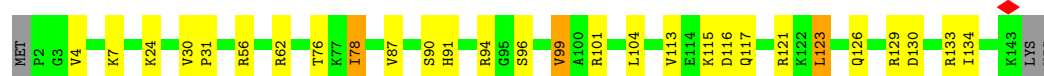
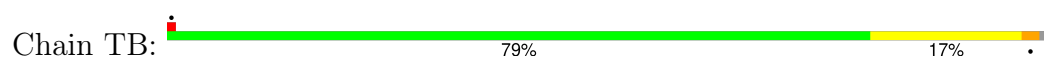




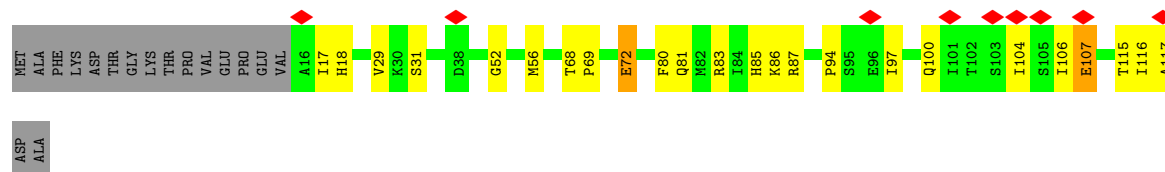
- Molecule 70: S18



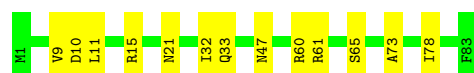
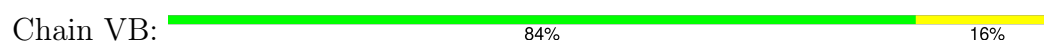
- Molecule 71: S19



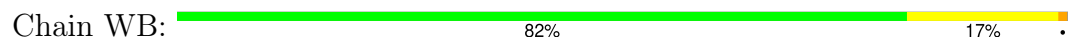
- Molecule 72: uS10



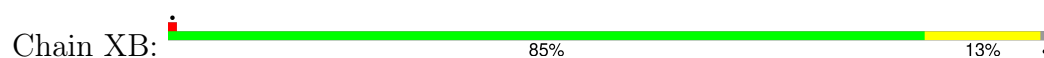
- Molecule 73: S21

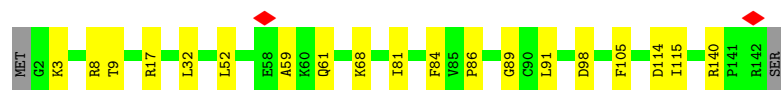


- Molecule 74: S15A

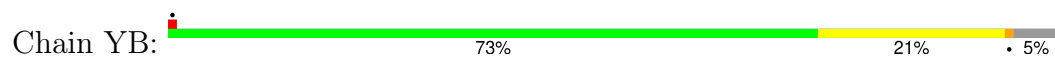


- Molecule 75: S23

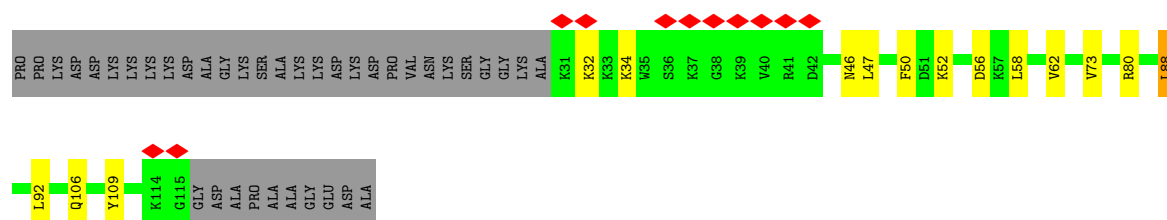




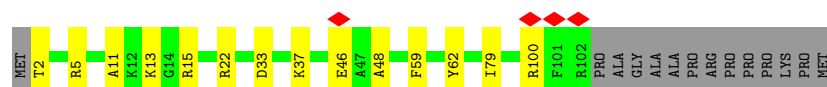
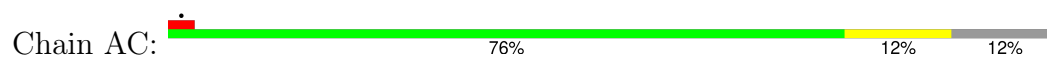
• Molecule 76: S24



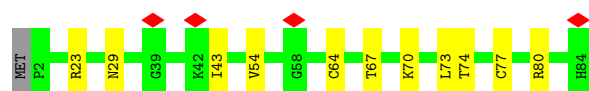
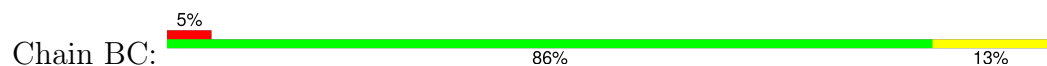
• Molecule 77: eS25



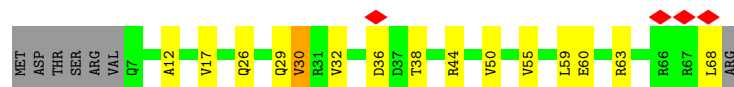
• Molecule 78: S26



• Molecule 79: S27

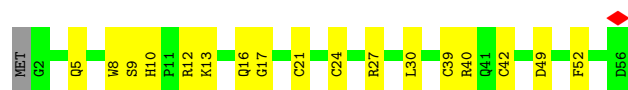


• Molecule 80: S28

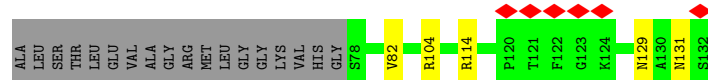
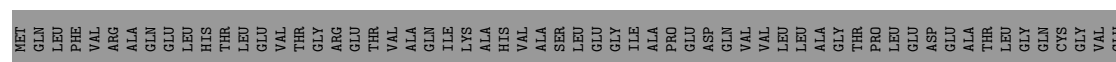


• Molecule 81: uS14

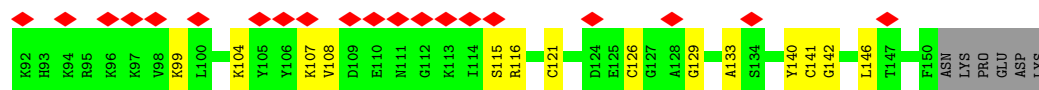
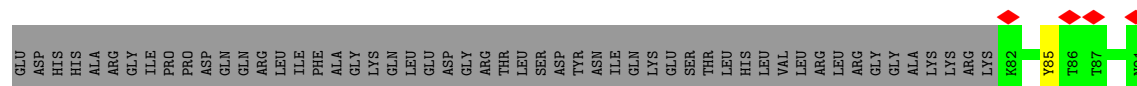
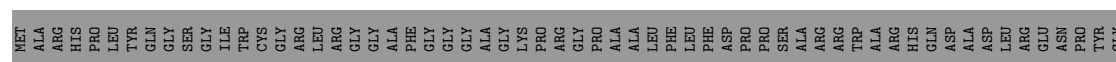




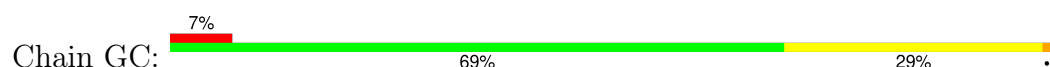
• Molecule 82: S30



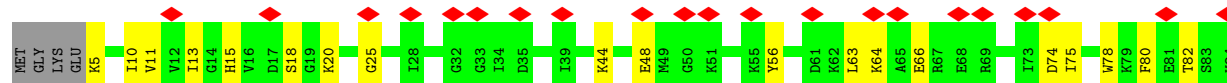
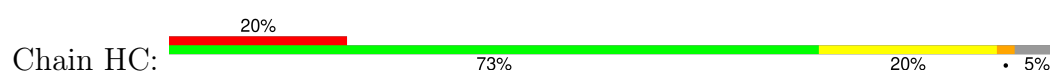
• Molecule 83: S27A



• Molecule 84: RACK1



• Molecule 85: eukaryotic elongation factor 1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37882	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 ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	43.279	Depositor
Minimum map value	-20.542	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.217	Depositor
Recommended contour level	4.45	Depositor
Map size (Å)	686.87994, 686.87994, 686.87994	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP, GTP, SPD, K, ZN, MG, ANM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/1952	0.33	0/2617
2	B	0.20	0/3264	0.30	0/4371
3	C	0.19	0/2937	0.29	0/3946
4	D	0.16	0/2441	0.27	0/3269
5	E	0.16	0/1859	0.30	0/2491
6	F	0.19	0/1933	0.29	0/2577
7	G	0.17	0/1881	0.29	0/2532
8	H	0.17	0/1535	0.27	0/2063
9	I	0.18	0/1702	0.27	0/2272
10	J	0.16	0/1395	0.30	0/1863
11	K	0.17	0/1733	0.26	0/2316
12	L	0.18	0/1158	0.30	0/1547
13	M	0.22	0/1746	0.31	0/2338
14	N	0.20	0/1662	0.31	0/2222
15	O	0.19	0/1292	0.31	0/1733
16	P	0.21	0/1539	0.30	0/2054
17	Q	0.17	0/1524	0.26	0/2013
18	R	0.20	0/1501	0.30	0/2012
19	S	0.19	0/1326	0.26	0/1770
20	T	0.16	0/840	0.31	0/1127
21	U	0.21	0/1018	0.31	0/1364
22	V	0.15	0/900	0.28	0/1194
23	W	0.18	0/984	0.27	0/1323
24	X	0.16	0/1132	0.26	0/1504
25	Y	0.18	0/1130	0.28	0/1507
26	Z	0.21	0/1191	0.31	0/1590
27	AA	0.15	0/886	0.22	0/1171
28	BA	0.18	0/779	0.25	0/1044
29	CA	0.19	0/908	0.31	0/1223
30	DA	0.21	0/1082	0.27	0/1443
31	EA	0.22	0/895	0.31	0/1198
32	FA	0.19	0/916	0.30	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	GA	0.17	0/1016	0.26	0/1341
34	HA	0.16	0/841	0.27	0/1112
35	IA	0.20	0/731	0.31	0/966
36	JA	0.16	0/575	0.26	0/761
37	KA	0.19	0/459	0.28	0/608
38	LA	0.18	0/435	0.30	0/575
39	MA	0.18	0/240	0.25	0/305
40	NA	0.19	0/864	0.26	0/1140
41	OA	0.20	0/718	0.33	0/953
42	PA	0.18	0/1010	0.31	0/1354
43	RA	0.11	0/1174	0.29	0/1582
44	SA	0.15	0/1815	0.27	0/2828
45	TA	0.12	0/1804	0.24	0/2810
46	UA	0.12	0/1771	0.29	0/2754
47	VA	0.13	0/278	0.24	0/428
48	WA	0.22	0/85840	0.29	0/133885
49	XA	0.20	0/2836	0.25	0/4421
50	YA	0.21	0/3701	0.26	0/5766
51	ZA	0.19	0/40949	0.28	0/63819
52	AB	0.16	0/1747	0.27	0/2374
53	BB	0.16	0/1756	0.28	0/2350
54	CB	0.18	0/1744	0.31	0/2358
55	DB	0.13	0/1796	0.26	0/2417
56	EB	0.16	0/2118	0.30	0/2849
57	FB	0.15	0/1492	0.30	0/2005
58	GB	0.13	0/1946	0.24	0/2590
59	HB	0.14	0/1511	0.28	0/2022
60	IB	0.17	0/1715	0.30	0/2287
61	JB	0.15	0/1550	0.27	0/2069
62	KB	0.12	0/834	0.26	0/1125
63	LB	0.18	0/1200	0.26	0/1604
64	MB	0.11	0/918	0.28	0/1233
65	NB	0.16	0/1226	0.25	0/1649
66	OB	0.18	0/1029	0.29	0/1380
67	PB	0.12	0/1079	0.26	0/1441
68	QB	0.16	0/1146	0.30	0/1534
69	RB	0.13	0/1082	0.26	0/1452
70	SB	0.13	0/1208	0.28	0/1618
71	TB	0.13	0/1123	0.26	0/1504
72	UB	0.14	0/818	0.28	0/1099
73	VB	0.15	0/643	0.27	0/860
74	WB	0.20	0/1051	0.35	0/1406
75	XB	0.18	0/1116	0.27	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YB	0.14	0/1028	0.28	0/1366
77	ZB	0.12	0/691	0.27	0/922
78	AC	0.19	0/828	0.29	0/1109
79	BC	0.15	0/665	0.24	0/891
80	CC	0.14	0/490	0.28	0/656
81	DC	0.15	0/470	0.29	0/623
82	EC	0.14	0/447	0.28	0/587
83	FC	0.09	0/576	0.24	0/764
84	GC	0.13	0/2493	0.31	0/3394
85	HC	0.12	0/3441	0.30	0/4657
86	IC	0.09	0/19	0.14	0/25
87	b	0.16	0/1298	0.36	0/1752
88	c	0.08	0/87	0.28	0/113
All	All	0.19	0/238479	0.29	0/349897

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
85	HC	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
85	HC	159	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1914	0	2013	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3196	0	3339	54	0
3	C	2883	0	3053	21	0
4	D	2395	0	2427	27	0
5	E	1823	0	1995	25	0
6	F	1897	0	2021	22	0
7	G	1850	0	1991	19	0
8	H	1516	0	1597	18	0
9	I	1664	0	1712	20	0
10	J	1372	0	1412	15	0
11	K	1702	0	1820	15	0
12	L	1137	0	1211	12	0
13	M	1701	0	1749	25	0
14	N	1630	0	1778	18	0
15	O	1266	0	1302	13	0
16	P	1515	0	1634	25	0
17	Q	1508	0	1664	14	0
18	R	1462	0	1508	23	0
19	S	1298	0	1366	19	0
20	T	826	0	852	10	0
21	U	1004	0	1063	14	0
22	V	887	0	935	9	0
23	W	967	0	1040	7	0
24	X	1115	0	1205	17	0
25	Y	1107	0	1182	16	0
26	Z	1162	0	1209	18	0
27	AA	873	0	949	11	0
28	BA	769	0	803	6	0
29	CA	893	0	932	12	0
30	DA	1064	0	1160	21	0
31	EA	876	0	912	9	0
32	FA	906	0	998	6	0
33	GA	1008	0	1142	15	0
34	HA	830	0	916	6	0
35	IA	716	0	750	8	0
36	JA	569	0	637	9	0
37	KA	447	0	480	9	0
38	LA	429	0	465	6	0
39	MA	239	0	289	3	0
40	NA	851	0	920	7	0
41	OA	708	0	757	6	0
42	PA	994	0	1051	17	0
43	RA	1160	0	1218	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	SA	1622	0	825	15	0
45	TA	1615	0	820	15	0
46	UA	1586	0	805	9	0
47	VA	249	0	125	1	0
48	WA	76735	0	38762	652	0
49	XA	2538	0	1286	20	0
50	YA	3314	0	1683	21	0
51	ZA	36623	0	18504	331	0
52	AB	1710	0	1711	25	0
53	BB	1729	0	1803	17	0
54	CB	1707	0	1793	24	0
55	DB	1768	0	1863	17	0
56	EB	2076	0	2177	38	0
57	FB	1471	0	1522	18	0
58	GB	1923	0	2089	21	0
59	HB	1489	0	1582	17	0
60	IB	1686	0	1772	26	0
61	JB	1525	0	1640	17	0
62	KB	810	0	836	12	0
63	LB	1180	0	1254	10	0
64	MB	908	0	939	21	0
65	NB	1202	0	1289	14	0
66	OB	1016	0	1039	14	0
67	PB	1058	0	1104	13	0
68	QB	1128	0	1195	21	0
69	RB	1068	0	1121	16	0
70	SB	1190	0	1249	20	0
71	TB	1104	0	1140	19	0
72	UB	808	0	878	13	0
73	VB	636	0	637	8	0
74	WB	1034	0	1080	16	0
75	XB	1098	0	1167	13	0
76	YB	1011	0	1083	17	0
77	ZB	683	0	761	10	0
78	AC	814	0	864	11	0
79	BC	651	0	672	4	0
80	CC	488	0	514	11	0
81	DC	459	0	449	11	0
82	EC	443	0	492	7	0
83	FC	564	0	577	10	0
84	GC	2436	0	2393	44	0
85	HC	3371	0	3428	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	IC	20	0	10	0	0
87	b	1279	0	1344	18	0
88	c	86	0	66	0	0
89	A	1	0	0	0	0
89	AC	1	0	0	0	0
89	B	1	0	0	0	0
89	DA	1	0	0	0	0
89	FA	1	0	0	0	0
89	HC	1	0	0	0	0
89	I	1	0	0	0	0
89	IA	1	0	0	0	0
89	LB	1	0	0	0	0
89	O	1	0	0	0	0
89	SA	1	0	0	0	0
89	U	1	0	0	0	0
89	WA	186	0	0	0	0
89	XA	6	0	0	0	0
89	YA	4	0	0	0	0
89	Z	1	0	0	0	0
89	ZA	80	0	0	0	0
89	b	1	0	0	0	0
90	AC	1	0	0	0	0
90	DC	1	0	0	0	0
90	FA	1	0	0	0	0
90	FC	1	0	0	0	0
90	IA	1	0	0	0	0
90	LA	1	0	0	0	0
90	NA	1	0	0	0	0
90	OA	1	0	0	0	0
91	UA	24	0	12	0	0
92	WA	19	0	19	3	0
93	WA	10	0	19	0	0
94	WA	1	0	0	0	0
95	HC	32	0	12	1	0
96	HC	6	0	4	1	0
All	All	222430	0	165866	1937	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 5.

All (1937) 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)
44:SA:50:U:H3	44:SA:64:G:H1	0.90	0.87
48:WA:2847:A:H61	48:WA:3845:C:H42	1.16	0.87
48:WA:986:U:H3	48:WA:1277:G:H1	1.22	0.86
48:WA:3694:A:H62	48:WA:3825:G:H21	1.24	0.85
48:WA:1761:G:H1	48:WA:1775:U:H3	1.24	0.83
48:WA:169:A:N6	48:WA:267:G:C6	2.49	0.81
51:ZA:1091:C:HO2'	74:WB:2:VAL:N	1.80	0.80
35:IA:2:THR:N	48:WA:3644:A:HO2'	1.79	0.80
48:WA:995:U:H3	48:WA:1071:G:H1	1.28	0.79
48:WA:169:A:N6	48:WA:267:G:C5	2.52	0.77
87:b:44:ARG:O	87:b:48:ARG:HB2	1.85	0.76
48:WA:2847:A:H61	48:WA:3845:C:N4	1.85	0.74
48:WA:762:G:H22	48:WA:905:U:H3	1.35	0.74
56:EB:87:MET:HE2	56:EB:123:LEU:HB2	1.71	0.73
60:IB:131:PRO:HD2	60:IB:134:GLU:HB2	1.71	0.73
45:TA:15:G:N2	45:TA:48:C:C2	2.56	0.73
85:HC:80:PHE:HB2	85:HC:87:VAL:HG22	1.70	0.73
48:WA:3946:G:H1	48:WA:4071:U:H3	1.36	0.72
48:WA:1526:A:H62	48:WA:1653:G:H1	1.37	0.72
48:WA:4874:G:H4'	48:WA:4875:G:H5'	1.71	0.72
51:ZA:1834:A:H2	51:ZA:1837:G:H1	1.35	0.72
11:K:56:ARG:O	11:K:116:ARG:NH1	2.23	0.71
2:B:329:ASP:OD1	2:B:329:ASP:N	2.24	0.71
51:ZA:1324:G:H1	51:ZA:1504:U:H3	1.39	0.71
51:ZA:1652:G:H1	51:ZA:1672:U:H3	1.38	0.71
48:WA:2847:A:N6	48:WA:3845:C:H42	1.89	0.71
51:ZA:1566:G:N7	71:TB:101:ARG:NH2	2.39	0.71
51:ZA:561:A:H5'	61:JB:171:GLY:HA3	1.73	0.70
48:WA:2649:A:H62	48:WA:2688:G:H8	1.39	0.69
51:ZA:1556:A:N6	81:DC:13:LYS:O	2.26	0.69
51:ZA:1396:A:O2'	51:ZA:1398:G:N7	2.26	0.69
1:A:70:LYS:NZ	48:WA:2505:G:N7	2.39	0.69
48:WA:4454:U:H3	48:WA:4533:U:H3	1.39	0.68
69:RB:111:PHE:HB3	69:RB:114:LEU:HD11	1.76	0.68
10:J:56:THR:HG22	10:J:64:ARG:H	1.58	0.68
5:E:159:ARG:NH1	48:WA:4942:C:OP1	2.27	0.68
44:SA:34:A:H61	47:VA:21:C:H42	1.41	0.67
48:WA:4993:U:H2'	48:WA:4994:G:H8	1.58	0.67
48:WA:3643:U:OP2	48:WA:3648:A:N6	2.27	0.67
84:GC:174:VAL:HB	84:GC:188:HIS:HB2	1.75	0.67
45:TA:15:G:N2	45:TA:48:C:O2	2.28	0.67
48:WA:1183:U:H2'	48:WA:1184:G:H8	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:3613:A:O2'	48:WA:5018:A:O2'	2.10	0.67
36:JA:35:LYS:NZ	48:WA:2695:G:OP1	2.28	0.66
51:ZA:925:G:H1	51:ZA:1017:U:H3	1.42	0.66
3:C:78:ARG:HB3	3:C:88:GLY:HA2	1.77	0.66
18:R:160:ARG:HH11	18:R:160:ARG:HA	1.61	0.66
10:J:75:ARG:NH1	49:XA:40:U:O2	2.29	0.66
44:SA:33:U:OP2	68:QB:172:ARG:NH2	2.29	0.66
25:Y:50:PRO:HD3	25:Y:68:ILE:HG13	1.77	0.66
16:P:16:LYS:O	16:P:33:ARG:NH2	2.28	0.66
3:C:143:ARG:NH1	48:WA:2302:A:N7	2.43	0.66
6:F:218:GLY:O	6:F:245:ARG:NH2	2.29	0.66
51:ZA:551:U:H2'	51:ZA:552:G:H8	1.61	0.66
30:DA:36:ARG:NH2	48:WA:2324:G:OP1	2.29	0.65
53:BB:122:GLU:HG2	53:BB:140:VAL:HG12	1.78	0.65
84:GC:31:ILE:HG23	84:GC:43:TRP:HB2	1.78	0.65
1:A:128:ARG:NH1	48:WA:3683:G:OP2	2.30	0.65
51:ZA:1864:U:H5'	78:AC:79:ILE:HD11	1.78	0.65
51:ZA:1858:G:OP2	66:OB:146:ARG:NH2	2.26	0.65
46:UA:17:G:O2'	46:UA:57:G:N2	2.29	0.65
51:ZA:64:A:H2	51:ZA:83:A:H62	1.43	0.65
51:ZA:377:G:H5'	60:IB:98:LYS:HB3	1.79	0.65
72:UB:31:SER:HB2	72:UB:107:GLU:HG2	1.77	0.65
51:ZA:168:C:OP1	58:GB:131:ARG:NH1	2.30	0.65
34:HA:48:CYS:SG	34:HA:49:GLY:N	2.70	0.65
72:UB:80:PHE:HB3	81:DC:52:PHE:HB3	1.78	0.65
5:E:185:ASN:ND2	5:E:274:LEU:O	2.30	0.64
11:K:35:ARG:NH1	48:WA:105:A:O2'	2.31	0.64
18:R:3:ALA:O	18:R:111:ARG:NH2	2.30	0.64
51:ZA:940:U:H3	51:ZA:1002:U:H3	1.43	0.64
71:TB:126:GLN:OE1	71:TB:129:ARG:NH2	2.31	0.64
6:F:95:ARG:NH2	48:WA:1897:G:OP1	2.30	0.64
54:CB:123:ARG:NH1	54:CB:143:CYS:SG	2.71	0.64
14:N:72:HIS:N	48:WA:4588:G:OP1	2.30	0.64
16:P:104:ARG:NH2	48:WA:1355:G:N7	2.45	0.64
26:Z:21:ARG:NH2	48:WA:1319:U:OP1	2.30	0.64
43:RA:16:ARG:NH1	48:WA:1977:G:O2'	2.30	0.64
53:BB:107:ARG:NH1	66:OB:133:THR:O	2.25	0.64
53:BB:149:GLN:HE22	53:BB:154:SER:HB3	1.62	0.64
44:SA:17:G:O2'	44:SA:57:G:N2	2.31	0.64
30:DA:36:ARG:NH1	48:WA:1663:C:OP1	2.31	0.64
14:N:116:LYS:HE3	18:R:169:THR:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1491:G:H1'	72:UB:72:GLU:HG2	1.80	0.63
21:U:92:ASP:OD1	21:U:92:ASP:N	2.30	0.63
14:N:42:ASN:HD22	14:N:125:LYS:HD3	1.62	0.63
84:GC:256:ILE:HG23	84:GC:270:LEU:HB2	1.79	0.63
42:PA:107:ARG:NH2	48:WA:2265:A:OP1	2.26	0.63
1:A:30:ARG:O	1:A:163:ARG:NH2	2.30	0.63
11:K:116:ARG:NH2	11:K:155:MET:O	2.30	0.63
51:ZA:639:C:H5'	82:EC:114:ARG:HH22	1.62	0.63
48:WA:1194:C:H2'	48:WA:1195:G:H8	1.63	0.63
58:GB:58:LYS:HA	58:GB:107:SER:HB2	1.80	0.63
4:D:65:ALA:HB2	4:D:74:ILE:HD13	1.80	0.63
51:ZA:1521:C:OP2	70:SB:136:THR:OG1	2.16	0.62
84:GC:4:GLN:HB3	84:GC:313:THR:HB	1.80	0.62
37:KA:20:ASN:O	37:KA:41:ARG:NH1	2.32	0.62
48:WA:1200:G:N2	48:WA:1201:G:O6	2.31	0.62
31:EA:50:VAL:HG22	31:EA:69:VAL:HG22	1.82	0.62
51:ZA:1497:G:N7	62:KB:25:LYS:NZ	2.46	0.62
48:WA:1976:U:H4'	48:WA:1977:G:H3'	1.81	0.62
48:WA:3665:A:N6	48:WA:4170:G:O2'	2.33	0.62
85:HC:281:ALA:HB2	85:HC:334:PRO:HB2	1.81	0.62
5:E:164:ARG:NH1	12:L:106:ASP:OD2	2.32	0.62
25:Y:64:LYS:NZ	48:WA:2762:G:O6	2.31	0.62
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.82	0.62
29:CA:19:GLU:HB3	29:CA:102:LEU:HD21	1.82	0.62
48:WA:1554:G:O2'	48:WA:1576:G:N2	2.30	0.62
87:b:47:LEU:O	87:b:51:ALA:N	2.23	0.62
30:DA:103:VAL:O	30:DA:128:ARG:NH1	2.33	0.61
1:A:198:ARG:NH2	48:WA:3690:U:OP2	2.33	0.61
9:I:203:ARG:NH1	49:XA:105:C:OP2	2.32	0.61
22:V:80:ARG:NH2	51:ZA:167:G:O2'	2.33	0.61
2:B:95:THR:HG22	48:WA:4912:A:H4'	1.80	0.61
35:IA:52:LYS:NZ	48:WA:364:G:O6	2.31	0.61
48:WA:1334:C:H2'	48:WA:1335:A:H8	1.66	0.61
48:WA:1678:C:H41	48:WA:4380:A:H2'	1.65	0.61
48:WA:2522:C:O2	48:WA:2642:G:N2	2.33	0.61
58:GB:69:THR:HG22	58:GB:71:GLY:H	1.64	0.61
1:A:27:ALA:O	1:A:128:ARG:NH2	2.33	0.61
13:M:90:ASN:ND2	48:WA:3930:A:OP1	2.33	0.61
13:M:184:ILE:O	13:M:194:ARG:NH2	2.33	0.61
48:WA:1205:G:H2'	48:WA:1206:G:H8	1.65	0.61
48:WA:5061:C:H1'	48:WA:5062:A:H5'	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:THR:HG23	8:H:86:LEU:HG	1.81	0.61
48:WA:3948:G:N1	48:WA:3949:A:N3	2.49	0.61
51:ZA:943:U:OP1	53:BB:214:LYS:NZ	2.33	0.61
57:FB:142:SER:HB3	80:CC:50:VAL:HG22	1.82	0.61
38:LA:74:TYR:O	48:WA:4474:G:O2'	2.18	0.61
48:WA:970:G:N2	48:WA:2098:G:O2'	2.33	0.61
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.83	0.61
48:WA:1092:C:H2'	48:WA:1093:A:H8	1.66	0.61
51:ZA:1228:A:H2'	51:ZA:1229:G:C8	2.35	0.61
54:CB:68:ARG:NH1	54:CB:72:ASP:OD1	2.34	0.61
79:BC:64:CYS:HB3	79:BC:73:LEU:HD23	1.82	0.61
13:M:178:HIS:ND1	48:WA:68:U:OP1	2.32	0.60
48:WA:974:C:H42	48:WA:2097:A:H61	1.47	0.60
66:OB:142:ARG:HB3	78:AC:22:ARG:HD3	1.83	0.60
70:SB:98:VAL:HG11	70:SB:106:LYS:HG3	1.83	0.60
85:HC:63:LEU:HD23	85:HC:66:GLU:HG3	1.83	0.60
11:K:31:ARG:HD2	11:K:35:ARG:HH21	1.66	0.60
18:R:112:ASP:OD1	18:R:116:ARG:NH1	2.33	0.60
26:Z:72:THR:HG22	26:Z:110:LYS:HB3	1.82	0.60
48:WA:926:C:H2'	48:WA:927:C:C6	2.35	0.60
56:EB:79:ASP:HB2	56:EB:82:TYR:HB2	1.83	0.60
80:CC:17:VAL:HA	80:CC:30:VAL:HG23	1.82	0.60
51:ZA:130:G:H1	51:ZA:182:C:H5	1.50	0.60
5:E:115:MET:O	42:PA:87:ARG:NH1	2.34	0.60
5:E:265:LYS:NZ	48:WA:4935:C:OP2	2.35	0.60
16:P:88:ASP:OD2	16:P:108:ARG:NH1	2.35	0.60
59:HB:289:ILE:HD12	59:HB:417:LYS:HG2	1.83	0.60
85:HC:208:MET:SD	85:HC:208:MET:N	2.74	0.60
43:RA:17:CYS:O	43:RA:57:ARG:HA	2.01	0.60
51:ZA:1781:A:H2'	51:ZA:1782:G:C8	2.37	0.60
74:WB:80:ASP:OD1	74:WB:124:LYS:NZ	2.33	0.60
44:SA:26:A:H61	44:SA:44:A:H61	1.50	0.60
51:ZA:1005:G:OP2	53:BB:162:ARG:NH1	2.34	0.60
68:QB:155:SER:O	68:QB:157:LYS:NZ	2.32	0.60
2:B:213:GLN:NE2	2:B:285:TYR:O	2.35	0.60
29:CA:24:GLU:OE2	29:CA:87:ARG:NH1	2.35	0.60
51:ZA:495:U:O2'	56:EB:27:PHE:O	2.20	0.60
48:WA:921:C:H2'	48:WA:922:C:C6	2.36	0.60
52:AB:51:LEU:HD23	69:RB:105:MET:HE1	1.84	0.60
48:WA:369:G:N2	48:WA:372:A:OP2	2.34	0.60
58:GB:2:LYS:HB2	58:GB:108:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:LEU:HB2	8:H:127:ARG:HH21	1.65	0.59
52:AB:77:ILE:HG12	52:AB:99:ILE:HB	1.84	0.59
61:JB:127:ARG:HD3	82:EC:104:ARG:HD3	1.84	0.59
37:KA:2:SER:N	48:WA:2408:G:N7	2.50	0.59
51:ZA:496:C:OP1	56:EB:49:ARG:NH2	2.31	0.59
51:ZA:1513:C:OP1	81:DC:12:ARG:NH1	2.35	0.59
52:AB:156:TYR:OH	73:VB:61:ARG:NH1	2.35	0.59
75:XB:68:LYS:HE2	82:EC:82:VAL:HG22	1.83	0.59
64:MB:89:VAL:HG11	64:MB:109:VAL:HG21	1.85	0.59
26:Z:132:ARG:NH1	48:WA:1470:C:OP1	2.35	0.59
48:WA:2467:C:H1'	48:WA:3674:G:H1	1.66	0.59
51:ZA:3:C:O2	61:JB:18:ARG:NH1	2.35	0.59
51:ZA:1228:A:H2'	51:ZA:1229:G:H8	1.67	0.59
69:RB:5:ARG:O	69:RB:10:LYS:NZ	2.36	0.59
41:OA:4:ARG:NH2	48:WA:1557:G:O6	2.36	0.59
43:RA:107:ASP:N	43:RA:107:ASP:OD1	2.35	0.59
48:WA:745:G:N2	48:WA:923:C:O2	2.36	0.59
48:WA:1671:A:N3	48:WA:1854:U:O2'	2.34	0.59
51:ZA:190:G:O2'	51:ZA:209:A:N6	2.35	0.59
51:ZA:1536:G:H2'	51:ZA:1537:A:H8	1.67	0.59
19:S:51:GLY:HA3	19:S:92:ARG:HG3	1.85	0.59
22:V:8:PHE:HZ	22:V:49:ILE:HD12	1.67	0.59
29:CA:59:THR:HG1	29:CA:104:THR:HG1	1.43	0.59
51:ZA:640:A:H2'	51:ZA:641:A:C8	2.37	0.59
56:EB:251:GLU:OE2	56:EB:255:ARG:NH2	2.36	0.59
65:NB:99:ARG:NH2	65:NB:119:GLU:OE2	2.35	0.59
85:HC:5:LYS:NZ	85:HC:82:THR:O	2.36	0.59
51:ZA:1654:G:OP1	71:TB:90:SER:OG	2.19	0.59
85:HC:272:LEU:HB3	85:HC:302:ALA:HB3	1.83	0.59
18:R:95:ARG:NH2	48:WA:1953:G:O2'	2.36	0.59
48:WA:2002:G:N2	48:WA:2002:G:OP2	2.35	0.59
51:ZA:1298:G:H4'	67:PB:78:THR:HA	1.84	0.59
12:L:5:ARG:NE	12:L:59:ASP:OD1	2.35	0.59
16:P:150:ARG:NH2	48:WA:1501:C:OP1	2.36	0.59
51:ZA:1513:C:H2'	51:ZA:1514:G:H8	1.68	0.59
65:NB:19:ARG:HH21	65:NB:21:SER:HB2	1.67	0.59
42:PA:6:GLN:HG3	42:PA:44:ILE:HD12	1.85	0.58
5:E:156:LEU:HD11	5:E:198:ILE:HG13	1.83	0.58
51:ZA:847:A:OP1	56:EB:108:ARG:NH2	2.36	0.58
51:ZA:1612:G:OP1	67:PB:18:ARG:NH2	2.36	0.58
67:PB:123:TYR:OH	70:SB:124:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RB:94:GLU:O	69:RB:116:ASN:ND2	2.36	0.58
71:TB:104:LEU:HB3	71:TB:121:ARG:HE	1.68	0.58
83:FC:121:CYS:CB	83:FC:126:CYS:SG	2.91	0.58
3:C:312:ARG:NH2	48:WA:2077:G:OP1	2.36	0.58
45:TA:22:G:H2'	45:TA:23:A:H8	1.68	0.58
55:DB:232:PRO:O	55:DB:239:LYS:NZ	2.37	0.58
17:Q:13:SER:OG	17:Q:38:ARG:NH2	2.37	0.58
24:X:1:MET:HE2	48:WA:1370:A:H1'	1.85	0.58
52:AB:2:SER:HB3	52:AB:59:LEU:HG	1.84	0.58
68:QB:96:VAL:HG11	68:QB:110:ILE:HG13	1.85	0.58
51:ZA:1403:C:N4	51:ZA:1433:C:OP1	2.36	0.58
52:AB:42:LYS:HE2	52:AB:46:ILE:HB	1.84	0.58
64:MB:96:ARG:HG3	64:MB:100:PRO:HG3	1.84	0.58
19:S:87:LYS:HD2	48:WA:4307:G:H1	1.68	0.58
21:U:50:ASN:ND2	48:WA:4459:U:OP1	2.37	0.58
48:WA:4993:U:H2'	48:WA:4994:G:C8	2.38	0.58
55:DB:69:GLU:O	55:DB:92:ARG:NH2	2.36	0.58
68:QB:79:GLU:OE1	68:QB:111:ARG:NH1	2.36	0.58
84:GC:24:THR:HB	84:GC:71:ILE:HG12	1.86	0.58
84:GC:132:TRP:CD1	84:GC:138:CYS:HA	2.39	0.58
87:b:53:VAL:HG22	87:b:89:VAL:HG12	1.85	0.58
75:XB:98:ASP:OD2	75:XB:140:ARG:NH2	2.36	0.58
40:NA:81:ARG:NH2	48:WA:4295:U:O2'	2.37	0.58
48:WA:4276:A:H2'	48:WA:4277:G:C8	2.39	0.58
51:ZA:562:U:H3	51:ZA:587:A:H2	1.52	0.58
4:D:88:VAL:HA	4:D:239:MET:HE3	1.85	0.58
8:H:94:SER:HB3	8:H:142:ASP:HB3	1.86	0.58
55:DB:144:ARG:HG3	55:DB:213:VAL:HG22	1.86	0.58
17:Q:21:LYS:NZ	48:WA:2823:U:OP1	2.33	0.58
20:T:111:GLU:OE1	20:T:113:ARG:NH1	2.36	0.58
25:Y:48:ARG:HB3	25:Y:69:LYS:HB3	1.86	0.58
25:Y:88:ASP:O	25:Y:121:ARG:NH1	2.37	0.58
48:WA:217:C:H4'	48:WA:218:A:H3'	1.86	0.58
5:E:144:ARG:NH1	31:EA:110:ILE:OXT	2.36	0.57
42:PA:67:ARG:NH1	48:WA:667:G:OP2	2.37	0.57
59:HB:355:PRO:HG2	59:HB:358:ARG:HG2	1.86	0.57
48:WA:2850:G:O2'	48:WA:3840:U:O4	2.19	0.57
48:WA:4451:A:H8	92:WA:5275:ANM:H61	1.68	0.57
51:ZA:872:A:O2'	51:ZA:874:G:OP2	2.22	0.57
9:I:77:VAL:HG23	9:I:82:LYS:HA	1.86	0.57
12:L:74:ARG:NH1	48:WA:737:C:OP1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:2522:C:H2'	48:WA:2523:G:H8	1.70	0.57
68:QB:156:LYS:NZ	68:QB:160:GLY:O	2.36	0.57
10:J:13:ARG:NH1	10:J:154:LYS:O	2.36	0.57
19:S:127:GLN:NE2	19:S:129:LYS:O	2.37	0.57
43:RA:121:LEU:HB2	87:b:45:MET:HE3	1.86	0.57
51:ZA:637:U:O2	82:EC:129:ASN:ND2	2.33	0.57
6:F:146:LEU:O	6:F:150:ASN:ND2	2.30	0.57
40:NA:15:CYS:SG	40:NA:19:GLN:NE2	2.77	0.57
48:WA:1446:G:H1	48:WA:2112:G:H22	1.50	0.57
48:WA:2603:A:N6	48:WA:2746:A:OP2	2.37	0.57
51:ZA:77:A:H2	58:GB:175:LYS:HG3	1.70	0.57
53:BB:90:ASP:OD2	53:BB:92:GLN:NE2	2.37	0.57
6:F:104:VAL:HG13	6:F:135:VAL:HG12	1.87	0.57
48:WA:746:G:N2	48:WA:922:C:O2	2.38	0.57
84:GC:67:SER:H	84:GC:82:SER:HA	1.70	0.57
9:I:61:SER:HA	9:I:126:VAL:HG12	1.85	0.57
38:LA:92:THR:HG22	38:LA:94:ASN:H	1.69	0.57
51:ZA:1665:G:OP1	71:TB:91:HIS:NE2	2.36	0.57
7:G:187:PRO:HB3	7:G:259:GLN:HG3	1.87	0.57
18:R:160:ARG:HB3	48:WA:1923:C:H1'	1.86	0.57
23:W:110:LYS:NZ	23:W:121:VAL:O	2.38	0.57
48:WA:2380:G:N2	48:WA:2383:A:OP2	2.38	0.57
48:WA:2795:G:H5'	48:WA:2796:C:H5''	1.86	0.57
51:ZA:1613:G:OP1	67:PB:42:ARG:NH2	2.38	0.57
57:FB:71:ARG:NH2	57:FB:148:ASN:OD1	2.34	0.57
43:RA:138:SER:HB3	48:WA:2004:A:N6	2.20	0.57
48:WA:2505:G:N2	48:WA:4086:G:O4'	2.38	0.57
51:ZA:1419:C:OP2	51:ZA:1420:G:N2	2.37	0.57
1:A:210:PRO:O	1:A:221:LYS:NZ	2.35	0.56
3:C:301:ALA:HB1	16:P:132:LYS:HE3	1.86	0.56
4:D:223:PHE:HB3	4:D:226:TYR:HB2	1.85	0.56
19:S:87:LYS:NZ	48:WA:4302:U:OP1	2.38	0.56
46:UA:18:G:H4'	46:UA:59:A:H61	1.69	0.56
48:WA:85:G:O2'	48:WA:97:G:O6	2.23	0.56
51:ZA:990:A:OP2	78:AC:37:LYS:NZ	2.38	0.56
76:YB:14:THR:HG22	76:YB:21:LYS:HD2	1.86	0.56
80:CC:36:ASP:OD1	80:CC:36:ASP:N	2.37	0.56
16:P:67:ILE:HD12	16:P:96:PRO:HD2	1.87	0.56
31:EA:100:ARG:NH1	48:WA:4755:U:OP1	2.38	0.56
48:WA:1929:U:OP1	48:WA:1951:U:O2'	2.21	0.56
51:ZA:375:U:OP2	63:LB:59:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JB:131:ARG:NH1	61:JB:143:ASN:OD1	2.38	0.56
8:H:120:GLU:HG2	48:WA:4613:A:H2	1.70	0.56
9:I:38:ARG:NH2	9:I:45:GLU:OE1	2.37	0.56
12:L:11:ARG:NH1	12:L:58:THR:O	2.38	0.56
12:L:94:LYS:NZ	48:WA:4874:G:OP2	2.37	0.56
19:S:70:HIS:NE2	48:WA:4329:C:OP1	2.37	0.56
31:EA:43:LEU:O	31:EA:109:ARG:NH1	2.38	0.56
48:WA:4355:U:H5''	48:WA:4356:U:H5'	1.88	0.56
51:ZA:919:A:OP2	65:NB:64:ARG:NH2	2.33	0.56
51:ZA:1130:G:OP2	51:ZA:1130:G:N2	2.37	0.56
61:JB:136:ARG:NH1	61:JB:159:PHE:O	2.39	0.56
70:SB:28:PHE:O	70:SB:31:THR:OG1	2.21	0.56
70:SB:118:ARG:HE	70:SB:123:LEU:HD21	1.70	0.56
84:GC:39:THR:HG22	84:GC:60:ARG:HG2	1.86	0.56
36:JA:24:LYS:HE2	36:JA:69:LEU:HD11	1.87	0.56
51:ZA:197:U:O2	51:ZA:202:G:O6	2.24	0.56
51:ZA:1203:G:H2'	51:ZA:1204:A:C8	2.40	0.56
84:GC:104:HIS:NE2	84:GC:122:SER:OG	2.34	0.56
85:HC:108:GLN:NE2	85:HC:251:GLN:OE1	2.37	0.56
51:ZA:846:G:OP2	56:EB:108:ARG:NH1	2.36	0.56
51:ZA:1527:C:OP1	68:QB:168:GLN:NE2	2.38	0.56
84:GC:87:LEU:HB2	84:GC:101:PHE:HB2	1.87	0.56
5:E:126:ARG:O	48:WA:963:G:O2'	2.24	0.56
12:L:34:ASN:ND2	48:WA:1927:G:OP1	2.39	0.56
36:JA:28:ASN:ND2	48:WA:2697:A:OP2	2.37	0.56
51:ZA:1658:G:OP2	51:ZA:1660:C:N4	2.38	0.56
64:MB:33:ARG:NH2	64:MB:89:VAL:O	2.39	0.56
76:YB:83:LYS:NZ	76:YB:96:LEU:O	2.39	0.56
1:A:101:VAL:HG22	1:A:165:VAL:HG22	1.88	0.56
15:O:154:MET:HB2	15:O:170:SER:HB3	1.88	0.56
48:WA:4476:A:OP2	48:WA:4478:C:N4	2.38	0.56
51:ZA:84:A:N3	51:ZA:150:A:O2'	2.36	0.56
2:B:249:ARG:NH1	48:WA:2839:U:OP1	2.36	0.56
31:EA:52:LYS:NZ	48:WA:4754:U:O4	2.38	0.56
55:DB:70:ASP:OD2	55:DB:103:ARG:NH1	2.39	0.56
5:E:141:ARG:NH1	5:E:172:SER:O	2.39	0.56
48:WA:1505:A:H4'	48:WA:1506:G:H5'	1.87	0.56
51:ZA:959:G:OP1	66:OB:104:ARG:NH2	2.33	0.56
56:EB:85:GLY:N	56:EB:88:ASP:OD2	2.37	0.56
68:QB:31:GLY:O	68:QB:53:ARG:NH2	2.39	0.56
87:b:128:THR:OG1	87:b:129:GLY:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:1:MET:HE3	24:X:2:LYS:H	1.71	0.55
48:WA:3666:G:H2'	48:WA:3667:G:H8	1.70	0.55
48:WA:4539:C:H2'	48:WA:4540:G:H8	1.71	0.55
53:BB:138:PHE:O	53:BB:213:ARG:N	2.38	0.55
57:FB:27:ASP:OD1	57:FB:107:ASN:ND2	2.38	0.55
62:KB:20:VAL:HG12	62:KB:70:TYR:HA	1.86	0.55
67:PB:81:ARG:NH1	67:PB:97:TYR:O	2.38	0.55
84:GC:132:TRP:HD1	84:GC:138:CYS:HA	1.70	0.55
17:Q:44:LEU:HD22	17:Q:49:LEU:HD12	1.87	0.55
24:X:112:ASP:H	24:X:115:ARG:HB2	1.70	0.55
43:RA:15:LEU:HD21	43:RA:31:LYS:HG3	1.88	0.55
51:ZA:70:G:N2	51:ZA:71:G:O6	2.40	0.55
57:FB:34:SER:HA	80:CC:55:VAL:HB	1.88	0.55
14:N:188:LYS:NZ	48:WA:4895:A:OP1	2.38	0.55
18:R:69:GLU:OE2	18:R:76:LYS:NZ	2.40	0.55
19:S:28:ALA:HA	19:S:31:MET:HG2	1.88	0.55
48:WA:2640:G:H1	48:WA:2699:A:H61	1.53	0.55
48:WA:4276:A:H2'	48:WA:4277:G:H8	1.71	0.55
52:AB:145:ILE:HG12	52:AB:159:ILE:HB	1.88	0.55
53:BB:32:ASP:OD1	53:BB:46:LYS:NZ	2.35	0.55
65:NB:4:MET:HE3	65:NB:121:ARG:HG2	1.87	0.55
83:FC:107:LYS:HD2	83:FC:115:SER:HB3	1.87	0.55
6:F:156:ARG:NH2	48:WA:2075:C:O2'	2.40	0.55
43:RA:119:ARG:NH2	48:WA:1975:G:O2'	2.39	0.55
48:WA:4240:G:H2'	48:WA:4241:A:H8	1.72	0.55
54:CB:199:PRO:HG3	61:JB:58:ARG:HD3	1.88	0.55
62:KB:91:PRO:HD2	62:KB:94:LEU:HD12	1.88	0.55
70:SB:91:LYS:NZ	70:SB:109:GLU:OE1	2.38	0.55
13:M:172:ARG:NH1	48:WA:62:A:OP1	2.36	0.55
28:BA:50:ASN:ND2	28:BA:75:SER:O	2.40	0.55
51:ZA:581:U:OP1	61:JB:133:ARG:NH2	2.39	0.55
51:ZA:587:A:H5'	51:ZA:592:C:H41	1.70	0.55
51:ZA:1711:U:H2'	51:ZA:1712:A:H8	1.71	0.55
56:EB:100:ARG:HH21	56:EB:118:GLU:HG2	1.72	0.55
68:QB:61:ASN:O	71:TB:7:LYS:NZ	2.32	0.55
71:TB:113:VAL:HG12	71:TB:123:LEU:HD23	1.88	0.55
14:N:27:VAL:HG13	14:N:98:ALA:HB1	1.87	0.55
48:WA:1330:G:O2'	48:WA:2351:A:OP1	2.24	0.55
48:WA:1334:C:H2'	48:WA:1335:A:C8	2.42	0.55
48:WA:1763:G:H1	48:WA:1773:U:H3	1.53	0.55
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:39:ARG:NH2	48:WA:1364:G:OP1	2.39	0.55
14:N:89:PRO:HD3	48:WA:1916:C:H4'	1.88	0.55
16:P:14:ARG:NH2	48:WA:2085:C:OP2	2.39	0.55
48:WA:382:G:N1	48:WA:385:A:OP2	2.37	0.55
48:WA:4596:U:H2'	48:WA:4597:G:H8	1.71	0.55
50:YA:122:G:OP2	50:YA:124:U:N3	2.40	0.55
51:ZA:1528:G:O2'	51:ZA:1666:C:OP1	2.24	0.55
70:SB:30:ILE:HG22	70:SB:36:VAL:HG11	1.88	0.55
18:R:23:ARG:HH12	48:WA:1206:G:H5'	1.72	0.55
48:WA:4539:C:H2'	48:WA:4540:G:C8	2.42	0.55
64:MB:43:ASP:OD1	83:FC:116:ARG:NH2	2.39	0.55
74:WB:30:CYS:SG	74:WB:31:SER:N	2.79	0.55
84:GC:8:ARG:HB3	84:GC:309:VAL:HG23	1.89	0.55
4:D:256:LYS:HD2	49:XA:117:G:H5'	1.89	0.55
11:K:140:SER:OG	11:K:143:GLU:OE1	2.24	0.55
13:M:157:LYS:O	13:M:162:ARG:NH1	2.36	0.55
51:ZA:1617:G:N1	51:ZA:1620:A:OP2	2.40	0.55
70:SB:22:GLY:HA2	70:SB:56:ALA:HB3	1.88	0.55
14:N:12:ARG:O	18:R:171:ARG:NH2	2.40	0.55
17:Q:117:ARG:NH2	48:WA:2662:A:OP1	2.40	0.55
48:WA:3719:A:H2'	48:WA:3720:A:C8	2.42	0.55
51:ZA:1536:G:H2'	51:ZA:1537:A:C8	2.42	0.55
54:CB:176:LYS:O	54:CB:200:ARG:NH2	2.40	0.55
84:GC:199:THR:HG21	84:GC:240:CYS:HA	1.89	0.55
85:HC:134:ARG:NH1	85:HC:177:TYR:OH	2.40	0.55
1:A:159:SER:OG	1:A:162:ASN:OD1	2.22	0.54
6:F:227:VAL:HA	18:R:39:VAL:HG12	1.90	0.54
32:FA:24:ARG:NH2	48:WA:2615:C:OP1	2.39	0.54
48:WA:2506:C:H4'	48:WA:2507:C:H5'	1.88	0.54
51:ZA:641:A:OP1	61:JB:40:LYS:NZ	2.35	0.54
63:LB:113:LEU:HD21	63:LB:120:VAL:HG11	1.89	0.54
85:HC:74:ASP:HA	85:HC:101:ASN:HD22	1.72	0.54
22:V:93:LYS:O	22:V:101:ARG:NH2	2.39	0.54
51:ZA:202:G:H2'	51:ZA:203:G:C8	2.42	0.54
51:ZA:212:C:H2'	51:ZA:213:G:C8	2.42	0.54
56:EB:199:GLU:HB3	56:EB:207:VAL:HG13	1.90	0.54
1:A:29:LEU:O	1:A:123:ARG:NH1	2.40	0.54
48:WA:2747:A:H2'	48:WA:2748:A:H8	1.72	0.54
51:ZA:1023:A:OP2	65:NB:124:ARG:NH1	2.41	0.54
53:BB:40:ASN:OD1	53:BB:75:GLN:NE2	2.40	0.54
64:MB:80:ASP:OD1	64:MB:80:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:681:U:H4'	75:XB:9:THR:HG22	1.89	0.54
51:ZA:1617:G:O6	67:PB:43:ARG:NH1	2.41	0.54
54:CB:273:LEU:O	54:CB:277:HIS:HB2	2.07	0.54
60:IB:157:LYS:NZ	60:IB:158:ILE:O	2.38	0.54
2:B:215:GLU:OE2	2:B:349:LYS:NZ	2.39	0.54
3:C:339:THR:HG22	3:C:342:ARG:HH22	1.72	0.54
6:F:148:SER:OG	6:F:244:ARG:NH2	2.41	0.54
7:G:142:ARG:NH1	50:YA:155:C:OP1	2.40	0.54
31:EA:89:ARG:NH2	48:WA:710:C:OP1	2.41	0.54
32:FA:76:ARG:NH1	48:WA:2585:C:OP2	2.37	0.54
51:ZA:616:A:OP1	75:XB:68:LYS:NZ	2.40	0.54
51:ZA:1758:G:H2'	51:ZA:1759:G:C8	2.42	0.54
61:JB:107:GLU:O	61:JB:113:GLN:NE2	2.41	0.54
67:PB:28:MET:HG3	67:PB:33:LEU:HD22	1.89	0.54
76:YB:55:ILE:HG12	76:YB:75:ILE:HG23	1.90	0.54
76:YB:102:THR:O	76:YB:107:ARG:NH2	2.39	0.54
21:U:74:LYS:NZ	48:WA:3800:U:OP2	2.40	0.54
23:W:64:SER:HB2	33:GA:69:LEU:HD13	1.88	0.54
48:WA:3762:A:N6	51:ZA:1826:G:OP2	2.41	0.54
51:ZA:928:G:H2'	51:ZA:929:G:C8	2.43	0.54
83:FC:121:CYS:SG	83:FC:126:CYS:HB3	2.47	0.54
26:Z:27:LYS:NZ	48:WA:1520:A:OP1	2.32	0.54
39:MA:1:MET:HB2	51:ZA:1706:G:H5'	1.89	0.54
48:WA:67:C:OP2	48:WA:312:G:N2	2.40	0.54
51:ZA:880:G:H1	51:ZA:906:U:H3	1.53	0.54
57:FB:114:ASN:OD1	57:FB:118:ASN:ND2	2.41	0.54
1:A:30:ARG:NH1	1:A:33:ASP:OD2	2.41	0.54
16:P:108:ARG:NH2	48:WA:1357:G:OP1	2.41	0.54
24:X:52:ASP:OD2	24:X:110:LYS:NZ	2.39	0.54
33:GA:3:LYS:NZ	50:YA:82:A:OP2	2.41	0.54
48:WA:982:G:OP2	48:WA:982:G:N2	2.36	0.54
71:TB:76:THR:HB	71:TB:94:ARG:HB3	1.90	0.54
51:ZA:1543:U:P	71:TB:62:ARG:HH22	2.30	0.54
52:AB:164:ASN:O	52:AB:170:SER:OG	2.24	0.54
74:WB:55:ASP:OD1	74:WB:57:ARG:NH1	2.40	0.54
85:HC:426:VAL:HB	85:HC:434:ALA:HB3	1.88	0.54
11:K:178:ALA:N	26:Z:134:GLU:OE2	2.38	0.54
51:ZA:396:U:OP2	63:LB:79:LYS:NZ	2.41	0.54
55:DB:80:THR:OG1	55:DB:83:ARG:O	2.21	0.54
74:WB:52:ILE:HG22	74:WB:61:ILE:HG12	1.89	0.54
81:DC:17:GLY:O	81:DC:27:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:GC:152:SER:H	84:GC:169:GLY:HA2	1.72	0.54
37:KA:2:SER:O	37:KA:5:LYS:NZ	2.41	0.53
48:WA:408:A:O2'	48:WA:411:G:OP2	2.22	0.53
48:WA:478:G:H2'	48:WA:479:G:H8	1.73	0.53
50:YA:67:U:H2'	50:YA:68:G:H8	1.72	0.53
51:ZA:1388:A:H61	55:DB:199:GLY:HA3	1.73	0.53
84:GC:109:LEU:HD23	84:GC:152:SER:HA	1.88	0.53
85:HC:15:HIS:O	85:HC:20:LYS:NZ	2.41	0.53
35:IA:49:TRP:O	48:WA:1648:A:O2'	2.27	0.53
45:TA:52:G:H2'	45:TA:53:G:H8	1.73	0.53
48:WA:4637:A:OP1	48:WA:4638:U:O2'	2.27	0.53
48:WA:4741:C:N4	48:WA:4742:G:O6	2.41	0.53
51:ZA:880:G:N2	51:ZA:906:U:O2	2.37	0.53
60:IB:12:ARG:HE	60:IB:18:ARG:HG3	1.73	0.53
60:IB:106:SER:HB3	60:IB:171:LEU:HG	1.90	0.53
79:BC:74:THR:OG1	79:BC:77:CYS:SG	2.66	0.53
16:P:22:ASP:OD1	16:P:22:ASP:N	2.41	0.53
27:AA:114:ARG:NH1	48:WA:1271:G:N7	2.56	0.53
30:DA:39:ARG:NH2	48:WA:1664:C:OP2	2.40	0.53
33:GA:79:LYS:HE3	48:WA:136:C:H41	1.72	0.53
53:BB:65:ARG:HH12	66:OB:51:GLU:HG2	1.74	0.53
54:CB:187:ARG:HE	54:CB:192:LEU:HD12	1.73	0.53
70:SB:13:LEU:HB2	70:SB:20:ILE:HB	1.89	0.53
6:F:130:ASN:ND2	48:WA:1729:U:OP1	2.41	0.53
14:N:125:LYS:HG3	14:N:129:LEU:HD12	1.89	0.53
26:Z:12:ARG:NH1	48:WA:2347:G:OP2	2.42	0.53
45:TA:42:G:H2'	45:TA:43:A:H8	1.74	0.53
51:ZA:107:A:H2'	51:ZA:108:G:C8	2.43	0.53
54:CB:244:ILE:O	54:CB:247:THR:OG1	2.27	0.53
70:SB:23:ARG:NH2	77:ZB:46:ASN:O	2.42	0.53
6:F:121:PHE:O	6:F:204:ASN:ND2	2.42	0.53
51:ZA:743:U:O4	51:ZA:798:G:N2	2.42	0.53
60:IB:76:THR:HG22	60:IB:108:PRO:HG2	1.90	0.53
70:SB:45:LEU:HD22	70:SB:50:ILE:HD12	1.89	0.53
4:D:53:VAL:HG11	4:D:159:VAL:HA	1.91	0.53
7:G:90:LYS:NZ	48:WA:4128:C:OP1	2.39	0.53
14:N:49:ARG:NH1	48:WA:1932:U:OP2	2.34	0.53
15:O:140:SER:OG	15:O:182:LYS:O	2.22	0.53
48:WA:4176:U:H2'	48:WA:4177:G:H8	1.74	0.53
51:ZA:453:C:O2'	58:GB:92:ARG:O	2.25	0.53
51:ZA:677:G:H21	51:ZA:1028:A:H62	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1245:G:O2'	51:ZA:1492:U:OP1	2.26	0.53
51:ZA:1674:G:OP1	57:FB:51:HIS:NE2	2.32	0.53
64:MB:49:LEU:HB3	64:MB:111:VAL:HG13	1.90	0.53
84:GC:259:TRP:HD1	84:GC:266:ILE:HA	1.73	0.53
85:HC:162:TYR:O	85:HC:210:TRP:NE1	2.41	0.53
51:ZA:5:U:H2'	51:ZA:6:G:H8	1.74	0.53
65:NB:29:THR:OG1	65:NB:31:ASP:OD1	2.25	0.53
85:HC:18:SER:O	85:HC:153:ASN:ND2	2.41	0.53
6:F:156:ARG:NH1	6:F:247:ASN:OXT	2.42	0.53
51:ZA:28:U:H2'	51:ZA:29:G:H8	1.74	0.53
55:DB:253:ASP:OD1	55:DB:253:ASP:N	2.42	0.53
8:H:129:ARG:NH1	8:H:156:ASN:OD1	2.41	0.53
13:M:114:ARG:HE	13:M:137:PRO:HG3	1.74	0.53
48:WA:2095:G:H4'	48:WA:2096:C:H5'	1.91	0.53
48:WA:2411:U:H4'	48:WA:2430:A:H4'	1.90	0.53
48:WA:4240:G:H2'	48:WA:4241:A:C8	2.43	0.53
48:WA:4763:G:H2'	48:WA:4764:A:H8	1.74	0.53
72:UB:69:PRO:O	81:DC:40:ARG:NH2	2.38	0.53
2:B:234:ARG:NH2	48:WA:4568:U:O2'	2.42	0.53
2:B:249:ARG:NH2	48:WA:3847:A:OP2	2.42	0.53
19:S:100:LYS:NZ	48:WA:1733:C:OP1	2.41	0.53
21:U:35:LYS:HB2	21:U:67:LYS:HG3	1.91	0.53
24:X:54:GLU:HB2	24:X:108:ARG:HB3	1.91	0.53
29:CA:64:ILE:HG23	29:CA:68:LEU:HD23	1.90	0.53
40:NA:26:TYR:HB3	40:NA:67:VAL:HB	1.92	0.53
48:WA:2031:A:H2'	48:WA:2032:A:C8	2.44	0.53
48:WA:3621:G:H22	48:WA:3626:A:H1'	1.74	0.53
51:ZA:1089:G:O6	75:XB:3:LYS:NZ	2.41	0.53
9:I:3:ARG:NH2	48:WA:4433:U:OP2	2.41	0.52
9:I:7:ARG:NH2	48:WA:4407:G:OP1	2.42	0.52
48:WA:153:G:H2'	48:WA:154:G:H8	1.73	0.52
48:WA:308:G:OP2	48:WA:308:G:N2	2.34	0.52
48:WA:2097:A:H2'	48:WA:2098:G:C8	2.45	0.52
48:WA:2589:A:H5'	48:WA:2772:C:H5'	1.91	0.52
51:ZA:981:A:H2'	51:ZA:982:G:C8	2.43	0.52
51:ZA:1588:A:H2'	51:ZA:1589:A:C8	2.44	0.52
51:ZA:1693:G:N2	51:ZA:1834:A:H8	2.07	0.52
56:EB:137:PRO:HB2	56:EB:150:PRO:HD2	1.90	0.52
5:E:144:ARG:NH2	5:E:194:GLN:O	2.42	0.52
48:WA:2051:G:HO2'	48:WA:3886:U:HO2'	1.57	0.52
48:WA:2413:C:H2'	48:WA:2414:A:H8	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:3738:A:H2'	48:WA:3739:A:C8	2.44	0.52
59:HB:284:THR:HG23	59:HB:303:PRO:HG3	1.91	0.52
64:MB:52:LEU:HD23	64:MB:76:LEU:HD11	1.90	0.52
83:FC:141:CYS:HB3	83:FC:146:LEU:H	1.74	0.52
8:H:113:GLU:OE1	8:H:115:ARG:NH2	2.42	0.52
10:J:40:LEU:HD12	10:J:70:VAL:HG22	1.91	0.52
17:Q:62:ARG:NH2	48:WA:4650:A:OP1	2.42	0.52
48:WA:1944:A:H2'	48:WA:1945:A:C8	2.44	0.52
56:EB:162:ILE:HG22	56:EB:169:ILE:HA	1.92	0.52
1:A:207:VAL:HG13	1:A:208:GLU:HG3	1.91	0.52
57:FB:122:ARG:N	57:FB:197:GLU:OE2	2.41	0.52
59:HB:274:LEU:HD21	59:HB:316:ARG:HD2	1.91	0.52
75:XB:91:LEU:HB3	82:EC:82:VAL:HG11	1.91	0.52
84:GC:107:ASP:N	84:GC:107:ASP:OD1	2.42	0.52
27:AA:111:ARG:NH2	48:WA:1270:G:O6	2.43	0.52
51:ZA:1474:A:H3'	51:ZA:1475:G:H21	1.75	0.52
85:HC:111:CYS:SG	85:HC:112:ALA:N	2.82	0.52
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.92	0.52
48:WA:1804:A:H5''	48:WA:1805:G:H5'	1.91	0.52
48:WA:1992:A:H2'	48:WA:1993:A:H8	1.75	0.52
56:EB:216:ASN:OD1	56:EB:216:ASN:N	2.42	0.52
60:IB:87:ASN:HB3	60:IB:90:LEU:HG	1.90	0.52
16:P:2:GLY:N	48:WA:2074:C:OP1	2.42	0.52
16:P:65:ARG:NH1	48:WA:1504:G:OP1	2.43	0.52
25:Y:90:PRO:O	25:Y:117:LYS:NZ	2.43	0.52
48:WA:1263:G:H2'	48:WA:1264:G:C8	2.45	0.52
51:ZA:433:A:H5''	60:IB:22:HIS:HB3	1.92	0.52
4:D:126:THR:HG22	4:D:128:ASP:H	1.73	0.52
48:WA:1183:U:H2'	48:WA:1184:G:C8	2.43	0.52
48:WA:2413:C:H2'	48:WA:2414:A:C8	2.45	0.52
48:WA:3813:G:O2'	48:WA:3816:U:OP2	2.28	0.52
58:GB:55:GLY:H	58:GB:63:MET:HE2	1.74	0.52
6:F:91:VAL:O	6:F:119:GLY:HA2	2.10	0.52
6:F:126:LYS:HB2	19:S:133:ALA:HB3	1.91	0.52
51:ZA:1562:C:H2'	51:ZA:1563:G:H8	1.75	0.52
54:CB:191:VAL:HG11	54:CB:236:PHE:HA	1.92	0.52
1:A:117:GLU:OE2	1:A:163:ARG:NH1	2.43	0.52
2:B:36:ASP:OD1	2:B:36:ASP:N	2.43	0.52
2:B:161:ARG:HE	2:B:184:GLN:HE21	1.58	0.52
3:C:4:ALA:O	3:C:29:LYS:NZ	2.41	0.52
20:T:100:LEU:HD13	20:T:112:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:1727:U:H2'	48:WA:1728:U:H6	1.75	0.52
48:WA:3724:G:H2'	48:WA:3725:A:H8	1.74	0.52
62:KB:15:LEU:HD22	62:KB:49:MET:HE1	1.91	0.52
84:GC:94:THR:HG23	84:GC:96:THR:H	1.74	0.52
21:U:21:PRO:HA	21:U:54:ALA:HA	1.93	0.51
48:WA:4469:A:O2'	48:WA:4512:A:N3	2.39	0.51
48:WA:5018:A:H2	48:WA:5035:G:H21	1.57	0.51
4:D:52:ILE:HD13	49:XA:6:C:H4'	1.92	0.51
8:H:129:ARG:HH12	48:WA:4706:C:H4'	1.75	0.51
18:R:95:ARG:NH1	18:R:112:ASP:OD2	2.43	0.51
25:Y:92:ASP:OD2	25:Y:94:THR:OG1	2.27	0.51
33:GA:97:LYS:HD3	48:WA:135:G:C6	2.45	0.51
59:HB:408:VAL:HG13	59:HB:425:PHE:HB2	1.92	0.51
1:A:179:ILE:O	48:WA:3655:A:O2'	2.24	0.51
7:G:96:GLN:O	48:WA:4126:G:N2	2.43	0.51
8:H:43:VAL:HG12	8:H:59:LYS:HD3	1.91	0.51
51:ZA:551:U:H2'	51:ZA:552:G:C8	2.43	0.51
52:AB:36:GLN:O	52:AB:53:ARG:NH1	2.44	0.51
74:WB:18:GLU:HG3	74:WB:69:LEU:HD23	1.92	0.51
17:Q:46:LYS:NZ	48:WA:2707:G:O6	2.32	0.51
19:S:63:ARG:NH2	27:AA:30:GLU:OE1	2.44	0.51
46:UA:23:C:H2'	46:UA:24:A:C8	2.44	0.51
48:WA:417:G:OP1	48:WA:2331:U:O2'	2.27	0.51
53:BB:180:ASP:OD1	53:BB:180:ASP:N	2.43	0.51
3:C:204:ARG:NH1	3:C:205:ARG:O	2.44	0.51
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.93	0.51
15:O:151:ALA:HB3	15:O:172:PRO:HG2	1.92	0.51
48:WA:2377:A:H2'	48:WA:2378:A:H8	1.74	0.51
52:AB:42:LYS:HD3	52:AB:48:ILE:HD11	1.93	0.51
59:HB:377:ILE:HG23	59:HB:394:VAL:HG13	1.91	0.51
79:BC:67:THR:OG1	79:BC:70:LYS:O	2.29	0.51
15:O:148:VAL:HG22	15:O:175:ILE:HG23	1.93	0.51
41:OA:4:ARG:NH1	48:WA:1556:A:OP2	2.34	0.51
48:WA:300:A:H2'	48:WA:301:G:H8	1.75	0.51
48:WA:483:G:O2'	48:WA:486:C:OP2	2.28	0.51
50:YA:102:G:OP2	50:YA:104:A:O2'	2.24	0.51
55:DB:252:LYS:NZ	55:DB:253:ASP:O	2.41	0.51
17:Q:70:ARG:NH2	48:WA:2813:G:OP1	2.44	0.51
20:T:28:PRO:HB2	20:T:34:MET:HG2	1.92	0.51
30:DA:104:SER:OG	48:WA:2307:U:O2'	2.27	0.51
51:ZA:891:G:H4'	51:ZA:892:U:H4'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:921:G:C5	74:WB:28:ARG:HD3	2.46	0.51
51:ZA:1332:A:O2'	55:DB:183:GLN:O	2.28	0.51
57:FB:40:ALA:HB1	57:FB:45:TYR:CG	2.46	0.51
87:b:221:ASN:OD1	87:b:221:ASN:N	2.34	0.51
11:K:46:ILE:HB	11:K:49:ARG:HB2	1.93	0.51
43:RA:47:ALA:O	43:RA:50:THR:OG1	2.29	0.51
48:WA:4190:U:H2'	48:WA:4191:U:C6	2.46	0.51
51:ZA:1232:U:H2'	51:ZA:1233:G:H8	1.76	0.51
51:ZA:1550:G:O2'	51:ZA:1558:C:O2	2.28	0.51
51:ZA:1692:U:H2'	51:ZA:1693:G:C8	2.45	0.51
58:GB:159:ARG:HG2	58:GB:173:ALA:HB2	1.93	0.51
76:YB:10:ARG:HH21	76:YB:24:VAL:HG11	1.76	0.51
3:C:323:ARG:HB2	48:WA:1283:G:H5'	1.93	0.51
33:GA:86:LYS:NZ	50:YA:38:U:O2'	2.44	0.51
48:WA:1256:A:H61	48:WA:1261:G:H1	1.57	0.51
51:ZA:1662:U:O4	51:ZA:1663:A:N6	2.42	0.51
60:IB:135:GLU:O	60:IB:139:LYS:HB2	2.11	0.51
5:E:160:HIS:HB3	5:E:163:LYS:HD2	1.93	0.51
33:GA:3:LYS:N	50:YA:80:A:N7	2.59	0.51
48:WA:4241:A:H2'	48:WA:4242:G:C8	2.46	0.51
51:ZA:860:G:H21	74:WB:107:SER:HB2	1.75	0.51
51:ZA:1285:G:O2'	83:FC:99:LYS:NZ	2.39	0.51
51:ZA:1477:U:OP2	69:RB:3:ARG:NH2	2.44	0.51
56:EB:112:HIS:NE2	56:EB:237:SER:O	2.43	0.51
64:MB:32:ALA:HB1	64:MB:37:GLU:HB3	1.92	0.51
64:MB:54:SER:HB2	64:MB:80:ASP:HA	1.93	0.51
74:WB:55:ASP:OD1	74:WB:56:HIS:N	2.43	0.51
8:H:177:ASP:OD1	8:H:177:ASP:N	2.43	0.50
36:JA:26:LYS:HE2	48:WA:2698:A:H5'	1.92	0.50
48:WA:1444:C:H2'	48:WA:1445:A:C8	2.46	0.50
54:CB:192:LEU:HB3	54:CB:227:ARG:HB3	1.93	0.50
13:M:49:ARG:HH12	48:WA:152:U:P	2.35	0.50
15:O:72:LYS:NZ	48:WA:5068:U:OP1	2.36	0.50
48:WA:1908:U:H2'	48:WA:1909:A:H8	1.76	0.50
48:WA:3950:C:H42	48:WA:4069:U:H1'	1.77	0.50
51:ZA:1079:C:O2'	51:ZA:1182:A:N1	2.45	0.50
51:ZA:1232:U:H2'	51:ZA:1233:G:C8	2.46	0.50
51:ZA:1447:G:OP1	72:UB:85:HIS:ND1	2.41	0.50
51:ZA:1743:G:H21	51:ZA:1791:A:H62	1.59	0.50
66:OB:105:THR:HG22	66:OB:107:THR:H	1.75	0.50
71:TB:116:ASP:OD1	71:TB:117:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:44:LYS:NZ	85:HC:48:GLU:OE2	2.44	0.50
3:C:69:THR:HG21	48:WA:3908:A:H2'	1.92	0.50
5:E:73:ARG:HD3	48:WA:989:C:C5	2.46	0.50
9:I:35:ASP:HA	9:I:87:ILE:O	2.11	0.50
29:CA:70:LYS:HG3	48:WA:2391:A:H4'	1.93	0.50
48:WA:2043:A:N7	48:WA:4436:C:O2'	2.45	0.50
51:ZA:476:A:N3	51:ZA:488:U:O2'	2.35	0.50
51:ZA:851:C:H5''	51:ZA:852:G:H5'	1.93	0.50
85:HC:247:ARG:NH2	85:HC:332:ASP:OD2	2.45	0.50
10:J:112:HIS:HE1	10:J:125:ILE:HA	1.75	0.50
23:W:139:ARG:NH1	48:WA:2535:C:OP1	2.45	0.50
48:WA:1341:U:H2'	48:WA:1342:C:C6	2.47	0.50
48:WA:3811:G:OP2	48:WA:3811:G:N2	2.34	0.50
56:EB:18:TRP:HB3	56:EB:20:LEU:HD13	1.92	0.50
56:EB:66:MET:SD	56:EB:78:THR:OG1	2.68	0.50
71:TB:130:ASP:OD1	71:TB:133:ARG:NH2	2.45	0.50
2:B:13:SER:HB2	48:WA:4624:A:H4'	1.94	0.50
5:E:48:ARG:HB2	5:E:64:MET:HE1	1.93	0.50
33:GA:112:ARG:NH1	48:WA:265:C:O2'	2.44	0.50
48:WA:456:C:H2'	48:WA:457:G:H8	1.77	0.50
48:WA:4305:C:H2'	48:WA:4307:G:H8	1.76	0.50
6:F:163:LYS:NZ	48:WA:1844:G:OP1	2.45	0.50
48:WA:137:G:H2'	48:WA:138:G:C8	2.45	0.50
48:WA:2811:G:O2'	48:WA:4646:G:OP1	2.26	0.50
62:KB:27:VAL:HG13	62:KB:43:LEU:HD13	1.93	0.50
64:MB:52:LEU:HD11	64:MB:78:LYS:HE3	1.93	0.50
85:HC:200:ASN:HB2	85:HC:208:MET:HE3	1.94	0.50
21:U:43:LYS:HD2	48:WA:4510:C:H5''	1.94	0.50
51:ZA:1018:U:O2'	65:NB:86:GLU:OE2	2.30	0.50
48:WA:173:C:H2'	48:WA:174:C:C6	2.47	0.50
51:ZA:1255:G:OP1	51:ZA:1256:G:O2'	2.26	0.50
70:SB:124:ARG:HB2	70:SB:131:VAL:HG13	1.93	0.50
84:GC:130:LYS:HG2	84:GC:141:THR:HB	1.93	0.50
85:HC:132:GLN:O	85:HC:136:HIS:ND1	2.45	0.50
8:H:66:GLU:O	8:H:69:THR:OG1	2.27	0.50
25:Y:103:ASP:HB3	25:Y:106:LEU:HB2	1.93	0.50
30:DA:76:LYS:NZ	30:DA:98:GLU:OE2	2.40	0.50
35:IA:82:THR:OG1	50:YA:94:G:N2	2.45	0.50
48:WA:4701:U:H1'	48:WA:4702:A:H5''	1.93	0.50
56:EB:185:GLY:H	56:EB:189:LEU:HD13	1.77	0.50
78:AC:59:PHE:HB2	78:AC:62:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:110:ASP:OD2	85:HC:240:ARG:NH2	2.44	0.50
4:D:33:ARG:HH11	19:S:27:LEU:HD12	1.77	0.49
11:K:91:ALA:HB1	11:K:96:ILE:HB	1.94	0.49
17:Q:15:LEU:HD13	17:Q:52:ARG:HB2	1.94	0.49
18:R:154:LEU:HB3	18:R:157:ARG:HD3	1.94	0.49
51:ZA:218:U:O2	60:IB:184:ARG:NH2	2.45	0.49
51:ZA:1156:U:O4	54:CB:194:ARG:NH1	2.45	0.49
52:AB:109:THR:O	54:CB:89:LYS:NZ	2.45	0.49
52:AB:109:THR:OG1	52:AB:136:GLU:OE1	2.27	0.49
52:AB:205:ARG:NH2	52:AB:213:GLU:OE1	2.41	0.49
2:B:220:ILE:HG12	2:B:278:THR:HG23	1.94	0.49
9:I:54:SER:HB2	9:I:135:ILE:HD11	1.95	0.49
15:O:130:ASN:OD1	48:WA:399:G:N2	2.46	0.49
38:LA:88:LYS:NZ	48:WA:4487:C:O2'	2.44	0.49
48:WA:712:A:H2'	48:WA:713:C:C6	2.47	0.49
48:WA:923:C:H2'	48:WA:924:C:C6	2.47	0.49
48:WA:1392:G:N2	48:WA:1395:G:OP2	2.38	0.49
51:ZA:866:U:H2'	51:ZA:867:G:C8	2.48	0.49
60:IB:64:ASN:O	60:IB:186:ASP:HA	2.12	0.49
66:OB:31:CYS:HB3	66:OB:44:VAL:HG22	1.93	0.49
72:UB:115:THR:HG22	72:UB:117:ALA:H	1.76	0.49
85:HC:294:MET:HB2	85:HC:308:VAL:HG12	1.94	0.49
48:WA:922:C:H2'	48:WA:923:C:C6	2.47	0.49
48:WA:1812:G:H1	48:WA:1830:C:H42	1.59	0.49
48:WA:3656:G:O2'	48:WA:3695:U:OP1	2.28	0.49
49:XA:92:C:H2'	49:XA:93:G:H8	1.77	0.49
51:ZA:1259:A:H1'	51:ZA:1264:C:H42	1.77	0.49
56:EB:31:PRO:HG3	56:EB:43:PRO:HG3	1.94	0.49
85:HC:178:ILE:HB	85:HC:183:TYR:HB2	1.93	0.49
87:b:107:VAL:HG12	87:b:109:ALA:H	1.78	0.49
1:A:225:ILE:HD11	1:A:233:ARG:HG3	1.94	0.49
7:G:148:LEU:HA	7:G:271:LEU:HD21	1.93	0.49
22:V:81:ALA:HB2	22:V:87:LEU:HD23	1.94	0.49
44:SA:12:G:H22	44:SA:23:G:H1	1.59	0.49
48:WA:955:G:H2'	48:WA:956:G:H8	1.77	0.49
48:WA:4063:C:H2'	48:WA:4064:A:H8	1.78	0.49
51:ZA:1016:U:H5''	65:NB:14:SER:HB2	1.94	0.49
51:ZA:1613:G:OP1	70:SB:88:LYS:NZ	2.42	0.49
54:CB:109:ILE:HD11	54:CB:151:ILE:HD11	1.94	0.49
54:CB:168:GLY:N	54:CB:179:THR:O	2.36	0.49
59:HB:258:GLU:HG3	59:HB:286:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HB3	1:A:123:ARG:HB3	1.93	0.49
7:G:139:VAL:HG21	7:G:238:LYS:HE3	1.94	0.49
7:G:218:GLU:OE2	13:M:26:ARG:NH1	2.45	0.49
18:R:127:MET:HG2	19:S:153:PRO:HB2	1.94	0.49
48:WA:35:U:O2'	48:WA:1527:A:N1	2.43	0.49
51:ZA:220:U:H2'	51:ZA:221:A:H8	1.78	0.49
51:ZA:1126:G:OP1	52:AB:41:ARG:NH1	2.46	0.49
51:ZA:1568:C:H2'	51:ZA:1569:A:C8	2.48	0.49
65:NB:33:VAL:HG21	65:NB:66:VAL:HG11	1.93	0.49
13:M:9:GLU:HB2	34:HA:44:ILE:HG13	1.94	0.49
15:O:164:ARG:NH2	48:WA:1598:U:O2'	2.46	0.49
48:WA:162:A:H2'	48:WA:163:A:H8	1.77	0.49
48:WA:456:C:H2'	48:WA:457:G:C8	2.48	0.49
51:ZA:1113:A:H2'	51:ZA:1114:U:C6	2.47	0.49
54:CB:169:TYR:OH	54:CB:175:GLY:O	2.30	0.49
21:U:87:SER:HB3	22:V:19:ARG:HH21	1.78	0.49
30:DA:64:LYS:NZ	48:WA:2081:G:OP2	2.38	0.49
30:DA:124:ASN:N	30:DA:124:ASN:OD1	2.45	0.49
48:WA:1335:A:H2'	48:WA:1336:A:C8	2.48	0.49
48:WA:4262:U:H2'	48:WA:4263:C:H6	1.77	0.49
51:ZA:1598:G:OP1	77:ZB:80:ARG:NH1	2.45	0.49
52:AB:157:VAL:O	73:VB:65:SER:OG	2.30	0.49
56:EB:124:CYS:HB3	56:EB:141:THR:HB	1.94	0.49
59:HB:338:ILE:HG12	59:HB:363:VAL:HG11	1.94	0.49
1:A:47:ASP:N	1:A:47:ASP:OD1	2.46	0.49
1:A:215:ASN:ND2	48:WA:4548:A:N7	2.61	0.49
48:WA:2081:G:H2'	48:WA:2082:U:C6	2.48	0.49
51:ZA:916:A:C5	65:NB:73:ARG:HD3	2.48	0.49
53:BB:124:HIS:HA	53:BB:137:LEU:O	2.11	0.49
58:GB:20:ASP:OD1	58:GB:20:ASP:N	2.44	0.49
72:UB:81:GLN:OE1	72:UB:83:ARG:NH1	2.45	0.49
74:WB:42:MET:HE2	74:WB:49:GLU:HA	1.95	0.49
8:H:128:MET:HE3	8:H:157:SER:HB2	1.95	0.49
14:N:46:ASN:O	14:N:50:ASN:ND2	2.45	0.49
30:DA:109:LYS:NZ	30:DA:128:ARG:O	2.45	0.49
48:WA:1335:A:H2'	48:WA:1336:A:H8	1.78	0.49
48:WA:2545:A:H2	48:WA:2775:G:H22	1.60	0.49
48:WA:2904:G:N1	48:WA:3599:G:OP1	2.38	0.49
56:EB:45:ILE:HA	56:EB:61:VAL:HG11	1.95	0.49
66:OB:33:ILE:HD11	66:OB:119:LEU:HD21	1.94	0.49
85:HC:13:ILE:HD12	85:HC:136:HIS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:b:48:ARG:NH2	87:b:53:VAL:H	2.10	0.49
1:A:188:LYS:NZ	48:WA:2741:C:O2	2.45	0.49
9:I:152:LEU:HB3	9:I:165:ILE:HD12	1.95	0.49
48:WA:424:U:H2'	48:WA:425:U:C6	2.48	0.49
48:WA:2531:A:O2'	48:WA:2533:C:OP2	2.30	0.49
48:WA:4994:G:H2'	48:WA:4995:G:C8	2.48	0.49
51:ZA:68:A:OP2	58:GB:164:LYS:NZ	2.41	0.49
51:ZA:1711:U:H2'	51:ZA:1712:A:C8	2.47	0.49
51:ZA:1797:U:H2'	51:ZA:1798:C:C6	2.48	0.49
2:B:228:TYR:O	48:WA:2837:A:O2'	2.29	0.48
6:F:33:ARG:NE	48:WA:1442:U:OP2	2.46	0.48
42:PA:66:ARG:NH2	48:WA:478:G:OP1	2.45	0.48
48:WA:478:G:H2'	48:WA:479:G:C8	2.48	0.48
48:WA:1975:G:H3'	48:WA:1976:U:H2'	1.95	0.48
48:WA:3947:A:H2'	48:WA:3948:G:C8	2.47	0.48
51:ZA:1221:G:H2'	51:ZA:1222:G:C8	2.47	0.48
60:IB:119:LEU:HD11	60:IB:153:LYS:HG3	1.95	0.48
64:MB:26:LEU:HD22	64:MB:33:ARG:HH22	1.77	0.48
84:GC:91:ASP:OD2	84:GC:93:THR:OG1	2.26	0.48
85:HC:11:VAL:HA	85:HC:90:ILE:HG23	1.95	0.48
85:HC:154:LYS:HE2	95:HC:601:GTP:H1'	1.95	0.48
2:B:52:GLY:HA2	2:B:341:LYS:HE3	1.95	0.48
5:E:275:ARG:NH2	48:WA:4886:G:N7	2.59	0.48
7:G:126:ARG:NH1	7:G:294:VAL:O	2.42	0.48
15:O:147:GLN:NE2	15:O:176:GLU:OE2	2.46	0.48
23:W:65:ALA:HB2	33:GA:69:LEU:HD11	1.95	0.48
24:X:30:MET:HB3	24:X:101:PRO:HG2	1.95	0.48
48:WA:126:C:H2'	48:WA:127:G:H8	1.77	0.48
48:WA:1205:G:H2'	48:WA:1206:G:C8	2.45	0.48
48:WA:2446:U:O2'	50:YA:112:G:O2'	2.26	0.48
51:ZA:1203:G:H4'	54:CB:116:THR:HA	1.95	0.48
68:QB:84:LEU:HB3	68:QB:88:ARG:HD2	1.95	0.48
85:HC:364:HIS:NE2	85:HC:411:CYS:O	2.45	0.48
2:B:57:VAL:HG22	2:B:73:VAL:HG22	1.94	0.48
16:P:178:ARG:N	26:Z:51:GLY:HA2	2.28	0.48
20:T:84:LYS:NZ	48:WA:2624:G:OP2	2.44	0.48
40:NA:64:LYS:HD2	48:WA:4372:G:H5''	1.95	0.48
45:TA:23:A:H2'	45:TA:24:G:C8	2.48	0.48
48:WA:4956:G:H2'	48:WA:4957:A:H8	1.77	0.48
51:ZA:980:A:H2'	51:ZA:981:A:C8	2.48	0.48
59:HB:245:LYS:NZ	59:HB:278:LEU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:IB:81:VAL:HG22	60:IB:102:VAL:HG12	1.95	0.48
78:AC:46:GLU:HG3	78:AC:48:ALA:H	1.77	0.48
11:K:18:TRP:NE1	48:WA:1518:G:O2'	2.44	0.48
13:M:68:ARG:HA	13:M:98:LEU:HD21	1.94	0.48
27:AA:10:HIS:NE2	48:WA:1879:G:O6	2.45	0.48
48:WA:1935:G:H2'	48:WA:1936:A:C8	2.49	0.48
48:WA:4241:A:H2'	48:WA:4242:G:H8	1.78	0.48
54:CB:81:ILE:HG23	54:CB:86:LEU:HB2	1.95	0.48
64:MB:92:CYS:SG	64:MB:102:LYS:NZ	2.84	0.48
68:QB:78:LEU:HB3	68:QB:82:LEU:HD13	1.96	0.48
84:GC:32:LEU:HD11	84:GC:92:LEU:HD21	1.94	0.48
6:F:154:TYR:OH	6:F:187:GLU:OE2	2.30	0.48
48:WA:652:C:H2'	48:WA:653:G:H8	1.78	0.48
48:WA:989:C:H42	48:WA:1077:C:H42	1.60	0.48
48:WA:1384:G:H2'	48:WA:1385:G:H8	1.78	0.48
48:WA:1874:G:O2'	48:WA:4221:A:N3	2.43	0.48
25:Y:5:MET:O	25:Y:28:ASN:ND2	2.47	0.48
45:TA:23:A:H2'	45:TA:24:G:H8	1.79	0.48
48:WA:759:G:H2'	48:WA:760:G:H8	1.78	0.48
48:WA:1664:C:H2'	48:WA:1665:C:C6	2.49	0.48
48:WA:4063:C:H2'	48:WA:4064:A:C8	2.49	0.48
49:XA:110:G:H2'	49:XA:111:C:C6	2.48	0.48
51:ZA:544:G:H2'	51:ZA:545:A:H8	1.78	0.48
51:ZA:1171:G:O2'	51:ZA:1187:G:O6	2.28	0.48
56:EB:192:ILE:HG12	56:EB:243:GLY:HA3	1.96	0.48
68:QB:123:GLN:OE1	84:GC:60:ARG:NE	2.41	0.48
83:FC:141:CYS:SG	83:FC:142:GLY:N	2.86	0.48
84:GC:41:ILE:HD11	84:GC:55:PRO:HB3	1.95	0.48
5:E:184:LEU:O	48:WA:4885:C:N4	2.46	0.48
16:P:181:ARG:NH2	48:WA:1393:A:OP1	2.34	0.48
22:V:80:ARG:HH22	51:ZA:167:G:HO2'	1.62	0.48
22:V:110:ARG:HA	22:V:113:LYS:HG2	1.96	0.48
48:WA:129:C:H2'	48:WA:130:C:C6	2.48	0.48
48:WA:652:C:H2'	48:WA:653:G:C8	2.48	0.48
48:WA:759:G:H2'	48:WA:760:G:C8	2.48	0.48
48:WA:3734:A:H2'	48:WA:3735:A:C8	2.49	0.48
51:ZA:943:U:OP2	53:BB:216:LYS:NZ	2.46	0.48
51:ZA:1297:U:O4	67:PB:59:ARG:NH2	2.47	0.48
51:ZA:1433:C:H1'	51:ZA:1434:C:H5	1.78	0.48
51:ZA:1447:G:OP1	72:UB:87:ARG:NH2	2.46	0.48
56:EB:87:MET:HE1	56:EB:236:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:38:ARG:NH1	48:WA:2529:A:OP1	2.47	0.48
19:S:75:VAL:HG22	19:S:88:ARG:HG2	1.95	0.48
19:S:108:ARG:NH1	48:WA:1839:A:OP1	2.47	0.48
51:ZA:165:G:OP2	51:ZA:165:G:N2	2.35	0.48
51:ZA:1513:C:H2'	51:ZA:1514:G:C8	2.49	0.48
60:IB:80:ASP:OD1	60:IB:81:VAL:N	2.46	0.48
69:RB:76:GLU:HA	69:RB:79:GLU:HG2	1.96	0.48
80:CC:44:ARG:NH2	80:CC:63:ARG:O	2.46	0.48
2:B:66:LYS:NZ	21:U:127:ASP:OD2	2.44	0.48
9:I:21:ARG:O	9:I:24:ARG:NH2	2.47	0.48
18:R:174:THR:HG1	48:WA:4765:U:HO2'	1.59	0.48
33:GA:31:LEU:HB3	33:GA:47:ILE:HG22	1.94	0.48
48:WA:2779:G:H5''	48:WA:2780:G:H5'	1.96	0.48
76:YB:10:ARG:HG2	76:YB:11:LYS:HG3	1.96	0.48
43:RA:20:GLY:N	43:RA:54:LYS:O	2.38	0.48
48:WA:1446:G:H22	48:WA:2112:G:H22	1.62	0.48
48:WA:3912:C:H2'	48:WA:3913:C:C6	2.49	0.48
48:WA:4460:C:H2'	48:WA:4461:U:C6	2.49	0.48
51:ZA:379:C:O2	60:IB:5:ARG:NH1	2.46	0.48
51:ZA:1199:A:OP1	78:AC:2:THR:N	2.46	0.48
51:ZA:1568:C:O2	51:ZA:1627:C:O2'	2.30	0.48
51:ZA:1798:C:H2'	51:ZA:1799:G:O4'	2.14	0.48
61:JB:107:GLU:HA	61:JB:112:THR:HG21	1.95	0.48
2:B:189:THR:HG23	2:B:192:GLU:H	1.79	0.47
13:M:63:ARG:NH1	13:M:131:GLU:OE2	2.47	0.47
17:Q:108:ARG:NH2	48:WA:2901:C:OP1	2.41	0.47
29:CA:57:MET:HG2	29:CA:88:LEU:HD23	1.96	0.47
48:WA:4:G:H2'	48:WA:5:A:H8	1.79	0.47
48:WA:2260:C:H5'	48:WA:2261:G:C8	2.49	0.47
48:WA:2747:A:H2'	48:WA:2748:A:C8	2.48	0.47
51:ZA:931:C:H2'	51:ZA:932:G:C8	2.47	0.47
51:ZA:942:G:H2'	51:ZA:943:U:C6	2.48	0.47
51:ZA:1204:A:O2'	51:ZA:1700:C:OP2	2.28	0.47
57:FB:140:ASP:OD2	80:CC:44:ARG:NH1	2.41	0.47
62:KB:11:ILE:HD11	62:KB:45:VAL:HG22	1.96	0.47
67:PB:53:GLN:HB3	67:PB:83:MET:HE1	1.95	0.47
76:YB:108:LYS:O	76:YB:112:ASN:ND2	2.47	0.47
30:DA:100:ALA:O	30:DA:108:ARG:NH2	2.47	0.47
32:FA:25:THR:OG1	48:WA:2523:G:O3'	2.31	0.47
54:CB:200:ARG:O	61:JB:54:ARG:NH2	2.47	0.47
55:DB:175:VAL:HG22	55:DB:189:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:85:ARG:HG3	14:N:99:LEU:HD11	1.95	0.47
20:T:39:PHE:HZ	20:T:87:THR:HG22	1.79	0.47
45:TA:9:A:O2'	45:TA:10:G:N7	2.38	0.47
51:ZA:639:C:H2'	51:ZA:640:A:H8	1.80	0.47
51:ZA:1389:C:OP1	69:RB:43:SER:OG	2.25	0.47
60:IB:114:GLU:OE2	60:IB:123:ARG:NH1	2.48	0.47
74:WB:105:THR:HG23	74:WB:126:LEU:HD11	1.96	0.47
81:DC:5:GLN:O	81:DC:9:SER:OG	2.30	0.47
3:C:144:ILE:HG21	3:C:150:LEU:HD13	1.96	0.47
48:WA:961:A:H1'	48:WA:2078:G:H5''	1.97	0.47
48:WA:2506:C:H1'	48:WA:2507:C:H2'	1.95	0.47
48:WA:4262:U:H2'	48:WA:4263:C:C6	2.49	0.47
51:ZA:1033:G:N1	51:ZA:1080:A:O2'	2.34	0.47
51:ZA:1277:C:OP1	62:KB:51:SER:OG	2.30	0.47
58:GB:67:VAL:HB	58:GB:99:GLY:HA2	1.96	0.47
4:D:28:THR:O	48:WA:4282:A:N6	2.44	0.47
8:H:155:SER:OG	48:WA:4690:C:O2'	2.32	0.47
10:J:25:CYS:SG	48:WA:4254:C:N4	2.87	0.47
19:S:88:ARG:NH2	27:AA:30:GLU:OE2	2.48	0.47
44:SA:22:A:H2'	44:SA:23:G:C8	2.49	0.47
48:WA:1246:G:H2'	48:WA:1247:C:C6	2.50	0.47
48:WA:1560:A:H2'	48:WA:1561:G:H8	1.78	0.47
48:WA:3951:A:N7	48:WA:3952:U:N3	2.63	0.47
53:BB:179:ASN:HB3	53:BB:183:GLU:HB2	1.95	0.47
1:A:179:ILE:HG23	1:A:184:ARG:HB2	1.95	0.47
1:A:223:SER:HG	48:WA:3750:A:HO2'	1.63	0.47
2:B:122:TRP:CH2	2:B:127:LYS:HG2	2.50	0.47
45:TA:69:G:H2'	45:TA:70:G:H8	1.79	0.47
48:WA:991:C:H2'	48:WA:992:C:C6	2.49	0.47
48:WA:1434:G:O2'	48:WA:1454:A:N6	2.48	0.47
48:WA:1872:C:H2'	48:WA:1873:A:H8	1.80	0.47
48:WA:2726:G:O2'	48:WA:2728:G:OP2	2.31	0.47
48:WA:4324:G:N2	48:WA:4327:A:OP2	2.41	0.47
48:WA:4524:G:O2'	48:WA:4527:C:OP2	2.31	0.47
51:ZA:520:A:O2'	51:ZA:825:A:N3	2.45	0.47
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.97	0.47
4:D:139:PRO:HB3	48:WA:1822:U:H5'	1.96	0.47
5:E:189:LEU:N	5:E:253:GLN:OE1	2.47	0.47
8:H:128:MET:HE2	8:H:134:CYS:HB2	1.96	0.47
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.97	0.47
29:CA:37:GLY:O	29:CA:41:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:PA:90:LEU:HG	42:PA:111:ILE:HG23	1.96	0.47
48:WA:747:G:H1	48:WA:920:G:H22	1.62	0.47
48:WA:2813:G:N1	48:WA:2816:C:OP2	2.27	0.47
48:WA:4574:U:HO2'	48:WA:4575:G:H8	1.63	0.47
51:ZA:332:G:O6	58:GB:189:ARG:NH2	2.41	0.47
51:ZA:1221:G:H2'	51:ZA:1222:G:H8	1.80	0.47
51:ZA:1221:G:O2'	51:ZA:1676:U:O2	2.30	0.47
51:ZA:1466:G:OP2	69:RB:5:ARG:NH1	2.48	0.47
51:ZA:1491:G:H2'	51:ZA:1492:U:C6	2.49	0.47
51:ZA:1635:C:OP1	77:ZB:34:LYS:NZ	2.48	0.47
58:GB:2:LYS:HB3	58:GB:15:LEU:HD11	1.97	0.47
59:HB:383:ARG:NH1	74:WB:49:GLU:OE2	2.48	0.47
63:LB:93:LEU:HD21	75:XB:8:ARG:HD3	1.97	0.47
64:MB:58:GLU:HB2	64:MB:62:VAL:HG12	1.96	0.47
68:QB:157:LYS:HB2	68:QB:166:ARG:HH22	1.78	0.47
84:GC:18:VAL:O	84:GC:287:THR:OG1	2.32	0.47
85:HC:378:LYS:HB2	85:HC:391:PRO:HG3	1.95	0.47
48:WA:462:G:H2'	48:WA:463:A:C8	2.50	0.47
48:WA:2337:C:H2'	48:WA:2338:G:H8	1.79	0.47
51:ZA:1226:G:N1	51:ZA:1639:G:OP2	2.36	0.47
51:ZA:1285:G:H4'	64:MB:35:ILE:HD11	1.97	0.47
73:VB:32:ILE:HG12	73:VB:60:ARG:HD2	1.97	0.47
84:GC:40:ILE:HB	84:GC:59:LEU:HB2	1.96	0.47
6:F:222:LYS:HE3	48:WA:1909:A:H4'	1.96	0.47
20:T:27:HIS:HB3	20:T:114:TYR:HE1	1.80	0.47
21:U:87:SER:HA	21:U:97:TYR:HB3	1.96	0.47
30:DA:19:LYS:HG3	30:DA:33:ARG:HH12	1.80	0.47
51:ZA:1438:A:H2'	51:ZA:1439:A:C8	2.49	0.47
63:LB:65:ASN:O	63:LB:132:ARG:NH1	2.46	0.47
85:HC:178:ILE:HD12	85:HC:188:VAL:HG21	1.96	0.47
2:B:77:THR:HG21	2:B:337:VAL:HG22	1.96	0.47
31:EA:45:LYS:HD2	31:EA:105:LEU:HA	1.97	0.47
42:PA:65:LYS:O	42:PA:102:TYR:OH	2.27	0.47
51:ZA:563:G:O2'	51:ZA:564:A:H8	1.97	0.47
51:ZA:608:C:O4'	82:EC:131:ASN:ND2	2.48	0.47
51:ZA:629:A:O2'	51:ZA:631:U:OP1	2.33	0.47
51:ZA:1608:U:O4	51:ZA:1632:G:N2	2.48	0.47
52:AB:198:MET:HG2	52:AB:200:ASP:H	1.79	0.47
55:DB:210:VAL:O	55:DB:211:ARG:NH1	2.40	0.47
56:EB:43:PRO:HD2	56:EB:46:ILE:HD11	1.95	0.47
60:IB:26:LYS:O	60:IB:29:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:OB:145:GLY:O	78:AC:22:ARG:NH2	2.48	0.47
69:RB:95:ILE:HD11	69:RB:118:GLN:HB2	1.97	0.47
2:B:165:HIS:ND1	2:B:166:THR:O	2.46	0.46
6:F:181:TYR:CZ	6:F:202:GLU:HG2	2.50	0.46
18:R:1:MET:HE2	18:R:43:ARG:HG3	1.96	0.46
26:Z:7:LYS:NZ	48:WA:2286:G:OP1	2.38	0.46
48:WA:3882:G:H2'	48:WA:3883:G:C8	2.50	0.46
51:ZA:28:U:H2'	51:ZA:29:G:C8	2.49	0.46
51:ZA:115:U:H2'	51:ZA:116:U:C6	2.50	0.46
51:ZA:964:A:H2'	51:ZA:965:U:H6	1.80	0.46
51:ZA:1619:A:OP2	67:PB:47:ARG:NH1	2.48	0.46
51:ZA:1801:A:H2'	51:ZA:1802:C:C6	2.50	0.46
60:IB:125:LYS:HE2	60:IB:125:LYS:HB3	1.84	0.46
73:VB:21:ASN:HB3	74:WB:67:GLY:HA3	1.97	0.46
84:GC:33:SER:HB2	84:GC:41:ILE:HG22	1.97	0.46
48:WA:1550:G:O2'	48:WA:2814:A:N3	2.43	0.46
48:WA:1664:C:H2'	48:WA:1665:C:H6	1.80	0.46
48:WA:3912:C:H2'	48:WA:3913:C:H6	1.79	0.46
48:WA:4450:G:H5''	48:WA:4451:A:H5'	1.97	0.46
51:ZA:522:A:H5''	61:JB:145:PRO:HD2	1.96	0.46
51:ZA:1263:U:O2	81:DC:16:GLN:NE2	2.41	0.46
56:EB:44:LEU:HD21	56:EB:70:ILE:HG21	1.97	0.46
59:HB:248:LYS:HG2	59:HB:252:GLU:HB3	1.97	0.46
7:G:253:THR:OG1	48:WA:150:U:OP2	2.23	0.46
15:O:91:ARG:NH1	48:WA:423:G:OP1	2.48	0.46
18:R:34:ALA:HB1	18:R:39:VAL:HG23	1.98	0.46
24:X:27:ARG:HB2	24:X:75:ARG:CZ	2.45	0.46
37:KA:23:ILE:HG23	37:KA:38:ASN:HB2	1.96	0.46
48:WA:162:A:H2'	48:WA:163:A:C8	2.51	0.46
48:WA:1382:G:H4'	48:WA:1383:U:H5'	1.98	0.46
48:WA:3863:A:H2'	48:WA:3864:A:H8	1.80	0.46
48:WA:4275:A:H2'	48:WA:4276:A:C8	2.50	0.46
48:WA:4725:A:H2'	48:WA:4726:A:C8	2.50	0.46
48:WA:4969:A:H2'	48:WA:4970:A:H8	1.81	0.46
51:ZA:824:C:C2	61:JB:144:ILE:HG12	2.51	0.46
51:ZA:1299:A:O2'	51:ZA:1301:A:OP1	2.29	0.46
73:VB:11:LEU:HD23	73:VB:11:LEU:H	1.79	0.46
84:GC:124:SER:OG	84:GC:125:ARG:N	2.48	0.46
87:b:21:LEU:HD12	87:b:68:HIS:CD2	2.50	0.46
3:C:218:VAL:O	3:C:222:ARG:HB3	2.14	0.46
4:D:146:LEU:HD21	4:D:159:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:ARG:HD3	9:I:83:ASP:HB3	1.97	0.46
48:WA:62:A:N3	48:WA:77:U:O2'	2.36	0.46
48:WA:2541:C:H2'	48:WA:2542:C:C6	2.51	0.46
51:ZA:674:C:H2'	51:ZA:675:U:C6	2.50	0.46
7:G:213:ASP:OD1	7:G:213:ASP:N	2.48	0.46
29:CA:50:ARG:NH2	48:WA:2375:C:OP1	2.49	0.46
29:CA:79:ASN:ND2	48:WA:4638:U:O4	2.46	0.46
48:WA:3850:U:H2'	48:WA:3851:A:H8	1.80	0.46
48:WA:4737:G:H1	48:WA:4967:U:H3	1.64	0.46
51:ZA:4:C:O2'	61:JB:18:ARG:NH2	2.48	0.46
51:ZA:106:C:H2'	51:ZA:107:A:H8	1.79	0.46
51:ZA:184:G:H2'	51:ZA:185:G:C8	2.51	0.46
51:ZA:1650:A:H5''	68:QB:165:ALA:HB2	1.97	0.46
64:MB:57:ASP:OD1	64:MB:57:ASP:N	2.49	0.46
66:OB:67:ASP:OD1	66:OB:67:ASP:N	2.44	0.46
74:WB:112:ASP:OD1	74:WB:112:ASP:N	2.43	0.46
8:H:59:LYS:HE2	8:H:66:GLU:HB3	1.98	0.46
9:I:118:ALA:O	48:WA:1866:G:O2'	2.28	0.46
25:Y:41:ALA:HB2	25:Y:77:TYR:HE1	1.80	0.46
44:SA:50:U:O4	44:SA:64:G:O6	2.33	0.46
48:WA:2416:G:H2'	48:WA:2417:U:H6	1.80	0.46
48:WA:3738:A:H2'	48:WA:3739:A:H8	1.81	0.46
51:ZA:797:C:N3	51:ZA:798:G:N1	2.64	0.46
52:AB:85:ARG:NH2	69:RB:82:ASP:O	2.48	0.46
53:BB:175:GLU:O	53:BB:187:LYS:NZ	2.40	0.46
58:GB:57:ASP:OD1	58:GB:58:LYS:N	2.46	0.46
77:ZB:73:VAL:HG21	77:ZB:88:LEU:HD11	1.97	0.46
85:HC:132:GLN:HB3	85:HC:136:HIS:CE1	2.51	0.46
2:B:240:LEU:HB3	2:B:244:THR:HG21	1.97	0.46
5:E:49:ASN:OD1	5:E:49:ASN:N	2.49	0.46
15:O:47:ARG:NH2	15:O:176:GLU:OE1	2.48	0.46
27:AA:12:GLN:NE2	48:WA:1672:G:OP1	2.42	0.46
42:PA:2:SER:O	42:PA:6:GLN:HG2	2.16	0.46
44:SA:35:A:OP2	68:QB:172:ARG:NH1	2.48	0.46
48:WA:2641:U:H2'	48:WA:2696:G:N1	2.31	0.46
48:WA:3850:U:H2'	48:WA:3851:A:C8	2.51	0.46
51:ZA:24:C:OP1	61:JB:11:LYS:NZ	2.31	0.46
51:ZA:880:G:H2'	51:ZA:881:G:H8	1.80	0.46
58:GB:121:ILE:N	58:GB:125:THR:OG1	2.46	0.46
59:HB:318:VAL:HG23	59:HB:330:VAL:HG13	1.98	0.46
68:QB:88:ARG:HD3	68:QB:134:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:ARG:NE	49:XA:7:G:OP1	2.39	0.46
7:G:210:ILE:HA	7:G:254:THR:HG22	1.98	0.46
16:P:57:ASN:O	16:P:143:ARG:NE	2.49	0.46
48:WA:2482:G:H2'	48:WA:2483:G:C8	2.51	0.46
48:WA:4090:C:H2'	48:WA:4091:G:H8	1.81	0.46
48:WA:4461:U:H2'	48:WA:4462:U:C6	2.51	0.46
48:WA:5008:U:H4'	48:WA:5009:A:H5'	1.97	0.46
51:ZA:1098:C:H2'	51:ZA:1099:G:C8	2.50	0.46
64:MB:38:ALA:HA	64:MB:110:VAL:HG11	1.97	0.46
68:QB:122:TYR:HA	68:QB:126:VAL:HG23	1.97	0.46
10:J:46:GLN:NE2	10:J:73:THR:O	2.46	0.46
23:W:135:LYS:NZ	48:WA:2438:U:OP2	2.49	0.46
25:Y:68:ILE:O	25:Y:115:LYS:NZ	2.49	0.46
29:CA:114:PHE:HA	29:CA:117:LEU:HD22	1.97	0.46
42:PA:49:VAL:HG11	42:PA:97:ILE:HD11	1.98	0.46
51:ZA:73:C:H2'	51:ZA:74:G:O4'	2.16	0.46
51:ZA:948:C:H2'	51:ZA:949:G:H8	1.81	0.46
51:ZA:1236:G:O2'	67:PB:131:PRO:O	2.23	0.46
51:ZA:1498:A:P	55:DB:65:ARG:HH22	2.38	0.46
71:TB:115:LYS:HE2	71:TB:121:ARG:HH12	1.81	0.46
2:B:384:GLU:OE2	22:V:14:TYR:OH	2.26	0.46
5:E:123:ASP:OD2	42:PA:112:ARG:NH2	2.49	0.46
12:L:11:ARG:HD3	12:L:57:LEU:HB3	1.97	0.46
27:AA:11:ASN:ND2	48:WA:1671:A:OP1	2.45	0.46
48:WA:86:U:H2'	48:WA:87:A:C8	2.51	0.46
48:WA:968:G:H2'	48:WA:969:A:C8	2.51	0.46
48:WA:2001:A:H2'	48:WA:2002:G:C4	2.51	0.46
48:WA:4350:A:O2'	48:WA:4352:C:OP2	2.30	0.46
51:ZA:996:A:H2'	51:ZA:997:A:C8	2.50	0.46
51:ZA:1160:U:O4	75:XB:3:LYS:NZ	2.41	0.46
51:ZA:1395:C:O2'	51:ZA:1396:A:H5''	2.16	0.46
62:KB:6:LYS:HE3	62:KB:6:LYS:HB3	1.77	0.46
2:B:252:ALA:HB3	48:WA:4459:U:H1'	1.98	0.45
4:D:215:ASP:OD1	4:D:215:ASP:N	2.49	0.45
20:T:66:SER:OG	20:T:67:LYS:N	2.49	0.45
26:Z:35:ALA:HB2	48:WA:38:A:H5''	1.99	0.45
42:PA:19:LYS:HB2	48:WA:2339:C:H4'	1.97	0.45
48:WA:3925:A:H2'	48:WA:3926:C:C6	2.50	0.45
48:WA:4596:U:H2'	48:WA:4597:G:C8	2.51	0.45
48:WA:4899:G:H1'	48:WA:4929:G:H22	1.80	0.45
51:ZA:570:C:O2'	76:YB:34:THR:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1217:A:H2'	51:ZA:1218:C:C6	2.51	0.45
52:AB:184:ARG:HD3	52:AB:191:ARG:HG2	1.98	0.45
76:YB:76:TYR:OH	76:YB:86:GLU:OE1	2.23	0.45
80:CC:12:ALA:HB1	80:CC:32:VAL:HB	1.98	0.45
4:D:146:LEU:HD22	4:D:163:LEU:HD13	1.98	0.45
5:E:186:ARG:HG3	48:WA:4940:A:H5'	1.98	0.45
34:HA:70:LEU:HD13	34:HA:87:ARG:HE	1.80	0.45
48:WA:1560:A:H2'	48:WA:1561:G:C8	2.51	0.45
48:WA:1820:G:OP2	48:WA:1820:G:N2	2.39	0.45
48:WA:2745:A:H2'	48:WA:2746:A:C8	2.51	0.45
48:WA:4090:C:H2'	48:WA:4091:G:C8	2.51	0.45
51:ZA:106:C:H2'	51:ZA:107:A:C8	2.52	0.45
51:ZA:155:G:H2'	51:ZA:156:G:H8	1.79	0.45
51:ZA:1277:C:H2'	51:ZA:1278:A:H8	1.81	0.45
56:EB:126:VAL:HG12	56:EB:158:ASP:O	2.17	0.45
68:QB:35:SER:HA	68:QB:51:CYS:O	2.17	0.45
76:YB:29:HIS:ND1	76:YB:29:HIS:O	2.50	0.45
76:YB:81:TYR:HD1	76:YB:84:LYS:HE2	1.81	0.45
2:B:55:HIS:HB2	2:B:369:ASP:HB3	1.98	0.45
2:B:252:ALA:HB1	48:WA:4526:G:C2	2.51	0.45
5:E:136:PHE:O	5:E:141:ARG:NH2	2.50	0.45
48:WA:4956:G:H2'	48:WA:4957:A:C8	2.51	0.45
51:ZA:17:C:H2'	51:ZA:18:C:C6	2.51	0.45
51:ZA:649:U:H2'	51:ZA:650:A:H8	1.81	0.45
76:YB:5:VAL:O	76:YB:43:LYS:NZ	2.40	0.45
85:HC:165:LYS:HE2	85:HC:165:LYS:HB3	1.83	0.45
85:HC:364:HIS:ND1	85:HC:364:HIS:O	2.50	0.45
1:A:194:ASN:HB2	48:WA:1541:G:H4'	1.99	0.45
48:WA:1082:C:H2'	48:WA:1083:C:C6	2.52	0.45
48:WA:2114:G:H2'	48:WA:2115:G:C8	2.52	0.45
51:ZA:5:U:H2'	51:ZA:6:G:C8	2.50	0.45
51:ZA:1144:A:H2'	51:ZA:1145:A:C8	2.51	0.45
51:ZA:1736:G:H2'	51:ZA:1737:G:C8	2.51	0.45
62:KB:86:PRO:HD2	62:KB:89:ILE:HD13	1.99	0.45
1:A:243:THR:HB	48:WA:3750:A:H5''	1.98	0.45
20:T:44:GLN:HG2	20:T:63:LEU:HD22	1.99	0.45
23:W:120:ASP:N	23:W:120:ASP:OD1	2.43	0.45
43:RA:109:ILE:HD11	43:RA:143:VAL:HG21	1.99	0.45
48:WA:180:C:H2'	48:WA:181:C:C6	2.52	0.45
48:WA:1886:C:H2'	48:WA:1887:G:H8	1.81	0.45
48:WA:2522:C:H2'	48:WA:2523:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:2864:G:N3	48:WA:3626:A:H2'	2.31	0.45
48:WA:2871:U:O2'	48:WA:2883:A:N7	2.43	0.45
48:WA:3870:G:H22	48:WA:3902:G:H1'	1.80	0.45
48:WA:4580:G:H2'	48:WA:4581:U:C6	2.52	0.45
48:WA:5004:U:H2'	48:WA:5005:U:C6	2.52	0.45
51:ZA:311:C:H5''	51:ZA:312:G:H5''	1.99	0.45
51:ZA:1486:A:O3'	54:CB:121:ARG:NH2	2.49	0.45
51:ZA:1712:A:H2'	51:ZA:1713:C:C6	2.51	0.45
84:GC:254:PRO:HB3	84:GC:283:PRO:HB2	1.98	0.45
11:K:141:ALA:HA	11:K:144:LEU:HB2	1.97	0.45
13:M:14:LYS:HE2	48:WA:280:G:H5''	1.98	0.45
16:P:62:SER:OG	48:WA:1504:G:OP2	2.27	0.45
24:X:11:ARG:HG3	48:WA:229:G:H5''	1.98	0.45
33:GA:96:ASN:N	33:GA:96:ASN:OD1	2.48	0.45
48:WA:20:U:H3'	48:WA:21:G:H8	1.81	0.45
48:WA:661:G:H2'	48:WA:662:C:C6	2.51	0.45
48:WA:1414:G:H2'	48:WA:1415:C:C6	2.52	0.45
48:WA:2902:U:H2'	48:WA:2903:G:C8	2.52	0.45
48:WA:3709:U:H2'	48:WA:3710:C:C6	2.52	0.45
56:EB:11:ARG:HA	56:EB:28:ALA:HB2	1.99	0.45
84:GC:214:GLY:HA2	84:GC:236:ILE:HG13	1.98	0.45
4:D:37:VAL:HG12	4:D:50:ARG:HD3	1.99	0.45
7:G:106:ARG:NH2	48:WA:4165:U:OP2	2.50	0.45
8:H:92:MET:HE2	8:H:179:ILE:HG22	1.98	0.45
11:K:48:PRO:HG3	33:GA:118:LYS:HE3	1.99	0.45
16:P:173:LYS:NZ	48:WA:88:A:N7	2.62	0.45
20:T:113:ARG:NH2	48:WA:2704:C:O3'	2.48	0.45
24:X:132:LYS:NZ	48:WA:246:G:O3'	2.49	0.45
46:UA:37:A:H2'	46:UA:38:C:C6	2.52	0.45
48:WA:137:G:H2'	48:WA:138:G:H8	1.82	0.45
48:WA:417:G:H1'	50:YA:17:A:H61	1.82	0.45
51:ZA:126:G:H5''	58:GB:195:LYS:HD3	1.99	0.45
51:ZA:307:G:H1'	60:IB:45:THR:HG22	1.98	0.45
52:AB:76:VAL:HG12	52:AB:123:VAL:HB	1.98	0.45
55:DB:60:ASN:OD1	55:DB:72:TYR:OH	2.27	0.45
57:FB:125:SER:HA	57:FB:138:ALA:HA	1.98	0.45
77:ZB:92:LEU:HD22	77:ZB:109:TYR:HE1	1.81	0.45
85:HC:363:CYS:HB3	85:HC:424:PHE:HB3	1.99	0.45
30:DA:89:LEU:HD13	30:DA:118:LEU:HD22	1.98	0.45
48:WA:407:A:O2'	48:WA:410:A:OP1	2.32	0.45
48:WA:2364:U:H2'	48:WA:2365:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:4323:U:H2'	48:WA:4324:G:C8	2.52	0.45
51:ZA:322:C:H3'	51:ZA:323:C:H5''	1.99	0.45
51:ZA:639:C:H2'	51:ZA:640:A:C8	2.52	0.45
51:ZA:848:U:H2'	51:ZA:849:A:H8	1.81	0.45
51:ZA:1693:G:H21	51:ZA:1834:A:H8	1.64	0.45
54:CB:196:ILE:HB	54:CB:223:TYR:HB2	1.98	0.45
55:DB:113:LYS:HZ3	62:KB:21:MET:HA	1.82	0.45
58:GB:54:GLY:O	58:GB:110:ASN:ND2	2.49	0.45
67:PB:108:LYS:HB3	67:PB:111:MET:HG3	1.99	0.45
1:A:178:PRO:HD2	41:OA:26:VAL:HG22	1.99	0.45
3:C:207:PRO:HB3	3:C:249:PHE:CD2	2.52	0.45
14:N:10:ASP:HB2	14:N:117:ARG:HG3	1.99	0.45
17:Q:105:LEU:HD13	17:Q:135:LYS:HE3	1.99	0.45
45:TA:43:A:H2'	45:TA:44:G:H8	1.82	0.45
45:TA:69:G:H2'	45:TA:70:G:C8	2.52	0.45
48:WA:223:G:H4'	48:WA:225:G:N7	2.32	0.45
48:WA:416:U:H4'	48:WA:2332:G:H4'	1.99	0.45
48:WA:1944:A:H2'	48:WA:1945:A:H8	1.81	0.45
48:WA:2494:C:H2'	48:WA:2495:G:C8	2.52	0.45
51:ZA:1598:G:H3'	77:ZB:80:ARG:HD2	1.98	0.45
58:GB:39:ASP:N	58:GB:39:ASP:OD1	2.50	0.45
64:MB:41:ALA:HA	64:MB:45:ARG:HD3	1.97	0.45
72:UB:100:GLN:O	72:UB:104:ILE:HG13	2.17	0.45
74:WB:27:ILE:HG13	74:WB:61:ILE:HB	1.98	0.45
1:A:102:LEU:HB2	1:A:107:MET:HE3	1.98	0.45
4:D:16:TYR:O	49:XA:11:A:N6	2.50	0.45
32:FA:6:THR:HG22	48:WA:2402:G:H21	1.82	0.45
43:RA:58:ILE:HD11	43:RA:75:PRO:HA	1.99	0.45
48:WA:23:C:H2'	48:WA:24:G:O4'	2.17	0.45
48:WA:1496:U:H2'	48:WA:1497:G:C8	2.52	0.45
48:WA:1751:A:H2'	48:WA:1752:G:C8	2.52	0.45
48:WA:2469:U:H4'	48:WA:2470:U:H5'	1.99	0.45
48:WA:4586:A:H2'	48:WA:4587:U:O4'	2.17	0.45
14:N:68:ARG:NH2	48:WA:4566:A:OP1	2.50	0.44
37:KA:2:SER:OG	48:WA:2406:A:OP2	2.34	0.44
48:WA:3913:C:H2'	48:WA:3914:U:H6	1.81	0.44
51:ZA:1010:G:H2'	51:ZA:1011:A:C8	2.52	0.44
51:ZA:1203:G:H2'	51:ZA:1204:A:H8	1.82	0.44
51:ZA:1411:G:OP1	51:ZA:1423:C:N4	2.50	0.44
63:LB:59:LYS:HD3	63:LB:134:LEU:HB3	1.98	0.44
72:UB:94:PRO:HD2	72:UB:97:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:GC:35:SER:OG	84:GC:36:ARG:N	2.50	0.44
1:A:152:SER:OG	48:WA:3663:G:N7	2.48	0.44
3:C:343:GLN:HG2	48:WA:725:C:H1'	2.00	0.44
5:E:96:THR:HG22	5:E:109:VAL:HG22	1.99	0.44
24:X:59:ARG:HD2	48:WA:209:U:H5'	1.98	0.44
31:EA:68:ARG:NH1	48:WA:442:G:OP1	2.46	0.44
43:RA:75:PRO:HB2	43:RA:80:LEU:HG	1.98	0.44
48:WA:1505:A:H1'	48:WA:1506:G:C8	2.53	0.44
48:WA:1826:G:H2'	48:WA:1827:A:C8	2.53	0.44
48:WA:2320:G:N2	48:WA:2323:G:OP2	2.40	0.44
48:WA:2734:G:H2'	48:WA:2735:C:C6	2.53	0.44
48:WA:3724:G:H2'	48:WA:3725:A:C8	2.51	0.44
48:WA:3954:A:O2'	48:WA:4063:C:O2	2.32	0.44
48:WA:5036:A:H2'	48:WA:5037:U:O4'	2.16	0.44
59:HB:401:GLN:O	59:HB:405:GLU:HB3	2.17	0.44
85:HC:63:LEU:HB3	85:HC:66:GLU:HB2	1.99	0.44
87:b:112:ARG:HE	87:b:121:VAL:HG11	1.82	0.44
2:B:331:VAL:HG21	2:B:347:LEU:HD21	2.00	0.44
4:D:156:GLY:HA2	4:D:181:PRO:HD3	1.99	0.44
30:DA:36:ARG:HA	30:DA:36:ARG:HD3	1.85	0.44
30:DA:44:ARG:NH2	48:WA:1314:A:O2'	2.51	0.44
38:LA:85:ARG:HG3	38:LA:86:LYS:HD2	1.97	0.44
42:PA:35:ARG:NH2	48:WA:2267:G:OP1	2.43	0.44
48:WA:164:G:H2'	48:WA:165:A:H8	1.82	0.44
48:WA:262:G:H2'	48:WA:263:G:C8	2.51	0.44
48:WA:4480:G:O2'	48:WA:4604:A:N1	2.46	0.44
60:IB:67:TRP:NE1	60:IB:191:GLU:OE2	2.49	0.44
64:MB:41:ALA:HA	64:MB:45:ARG:HB2	1.98	0.44
70:SB:101:ASN:O	70:SB:105:ASN:ND2	2.35	0.44
3:C:159:GLU:HA	3:C:217:ILE:HB	1.99	0.44
25:Y:46:ILE:HG23	25:Y:68:ILE:HG23	1.99	0.44
30:DA:48:ARG:O	48:WA:1885:G:O2'	2.27	0.44
31:EA:36:ARG:HG3	31:EA:80:ASN:HA	1.99	0.44
48:WA:268:G:H2'	48:WA:269:G:H8	1.83	0.44
48:WA:912:G:H2'	48:WA:913:U:H6	1.83	0.44
48:WA:1808:G:H2'	48:WA:1809:C:H6	1.83	0.44
48:WA:3699:U:H5''	48:WA:3700:G:H5'	1.99	0.44
48:WA:3892:A:N6	48:WA:4572:G:O2'	2.48	0.44
48:WA:4305:C:H2'	48:WA:4307:G:C8	2.53	0.44
48:WA:4950:C:OP2	48:WA:4951:G:O2'	2.24	0.44
48:WA:4969:A:H2'	48:WA:4970:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1201:U:H2'	51:ZA:1202:U:C6	2.51	0.44
73:VB:10:ASP:N	73:VB:10:ASP:OD1	2.48	0.44
4:D:136:ASP:OD1	4:D:136:ASP:N	2.50	0.44
9:I:35:ASP:HB2	9:I:86:HIS:HE2	1.81	0.44
11:K:62:PRO:O	48:WA:71:C:H1'	2.18	0.44
48:WA:761:G:H2'	48:WA:762:G:H8	1.83	0.44
48:WA:3691:G:O2'	48:WA:3820:U:OP2	2.30	0.44
48:WA:4095:G:H1	48:WA:4117:G:H1	1.65	0.44
48:WA:4639:G:H2'	48:WA:4640:U:C6	2.52	0.44
51:ZA:155:G:H2'	51:ZA:156:G:C8	2.52	0.44
51:ZA:388:U:H2'	51:ZA:389:A:C8	2.53	0.44
51:ZA:1605:G:H22	51:ZA:1635:C:H42	1.65	0.44
56:EB:40:GLU:OE1	56:EB:103:TYR:OH	2.32	0.44
69:RB:60:ARG:HD2	69:RB:63:ARG:HH21	1.81	0.44
44:SA:12:G:H1	44:SA:23:G:H1	1.65	0.44
48:WA:1260:G:H3'	48:WA:1261:G:H8	1.82	0.44
50:YA:67:U:H2'	50:YA:68:G:C8	2.51	0.44
51:ZA:689:U:H2'	51:ZA:690:G:C8	2.53	0.44
51:ZA:1010:G:H2'	51:ZA:1011:A:H8	1.82	0.44
51:ZA:1597:C:H4'	51:ZA:1603:G:O6	2.17	0.44
51:ZA:1631:U:O4	51:ZA:1632:G:N1	2.50	0.44
56:EB:175:PHE:HE2	56:EB:198:ARG:HD2	1.83	0.44
67:PB:17:TYR:HB3	67:PB:25:LEU:HD11	1.98	0.44
87:b:143:ILE:HD11	87:b:219:VAL:HB	1.99	0.44
12:L:63:LYS:HE2	12:L:63:LYS:HB2	1.87	0.44
48:WA:1446:G:H22	48:WA:2112:G:N2	2.16	0.44
48:WA:2523:G:H2'	48:WA:2524:G:H8	1.83	0.44
48:WA:2760:G:H2'	48:WA:2761:G:C8	2.53	0.44
48:WA:3879:A:N3	48:WA:4403:G:O2'	2.35	0.44
48:WA:5032:U:H2'	48:WA:5033:G:H8	1.82	0.44
51:ZA:388:U:H2'	51:ZA:389:A:H8	1.82	0.44
51:ZA:913:A:N6	59:HB:357:SER:O	2.48	0.44
51:ZA:1395:C:O2'	51:ZA:1396:A:N3	2.38	0.44
51:ZA:1862:G:O2'	78:AC:5:ARG:NH2	2.49	0.44
52:AB:51:LEU:HD13	52:AB:51:LEU:HA	1.88	0.44
56:EB:141:THR:OG1	56:EB:143:ASP:OD1	2.24	0.44
57:FB:176:GLU:OE2	57:FB:187:SER:OG	2.30	0.44
58:GB:7:PHE:HB3	58:GB:10:THR:HG22	2.00	0.44
70:SB:60:THR:OG1	70:SB:62:ASP:OD1	2.30	0.44
85:HC:193:ILE:HD13	85:HC:228:LEU:HD22	2.00	0.44
85:HC:205:SER:HB2	85:HC:208:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:NH2	1:A:243:THR:O	2.50	0.44
24:X:82:ILE:HD12	24:X:85:VAL:HG21	2.00	0.44
25:Y:51:ARG:HB2	25:Y:65:ARG:HE	1.83	0.44
44:SA:21:A:O2'	44:SA:22:A:O5'	2.32	0.44
48:WA:1095:G:H2'	48:WA:1096:G:H8	1.83	0.44
48:WA:1775:U:H2'	48:WA:1776:C:C6	2.53	0.44
48:WA:1980:C:H2'	48:WA:1981:A:O4'	2.18	0.44
48:WA:3643:U:H5	48:WA:3648:A:N7	2.15	0.44
51:ZA:1101:U:H2'	51:ZA:1102:G:C8	2.53	0.44
51:ZA:1401:A:H4'	72:UB:52:GLY:HA3	1.99	0.44
51:ZA:1529:C:O2'	71:TB:87:VAL:O	2.31	0.44
51:ZA:1541:G:OP1	71:TB:56:ARG:NE	2.47	0.44
57:FB:16:ASP:OD1	57:FB:16:ASP:N	2.51	0.44
84:GC:286:CYS:HA	84:GC:302:TYR:HA	2.00	0.44
19:S:91:VAL:HB	19:S:96:ILE:HD11	2.00	0.44
30:DA:104:SER:OG	30:DA:105:SER:N	2.51	0.44
40:NA:4:VAL:O	40:NA:94:GLY:N	2.46	0.44
45:TA:22:G:H2'	45:TA:23:A:C8	2.51	0.44
48:WA:469:C:H2'	48:WA:470:A:H8	1.83	0.44
48:WA:1859:C:H2'	48:WA:1860:A:C8	2.52	0.44
48:WA:3734:A:H2'	48:WA:3735:A:H8	1.82	0.44
48:WA:3863:A:H2'	48:WA:3864:A:C8	2.53	0.44
49:XA:92:C:H2'	49:XA:93:G:C8	2.53	0.44
51:ZA:375:U:H2'	51:ZA:376:A:C8	2.53	0.44
54:CB:202:THR:HA	61:JB:54:ARG:HH12	1.82	0.44
63:LB:126:VAL:HG22	63:LB:145:VAL:HG22	2.00	0.44
64:MB:36:ARG:NH2	83:FC:129:GLY:O	2.51	0.44
65:NB:136:PRO:HG2	65:NB:139:TRP:HB2	1.99	0.44
66:OB:149:ARG:HH12	66:OB:151:LEU:HD13	1.82	0.44
16:P:179:GLY:H	26:Z:51:GLY:HA2	1.83	0.43
21:U:41:SER:OG	48:WA:4509:A:O2'	2.33	0.43
21:U:48:ARG:HB3	21:U:51:ARG:HE	1.83	0.43
25:Y:67:LYS:HD3	25:Y:67:LYS:HA	1.85	0.43
28:BA:77:ASN:H	28:BA:80:GLU:HG3	1.83	0.43
34:HA:66:ASP:OD1	34:HA:66:ASP:N	2.48	0.43
34:HA:76:ARG:HA	34:HA:76:ARG:HD2	1.81	0.43
43:RA:124:GLU:OE2	43:RA:126:SER:OG	2.35	0.43
46:UA:76:A:OP2	85:HC:296:HIS:NE2	2.45	0.43
48:WA:1962:A:H1'	87:b:14:PHE:HZ	1.83	0.43
48:WA:2559:G:H1	48:WA:2572:U:H3	1.64	0.43
51:ZA:15:U:H2'	51:ZA:16:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:527:C:H2'	51:ZA:528:A:H8	1.83	0.43
51:ZA:929:G:H2'	51:ZA:930:C:O4'	2.18	0.43
55:DB:234:GLY:HA3	55:DB:239:LYS:HG2	2.00	0.43
59:HB:246:ILE:HG12	59:HB:262:SER:HB3	2.00	0.43
59:HB:378:VAL:HG11	59:HB:431:GLN:HG3	1.99	0.43
70:SB:120:HIS:CE1	70:SB:124:ARG:HD2	2.53	0.43
78:AC:11:ALA:HB3	78:AC:33:ASP:HB2	2.00	0.43
85:HC:75:ILE:HB	85:HC:90:ILE:HD11	2.00	0.43
4:D:286:SER:OG	48:WA:1186:C:OP2	2.33	0.43
10:J:136:ARG:HG3	10:J:157:ILE:HD11	1.99	0.43
25:Y:42:LEU:HD21	25:Y:96:VAL:HG12	2.00	0.43
26:Z:125:LYS:HG2	26:Z:145:VAL:HB	1.99	0.43
48:WA:989:C:N4	48:WA:1077:C:H42	2.16	0.43
48:WA:1599:G:O2'	48:WA:1600:C:H3'	2.18	0.43
50:YA:5:U:H2'	50:YA:6:C:H6	1.83	0.43
51:ZA:1277:C:H2'	51:ZA:1278:A:C8	2.53	0.43
51:ZA:1628:C:H2'	51:ZA:1629:C:C6	2.54	0.43
56:EB:55:ALA:HB1	56:EB:60:GLU:HB2	1.99	0.43
65:NB:24:THR:O	65:NB:27:LYS:NZ	2.43	0.43
87:b:57:LYS:HG2	87:b:60:MET:H	1.83	0.43
3:C:140:LYS:HE3	3:C:245:HIS:HB2	2.00	0.43
42:PA:38:PHE:O	42:PA:45:HIS:NE2	2.36	0.43
43:RA:141:CYS:SG	43:RA:142:ASN:N	2.91	0.43
46:UA:27:U:H2'	46:UA:28:U:C6	2.53	0.43
48:WA:919:A:H2'	48:WA:920:G:H8	1.83	0.43
48:WA:1394:A:H2'	48:WA:1395:G:C8	2.53	0.43
48:WA:2492:U:H3'	48:WA:2493:C:C6	2.53	0.43
48:WA:2609:C:H2'	48:WA:2610:G:H8	1.83	0.43
48:WA:3719:A:H2'	48:WA:3720:A:H8	1.80	0.43
51:ZA:49:C:H2'	51:ZA:472:C:H41	1.83	0.43
51:ZA:1568:C:OP1	71:TB:96:SER:OG	2.28	0.43
51:ZA:1778:C:H2'	51:ZA:1779:G:C8	2.53	0.43
8:H:115:ARG:HE	8:H:115:ARG:HB2	1.66	0.43
37:KA:21:ARG:NH1	50:YA:52:A:OP1	2.51	0.43
44:SA:9:A:O2'	44:SA:10:G:N7	2.47	0.43
46:UA:55:U:H2'	46:UA:57:G:N7	2.33	0.43
48:WA:675:G:H2'	48:WA:676:C:C6	2.53	0.43
48:WA:1820:G:O2'	48:WA:1821:G:OP1	2.32	0.43
48:WA:2377:A:H2'	48:WA:2378:A:C8	2.52	0.43
48:WA:2544:G:H2'	48:WA:2545:A:C8	2.53	0.43
48:WA:3872:C:H2'	48:WA:3873:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AB:102:ARG:HA	52:AB:102:ARG:HD2	1.71	0.43
66:OB:54:CYS:HB2	66:OB:84:ARG:HG2	2.00	0.43
84:GC:45:LEU:HB3	84:GC:47:ARG:HD3	1.99	0.43
10:J:151:ILE:O	49:XA:55:A:O2'	2.28	0.43
25:Y:47:ASP:OD2	25:Y:69:LYS:NZ	2.49	0.43
40:NA:19:GLN:NE2	40:NA:72:CYS:SG	2.92	0.43
48:WA:422:C:H2'	48:WA:423:G:H8	1.83	0.43
48:WA:2081:G:H2'	48:WA:2082:U:H6	1.81	0.43
51:ZA:383:G:O2'	63:LB:133:PRO:O	2.36	0.43
51:ZA:1198:G:H2'	51:ZA:1199:A:C8	2.54	0.43
68:QB:142:ASP:OD2	68:QB:144:THR:OG1	2.34	0.43
75:XB:84:PHE:CE2	75:XB:86:PRO:HA	2.53	0.43
2:B:261:ARG:HB2	14:N:64:THR:HG21	2.01	0.43
35:IA:20:ARG:NH1	35:IA:39:TYR:OH	2.52	0.43
48:WA:1657:C:O2	48:WA:4392:A:O2'	2.37	0.43
48:WA:4682:G:H2'	48:WA:4683:A:C8	2.53	0.43
51:ZA:496:C:H2'	51:ZA:497:C:H6	1.84	0.43
51:ZA:656:G:H5'	51:ZA:662:G:N2	2.33	0.43
60:IB:162:LEU:HD11	60:IB:191:GLU:HG2	1.99	0.43
85:HC:282:PRO:HG2	85:HC:324:ASN:HD22	1.83	0.43
4:D:53:VAL:HB	4:D:159:VAL:HG23	2.01	0.43
9:I:158:LYS:NZ	48:WA:4431:C:N3	2.65	0.43
16:P:122:THR:OG1	16:P:124:ASP:OD1	2.32	0.43
16:P:172:ARG:HD2	26:Z:57:GLY:HA3	2.00	0.43
19:S:17:ARG:HD3	19:S:47:THR:HG23	2.01	0.43
44:SA:2:U:HO2'	48:WA:4202:G:HO2'	1.63	0.43
48:WA:1806:A:H4'	48:WA:1807:A:O5'	2.19	0.43
50:YA:64:U:H2'	50:YA:65:A:H8	1.83	0.43
51:ZA:223:C:H2'	51:ZA:224:A:C8	2.54	0.43
51:ZA:371:A:OP2	60:IB:10:LYS:HB2	2.18	0.43
51:ZA:1293:A:N6	51:ZA:1294:G:O6	2.52	0.43
51:ZA:1854:U:H2'	51:ZA:1855:G:H8	1.84	0.43
56:EB:212:ASP:OD1	56:EB:213:ALA:N	2.52	0.43
68:QB:68:ILE:HG22	68:QB:70:PRO:HD2	2.01	0.43
7:G:116:LEU:HD11	13:M:29:GLN:HG3	2.01	0.43
27:AA:95:ARG:NH1	48:WA:1267:G:OP2	2.46	0.43
45:TA:43:A:H2'	45:TA:44:G:C8	2.54	0.43
48:WA:926:C:O2'	48:WA:927:C:O4'	2.35	0.43
48:WA:3615:U:O2'	48:WA:5037:U:O2'	2.34	0.43
48:WA:4100:A:H61	48:WA:4113:U:H3	1.66	0.43
48:WA:4509:A:H2'	48:WA:4510:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:29:G:H2'	51:ZA:30:C:C6	2.54	0.43
51:ZA:220:U:H2'	51:ZA:221:A:C8	2.53	0.43
51:ZA:744:G:H2'	51:ZA:745:C:C6	2.53	0.43
51:ZA:1406:G:H2'	51:ZA:1407:U:C6	2.54	0.43
13:M:116:LEU:HD22	13:M:135:ILE:HD11	1.99	0.43
19:S:2:THR:N	48:WA:4222:A:OP2	2.51	0.43
26:Z:90:ALA:HB3	26:Z:120:GLN:HE21	1.83	0.43
48:WA:93:G:H2'	48:WA:94:A:C8	2.54	0.43
48:WA:1300:C:H2'	48:WA:1301:G:C8	2.54	0.43
48:WA:1516:U:H2'	48:WA:1517:A:C8	2.53	0.43
48:WA:1540:U:H2'	48:WA:1541:G:H8	1.84	0.43
48:WA:4072:U:H2'	48:WA:4073:U:C6	2.54	0.43
51:ZA:446:G:P	60:IB:47:ARG:HH22	2.42	0.43
51:ZA:1550:G:H3'	51:ZA:1579:A:H61	1.84	0.43
51:ZA:1589:A:N3	51:ZA:1653:U:O2'	2.50	0.43
52:AB:200:ASP:N	52:AB:200:ASP:OD1	2.52	0.43
62:KB:37:ASP:N	62:KB:37:ASP:OD1	2.51	0.43
66:OB:54:CYS:SG	66:OB:55:ARG:N	2.92	0.43
1:A:117:GLU:HG2	1:A:124:GLY:H	1.83	0.43
2:B:268:ARG:NH1	48:WA:3898:C:O2'	2.41	0.43
7:G:87:LYS:HG3	48:WA:4130:A:H2	1.84	0.43
9:I:51:HIS:CD2	9:I:168:SER:HB2	2.53	0.43
15:O:84:LYS:HD3	15:O:84:LYS:HA	1.83	0.43
15:O:123:MET:HE2	15:O:123:MET:HB3	1.94	0.43
16:P:181:ARG:HH12	48:WA:1393:A:P	2.42	0.43
32:FA:19:LYS:HD3	32:FA:19:LYS:HA	1.78	0.43
41:OA:30:GLU:HA	41:OA:33:GLN:HG2	2.01	0.43
43:RA:46:ILE:HD11	43:RA:62:LEU:HD21	2.01	0.43
48:WA:1689:U:H2'	48:WA:1690:G:C8	2.54	0.43
48:WA:2396:G:O2'	48:WA:2821:U:O4	2.33	0.43
48:WA:2555:A:H2	48:WA:2767:A:H62	1.64	0.43
48:WA:4451:A:C8	92:WA:5275:ANM:H61	2.51	0.43
48:WA:4640:U:H2'	48:WA:4641:G:N3	2.34	0.43
49:XA:4:U:H2'	49:XA:5:A:H8	1.84	0.43
51:ZA:1616:U:H2'	51:ZA:1617:G:C8	2.54	0.43
87:b:17:ILE:HD13	87:b:17:ILE:HA	1.90	0.43
3:C:170:LEU:HD23	3:C:221:PHE:HZ	1.84	0.42
4:D:40:ASP:HB2	4:D:43:LYS:HG2	2.00	0.42
5:E:216:THR:OG1	5:E:217:ASP:N	2.52	0.42
7:G:126:ARG:NE	48:WA:4078:G:OP1	2.34	0.42
13:M:124:ASP:OD1	48:WA:3939:C:O2'	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:174:THR:OG1	48:WA:4765:U:O2'	2.32	0.42
48:WA:1348:C:H2'	48:WA:1349:G:H8	1.84	0.42
48:WA:1606:G:H2'	48:WA:1607:G:C8	2.53	0.42
48:WA:3934:U:H2'	48:WA:3935:G:H8	1.84	0.42
51:ZA:553:U:O2'	51:ZA:554:A:H8	2.01	0.42
51:ZA:1137:U:O2'	51:ZA:1138:C:OP1	2.30	0.42
57:FB:127:ARG:O	80:CC:26:GLN:NE2	2.52	0.42
69:RB:29:HIS:HA	69:RB:32:LYS:HE2	1.99	0.42
85:HC:184:ASN:ND2	85:HC:186:ASP:OD1	2.52	0.42
85:HC:342:ALA:HA	85:HC:438:ILE:HA	2.01	0.42
85:HC:343:GLN:HE21	85:HC:379:ILE:HD11	1.85	0.42
4:D:271:MET:HE3	4:D:275:GLN:HB3	2.02	0.42
5:E:224:LYS:NZ	48:WA:697:C:N3	2.67	0.42
10:J:99:PHE:O	10:J:159:LYS:NZ	2.50	0.42
16:P:119:LYS:HE3	16:P:121:LEU:HD21	2.00	0.42
48:WA:287:U:H2'	48:WA:288:G:C8	2.55	0.42
48:WA:1727:U:H2'	48:WA:1728:U:C6	2.54	0.42
50:YA:141:C:H2'	50:YA:142:U:C6	2.54	0.42
51:ZA:65:C:C6	58:GB:174:PRO:HB3	2.54	0.42
51:ZA:65:C:C2	58:GB:133:LEU:HD22	2.54	0.42
51:ZA:98:C:OP2	51:ZA:426:A:O2'	2.27	0.42
51:ZA:1025:U:H2'	51:ZA:1026:C:O4'	2.18	0.42
51:ZA:1752:C:H2'	51:ZA:1753:C:C6	2.54	0.42
57:FB:99:ILE:HD11	77:ZB:106:GLN:HE22	1.84	0.42
84:GC:87:LEU:HD22	84:GC:132:TRP:HZ3	1.85	0.42
26:Z:71:PRO:HG2	26:Z:108:TYR:HA	2.01	0.42
28:BA:99:PRO:HG3	28:BA:105:ILE:HG12	2.00	0.42
43:RA:35:LEU:HD13	43:RA:64:ILE:HD12	2.01	0.42
48:WA:1310:C:H2'	48:WA:1311:C:C6	2.55	0.42
51:ZA:1836:G:OP1	51:ZA:1839:U:H4'	2.19	0.42
53:BB:86:LEU:HB3	53:BB:98:THR:HB	2.02	0.42
59:HB:246:ILE:HG21	59:HB:254:PRO:HB3	2.02	0.42
70:SB:84:LEU:HD12	70:SB:95:TYR:HB3	1.99	0.42
70:SB:89:ASP:N	70:SB:89:ASP:OD1	2.52	0.42
2:B:231:VAL:HG11	2:B:251:VAL:HG23	2.01	0.42
4:D:166:ALA:HB1	4:D:171:LEU:HD12	2.02	0.42
13:M:53:TYR:HB2	13:M:133:ILE:HD13	2.00	0.42
26:Z:117:LEU:HD12	26:Z:118:PRO:HD2	2.00	0.42
26:Z:117:LEU:HB3	26:Z:140:VAL:HG21	2.02	0.42
27:AA:5:LYS:HE3	27:AA:8:THR:HB	2.00	0.42
28:BA:52:CYS:SG	28:BA:56:ARG:HG2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DA:98:GLU:OE1	48:WA:2326:C:O2'	2.34	0.42
33:GA:87:LYS:HB3	33:GA:87:LYS:HE2	1.81	0.42
48:WA:197:A:N1	48:WA:225:G:O2'	2.45	0.42
48:WA:4176:U:H2'	48:WA:4177:G:C8	2.54	0.42
51:ZA:303:C:H5''	60:IB:75:LYS:HE3	2.01	0.42
51:ZA:1587:G:C8	71:TB:78:ILE:HD11	2.54	0.42
51:ZA:1673:U:O2'	57:FB:84:GLY:O	2.31	0.42
76:YB:28:LEU:HD21	76:YB:68:LYS:HE2	2.01	0.42
85:HC:256:ILE:HB	85:HC:259:ILE:HB	2.01	0.42
87:b:21:LEU:HD23	87:b:21:LEU:HA	1.81	0.42
2:B:11:HIS:NE2	48:WA:4460:C:OP1	2.51	0.42
2:B:47:LEU:HD12	2:B:47:LEU:HA	1.87	0.42
3:C:284:MET:HE3	16:P:124:ASP:HB3	2.01	0.42
13:M:49:ARG:HH21	48:WA:114:G:P	2.42	0.42
27:AA:4:SER:HB2	48:WA:1857:G:OP1	2.19	0.42
30:DA:107:ASN:OD1	30:DA:107:ASN:N	2.53	0.42
36:JA:47:ILE:HG22	36:JA:49:ASP:H	1.84	0.42
48:WA:488:G:H2'	48:WA:489:G:H8	1.85	0.42
48:WA:1266:C:H2'	48:WA:1267:G:C8	2.54	0.42
48:WA:1506:G:H2'	48:WA:1507:C:C6	2.54	0.42
48:WA:3913:C:H2'	48:WA:3914:U:C6	2.54	0.42
48:WA:4632:G:H2'	48:WA:4633:G:H8	1.84	0.42
51:ZA:16:G:H2'	51:ZA:17:C:C6	2.54	0.42
51:ZA:1839:U:H2'	51:ZA:1840:U:C6	2.54	0.42
56:EB:54:TYR:O	76:YB:15:ASN:ND2	2.53	0.42
56:EB:232:ASN:OD1	56:EB:232:ASN:N	2.53	0.42
75:XB:68:LYS:HG2	75:XB:91:LEU:HD22	2.00	0.42
87:b:119:CYS:SG	87:b:120:GLU:N	2.92	0.42
1:A:241:ARG:NH1	48:WA:3661:G:OP1	2.50	0.42
5:E:53:VAL:HG11	48:WA:952:C:H5''	2.00	0.42
41:OA:83:ILE:HD13	41:OA:83:ILE:HA	1.89	0.42
48:WA:1192:U:H2'	48:WA:1193:G:N3	2.34	0.42
48:WA:1307:C:OP1	50:YA:7:U:O2'	2.38	0.42
48:WA:2363:G:O2'	48:WA:3861:G:O6	2.35	0.42
48:WA:2488:G:H2'	48:WA:2489:G:O4'	2.18	0.42
48:WA:3779:G:O2'	48:WA:3817:G:O6	2.34	0.42
48:WA:4260:C:H2'	48:WA:4261:C:C6	2.55	0.42
48:WA:4908:C:H2'	48:WA:4909:G:C8	2.54	0.42
51:ZA:1356:G:O3'	54:CB:125:LYS:NZ	2.43	0.42
51:ZA:1628:C:H2'	51:ZA:1629:C:H6	1.84	0.42
84:GC:107:ASP:OD2	84:GC:125:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:GC:296:GLN:HG3	84:GC:312:VAL:HB	2.01	0.42
3:C:328:LEU:HD13	6:F:186:MET:HE2	2.02	0.42
14:N:54:TYR:OH	14:N:73:PHE:O	2.37	0.42
27:AA:31:SER:HB2	48:WA:1465:C:H5''	2.02	0.42
35:IA:2:THR:O	35:IA:7:SER:OG	2.27	0.42
42:PA:17:LEU:HD13	42:PA:19:LYS:HE3	2.02	0.42
48:WA:1082:C:H2'	48:WA:1083:C:H6	1.85	0.42
48:WA:2519:A:N3	48:WA:2541:C:O2'	2.50	0.42
48:WA:2523:G:H2'	48:WA:2524:G:C8	2.53	0.42
48:WA:3934:U:H2'	48:WA:3935:G:C8	2.55	0.42
48:WA:5006:C:H2'	48:WA:5007:G:O4'	2.20	0.42
49:XA:12:U:OP2	49:XA:67:C:O2'	2.34	0.42
50:YA:47:C:H1'	50:YA:61:A:H2'	2.02	0.42
51:ZA:671:A:H4'	51:ZA:672:A:H5''	2.01	0.42
51:ZA:1758:G:H2'	51:ZA:1759:G:H8	1.85	0.42
56:EB:100:ARG:HB2	56:EB:114:ILE:HD13	2.01	0.42
2:B:301:ASN:OD1	2:B:301:ASN:N	2.53	0.42
2:B:373:LYS:HD2	48:WA:4629:U:H4'	2.02	0.42
15:O:45:LYS:HB3	15:O:178:ILE:HG12	2.02	0.42
17:Q:108:ARG:HH22	48:WA:2901:C:P	2.43	0.42
21:U:15:ARG:HB2	48:WA:4620:G:H5''	2.01	0.42
48:WA:752:U:H1'	48:WA:918:C:C5	2.54	0.42
48:WA:992:C:H2'	48:WA:993:C:C6	2.55	0.42
48:WA:1194:C:H2'	48:WA:1195:G:C8	2.48	0.42
51:ZA:807:G:H2'	51:ZA:808:A:H8	1.85	0.42
51:ZA:1109:C:N3	69:RB:126:MET:HG3	2.34	0.42
51:ZA:1124:C:O2'	69:RB:126:MET:O	2.37	0.42
51:ZA:1259:A:H1'	51:ZA:1264:C:N4	2.35	0.42
51:ZA:1809:A:H2'	51:ZA:1810:U:C6	2.55	0.42
52:AB:190:SER:OG	52:AB:192:GLU:OE1	2.36	0.42
68:QB:126:VAL:HG12	68:QB:127:ASP:H	1.84	0.42
79:BC:23:ARG:NH2	79:BC:29:ASN:OD1	2.40	0.42
83:FC:133:ALA:N	83:FC:140:TYR:O	2.33	0.42
85:HC:187:THR:HA	85:HC:216:VAL:HG13	2.01	0.42
85:HC:307:ASN:O	96:HC:603:SER:N	2.53	0.42
2:B:224:LYS:HG2	2:B:340:THR:HB	2.01	0.42
2:B:342:LYS:O	48:WA:4978:U:N3	2.53	0.42
9:I:86:HIS:HB3	9:I:139:ARG:HG2	2.01	0.42
19:S:4:THR:OG1	48:WA:4210:U:OP2	2.33	0.42
24:X:50:ARG:HB2	24:X:115:ARG:NH2	2.34	0.42
32:FA:21:ARG:NH2	48:WA:2643:A:OP1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:347:A:H2'	48:WA:348:G:C8	2.55	0.42
48:WA:1348:C:H2'	48:WA:1349:G:C8	2.54	0.42
48:WA:1547:G:H2'	48:WA:1548:C:C6	2.54	0.42
48:WA:1619:G:H1'	48:WA:2515:A:N6	2.35	0.42
48:WA:1679:U:H4'	48:WA:1682:G:N1	2.35	0.42
51:ZA:350:C:O2'	51:ZA:383:G:N1	2.52	0.42
54:CB:78:LEU:HD23	54:CB:81:ILE:HD12	2.02	0.42
2:B:30:LYS:HG3	48:WA:4718:C:OP2	2.19	0.42
5:E:193:HIS:HB3	5:E:196:PHE:HD2	1.85	0.42
6:F:79:ASN:HA	19:S:143:THR:HG22	2.01	0.42
7:G:136:PHE:HA	7:G:236:ILE:HD13	2.01	0.42
10:J:151:ILE:HG22	10:J:155:HIS:HB3	2.00	0.42
25:Y:30:ASP:OD1	25:Y:30:ASP:N	2.52	0.42
26:Z:21:ARG:HB2	48:WA:1320:C:OP1	2.19	0.42
30:DA:87:VAL:HG11	42:PA:25:TYR:HB3	2.02	0.42
41:OA:13:LYS:HE3	41:OA:14:TYR:CZ	2.55	0.42
48:WA:1346:C:H2'	48:WA:1347:A:C8	2.54	0.42
48:WA:4776:C:H2'	48:WA:4777:C:C6	2.55	0.42
48:WA:5004:U:H2'	48:WA:5005:U:H6	1.84	0.42
51:ZA:1317:C:H2'	51:ZA:1318:G:C8	2.54	0.42
51:ZA:1670:C:H2'	51:ZA:1671:G:C8	2.55	0.42
53:BB:144:LYS:HE2	53:BB:206:PRO:HB2	2.02	0.42
69:RB:37:GLU:HG3	84:GC:150:TRP:HE1	1.83	0.42
75:XB:32:LEU:HD12	75:XB:32:LEU:HA	1.90	0.42
85:HC:120:VAL:HG13	85:HC:121:GLY:H	1.85	0.42
85:HC:370:CYS:HA	85:HC:406:PRO:HA	2.02	0.42
2:B:385:LYS:NZ	48:WA:5004:U:OP2	2.47	0.41
3:C:150:LEU:O	3:C:152:LEU:N	2.53	0.41
10:J:44:THR:O	10:J:78:LYS:NZ	2.44	0.41
13:M:35:ALA:HA	13:M:65:ARG:HG2	2.01	0.41
13:M:172:ARG:HG2	48:WA:29:G:H5''	2.02	0.41
13:M:181:HIS:CD2	48:WA:99:A:H4'	2.55	0.41
33:GA:85:PRO:HB3	48:WA:134:G:H1'	2.02	0.41
48:WA:1474:C:H2'	48:WA:1475:U:C6	2.54	0.41
48:WA:1671:A:H4'	48:WA:1687:G:N2	2.35	0.41
48:WA:2650:G:H2'	48:WA:2651:G:H8	1.85	0.41
48:WA:3895:C:H2'	48:WA:3896:A:C8	2.54	0.41
48:WA:4171:G:H4'	48:WA:4173:C:C2	2.55	0.41
49:XA:57:C:H2'	49:XA:58:A:H8	1.85	0.41
51:ZA:14:C:H2'	51:ZA:15:U:C6	2.55	0.41
51:ZA:181:A:H5''	51:ZA:182:C:H2'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1004:U:H2'	51:ZA:1005:G:H8	1.85	0.41
51:ZA:1215:C:O2'	51:ZA:1645:C:OP2	2.30	0.41
51:ZA:1545:A:H2'	51:ZA:1546:G:C8	2.54	0.41
55:DB:173:GLU:HG2	55:DB:191:VAL:HG13	2.00	0.41
85:HC:25:GLY:HA3	85:HC:56:TYR:HB3	2.02	0.41
9:I:47:PRO:HD2	9:I:141:LYS:HA	2.02	0.41
12:L:29:ASP:OD1	12:L:30:VAL:N	2.50	0.41
24:X:74:TYR:OH	50:YA:75:G:OP2	2.31	0.41
33:GA:89:ARG:O	33:GA:93:ARG:HG2	2.21	0.41
43:RA:134:GLY:HA3	48:WA:1995:C:H1'	2.01	0.41
48:WA:36:U:OP1	48:WA:1653:G:N2	2.41	0.41
48:WA:106:A:H2'	48:WA:107:G:O4'	2.20	0.41
48:WA:1343:U:H2'	48:WA:1344:A:H8	1.85	0.41
48:WA:2082:U:H2'	48:WA:2083:C:C6	2.55	0.41
48:WA:2415:U:H2'	48:WA:2416:G:H8	1.85	0.41
48:WA:4729:A:H2'	48:WA:4730:U:O4'	2.20	0.41
48:WA:4899:G:H1'	48:WA:4929:G:N2	2.35	0.41
51:ZA:195:C:O2	51:ZA:204:G:N2	2.53	0.41
51:ZA:222:U:H5''	63:LB:17:PHE:CG	2.55	0.41
51:ZA:952:G:H2'	51:ZA:953:C:C6	2.54	0.41
51:ZA:1643:U:H2'	51:ZA:1644:C:C6	2.55	0.41
54:CB:60:TRP:O	54:CB:71:LYS:NZ	2.37	0.41
60:IB:74:ARG:HA	60:IB:74:ARG:HD3	1.90	0.41
84:GC:7:LEU:HD13	84:GC:7:LEU:HA	1.93	0.41
2:B:163:LEU:HG	2:B:180:LEU:HD11	2.02	0.41
14:N:74:ARG:HG3	14:N:145:VAL:HG12	2.02	0.41
24:X:56:GLN:HG3	24:X:105:VAL:HG13	2.02	0.41
36:JA:35:LYS:HG2	36:JA:44:THR:HG22	2.02	0.41
37:KA:13:LEU:HD22	48:WA:2409:G:H2'	2.01	0.41
37:KA:44:TRP:CZ3	37:KA:45:ARG:HD3	2.55	0.41
48:WA:1763:G:H2'	48:WA:1764:C:H6	1.85	0.41
48:WA:1848:G:H2'	48:WA:1849:C:H6	1.84	0.41
48:WA:4580:G:H2'	48:WA:4581:U:H6	1.84	0.41
51:ZA:385:G:O2'	60:IB:10:LYS:NZ	2.47	0.41
51:ZA:984:C:O2'	66:OB:138:ASP:HB3	2.20	0.41
56:EB:198:ARG:HE	56:EB:222:LEU:HD11	1.86	0.41
72:UB:56:MET:HB2	72:UB:86:LYS:HB3	2.00	0.41
75:XB:59:ALA:HB1	75:XB:114:ASP:HB3	2.02	0.41
84:GC:84:ASP:OD1	84:GC:86:THR:OG1	2.31	0.41
2:B:41:VAL:HA	2:B:187:GLY:HA3	2.03	0.41
2:B:77:THR:OG1	2:B:335:GLY:O	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:27:ASN:HB3	50:YA:29:G:H5''	2.02	0.41
18:R:68:PHE:N	48:WA:730:G:O6	2.52	0.41
36:JA:61:PRO:HA	36:JA:62:PRO:HD3	1.94	0.41
38:LA:99:LYS:HD2	48:WA:4476:A:H5''	2.02	0.41
43:RA:24:ALA:HB2	43:RA:40:LYS:HE3	2.02	0.41
48:WA:272:U:H2'	48:WA:273:U:C6	2.55	0.41
48:WA:1176:G:H2'	48:WA:1177:G:C8	2.55	0.41
48:WA:1496:U:H2'	48:WA:1497:G:H8	1.84	0.41
48:WA:1761:G:O6	48:WA:1775:U:O4	2.38	0.41
48:WA:4565:U:H2'	48:WA:4566:A:H8	1.84	0.41
48:WA:4763:G:H2'	48:WA:4764:A:C8	2.55	0.41
48:WA:4908:C:H2'	48:WA:4909:G:H8	1.85	0.41
92:WA:5275:ANM:H11	92:WA:5275:ANM:H16	1.86	0.41
49:XA:111:C:H2'	49:XA:112:U:O4'	2.21	0.41
51:ZA:886:A:H5''	51:ZA:887:U:C5	2.55	0.41
51:ZA:1447:G:H2'	51:ZA:1448:A:C8	2.55	0.41
51:ZA:1605:G:H2'	51:ZA:1606:G:C4	2.56	0.41
51:ZA:1667:U:H2'	51:ZA:1668:U:C6	2.56	0.41
51:ZA:1801:A:H2'	51:ZA:1802:C:H6	1.84	0.41
78:AC:13:LYS:H	78:AC:15:ARG:NH1	2.19	0.41
2:B:128:LYS:O	2:B:131:THR:OG1	2.32	0.41
2:B:369:ASP:OD2	2:B:373:LYS:NZ	2.52	0.41
13:M:12:ARG:NH1	48:WA:308:G:O6	2.54	0.41
17:Q:88:ARG:O	48:WA:2727:A:N6	2.54	0.41
17:Q:116:ASP:OD1	17:Q:116:ASP:N	2.48	0.41
48:WA:164:G:H2'	48:WA:165:A:C8	2.55	0.41
48:WA:286:U:H2'	48:WA:287:U:C6	2.55	0.41
48:WA:1352:C:H2'	48:WA:1353:G:C8	2.56	0.41
48:WA:2499:C:H2'	48:WA:2500:C:C6	2.55	0.41
48:WA:4194:A:H2'	48:WA:4195:C:H6	1.86	0.41
48:WA:4321:C:H2'	48:WA:4322:G:H8	1.85	0.41
51:ZA:1673:U:H2'	51:ZA:1674:G:O4'	2.20	0.41
57:FB:122:ARG:HE	80:CC:59:LEU:HD21	1.85	0.41
64:MB:42:LEU:HD22	64:MB:74:ILE:HG13	2.03	0.41
64:MB:42:LEU:O	64:MB:72:HIS:ND1	2.49	0.41
68:QB:63:ARG:HG2	71:TB:7:LYS:HB3	2.01	0.41
73:VB:73:ALA:HB1	73:VB:78:ILE:HB	2.02	0.41
85:HC:392:LYS:HG3	85:HC:393:PHE:HD1	1.85	0.41
87:b:125:ALA:HA	87:b:218:GLY:HA2	2.02	0.41
1:A:132:ASN:ND2	48:WA:3685:C:OP1	2.52	0.41
10:J:19:LYS:HD3	10:J:75:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:132:ARG:NH2	48:WA:4898:G:OP1	2.54	0.41
13:M:140:LYS:HD2	13:M:144:ARG:HE	1.86	0.41
18:R:76:LYS:HE3	18:R:76:LYS:HB2	1.89	0.41
36:JA:11:PHE:CE2	36:JA:56:LEU:HD21	2.56	0.41
48:WA:692:C:H2'	48:WA:693:A:C8	2.55	0.41
48:WA:2445:G:OP2	48:WA:2518:G:N2	2.46	0.41
48:WA:2846:A:N6	48:WA:3841:G:O2'	2.54	0.41
48:WA:4147:C:H2'	48:WA:4148:G:C8	2.55	0.41
49:XA:22:A:H2'	49:XA:23:A:C8	2.55	0.41
49:XA:58:A:H2'	49:XA:59:G:C8	2.56	0.41
51:ZA:634:A:H2'	51:ZA:635:G:H8	1.85	0.41
51:ZA:1261:C:O2	81:DC:10:HIS:NE2	2.51	0.41
71:TB:96:SER:HB3	71:TB:99:VAL:HG22	2.01	0.41
84:GC:191:HIS:NE2	84:GC:215:GLN:O	2.53	0.41
85:HC:113:VAL:HA	85:HC:149:ILE:O	2.21	0.41
85:HC:392:LYS:HG3	85:HC:393:PHE:CD1	2.56	0.41
13:M:85:VAL:HG23	48:WA:43:U:OP1	2.21	0.41
14:N:10:ASP:OD2	14:N:37:ARG:NH2	2.53	0.41
18:R:35:PRO:HD2	18:R:39:VAL:HG21	2.02	0.41
43:RA:90:ARG:NH2	43:RA:95:GLN:OE1	2.43	0.41
48:WA:1319:U:H2'	48:WA:1320:C:C6	2.55	0.41
48:WA:1741:G:H2'	48:WA:1742:C:C6	2.56	0.41
48:WA:4462:U:H2'	48:WA:4463:C:C6	2.56	0.41
48:WA:4996:G:H2'	48:WA:4997:U:C6	2.56	0.41
51:ZA:694:G:H22	51:ZA:732:U:H3	1.67	0.41
51:ZA:1420:G:H1'	51:ZA:1422:G:C2	2.55	0.41
51:ZA:1681:U:H2'	51:ZA:1682:C:C6	2.56	0.41
51:ZA:1716:C:H2'	51:ZA:1717:C:H6	1.85	0.41
56:EB:185:GLY:N	56:EB:189:LEU:HD13	2.34	0.41
84:GC:207:CYS:HB2	84:GC:221:LEU:HD21	2.01	0.41
84:GC:246:TYR:HB3	84:GC:261:LEU:HB2	2.03	0.41
1:A:117:GLU:HG2	1:A:124:GLY:N	2.34	0.41
2:B:86:VAL:HG13	2:B:162:VAL:HG13	2.03	0.41
2:B:90:VAL:HG22	2:B:104:THR:HG23	2.02	0.41
6:F:135:VAL:HG23	6:F:139:ILE:HD13	2.03	0.41
13:M:44:ARG:NH1	48:WA:280:G:OP2	2.49	0.41
22:V:97:LYS:HG3	22:V:99:GLU:H	1.86	0.41
48:WA:436:C:H2'	48:WA:437:G:H8	1.86	0.41
48:WA:1656:G:C6	48:WA:3916:U:H5'	2.56	0.41
48:WA:2450:G:H2'	48:WA:2451:A:C8	2.55	0.41
48:WA:2485:G:H2'	48:WA:2486:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:4706:C:H2'	48:WA:4707:A:H8	1.86	0.41
51:ZA:912:C:H3'	51:ZA:913:A:H3'	2.03	0.41
80:CC:60:GLU:OE2	80:CC:63:ARG:NH1	2.43	0.41
2:B:92:TYR:HB2	2:B:159:VAL:HB	2.02	0.41
2:B:181:MET:HE2	2:B:181:MET:HB3	1.92	0.41
2:B:276:HIS:ND1	48:WA:4718:C:OP1	2.48	0.41
2:B:291:TYR:HB3	2:B:298:LEU:HD11	2.02	0.41
8:H:21:LYS:HB3	8:H:24:THR:HB	2.03	0.41
9:I:150:GLU:OE2	9:I:153:ARG:NH2	2.36	0.41
10:J:96:LYS:O	10:J:159:LYS:NZ	2.51	0.41
12:L:72:TYR:CE2	48:WA:919:A:H5'	2.56	0.41
13:M:46:ASP:OD1	13:M:46:ASP:N	2.53	0.41
16:P:12:LYS:HB2	16:P:14:ARG:NH1	2.36	0.41
16:P:14:ARG:HE	48:WA:2086:U:H1'	1.85	0.41
20:T:83:LEU:HD23	20:T:83:LEU:HA	1.87	0.41
21:U:42:VAL:HB	21:U:45:ILE:HG13	2.02	0.41
23:W:122:ALA:HB3	23:W:139:ARG:HG3	2.01	0.41
26:Z:77:LYS:NZ	48:WA:1504:G:H22	2.19	0.41
28:BA:13:SER:OG	28:BA:17:ARG:NH1	2.53	0.41
28:BA:47:ILE:HD12	28:BA:94:LEU:HD13	2.02	0.41
30:DA:19:LYS:HE2	30:DA:19:LYS:HB3	1.93	0.41
34:HA:63:VAL:HG23	34:HA:65:LYS:HG3	2.03	0.41
35:IA:22:CYS:HB3	35:IA:37:CYS:SG	2.60	0.41
37:KA:37:TYR:O	48:WA:362:A:N6	2.49	0.41
38:LA:60:ALA:O	38:LA:64:ASN:HB2	2.21	0.41
39:MA:1:MET:HE2	39:MA:9:ARG:HE	1.86	0.41
39:MA:2:ARG:HD3	39:MA:5:TRP:NE1	2.36	0.41
44:SA:11:U:H2'	44:SA:12:G:C8	2.56	0.41
46:UA:14:A:C2	46:UA:15:G:H1'	2.56	0.41
48:WA:324:A:H2'	48:WA:325:U:C6	2.56	0.41
48:WA:1346:C:H2'	48:WA:1347:A:H8	1.86	0.41
48:WA:2295:U:H2'	48:WA:2296:G:C8	2.56	0.41
48:WA:2540:U:H2'	48:WA:2541:C:C6	2.56	0.41
48:WA:3709:U:H2'	48:WA:3710:C:H6	1.85	0.41
48:WA:3949:A:C4	48:WA:3950:C:H5	2.38	0.41
48:WA:4553:U:H2'	48:WA:4554:U:C6	2.56	0.41
48:WA:4957:A:H2'	48:WA:4958:A:C8	2.56	0.41
51:ZA:96:C:H2'	51:ZA:97:U:C6	2.55	0.41
51:ZA:495:U:H2'	51:ZA:496:C:O4'	2.21	0.41
51:ZA:1158:G:H5''	74:WB:76:SER:HB2	2.02	0.41
51:ZA:1189:A:H2'	51:ZA:1190:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1454:A:C8	69:RB:3:ARG:HD2	2.55	0.41
51:ZA:1512:C:H5''	81:DC:8:TRP:HZ3	1.86	0.41
51:ZA:1588:A:H2'	51:ZA:1589:A:H8	1.85	0.41
52:AB:37:TYR:OH	52:AB:57:LYS:NZ	2.45	0.41
56:EB:155:LYS:HA	56:EB:155:LYS:HD3	1.80	0.41
57:FB:35:LEU:HD13	57:FB:146:ARG:HH21	1.86	0.41
62:KB:41:PRO:HD2	62:KB:44:HIS:ND1	2.36	0.41
65:NB:4:MET:SD	65:NB:124:ARG:NH1	2.94	0.41
75:XB:89:GLY:HA2	82:EC:82:VAL:HG12	2.03	0.41
77:ZB:52:LYS:NZ	77:ZB:56:ASP:OD2	2.51	0.41
80:CC:29:GLN:HE22	80:CC:68:LEU:HD23	1.86	0.41
84:GC:17:TRP:HB2	84:GC:36:ARG:HG3	2.02	0.41
85:HC:11:VAL:HB	85:HC:109:ALA:HB2	2.03	0.41
85:HC:211:PHE:HZ	85:HC:214:TRP:HD1	1.68	0.41
2:B:300:LYS:O	2:B:302:ASN:N	2.52	0.41
3:C:273:LEU:HD13	3:C:273:LEU:HA	1.91	0.41
4:D:116:ASP:OD1	4:D:116:ASP:N	2.54	0.41
21:U:13:LYS:HD2	21:U:128:LEU:HD11	2.03	0.41
30:DA:106:LYS:HE3	30:DA:106:LYS:HB2	1.89	0.41
45:TA:49:C:H2'	45:TA:50:A:H8	1.85	0.41
46:UA:62:C:H2'	46:UA:63:G:C8	2.56	0.41
48:WA:268:G:H2'	48:WA:269:G:C8	2.56	0.41
48:WA:269:G:H2'	48:WA:270:U:C6	2.55	0.41
48:WA:1343:U:H2'	48:WA:1344:A:C8	2.56	0.41
48:WA:1474:C:H2'	48:WA:1475:U:H6	1.86	0.41
48:WA:1507:C:H2'	48:WA:1508:G:C8	2.55	0.41
48:WA:1848:G:H2'	48:WA:1849:C:C6	2.56	0.41
48:WA:3918:G:H2'	48:WA:3919:A:C8	2.56	0.41
48:WA:4540:G:H2'	48:WA:4541:U:C6	2.56	0.41
48:WA:4593:U:H2'	48:WA:4594:C:C6	2.56	0.41
49:XA:24:C:H2'	49:XA:25:G:O4'	2.21	0.41
51:ZA:429:C:H2'	51:ZA:430:C:H6	1.86	0.41
51:ZA:857:U:H2'	51:ZA:858:A:C8	2.56	0.41
51:ZA:1562:C:H2'	51:ZA:1563:G:C8	2.53	0.41
52:AB:6:ASP:OD1	52:AB:6:ASP:N	2.54	0.41
54:CB:104:ASP:HB3	54:CB:130:ILE:HG13	2.03	0.41
70:SB:36:VAL:HG21	70:SB:71:MET:HE3	2.03	0.41
84:GC:248:LEU:HB2	84:GC:261:LEU:HD21	2.03	0.41
85:HC:102:MET:HE3	85:HC:102:MET:HB3	1.96	0.41
2:B:50:LYS:NZ	2:B:339:GLY:O	2.40	0.40
2:B:54:THR:OG1	2:B:369:ASP:O	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:ILE:HB	4:D:80:ALA:HB2	2.03	0.40
6:F:114:ARG:NH1	16:P:4:ASP:O	2.51	0.40
36:JA:26:LYS:HD3	36:JA:69:LEU:HD23	2.03	0.40
43:RA:32:ILE:HA	43:RA:35:LEU:HD12	2.02	0.40
48:WA:417:G:O2'	50:YA:17:A:N6	2.54	0.40
48:WA:1083:C:H2'	48:WA:1084:A:H8	1.86	0.40
48:WA:1463:C:H2'	48:WA:1464:A:C8	2.55	0.40
48:WA:2703:U:H2'	48:WA:2704:C:C6	2.56	0.40
48:WA:4099:G:O2'	48:WA:4100:A:H8	2.03	0.40
48:WA:4772:U:H2'	48:WA:4773:C:C5	2.56	0.40
50:YA:5:U:H2'	50:YA:6:C:C6	2.56	0.40
51:ZA:12:U:H2'	51:ZA:13:C:C6	2.56	0.40
56:EB:95:THR:HG22	76:YB:16:ARG:HB2	2.03	0.40
61:JB:111:GLN:NE2	61:JB:127:ARG:HB2	2.36	0.40
73:VB:15:ARG:NH1	73:VB:33:GLN:OE1	2.47	0.40
81:DC:49:ASP:OD1	81:DC:49:ASP:N	2.50	0.40
85:HC:417:ASP:N	85:HC:417:ASP:OD1	2.54	0.40
2:B:117:ARG:NH2	48:WA:4987:U:OP1	2.38	0.40
3:C:83:GLY:H	48:WA:368:C:H1'	1.87	0.40
4:D:270:LYS:HE3	4:D:270:LYS:HB2	1.93	0.40
6:F:30:LYS:O	6:F:34:LYS:HG3	2.21	0.40
7:G:128:LYS:HB3	7:G:128:LYS:HE2	1.86	0.40
8:H:88:PHE:CE2	8:H:151:ILE:HB	2.56	0.40
18:R:53:LYS:NZ	49:XA:74:A:O2'	2.54	0.40
29:CA:46:LEU:HD13	29:CA:46:LEU:HA	1.88	0.40
42:PA:39:ARG:NH1	48:WA:2268:C:O2'	2.54	0.40
45:TA:14:A:H3'	45:TA:15:G:H8	1.86	0.40
48:WA:128:C:H2'	48:WA:129:C:C6	2.56	0.40
48:WA:699:G:H2'	48:WA:700:C:C6	2.56	0.40
48:WA:1309:A:H2'	48:WA:1310:C:C6	2.56	0.40
48:WA:1400:A:H62	48:WA:1421:G:H21	1.69	0.40
48:WA:2000:A:H2'	48:WA:2001:A:C8	2.56	0.40
48:WA:4761:C:H2'	48:WA:4762:G:C8	2.56	0.40
51:ZA:51:U:H2'	51:ZA:52:G:C8	2.56	0.40
51:ZA:219:U:H2'	51:ZA:220:U:C6	2.57	0.40
51:ZA:383:G:H4'	63:LB:132:ARG:HD2	2.03	0.40
51:ZA:429:C:H2'	51:ZA:430:C:C6	2.56	0.40
51:ZA:880:G:H2'	51:ZA:881:G:C8	2.56	0.40
51:ZA:1230:C:H2'	51:ZA:1231:C:H6	1.86	0.40
77:ZB:58:LEU:HD12	77:ZB:62:VAL:HG21	2.01	0.40
81:DC:21:CYS:SG	81:DC:39:CYS:N	2.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD11	1:A:149:LYS:HB2	2.02	0.40
9:I:101:LYS:NZ	9:I:102:MET:O	2.46	0.40
18:R:99:ASP:OD1	18:R:100:LEU:N	2.43	0.40
24:X:34:LEU:HD23	24:X:38:LEU:HB3	2.02	0.40
29:CA:88:LEU:HD12	29:CA:106:VAL:HG13	2.03	0.40
43:RA:81:ILE:HG21	43:RA:139:VAL:HG21	2.04	0.40
48:WA:737:C:H2'	48:WA:738:C:C6	2.56	0.40
48:WA:1078:C:H42	48:WA:1245:C:H42	1.68	0.40
48:WA:1735:G:N3	48:WA:4216:A:H2'	2.36	0.40
48:WA:2866:A:H2'	48:WA:2867:U:C6	2.56	0.40
48:WA:5032:U:H2'	48:WA:5033:G:C8	2.56	0.40
49:XA:3:C:H2'	49:XA:4:U:C6	2.57	0.40
49:XA:58:A:H2'	49:XA:59:G:H8	1.86	0.40
51:ZA:935:G:O2'	65:NB:108:ASP:OD1	2.36	0.40
51:ZA:1309:C:OP1	83:FC:104:LYS:NZ	2.50	0.40
51:ZA:1712:A:H2'	51:ZA:1713:C:H6	1.86	0.40
51:ZA:1865:C:OP2	78:AC:5:ARG:NH1	2.53	0.40
55:DB:171:GLY:HA3	55:DB:194:LEU:O	2.21	0.40
71:TB:30:VAL:HA	71:TB:31:PRO:HD3	1.96	0.40
76:YB:17:LEU:HD23	76:YB:17:LEU:HA	1.94	0.40
87:b:148:SER:HB2	87:b:153:GLU:HB2	2.04	0.40
2:B:252:ALA:HB1	48:WA:4526:G:N3	2.36	0.40
14:N:130:LYS:HB2	14:N:133:ARG:HG2	2.04	0.40
24:X:82:ILE:HG22	24:X:83:GLU:H	1.86	0.40
35:IA:22:CYS:SG	35:IA:24:SER:OG	2.69	0.40
40:NA:63:THR:O	40:NA:87:ARG:NH1	2.55	0.40
44:SA:43:A:H2'	44:SA:44:A:C8	2.56	0.40
48:WA:161:G:H2'	48:WA:162:A:H8	1.86	0.40
48:WA:932:C:H2'	48:WA:933:A:C8	2.57	0.40
48:WA:3602:G:H2'	48:WA:3603:C:C6	2.56	0.40
51:ZA:571:U:O2'	76:YB:60:PHE:O	2.37	0.40
51:ZA:1097:G:H4'	52:AB:32:PHE:CD1	2.57	0.40
51:ZA:1733:U:H2'	51:ZA:1734:G:O4'	2.22	0.40
57:FB:77:MET:H	57:FB:77:MET:HG3	1.51	0.40
72:UB:116:ILE:HD12	72:UB:116:ILE:HA	1.97	0.40
2:B:285:TYR:N	2:B:332:MET:O	2.49	0.40
7:G:241:ALA:HB2	48:WA:6:C:H1'	2.02	0.40
11:K:127:PHE:O	33:GA:117:ARG:NH2	2.46	0.40
12:L:121:ARG:NH2	48:WA:4883:U:OP1	2.38	0.40
18:R:23:ARG:HG3	18:R:24:THR:HG23	2.03	0.40
24:X:42:TYR:HB3	24:X:119:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:PA:105:ASP:N	42:PA:105:ASP:OD1	2.55	0.40
48:WA:1481:G:H2'	48:WA:1482:C:C6	2.57	0.40
48:WA:3857:C:H2'	48:WA:3858:A:H8	1.86	0.40
48:WA:4501:G:C2	48:WA:4531:G:H1'	2.56	0.40
48:WA:5003:U:H2'	48:WA:5004:U:O4'	2.21	0.40
51:ZA:944:A:H2'	51:ZA:945:U:H6	1.87	0.40
51:ZA:1195:A:H2'	51:ZA:1196:A:H8	1.86	0.40
70:SB:5:ILE:N	77:ZB:50:PHE:O	2.53	0.40
84:GC:89:LEU:HB3	84:GC:99:ARG:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/257 (96%)	235 (95%)	13 (5%)	0	100	100
2	B	395/403 (98%)	382 (97%)	13 (3%)	0	100	100
3	C	360/413 (87%)	349 (97%)	11 (3%)	0	100	100
4	D	292/297 (98%)	288 (99%)	4 (1%)	0	100	100
5	E	222/291 (76%)	212 (96%)	10 (4%)	0	100	100
6	F	225/249 (90%)	219 (97%)	6 (3%)	0	100	100
7	G	225/319 (70%)	220 (98%)	5 (2%)	0	100	100
8	H	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
9	I	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
10	J	169/178 (95%)	168 (99%)	1 (1%)	0	100	100
11	K	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
12	L	136/218 (62%)	131 (96%)	5 (4%)	0	100	100
13	M	201/204 (98%)	198 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
15	O	154/213 (72%)	151 (98%)	3 (2%)	0	100	100
16	P	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
17	Q	178/212 (84%)	173 (97%)	5 (3%)	0	100	100
18	R	174/224 (78%)	167 (96%)	7 (4%)	0	100	100
19	S	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
20	T	99/128 (77%)	96 (97%)	3 (3%)	0	100	100
21	U	133/140 (95%)	128 (96%)	5 (4%)	0	100	100
22	V	106/157 (68%)	105 (99%)	1 (1%)	0	100	100
23	W	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
24	X	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
25	Y	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
26	Z	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
27	AA	103/245 (42%)	100 (97%)	3 (3%)	0	100	100
28	BA	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
29	CA	106/125 (85%)	102 (96%)	4 (4%)	0	100	100
30	DA	127/135 (94%)	123 (97%)	4 (3%)	0	100	100
31	EA	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
32	FA	112/129 (87%)	108 (96%)	4 (4%)	0	100	100
33	GA	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
34	HA	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
35	IA	85/97 (88%)	84 (99%)	1 (1%)	0	100	100
36	JA	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
37	KA	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
38	LA	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
39	MA	23/25 (92%)	23 (100%)	0	0	100	100
40	NA	102/106 (96%)	99 (97%)	3 (3%)	0	100	100
41	OA	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
42	PA	122/137 (89%)	114 (93%)	8 (7%)	0	100	100
43	RA	151/165 (92%)	143 (95%)	8 (5%)	0	100	100
52	AB	215/295 (73%)	207 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BB	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
54	CB	218/293 (74%)	214 (98%)	4 (2%)	0	100	100
55	DB	226/281 (80%)	225 (100%)	1 (0%)	0	100	100
56	EB	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
57	FB	181/204 (89%)	176 (97%)	5 (3%)	0	100	100
58	GB	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
59	HB	181/432 (42%)	175 (97%)	6 (3%)	0	100	100
60	IB	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
61	JB	183/194 (94%)	182 (100%)	1 (0%)	0	100	100
62	KB	94/165 (57%)	90 (96%)	4 (4%)	0	100	100
63	LB	140/158 (89%)	139 (99%)	1 (1%)	0	100	100
64	MB	115/132 (87%)	108 (94%)	7 (6%)	0	100	100
65	NB	147/151 (97%)	147 (100%)	0	0	100	100
66	OB	134/151 (89%)	130 (97%)	4 (3%)	0	100	100
67	PB	127/145 (88%)	127 (100%)	0	0	100	100
68	QB	140/172 (81%)	136 (97%)	4 (3%)	0	100	100
69	RB	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
70	SB	142/152 (93%)	141 (99%)	1 (1%)	0	100	100
71	TB	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
72	UB	100/119 (84%)	95 (95%)	5 (5%)	0	100	100
73	VB	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
74	WB	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
75	XB	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
76	YB	122/131 (93%)	120 (98%)	2 (2%)	0	100	100
77	ZB	83/124 (67%)	83 (100%)	0	0	100	100
78	AC	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
79	BC	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
80	CC	60/69 (87%)	60 (100%)	0	0	100	100
81	DC	53/56 (95%)	53 (100%)	0	0	100	100
82	EC	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	FC	67/188 (36%)	65 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	GC	311/317 (98%)	299 (96%)	12 (4%)	0	100	100
85	HC	438/462 (95%)	418 (95%)	19 (4%)	1 (0%)	43	68
86	IC	2/4 (50%)	2 (100%)	0	0	100	100
87	b	165/318 (52%)	150 (91%)	14 (8%)	1 (1%)	21	44
88	c	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
All	All	12000/14293 (84%)	11655 (97%)	343 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
85	HC	160	PRO
87	b	225	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/199 (96%)	187 (97%)	5 (3%)	40	70
2	B	344/348 (99%)	337 (98%)	7 (2%)	48	76
3	C	302/337 (90%)	299 (99%)	3 (1%)	68	86
4	D	247/250 (99%)	244 (99%)	3 (1%)	63	84
5	E	201/251 (80%)	198 (98%)	3 (2%)	57	81
6	F	198/218 (91%)	197 (100%)	1 (0%)	81	92
7	G	197/273 (72%)	194 (98%)	3 (2%)	57	81
8	H	169/171 (99%)	164 (97%)	5 (3%)	36	66
9	I	175/181 (97%)	169 (97%)	6 (3%)	32	62
10	J	144/149 (97%)	140 (97%)	4 (3%)	38	68
11	K	175/176 (99%)	174 (99%)	1 (1%)	78	91
12	L	117/161 (73%)	115 (98%)	2 (2%)	53	79
13	M	171/172 (99%)	170 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	171/173 (99%)	168 (98%)	3 (2%)	51	78
15	O	137/190 (72%)	136 (99%)	1 (1%)	76	90
16	P	164/165 (99%)	162 (99%)	2 (1%)	63	84
17	Q	159/191 (83%)	159 (100%)	0	100	100
18	R	157/192 (82%)	153 (98%)	4 (2%)	42	71
19	S	139/140 (99%)	138 (99%)	1 (1%)	76	90
20	T	91/114 (80%)	91 (100%)	0	100	100
21	U	103/107 (96%)	101 (98%)	2 (2%)	50	77
22	V	89/126 (71%)	88 (99%)	1 (1%)	65	85
23	W	106/134 (79%)	104 (98%)	2 (2%)	50	77
24	X	124/135 (92%)	119 (96%)	5 (4%)	28	56
25	Y	117/118 (99%)	116 (99%)	1 (1%)	70	87
26	Z	119/120 (99%)	118 (99%)	1 (1%)	73	88
27	AA	87/184 (47%)	85 (98%)	2 (2%)	44	73
28	BA	85/98 (87%)	84 (99%)	1 (1%)	63	84
29	CA	98/110 (89%)	95 (97%)	3 (3%)	35	65
30	DA	115/121 (95%)	113 (98%)	2 (2%)	53	79
31	EA	88/89 (99%)	87 (99%)	1 (1%)	65	85
32	FA	98/109 (90%)	98 (100%)	0	100	100
33	GA	109/110 (99%)	105 (96%)	4 (4%)	30	59
34	HA	86/89 (97%)	84 (98%)	2 (2%)	44	73
35	IA	74/80 (92%)	73 (99%)	1 (1%)	59	82
36	JA	64/65 (98%)	63 (98%)	1 (2%)	55	80
37	KA	47/48 (98%)	46 (98%)	1 (2%)	47	75
38	LA	48/116 (41%)	47 (98%)	1 (2%)	47	75
39	MA	24/24 (100%)	24 (100%)	0	100	100
40	NA	92/94 (98%)	92 (100%)	0	100	100
41	OA	74/75 (99%)	72 (97%)	2 (3%)	39	69
42	PA	108/121 (89%)	105 (97%)	3 (3%)	38	68
43	RA	126/137 (92%)	117 (93%)	9 (7%)	13	33
52	AB	180/244 (74%)	178 (99%)	2 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BB	194/231 (84%)	191 (98%)	3 (2%)	57	81
54	CB	186/225 (83%)	183 (98%)	3 (2%)	55	80
55	DB	190/232 (82%)	186 (98%)	4 (2%)	47	75
56	EB	224/225 (100%)	218 (97%)	6 (3%)	39	69
57	FB	158/170 (93%)	154 (98%)	4 (2%)	42	71
58	GB	207/218 (95%)	202 (98%)	5 (2%)	43	72
59	HB	165/360 (46%)	163 (99%)	2 (1%)	63	84
60	IB	178/180 (99%)	176 (99%)	2 (1%)	65	85
61	JB	161/168 (96%)	159 (99%)	2 (1%)	63	84
62	KB	87/136 (64%)	85 (98%)	2 (2%)	44	73
63	LB	130/142 (92%)	128 (98%)	2 (2%)	57	81
64	MB	99/108 (92%)	93 (94%)	6 (6%)	17	40
65	NB	130/131 (99%)	129 (99%)	1 (1%)	73	88
66	OB	106/119 (89%)	104 (98%)	2 (2%)	50	77
67	PB	115/130 (88%)	113 (98%)	2 (2%)	53	79
68	QB	117/140 (84%)	115 (98%)	2 (2%)	53	79
69	RB	119/121 (98%)	117 (98%)	2 (2%)	53	79
70	SB	125/132 (95%)	123 (98%)	2 (2%)	55	80
71	TB	112/115 (97%)	106 (95%)	6 (5%)	20	45
72	UB	93/107 (87%)	86 (92%)	7 (8%)	12	31
73	VB	67/67 (100%)	65 (97%)	2 (3%)	36	66
74	WB	112/113 (99%)	110 (98%)	2 (2%)	51	78
75	XB	113/115 (98%)	107 (95%)	6 (5%)	20	46
76	YB	107/113 (95%)	105 (98%)	2 (2%)	50	77
77	ZB	75/102 (74%)	72 (96%)	3 (4%)	28	56
78	AC	88/98 (90%)	87 (99%)	1 (1%)	65	85
79	BC	75/76 (99%)	72 (96%)	3 (4%)	28	56
80	CC	55/62 (89%)	53 (96%)	2 (4%)	31	60
81	DC	48/49 (98%)	45 (94%)	3 (6%)	16	39
82	EC	46/106 (43%)	46 (100%)	0	100	100
83	FC	62/154 (40%)	60 (97%)	2 (3%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	GC	272/275 (99%)	246 (90%)	26 (10%)	8	20
85	HC	366/379 (97%)	342 (93%)	24 (7%)	15	36
87	b	138/258 (54%)	122 (88%)	16 (12%)	5	13
88	c	9/12 (75%)	9 (100%)	0	100	100
All	All	10440/12074 (86%)	10181 (98%)	259 (2%)	42	71

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	181	LYS
1	A	225	ILE
1	A	226	ARG
1	A	235	VAL
2	B	162	VAL
2	B	248	LEU
2	B	292	LEU
2	B	329	ASP
2	B	338	VAL
2	B	344	VAL
2	B	353	VAL
3	C	71	ARG
3	C	215	ASN
3	C	232	VAL
4	D	7	VAL
4	D	150	LEU
4	D	163	LEU
5	E	178	VAL
5	E	242	LYS
5	E	290	VAL
6	F	173	LEU
7	G	167	LEU
7	G	193	VAL
7	G	271	LEU
8	H	48	LEU
8	H	95	VAL
8	H	123	ILE
8	H	167	VAL
8	H	177	ASP
9	I	43	VAL
9	I	44	ASP

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Mol	Chain	Res	Type
9	I	142	LEU
9	I	180	GLU
9	I	184	MET
9	I	197	VAL
10	J	15	LEU
10	J	20	LEU
10	J	93	GLU
10	J	128	LEU
11	K	70	VAL
12	L	25	VAL
12	L	56	GLN
13	M	142	ILE
14	N	27	VAL
14	N	53	LYS
14	N	186	GLU
15	O	142	VAL
16	P	83	VAL
16	P	92	VAL
18	R	39	VAL
18	R	149	LYS
18	R	154	LEU
18	R	160	ARG
19	S	80	VAL
21	U	20	LEU
21	U	92	ASP
22	V	87	LEU
23	W	52	LEU
23	W	155	ILE
24	X	58	VAL
24	X	79	VAL
24	X	82	ILE
24	X	104	VAL
24	X	105	VAL
25	Y	53	VAL
26	Z	122	VAL
27	AA	103	LYS
27	AA	107	ARG
28	BA	14	ILE
29	CA	46	LEU
29	CA	87	ARG
29	CA	100	ASN
30	DA	21	ILE

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Mol	Chain	Res	Type
30	DA	78	LEU
31	EA	76	ARG
33	GA	47	ILE
33	GA	81	LEU
33	GA	87	LYS
33	GA	96	ASN
34	HA	66	ASP
34	HA	90	LEU
35	IA	82	THR
36	JA	69	LEU
37	KA	51	LEU
38	LA	58	GLN
41	OA	30	GLU
41	OA	52	VAL
42	PA	31	ASN
42	PA	103	HIS
42	PA	124	VAL
43	RA	13	VAL
43	RA	37	LEU
43	RA	40	LYS
43	RA	56	LEU
43	RA	92	ARG
43	RA	107	ASP
43	RA	147	HIS
43	RA	151	ILE
43	RA	154	ASP
52	AB	16	LEU
52	AB	51	LEU
53	BB	105	LEU
53	BB	180	ASP
53	BB	191	ASP
54	CB	248	TYR
54	CB	255	LEU
54	CB	271	ASP
55	DB	123	GLU
55	DB	206	VAL
55	DB	220	LEU
55	DB	253	ASP
56	EB	12	VAL
56	EB	181	CYS
56	EB	207	VAL
56	EB	216	ASN

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Mol	Chain	Res	Type
56	EB	220	THR
56	EB	222	LEU
57	FB	69	VAL
57	FB	77	MET
57	FB	102	LEU
57	FB	194	ASP
58	GB	50	VAL
58	GB	77	LEU
58	GB	116	LYS
58	GB	120	ASP
58	GB	213	LEU
59	HB	330	VAL
59	HB	372	VAL
60	IB	82	VAL
60	IB	125	LYS
61	JB	123	ILE
61	JB	154	GLN
62	KB	1	MET
62	KB	52	LEU
63	LB	84	ARG
63	LB	120	VAL
64	MB	28	HIS
64	MB	31	LEU
64	MB	62	VAL
64	MB	77	ILE
64	MB	110	VAL
64	MB	111	VAL
65	NB	134	VAL
66	OB	30	VAL
66	OB	38	ASN
67	PB	26	LEU
67	PB	30	TYR
68	QB	96	VAL
68	QB	126	VAL
69	RB	99	ASP
69	RB	127	ASN
70	SB	131	VAL
70	SB	145	THR
71	TB	4	VAL
71	TB	24	LYS
71	TB	78	ILE
71	TB	99	VAL

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Mol	Chain	Res	Type
71	TB	123	LEU
71	TB	134	ILE
72	UB	17	ILE
72	UB	18	HIS
72	UB	29	VAL
72	UB	68	THR
72	UB	72	GLU
72	UB	106	ILE
72	UB	107	GLU
73	VB	9	VAL
73	VB	47	ASN
74	WB	78	ARG
74	WB	105	THR
75	XB	17	ARG
75	XB	52	LEU
75	XB	61	GLN
75	XB	81	ILE
75	XB	105	PHE
75	XB	115	ILE
76	YB	51	THR
76	YB	75	ILE
77	ZB	32	LYS
77	ZB	47	LEU
77	ZB	88	LEU
78	AC	100	ARG
79	BC	43	ILE
79	BC	54	VAL
79	BC	80	ARG
80	CC	30	VAL
80	CC	38	THR
81	DC	24	CYS
81	DC	30	LEU
81	DC	42	CYS
83	FC	85	TYR
83	FC	108	VAL
84	GC	7	LEU
84	GC	11	LEU
84	GC	31	ILE
84	GC	38	LYS
84	GC	46	THR
84	GC	54	ILE
84	GC	64	HIS

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Mol	Chain	Res	Type
84	GC	68	ASP
84	GC	74	ASP
84	GC	90	TRP
84	GC	113	PHE
84	GC	120	ILE
84	GC	141	THR
84	GC	142	VAL
84	GC	162	ASN
84	GC	179	LEU
84	GC	185	LYS
84	GC	186	THR
84	GC	192	THR
84	GC	198	VAL
84	GC	256	ILE
84	GC	274	VAL
84	GC	275	ILE
84	GC	280	LYS
84	GC	297	THR
84	GC	306	LEU
85	HC	10	ILE
85	HC	64	LYS
85	HC	78	TRP
85	HC	87	VAL
85	HC	90	ILE
85	HC	120	VAL
85	HC	165	LYS
85	HC	177	TYR
85	HC	193	ILE
85	HC	208	MET
85	HC	212	LYS
85	HC	217	THR
85	HC	239	THR
85	HC	247	ARG
85	HC	290	LYS
85	HC	318	LYS
85	HC	347	LEU
85	HC	376	LYS
85	HC	387	LEU
85	HC	392	LYS
85	HC	398	ASP
85	HC	432	THR
85	HC	433	VAL

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Mol	Chain	Res	Type
85	HC	438	ILE
87	b	28	PHE
87	b	30	VAL
87	b	41	GLN
87	b	48	ARG
87	b	60	MET
87	b	75	LEU
87	b	89	VAL
87	b	105	ASN
87	b	112	ARG
87	b	121	VAL
87	b	135	THR
87	b	149	ARG
87	b	155	LEU
87	b	219	VAL
87	b	221	ASN
87	b	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	38	HIS
1	A	205	ASN
2	B	184	GLN
2	B	186	ASN
2	B	203	GLN
2	B	236	HIS
3	C	38	ASN
3	C	187	GLN
3	C	329	ASN
4	D	81	HIS
5	E	185	ASN
5	E	269	GLN
6	F	57	HIS
6	F	238	GLN
7	G	96	GLN
8	H	140	GLN
9	I	73	ASN
10	J	65	ASN
10	J	167	GLN
12	L	20	HIS

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Mol	Chain	Res	Type
12	L	48	GLN
13	M	32	GLN
14	N	26	GLN
14	N	42	ASN
15	O	145	HIS
16	P	7	HIS
16	P	188	ASN
17	Q	34	ASN
17	Q	141	HIS
17	Q	143	HIS
20	T	50	ASN
22	V	45	ASN
24	X	14	ASN
26	Z	60	HIS
26	Z	66	ASN
27	AA	6	ASN
30	DA	126	ASN
31	EA	55	ASN
35	IA	66	HIS
36	JA	31	ASN
37	KA	33	ASN
40	NA	19	GLN
42	PA	21	ASN
53	BB	75	GLN
53	BB	186	ASN
54	CB	136	HIS
55	DB	95	ASN
55	DB	139	GLN
55	DB	197	HIS
55	DB	245	HIS
56	EB	188	ASN
56	EB	224	ASN
57	FB	79	HIS
57	FB	101	HIS
58	GB	56	ASN
58	GB	177	GLN
58	GB	187	HIS
59	HB	335	GLN
60	IB	22	HIS
61	JB	75	ASN
61	JB	140	GLN
63	LB	19	ASN

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Mol	Chain	Res	Type
63	LB	39	ASN
63	LB	100	ASN
64	MB	19	GLN
64	MB	55	ASN
70	SB	125	HIS
71	TB	51	ASN
71	TB	85	ASN
74	WB	15	ASN
74	WB	91	ASN
74	WB	120	HIS
75	XB	16	HIS
75	XB	77	ASN
75	XB	92	ASN
77	ZB	112	ASN
78	AC	8	ASN
80	CC	7	GLN
80	CC	29	GLN
80	CC	45	ASN
84	GC	187	ASN
85	HC	136	HIS
85	HC	184	ASN
85	HC	200	ASN
85	HC	343	GLN
87	b	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	SA	75/76 (98%)	16 (21%)	3 (4%)
45	TA	75/76 (98%)	16 (21%)	0
46	UA	74/75 (98%)	26 (35%)	1 (1%)
47	VA	11/12 (91%)	3 (27%)	0
48	WA	3558/3584 (99%)	701 (19%)	20 (0%)
49	XA	118/120 (98%)	11 (9%)	0
50	YA	155/156 (99%)	33 (21%)	0
51	ZA	1707/1869 (91%)	317 (18%)	7 (0%)
All	All	5773/5968 (96%)	1123 (19%)	31 (0%)

All (1123) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	SA	9	A
44	SA	17	G
44	SA	19	C
44	SA	20	A
44	SA	21	A
44	SA	22	A
44	SA	46	G
44	SA	47	U
44	SA	48	C
44	SA	57	G
44	SA	58	A
44	SA	60	A
44	SA	61	C
44	SA	70	A
44	SA	73	A
44	SA	76	A
45	TA	6	G
45	TA	7	A
45	TA	13	C
45	TA	16	C
45	TA	17	U
45	TA	18	G
45	TA	19	A
45	TA	20	U
45	TA	22	G
45	TA	31	A
45	TA	34	U
45	TA	35	U
45	TA	46	G
45	TA	47	U
45	TA	58	A
45	TA	76	A
46	UA	8	U
46	UA	9	A
46	UA	16	C
46	UA	17	G
46	UA	18	G
46	UA	19	U
46	UA	20	U
46	UA	21	A
46	UA	24	A
46	UA	25	C
46	UA	26	G

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Mol	Chain	Res	Type
46	UA	31	C
46	UA	32	C
46	UA	33	U
46	UA	34	C
46	UA	40	C
46	UA	42	A
46	UA	43	A
46	UA	47	U
46	UA	48	C
46	UA	55	U
46	UA	59	A
46	UA	60	A
46	UA	63	G
46	UA	70	A
46	UA	76	A
47	VA	22	G
47	VA	24	U
47	VA	26	A
48	WA	12	A
48	WA	13	U
48	WA	17	A
48	WA	25	A
48	WA	39	A
48	WA	42	A
48	WA	48	G
48	WA	58	G
48	WA	59	A
48	WA	64	A
48	WA	65	A
48	WA	76	A
48	WA	91	G
48	WA	108	A
48	WA	110	C
48	WA	119	G
48	WA	120	A
48	WA	131	C
48	WA	134	G
48	WA	135	G
48	WA	136	C
48	WA	142	G
48	WA	143	C
48	WA	144	G

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Mol	Chain	Res	Type
48	WA	157	U
48	WA	159	C
48	WA	169	A
48	WA	170	C
48	WA	171	U
48	WA	172	C
48	WA	173	C
48	WA	179	G
48	WA	200	U
48	WA	201	C
48	WA	209	U
48	WA	210	C
48	WA	216	C
48	WA	217	C
48	WA	218	A
48	WA	219	G
48	WA	224	U
48	WA	225	G
48	WA	233	U
48	WA	234	G
48	WA	256	G
48	WA	258	G
48	WA	266	C
48	WA	280	G
48	WA	297	U
48	WA	306	A
48	WA	309	C
48	WA	315	G
48	WA	316	U
48	WA	322	C
48	WA	334	A
48	WA	340	C
48	WA	350	C
48	WA	363	A
48	WA	386	A
48	WA	387	G
48	WA	409	G
48	WA	410	A
48	WA	412	G
48	WA	413	G
48	WA	414	C
48	WA	417	G

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Mol	Chain	Res	Type
48	WA	449	C
48	WA	450	G
48	WA	452	A
48	WA	453	G
48	WA	454	U
48	WA	455	C
48	WA	462	G
48	WA	467	U
48	WA	468	U
48	WA	469	C
48	WA	470	A
48	WA	482	C
48	WA	483	G
48	WA	484	G
48	WA	485	U
48	WA	486	C
48	WA	490	C
48	WA	493	U
48	WA	494	G
48	WA	495	C
48	WA	497	G
48	WA	499	C
48	WA	500	G
48	WA	506	G
48	WA	511	U
48	WA	517	C
48	WA	519	G
48	WA	521	U
48	WA	522	C
48	WA	523	C
48	WA	524	C
48	WA	640	U
48	WA	641	C
48	WA	642	G
48	WA	645	G
48	WA	650	A
48	WA	661	G
48	WA	665	G
48	WA	667	G
48	WA	688	U
48	WA	696	G
48	WA	697	C

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Mol	Chain	Res	Type
48	WA	698	G
48	WA	699	G
48	WA	705	C
48	WA	706	G
48	WA	720	C
48	WA	732	G
48	WA	738	C
48	WA	739	C
48	WA	741	G
48	WA	744	G
48	WA	751	G
48	WA	752	U
48	WA	753	G
48	WA	756	U
48	WA	762	G
48	WA	763	G
48	WA	905	U
48	WA	907	C
48	WA	915	U
48	WA	917	A
48	WA	918	C
48	WA	919	A
48	WA	920	G
48	WA	921	C
48	WA	922	C
48	WA	926	C
48	WA	927	C
48	WA	929	C
48	WA	931	G
48	WA	936	A
48	WA	937	G
48	WA	938	C
48	WA	939	A
48	WA	940	G
48	WA	941	C
48	WA	946	C
48	WA	948	A
48	WA	949	A
48	WA	950	U
48	WA	964	G
48	WA	965	A
48	WA	966	G

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Mol	Chain	Res	Type
48	WA	971	A
48	WA	972	C
48	WA	978	C
48	WA	989	C
48	WA	991	C
48	WA	1072	G
48	WA	1076	G
48	WA	1078	C
48	WA	1079	G
48	WA	1085	C
48	WA	1099	C
48	WA	1101	A
48	WA	1102	C
48	WA	1103	C
48	WA	1104	G
48	WA	1175	G
48	WA	1177	G
48	WA	1178	C
48	WA	1186	C
48	WA	1190	A
48	WA	1197	C
48	WA	1200	G
48	WA	1201	G
48	WA	1202	G
48	WA	1216	C
48	WA	1217	G
48	WA	1221	C
48	WA	1225	G
48	WA	1243	C
48	WA	1244	A
48	WA	1250	C
48	WA	1252	C
48	WA	1253	C
48	WA	1255	G
48	WA	1257	A
48	WA	1258	A
48	WA	1259	A
48	WA	1260	G
48	WA	1261	G
48	WA	1262	G
48	WA	1265	A
48	WA	1268	G

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Mol	Chain	Res	Type
48	WA	1270	G
48	WA	1271	G
48	WA	1272	A
48	WA	1274	C
48	WA	1275	G
48	WA	1277	G
48	WA	1279	G
48	WA	1282	C
48	WA	1286	G
48	WA	1287	U
48	WA	1289	G
48	WA	1290	G
48	WA	1294	C
48	WA	1295	G
48	WA	1298	G
48	WA	1303	C
48	WA	1305	A
48	WA	1316	C
48	WA	1328	A
48	WA	1356	A
48	WA	1360	G
48	WA	1361	G
48	WA	1379	G
48	WA	1383	U
48	WA	1389	A
48	WA	1396	G
48	WA	1399	A
48	WA	1400	A
48	WA	1405	G
48	WA	1406	G
48	WA	1413	C
48	WA	1414	G
48	WA	1416	C
48	WA	1422	A
48	WA	1423	G
48	WA	1437	G
48	WA	1438	C
48	WA	1442	U
48	WA	1443	C
48	WA	1485	C
48	WA	1499	A
48	WA	1500	G

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Mol	Chain	Res	Type
48	WA	1504	G
48	WA	1525	A
48	WA	1527	A
48	WA	1536	A
48	WA	1549	A
48	WA	1568	C
48	WA	1580	U
48	WA	1593	U
48	WA	1598	U
48	WA	1599	G
48	WA	1604	U
48	WA	1614	G
48	WA	1626	G
48	WA	1627	G
48	WA	1633	A
48	WA	1635	G
48	WA	1636	A
48	WA	1640	A
48	WA	1642	C
48	WA	1643	G
48	WA	1656	G
48	WA	1663	C
48	WA	1678	C
48	WA	1679	U
48	WA	1693	G
48	WA	1696	C
48	WA	1733	C
48	WA	1736	G
48	WA	1743	G
48	WA	1744	A
48	WA	1757	C
48	WA	1758	U
48	WA	1763	G
48	WA	1765	C
48	WA	1766	G
48	WA	1768	A
48	WA	1772	A
48	WA	1782	A
48	WA	1783	U
48	WA	1789	A
48	WA	1806	A
48	WA	1807	A

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Mol	Chain	Res	Type
48	WA	1817	G
48	WA	1821	G
48	WA	1822	U
48	WA	1823	G
48	WA	1830	C
48	WA	1835	G
48	WA	1836	U
48	WA	1838	G
48	WA	1839	A
48	WA	1844	G
48	WA	1857	G
48	WA	1871	G
48	WA	1884	U
48	WA	1899	A
48	WA	1900	C
48	WA	1912	G
48	WA	1920	U
48	WA	1922	C
48	WA	1923	C
48	WA	1924	G
48	WA	1933	C
48	WA	1937	C
48	WA	1943	A
48	WA	1950	G
48	WA	1961	U
48	WA	1962	A
48	WA	1964	A
48	WA	1965	C
48	WA	1970	G
48	WA	1975	G
48	WA	1976	U
48	WA	1977	G
48	WA	1983	G
48	WA	1984	G
48	WA	1985	A
48	WA	1986	A
48	WA	1987	G
48	WA	1988	U
48	WA	1989	C
48	WA	1990	G
48	WA	1997	G
48	WA	1998	C

Continued on next page...

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Mol	Chain	Res	Type
48	WA	1999	U
48	WA	2003	G
48	WA	2004	A
48	WA	2005	G
48	WA	2007	G
48	WA	2010	U
48	WA	2012	A
48	WA	2013	C
48	WA	2022	U
48	WA	2023	G
48	WA	2027	A
48	WA	2028	A
48	WA	2033	C
48	WA	2034	U
48	WA	2048	G
48	WA	2049	A
48	WA	2050	U
48	WA	2054	G
48	WA	2057	G
48	WA	2058	G
48	WA	2064	C
48	WA	2071	A
48	WA	2086	U
48	WA	2095	G
48	WA	2096	C
48	WA	2097	A
48	WA	2099	A
48	WA	2102	G
48	WA	2103	A
48	WA	2104	G
48	WA	2106	A
48	WA	2107	A
48	WA	2108	G
48	WA	2109	A
48	WA	2110	G
48	WA	2118	C
48	WA	2261	G
48	WA	2262	C
48	WA	2268	C
48	WA	2269	U
48	WA	2270	A
48	WA	2277	G

Continued on next page...

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Mol	Chain	Res	Type
48	WA	2281	A
48	WA	2291	C
48	WA	2302	A
48	WA	2303	G
48	WA	2308	G
48	WA	2315	A
48	WA	2333	G
48	WA	2335	G
48	WA	2350	G
48	WA	2353	C
48	WA	2362	A
48	WA	2397	A
48	WA	2412	C
48	WA	2424	C
48	WA	2427	U
48	WA	2435	G
48	WA	2436	G
48	WA	2443	C
48	WA	2455	A
48	WA	2473	G
48	WA	2477	G
48	WA	2486	A
48	WA	2489	G
48	WA	2490	C
48	WA	2491	C
48	WA	2492	U
48	WA	2493	C
48	WA	2495	G
48	WA	2496	U
48	WA	2498	G
48	WA	2505	G
48	WA	2506	C
48	WA	2507	C
48	WA	2508	G
48	WA	2514	A
48	WA	2515	A
48	WA	2531	A
48	WA	2539	A
48	WA	2546	G
48	WA	2547	U
48	WA	2548	G
48	WA	2549	G

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Mol	Chain	Res	Type
48	WA	2556	U
48	WA	2561	G
48	WA	2567	A
48	WA	2568	G
48	WA	2577	U
48	WA	2585	C
48	WA	2588	G
48	WA	2591	C
48	WA	2603	A
48	WA	2627	U
48	WA	2629	C
48	WA	2640	G
48	WA	2655	C
48	WA	2662	A
48	WA	2664	G
48	WA	2671	C
48	WA	2672	C
48	WA	2678	A
48	WA	2688	G
48	WA	2689	U
48	WA	2697	A
48	WA	2698	A
48	WA	2705	G
48	WA	2708	G
48	WA	2709	U
48	WA	2710	U
48	WA	2711	C
48	WA	2712	C
48	WA	2713	G
48	WA	2723	G
48	WA	2726	G
48	WA	2727	A
48	WA	2728	G
48	WA	2737	G
48	WA	2742	U
48	WA	2745	A
48	WA	2746	A
48	WA	2760	G
48	WA	2761	G
48	WA	2771	U
48	WA	2789	A
48	WA	2790	U

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Mol	Chain	Res	Type
48	WA	2792	U
48	WA	2796	C
48	WA	2800	A
48	WA	2828	U
48	WA	2829	G
48	WA	2830	U
48	WA	2844	G
48	WA	2857	G
48	WA	3599	G
48	WA	3600	C
48	WA	3627	G
48	WA	3628	G
48	WA	3637	A
48	WA	3646	U
48	WA	3650	A
48	WA	3664	A
48	WA	3666	G
48	WA	3674	G
48	WA	3675	C
48	WA	3676	G
48	WA	3714	A
48	WA	3716	G
48	WA	3755	G
48	WA	3762	A
48	WA	3763	C
48	WA	3775	U
48	WA	3776	A
48	WA	3778	G
48	WA	3779	G
48	WA	3786	A
48	WA	3788	U
48	WA	3801	A
48	WA	3804	U
48	WA	3812	C
48	WA	3813	G
48	WA	3814	C
48	WA	3815	A
48	WA	3816	U
48	WA	3819	A
48	WA	3821	G
48	WA	3840	U
48	WA	3841	G

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Mol	Chain	Res	Type
48	WA	3842	U
48	WA	3879	A
48	WA	3880	C
48	WA	3881	G
48	WA	3891	G
48	WA	3894	U
48	WA	3899	G
48	WA	3900	G
48	WA	3903	A
48	WA	3908	A
48	WA	3909	G
48	WA	3910	A
48	WA	3916	U
48	WA	3917	U
48	WA	3918	G
48	WA	3919	A
48	WA	3940	G
48	WA	3941	G
48	WA	3945	A
48	WA	3948	G
48	WA	3949	A
48	WA	3950	C
48	WA	3953	G
48	WA	4066	C
48	WA	4075	A
48	WA	4078	G
48	WA	4088	G
48	WA	4090	C
48	WA	4093	G
48	WA	4097	G
48	WA	4099	G
48	WA	4100	A
48	WA	4101	G
48	WA	4102	C
48	WA	4110	G
48	WA	4111	G
48	WA	4113	U
48	WA	4114	C
48	WA	4118	C
48	WA	4119	U
48	WA	4120	U
48	WA	4121	C

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Mol	Chain	Res	Type
48	WA	4123	G
48	WA	4124	G
48	WA	4129	A
48	WA	4135	C
48	WA	4140	C
48	WA	4141	G
48	WA	4142	C
48	WA	4143	G
48	WA	4144	C
48	WA	4145	C
48	WA	4146	G
48	WA	4154	G
48	WA	4165	U
48	WA	4168	G
48	WA	4172	A
48	WA	4185	G
48	WA	4186	G
48	WA	4193	G
48	WA	4205	A
48	WA	4214	A
48	WA	4227	G
48	WA	4231	U
48	WA	4235	A
48	WA	4236	A
48	WA	4253	A
48	WA	4256	G
48	WA	4268	G
48	WA	4270	A
48	WA	4273	A
48	WA	4275	A
48	WA	4283	A
48	WA	4293	G
48	WA	4298	U
48	WA	4306	A
48	WA	4307	G
48	WA	4308	U
48	WA	4316	C
48	WA	4328	G
48	WA	4331	G
48	WA	4332	G
48	WA	4334	C
48	WA	4338	A

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Mol	Chain	Res	Type
48	WA	4351	C
48	WA	4352	C
48	WA	4356	U
48	WA	4375	G
48	WA	4379	G
48	WA	4380	A
48	WA	4381	A
48	WA	4389	C
48	WA	4395	G
48	WA	4396	A
48	WA	4397	U
48	WA	4398	A
48	WA	4417	A
48	WA	4421	U
48	WA	4422	U
48	WA	4424	A
48	WA	4440	U
48	WA	4446	C
48	WA	4450	G
48	WA	4451	A
48	WA	4466	A
48	WA	4468	C
48	WA	4477	G
48	WA	4502	U
48	WA	4514	U
48	WA	4515	A
48	WA	4521	C
48	WA	4522	G
48	WA	4524	G
48	WA	4526	G
48	WA	4531	G
48	WA	4533	U
48	WA	4550	A
48	WA	4562	C
48	WA	4569	G
48	WA	4575	G
48	WA	4577	G
48	WA	4579	U
48	WA	4586	A
48	WA	4588	G
48	WA	4592	A
48	WA	4601	A

Continued on next page...

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Mol	Chain	Res	Type
48	WA	4602	G
48	WA	4629	U
48	WA	4638	U
48	WA	4639	G
48	WA	4641	G
48	WA	4654	G
48	WA	4658	A
48	WA	4672	C
48	WA	4674	A
48	WA	4679	U
48	WA	4702	A
48	WA	4711	U
48	WA	4739	G
48	WA	4740	C
48	WA	4741	C
48	WA	4756	G
48	WA	4759	C
48	WA	4761	C
48	WA	4763	G
48	WA	4767	G
48	WA	4773	C
48	WA	4774	C
48	WA	4775	C
48	WA	4777	C
48	WA	4778	G
48	WA	4863	G
48	WA	4867	C
48	WA	4870	G
48	WA	4872	G
48	WA	4873	C
48	WA	4875	G
48	WA	4876	A
48	WA	4877	G
48	WA	4878	A
48	WA	4879	G
48	WA	4881	C
48	WA	4884	U
48	WA	4885	C
48	WA	4887	U
48	WA	4888	C
48	WA	4897	C
48	WA	4898	G

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Mol	Chain	Res	Type
48	WA	4904	C
48	WA	4905	G
48	WA	4906	G
48	WA	4914	G
48	WA	4915	G
48	WA	4916	G
48	WA	4917	G
48	WA	4922	C
48	WA	4924	C
48	WA	4926	C
48	WA	4927	U
48	WA	4928	C
48	WA	4930	C
48	WA	4939	C
48	WA	4941	C
48	WA	4942	C
48	WA	4945	A
48	WA	4946	C
48	WA	4951	G
48	WA	4952	U
48	WA	4953	G
48	WA	4959	C
48	WA	4960	C
48	WA	4962	G
48	WA	4965	G
48	WA	4968	A
48	WA	4978	U
48	WA	4981	A
48	WA	4991	U
48	WA	4992	C
48	WA	4995	G
48	WA	5008	U
48	WA	5009	A
48	WA	5018	A
48	WA	5019	G
48	WA	5024	U
48	WA	5040	A
48	WA	5041	U
48	WA	5042	U
48	WA	5043	G
48	WA	5049	C
48	WA	5052	C

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Mol	Chain	Res	Type
48	WA	5055	U
48	WA	5056	C
48	WA	5062	A
48	WA	5063	A
48	WA	5064	G
49	XA	7	G
49	XA	11	A
49	XA	21	G
49	XA	22	A
49	XA	33	U
49	XA	41	G
49	XA	53	U
49	XA	54	A
49	XA	64	G
49	XA	100	A
49	XA	110	G
50	YA	34	U
50	YA	35	C
50	YA	39	G
50	YA	59	A
50	YA	62	A
50	YA	63	U
50	YA	72	A
50	YA	75	G
50	YA	78	G
50	YA	80	A
50	YA	81	C
50	YA	82	A
50	YA	84	A
50	YA	85	U
50	YA	86	U
50	YA	90	C
50	YA	94	G
50	YA	95	A
50	YA	103	A
50	YA	105	C
50	YA	110	U
50	YA	111	U
50	YA	113	C
50	YA	114	G
50	YA	123	U
50	YA	124	U

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Mol	Chain	Res	Type
50	YA	125	C
50	YA	126	C
50	YA	137	A
50	YA	147	G
50	YA	150	C
50	YA	153	C
50	YA	155	C
51	ZA	3	C
51	ZA	4	C
51	ZA	25	A
51	ZA	33	G
51	ZA	41	G
51	ZA	44	U
51	ZA	45	A
51	ZA	46	A
51	ZA	56	G
51	ZA	58	C
51	ZA	59	U
51	ZA	67	C
51	ZA	68	A
51	ZA	70	G
51	ZA	72	C
51	ZA	75	G
51	ZA	76	U
51	ZA	79	A
51	ZA	99	A
51	ZA	103	A
51	ZA	113	G
51	ZA	115	U
51	ZA	116	U
51	ZA	126	G
51	ZA	143	U
51	ZA	155	G
51	ZA	160	U
51	ZA	162	C
51	ZA	173	A
51	ZA	178	C
51	ZA	180	G
51	ZA	181	A
51	ZA	182	C
51	ZA	183	G
51	ZA	184	G

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Mol	Chain	Res	Type
51	ZA	187	G
51	ZA	188	C
51	ZA	189	U
51	ZA	192	C
51	ZA	193	C
51	ZA	194	C
51	ZA	195	C
51	ZA	196	C
51	ZA	197	U
51	ZA	199	C
51	ZA	200	G
51	ZA	202	G
51	ZA	206	G
51	ZA	207	G
51	ZA	209	A
51	ZA	215	G
51	ZA	292	A
51	ZA	307	G
51	ZA	308	G
51	ZA	309	G
51	ZA	319	C
51	ZA	323	C
51	ZA	324	U
51	ZA	325	C
51	ZA	326	C
51	ZA	327	G
51	ZA	328	U
51	ZA	335	G
51	ZA	347	G
51	ZA	351	G
51	ZA	362	C
51	ZA	364	A
51	ZA	369	C
51	ZA	370	G
51	ZA	380	G
51	ZA	381	C
51	ZA	385	G
51	ZA	386	C
51	ZA	400	C
51	ZA	409	C
51	ZA	418	A
51	ZA	438	G

Continued on next page...

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Mol	Chain	Res	Type
51	ZA	441	C
51	ZA	448	A
51	ZA	449	A
51	ZA	450	C
51	ZA	464	A
51	ZA	466	G
51	ZA	471	G
51	ZA	472	C
51	ZA	473	A
51	ZA	474	G
51	ZA	476	A
51	ZA	482	G
51	ZA	485	A
51	ZA	487	U
51	ZA	492	C
51	ZA	493	A
51	ZA	508	A
51	ZA	531	A
51	ZA	532	C
51	ZA	536	A
51	ZA	541	U
51	ZA	544	G
51	ZA	547	G
51	ZA	548	C
51	ZA	549	C
51	ZA	554	A
51	ZA	555	A
51	ZA	556	U
51	ZA	559	G
51	ZA	560	A
51	ZA	561	A
51	ZA	562	U
51	ZA	564	A
51	ZA	568	C
51	ZA	576	A
51	ZA	583	A
51	ZA	587	A
51	ZA	588	G
51	ZA	590	A
51	ZA	591	U
51	ZA	594	A
51	ZA	595	U

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Mol	Chain	Res	Type
51	ZA	604	A
51	ZA	606	G
51	ZA	608	C
51	ZA	614	C
51	ZA	617	G
51	ZA	626	G
51	ZA	627	U
51	ZA	631	U
51	ZA	643	A
51	ZA	644	G
51	ZA	655	A
51	ZA	660	C
51	ZA	668	A
51	ZA	669	A
51	ZA	671	A
51	ZA	672	A
51	ZA	673	G
51	ZA	684	G
51	ZA	689	U
51	ZA	752	G
51	ZA	753	C
51	ZA	754	G
51	ZA	799	U
51	ZA	809	A
51	ZA	821	G
51	ZA	822	U
51	ZA	834	C
51	ZA	835	C
51	ZA	840	C
51	ZA	841	G
51	ZA	845	G
51	ZA	847	A
51	ZA	859	G
51	ZA	869	A
51	ZA	870	A
51	ZA	871	U
51	ZA	872	A
51	ZA	873	G
51	ZA	875	A
51	ZA	878	G
51	ZA	885	U
51	ZA	886	A

Continued on next page...

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Mol	Chain	Res	Type
51	ZA	887	U
51	ZA	888	U
51	ZA	889	U
51	ZA	890	U
51	ZA	891	G
51	ZA	892	U
51	ZA	894	G
51	ZA	898	U
51	ZA	901	G
51	ZA	905	C
51	ZA	907	G
51	ZA	913	A
51	ZA	914	U
51	ZA	920	A
51	ZA	933	G
51	ZA	934	G
51	ZA	943	U
51	ZA	971	G
51	ZA	985	G
51	ZA	990	A
51	ZA	992	A
51	ZA	999	G
51	ZA	1008	A
51	ZA	1017	U
51	ZA	1023	A
51	ZA	1061	U
51	ZA	1062	A
51	ZA	1083	A
51	ZA	1085	C
51	ZA	1115	U
51	ZA	1116	C
51	ZA	1117	C
51	ZA	1118	C
51	ZA	1126	G
51	ZA	1133	A
51	ZA	1138	C
51	ZA	1148	A
51	ZA	1149	A
51	ZA	1153	C
51	ZA	1154	U
51	ZA	1195	A
51	ZA	1207	G

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Mol	Chain	Res	Type
51	ZA	1208	A
51	ZA	1215	C
51	ZA	1220	A
51	ZA	1224	G
51	ZA	1242	U
51	ZA	1251	A
51	ZA	1253	A
51	ZA	1256	G
51	ZA	1257	G
51	ZA	1259	A
51	ZA	1274	G
51	ZA	1275	G
51	ZA	1282	A
51	ZA	1285	G
51	ZA	1286	G
51	ZA	1298	G
51	ZA	1299	A
51	ZA	1300	U
51	ZA	1301	A
51	ZA	1302	G
51	ZA	1303	C
51	ZA	1312	G
51	ZA	1313	A
51	ZA	1342	U
51	ZA	1348	G
51	ZA	1354	G
51	ZA	1371	U
51	ZA	1372	U
51	ZA	1378	A
51	ZA	1396	A
51	ZA	1397	U
51	ZA	1405	A
51	ZA	1406	G
51	ZA	1416	C
51	ZA	1418	C
51	ZA	1419	C
51	ZA	1420	G
51	ZA	1421	A
51	ZA	1422	G
51	ZA	1423	C
51	ZA	1424	G
51	ZA	1428	G

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Mol	Chain	Res	Type
51	ZA	1433	C
51	ZA	1434	C
51	ZA	1435	C
51	ZA	1436	C
51	ZA	1437	C
51	ZA	1438	A
51	ZA	1454	A
51	ZA	1466	G
51	ZA	1475	G
51	ZA	1476	A
51	ZA	1477	U
51	ZA	1489	A
51	ZA	1490	G
51	ZA	1497	G
51	ZA	1498	A
51	ZA	1509	U
51	ZA	1521	C
51	ZA	1522	A
51	ZA	1531	A
51	ZA	1533	A
51	ZA	1535	U
51	ZA	1544	C
51	ZA	1548	G
51	ZA	1551	U
51	ZA	1552	G
51	ZA	1553	C
51	ZA	1556	A
51	ZA	1557	C
51	ZA	1560	U
51	ZA	1567	G
51	ZA	1570	G
51	ZA	1578	U
51	ZA	1580	A
51	ZA	1585	U
51	ZA	1587	G
51	ZA	1588	A
51	ZA	1601	A
51	ZA	1605	G
51	ZA	1606	G
51	ZA	1607	A
51	ZA	1621	U
51	ZA	1623	A

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Mol	Chain	Res	Type
51	ZA	1648	G
51	ZA	1665	G
51	ZA	1698	C
51	ZA	1699	A
51	ZA	1721	U
51	ZA	1722	G
51	ZA	1726	G
51	ZA	1744	G
51	ZA	1745	A
51	ZA	1748	G
51	ZA	1753	C
51	ZA	1757	G
51	ZA	1773	C
51	ZA	1774	C
51	ZA	1780	G
51	ZA	1783	C
51	ZA	1784	G
51	ZA	1825	A
51	ZA	1829	G
51	ZA	1831	A
51	ZA	1835	A
51	ZA	1836	G
51	ZA	1838	U
51	ZA	1849	G
51	ZA	1851	A
51	ZA	1861	G
51	ZA	1862	G
51	ZA	1863	A
51	ZA	1865	C
51	ZA	1869	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	SA	20	A
44	SA	21	A
44	SA	57	G
46	UA	19	U
48	WA	12	A
48	WA	385	A
48	WA	505	G
48	WA	971	A

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Mol	Chain	Res	Type
48	WA	1293	G
48	WA	1635	G
48	WA	1677	C
48	WA	1806	A
48	WA	1820	G
48	WA	1963	G
48	WA	2048	G
48	WA	2268	C
48	WA	2697	A
48	WA	3627	G
48	WA	4117	G
48	WA	4450	G
48	WA	4701	U
48	WA	4886	G
48	WA	4951	G
48	WA	5040	A
51	ZA	24	C
51	ZA	553	U
51	ZA	561	A
51	ZA	752	G
51	ZA	870	A
51	ZA	874	G
51	ZA	1137	U

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 304 ligands modelled in this entry, 299 are monoatomic - leaving 5 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	$\# Z > 2$
96	SER	HC	603	-	4,5,6	0.57	0	1,5,7	0.55	0
91	5GP	UA	101	-	26,26,26	1.00	2 (7%)	39,40,40	1.72	7 (17%)
95	GTP	HC	601	89	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
92	ANM	WA	5275	94	20,20,20	4.09	7 (35%)	24,27,27	1.42	1 (4%)
93	SPD	WA	5276	-	9,9,9	0.28	0	8,8,8	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	SER	HC	603	-	-	0/2/4/6	-
91	5GP	UA	101	-	-	1/10/26/26	0/3/3/3
95	GTP	HC	601	89	-	8/22/38/38	0/3/3/3
92	ANM	WA	5275	94	-	6/10/23/23	0/2/2/2
93	SPD	WA	5276	-	-	0/7/7/7	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	WA	5275	ANM	C3-C2	-11.90	1.32	1.53
92	WA	5275	ANM	C16-N1	-8.84	1.30	1.47
92	WA	5275	ANM	C2-C16	7.41	1.68	1.53
92	WA	5275	ANM	C4-C3	3.96	1.58	1.53
92	WA	5275	ANM	C4-N1	3.86	1.60	1.47
92	WA	5275	ANM	O2-C5	3.58	1.43	1.35
91	UA	101	5GP	C6-N1	-2.61	1.34	1.38
92	WA	5275	ANM	C6-C5	2.43	1.57	1.49
95	HC	601	GTP	C2-N3	2.16	1.38	1.33
91	UA	101	5GP	C5-N7	-2.05	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	UA	101	5GP	C5-C4-N3	-5.86	119.07	128.39
92	WA	5275	ANM	O2-C5-C6	5.44	120.79	111.09
95	HC	601	GTP	C5-C4-N3	-5.34	119.90	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
95	HC	601	GTP	C2-N3-C4	4.76	120.50	112.30
91	UA	101	5GP	C2-N3-C4	4.51	120.07	112.30
91	UA	101	5GP	N9-C4-N3	3.70	133.35	125.95
95	HC	601	GTP	N9-C4-N3	3.49	132.94	125.95
95	HC	601	GTP	C2-N1-C6	-3.00	119.67	125.11
95	HC	601	GTP	C5-C6-N1	2.53	119.69	113.25
91	UA	101	5GP	C5-C6-N1	2.46	119.51	113.25
95	HC	601	GTP	O6-C6-C5	-2.45	120.08	126.53
95	HC	601	GTP	N9-C8-N7	-2.42	108.91	113.40
95	HC	601	GTP	C8-N7-C5	2.41	108.55	104.26
91	UA	101	5GP	C2-N1-C6	-2.41	120.75	125.11
91	UA	101	5GP	O6-C6-C5	-2.40	120.21	126.53
91	UA	101	5GP	N9-C8-N7	-2.20	109.31	113.40
95	HC	601	GTP	C3'-C2'-C1'	2.15	105.52	101.46

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
95	HC	601	GTP	C5'-O5'-PA-O3A
95	HC	601	GTP	C5'-O5'-PA-O1A
95	HC	601	GTP	C5'-O5'-PA-O2A
92	WA	5275	ANM	C6-C5-O2-C2
92	WA	5275	ANM	O3-C5-O2-C2
92	WA	5275	ANM	C1-C9-O1-C14
92	WA	5275	ANM	C10-C9-O1-C14
95	HC	601	GTP	C3'-C4'-C5'-O5'
95	HC	601	GTP	O4'-C4'-C5'-O5'
91	UA	101	5GP	O4'-C4'-C5'-O5'
92	WA	5275	ANM	C11-C12-C15-C16
92	WA	5275	ANM	C13-C12-C15-C16
95	HC	601	GTP	C4'-C5'-O5'-PA
95	HC	601	GTP	PA-O3A-PB-O1B
95	HC	601	GTP	PA-O3A-PB-O2B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

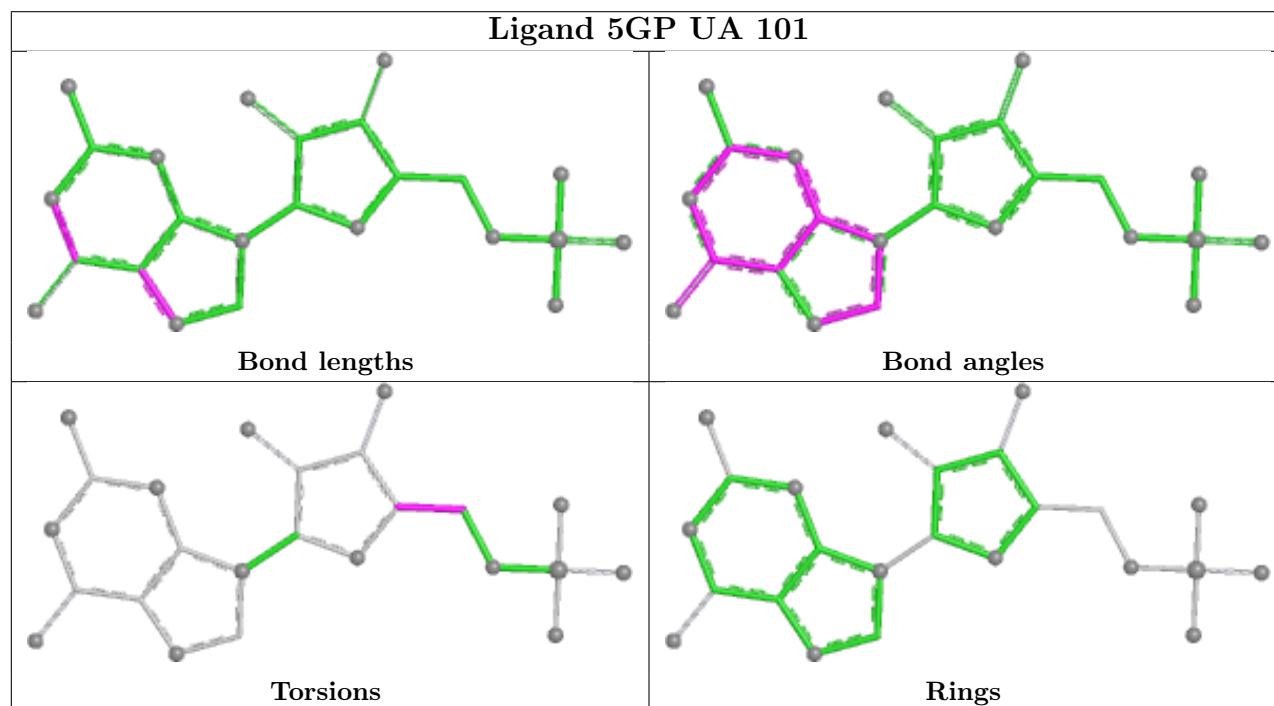
Mol	Chain	Res	Type	Clashes	Symm-Clashes
96	HC	603	SER	1	0
95	HC	601	GTP	1	0

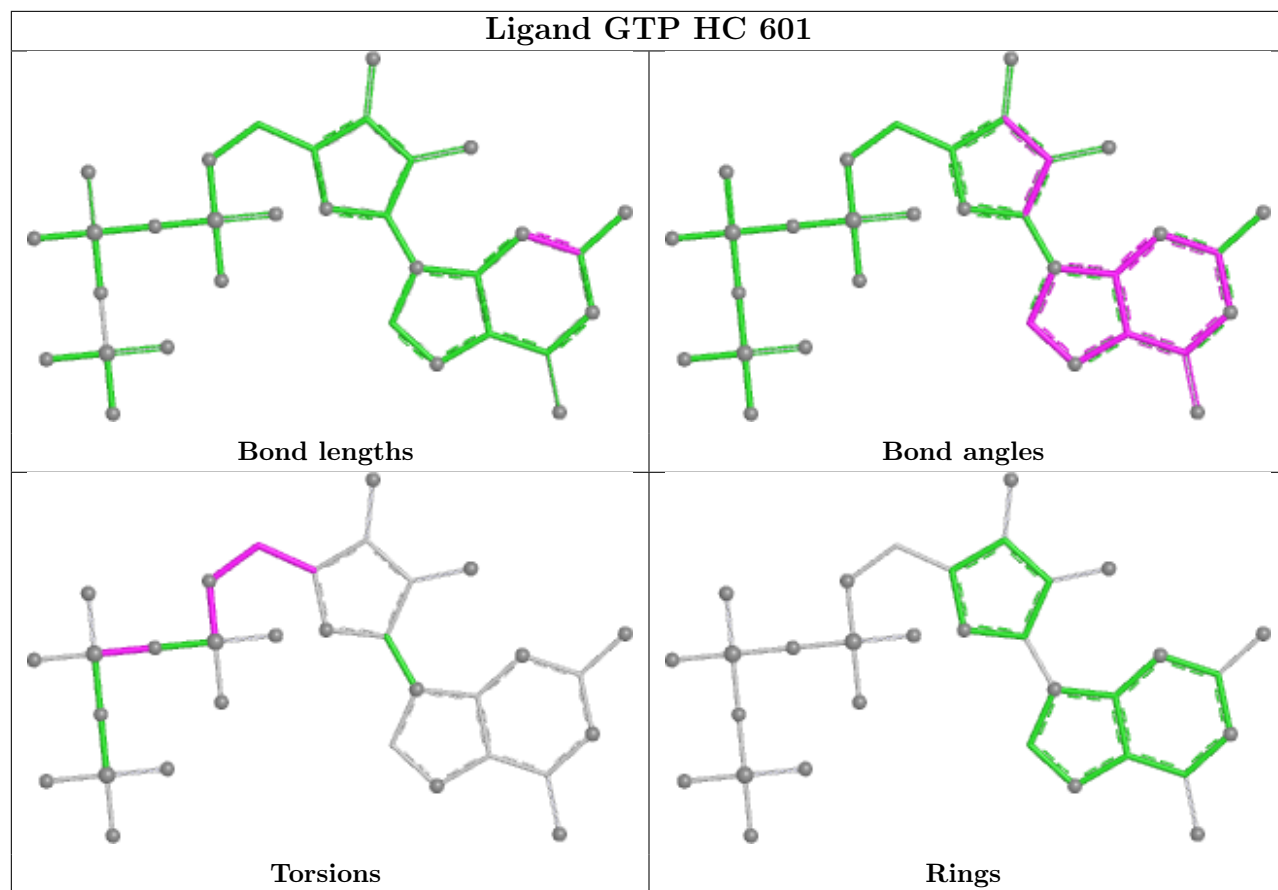
Continued on next page...

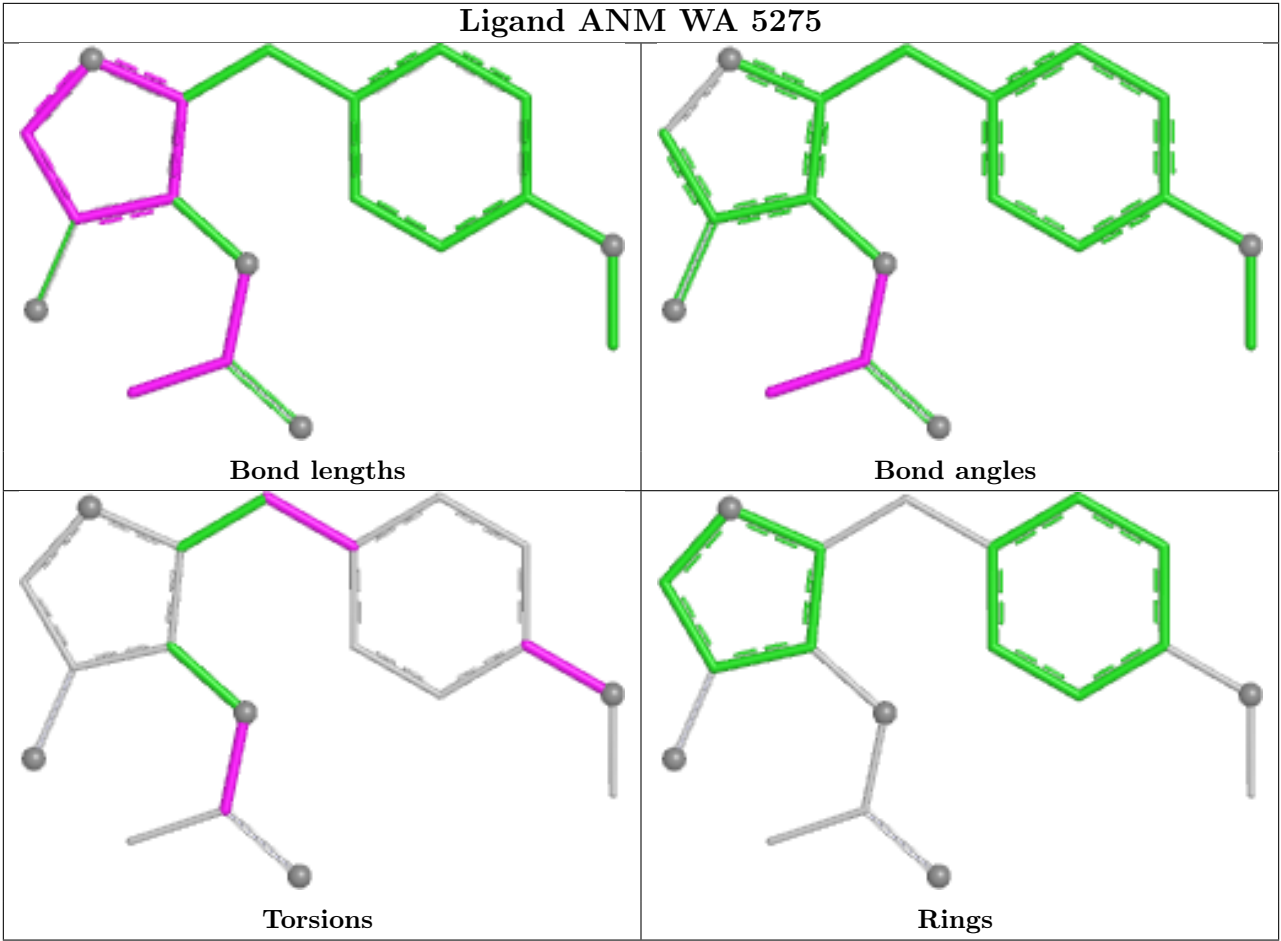
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	WA	5275	ANM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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
48	WA	20

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	WA	2118:C	O3'	2260:C	P	36.21
1	WA	1225:G	O3'	1239:G	P	21.47
1	WA	4103:C	O3'	4109:G	P	19.88
1	WA	524:C	O3'	639:G	P	17.34
1	WA	996:C	O3'	1070:G	P	16.49

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	WA	763:G	O3'	904:C	P	15.18
1	WA	5024:U	O3'	5030:G	P	13.76
1	WA	1366:U	O3'	1370:A	P	13.37
1	WA	1698:C	O3'	1722:C	P	12.75
1	WA	4779:C	O3'	4861:C	P	11.96
1	WA	4731:A	O3'	4737:G	P	11.92
1	WA	2904:G	O3'	3598:A	P	11.60
1	WA	1186:C	O3'	1189:C	P	11.03
1	WA	3954:A	O3'	4063:C	P	10.76
1	WA	182:G	O3'	189:G	P	10.22
1	WA	513:U	O3'	516:C	P	8.57
1	WA	4742:G	O3'	4745:G	P	8.29
1	WA	1106:U	O3'	1174:G	P	5.55
1	WA	501:G	O3'	505:G	P	5.40
1	WA	4901:G	O3'	4904:C	P	3.37

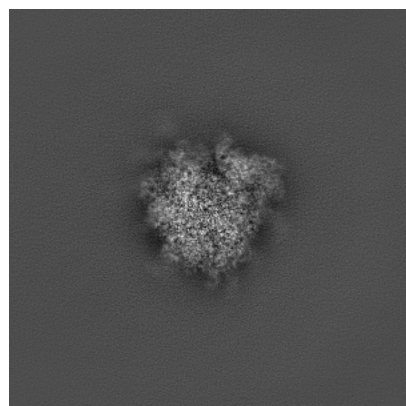
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43565. These allow visual inspection of the internal detail of the map and identification of artifacts.

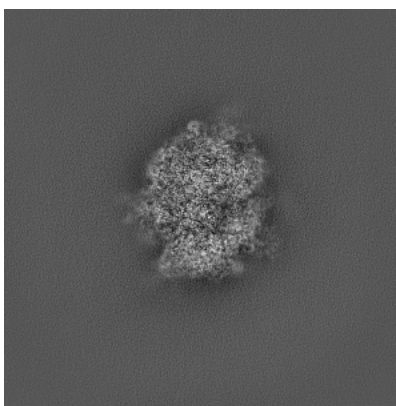
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

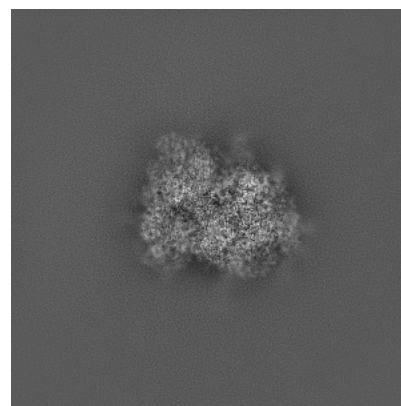
6.1.1 Primary map



X

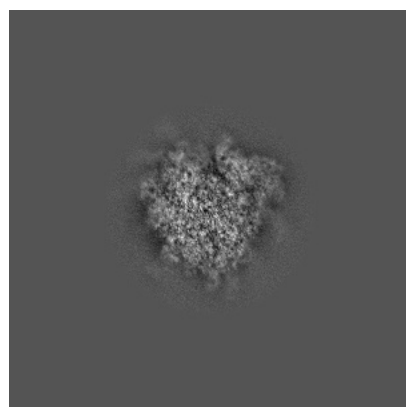


Y

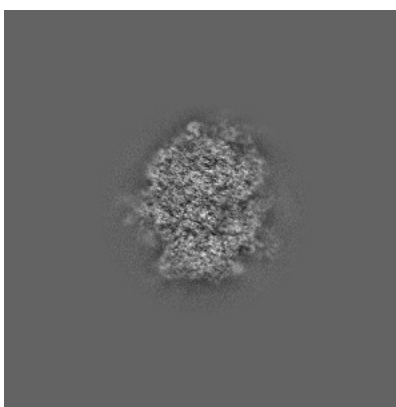


Z

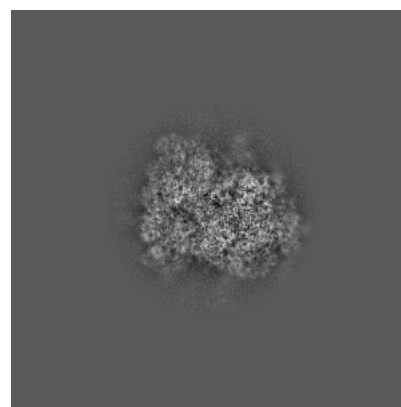
6.1.2 Raw map



X



Y

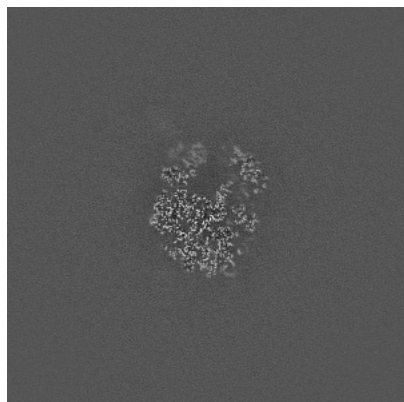


Z

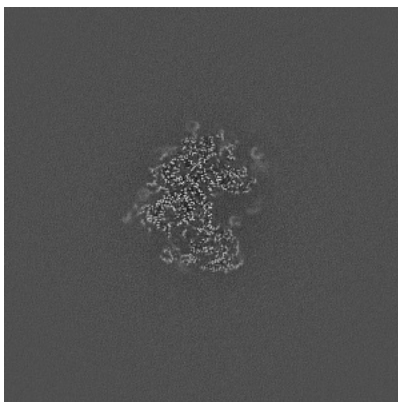
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

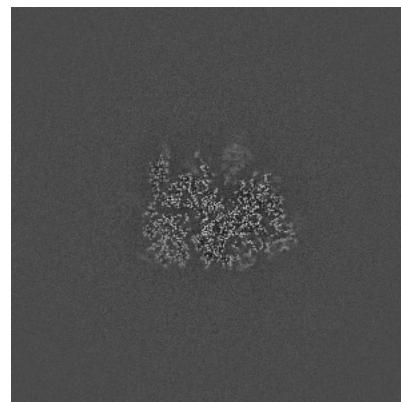
6.2.1 Primary map



X Index: 324

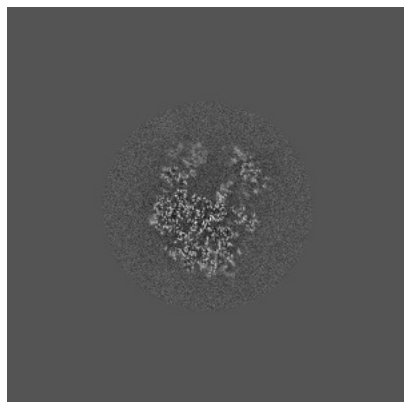


Y Index: 324

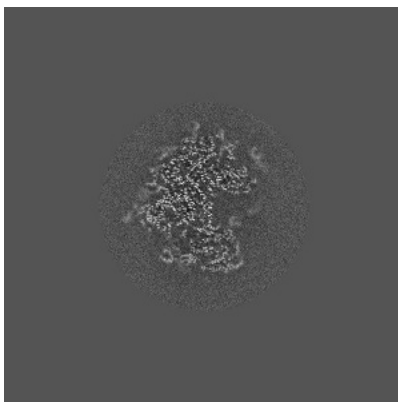


Z Index: 324

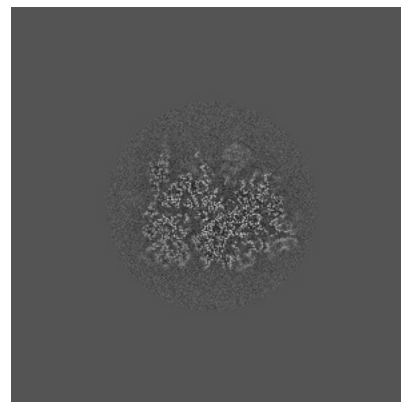
6.2.2 Raw map



X Index: 324



Y Index: 324

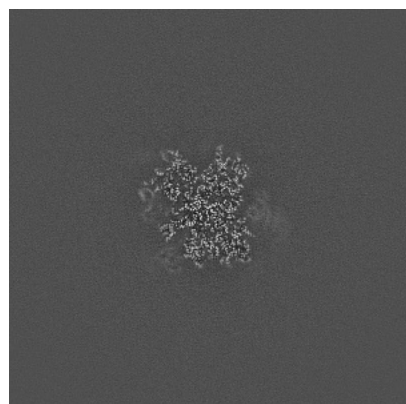


Z Index: 324

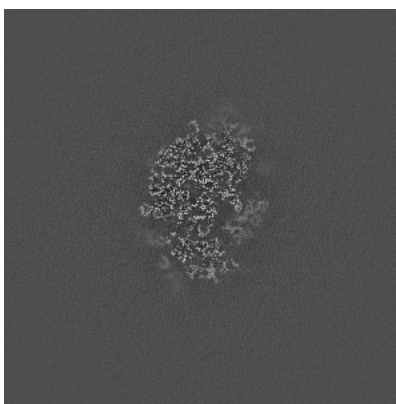
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

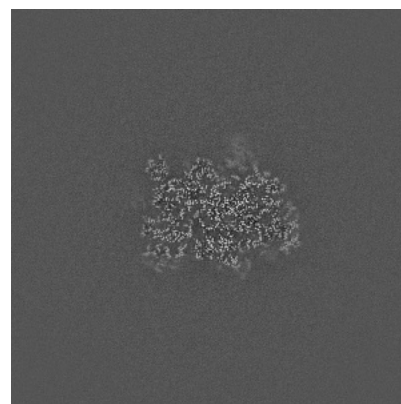
6.3.1 Primary map



X Index: 376

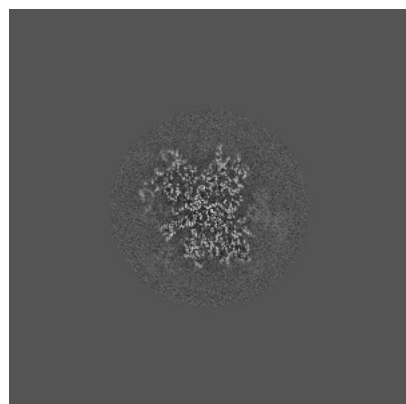


Y Index: 300

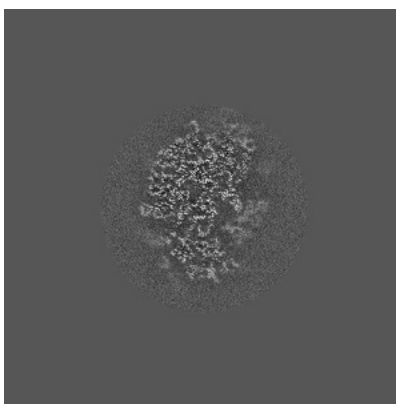


Z Index: 313

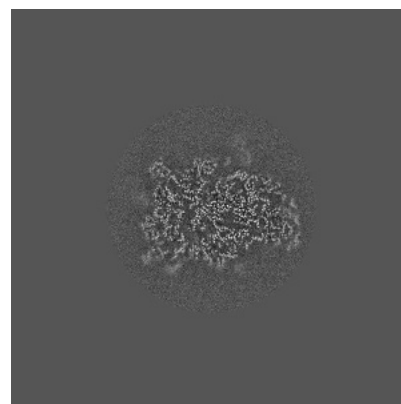
6.3.2 Raw map



X Index: 376



Y Index: 300



Z Index: 306

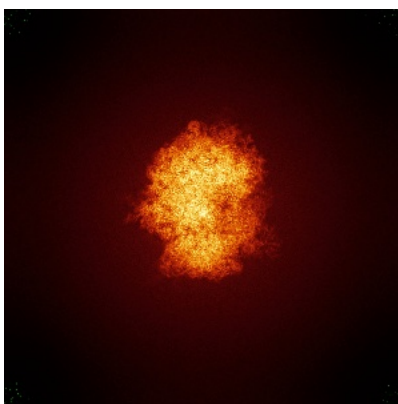
The images above show the largest variance slices of the map in three orthogonal directions.

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

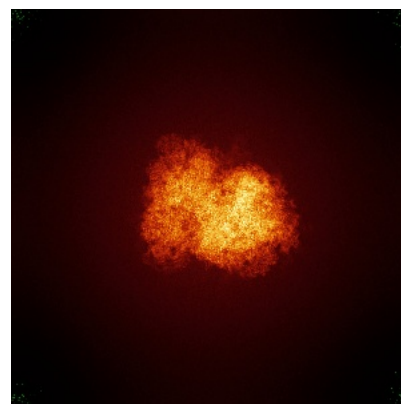
6.4.1 Primary map



X

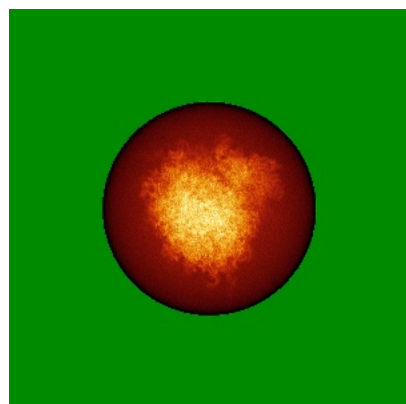


Y

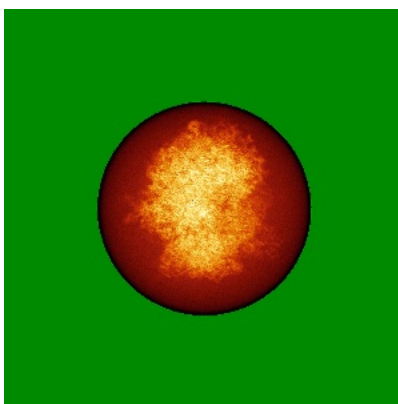


Z

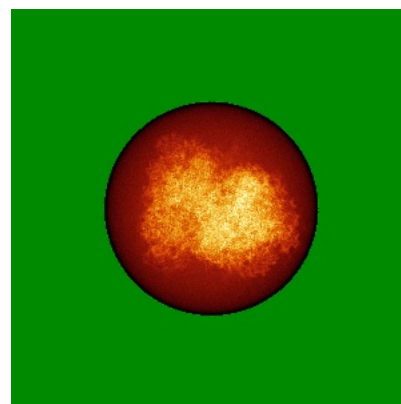
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



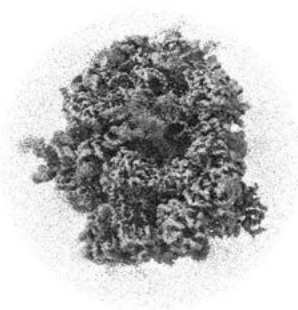
Z

The images above show the 3D surface view of the map at the recommended contour level 4.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

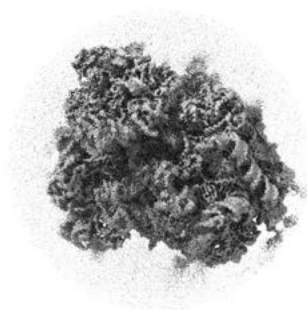
6.5.2 Raw map



X



Y



Z

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

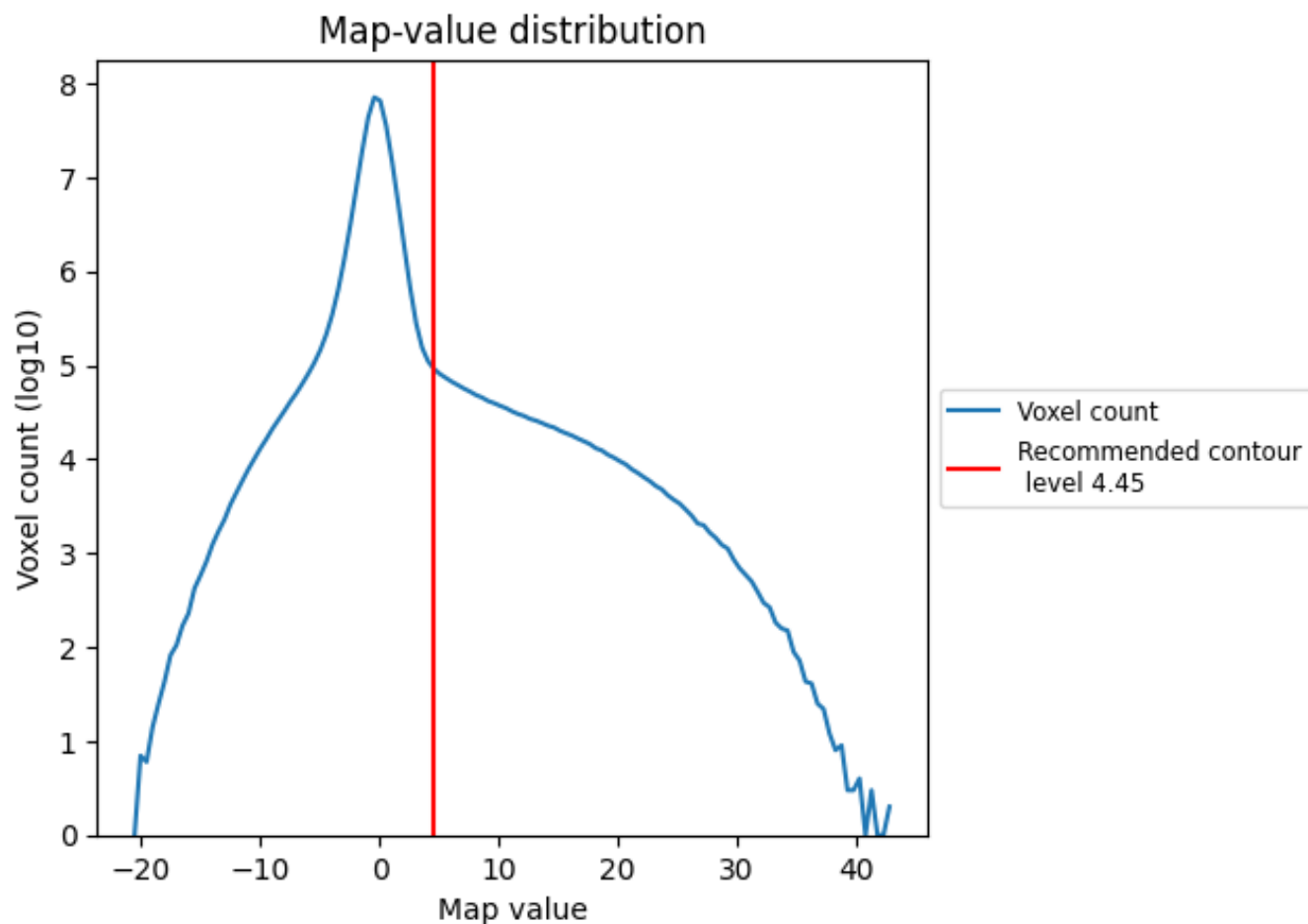
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

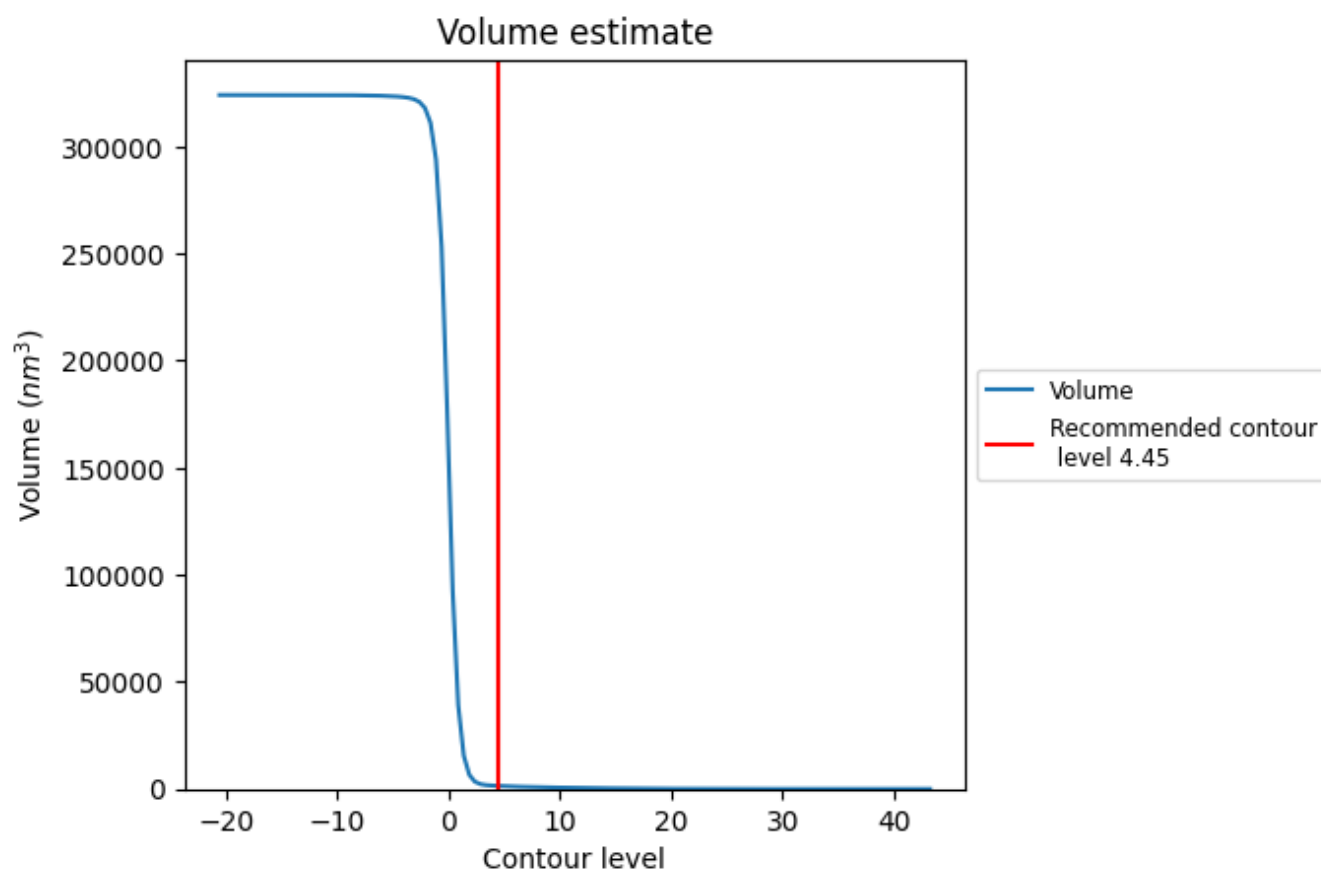
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

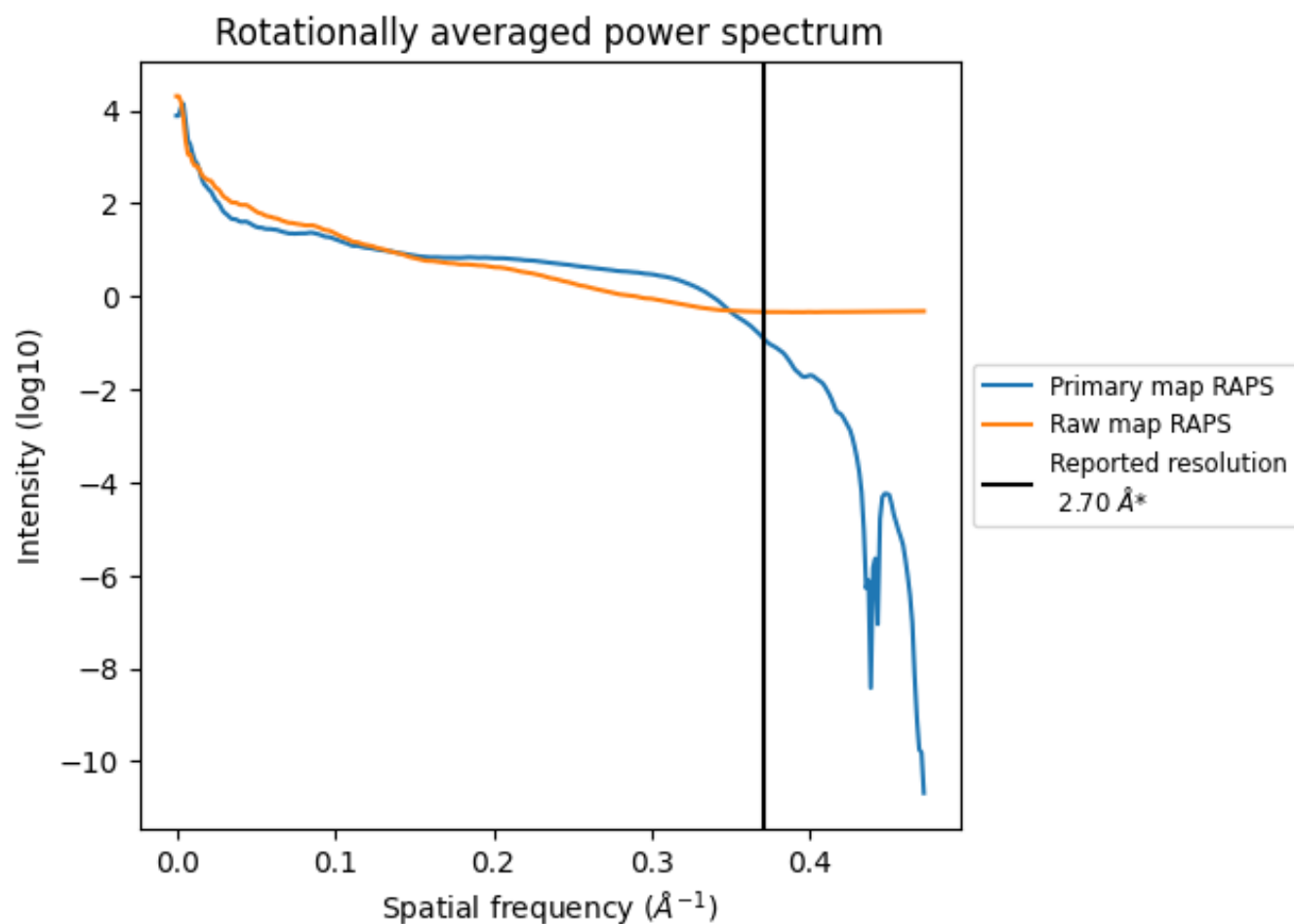
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1435 nm^3 ; this corresponds to an approximate mass of 1296 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 ⓘ

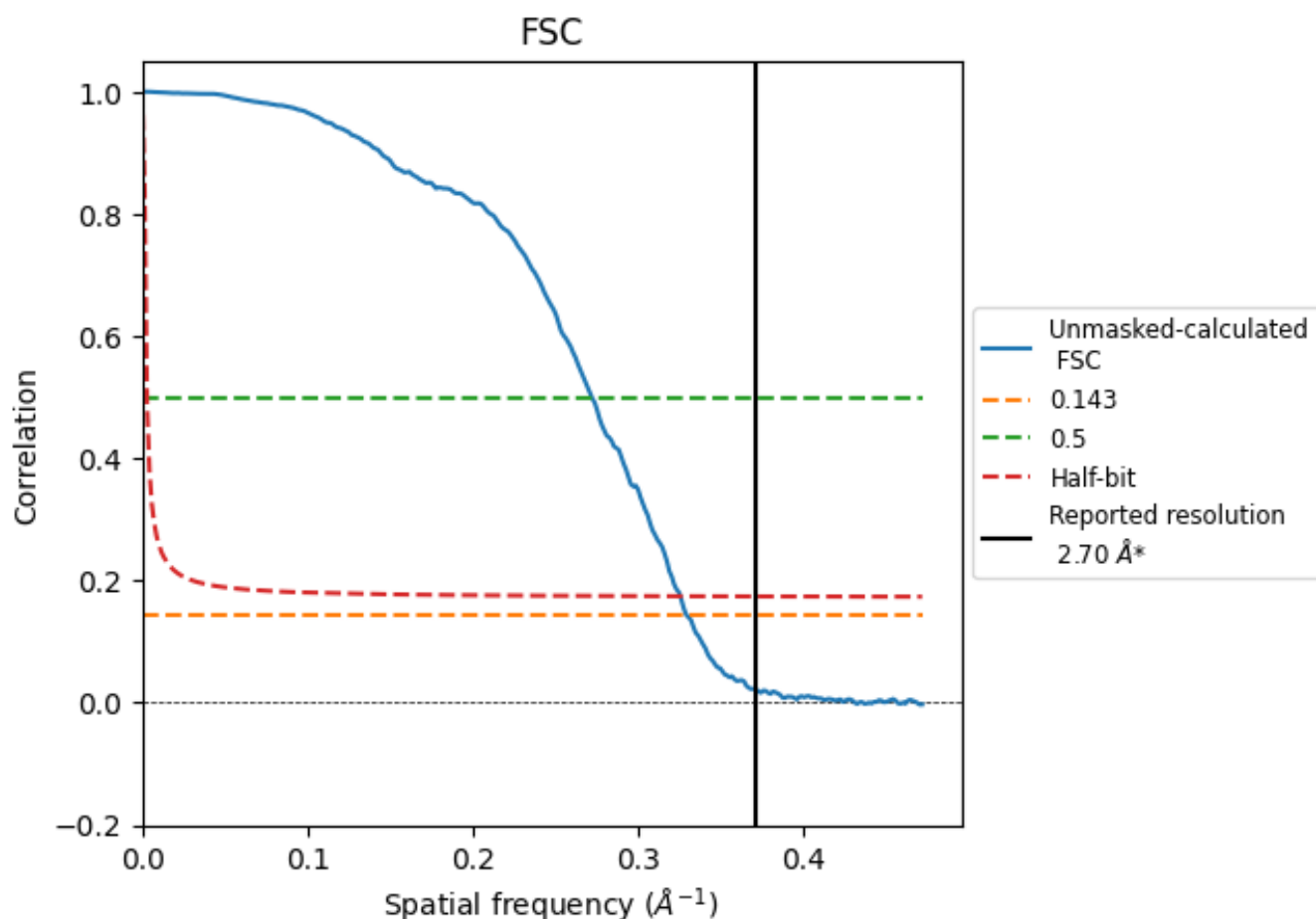


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

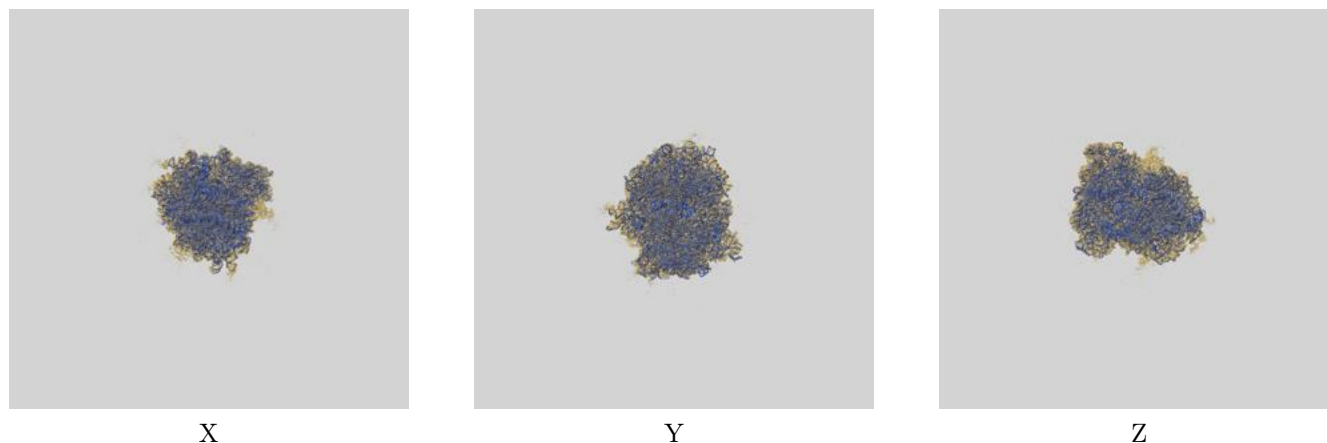
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.68	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

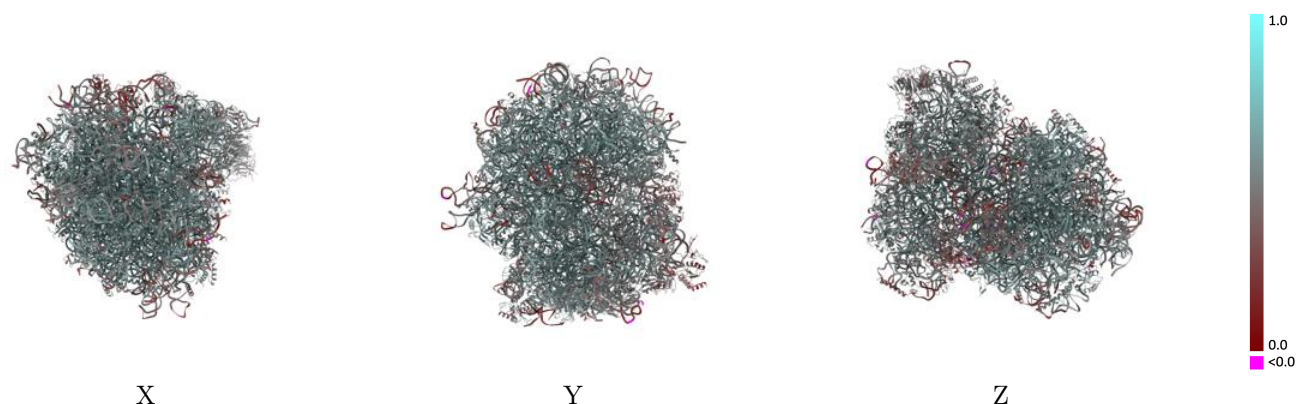
This section contains information regarding the fit between EMDB map EMD-43565 and PDB model 8VVQ. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



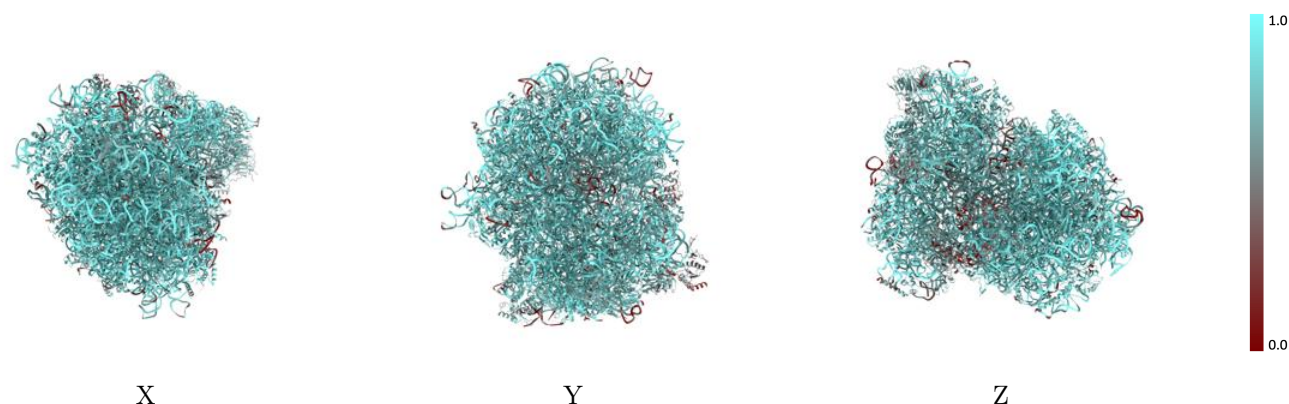
The images above show the 3D surface view of the map at the recommended contour level 4.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



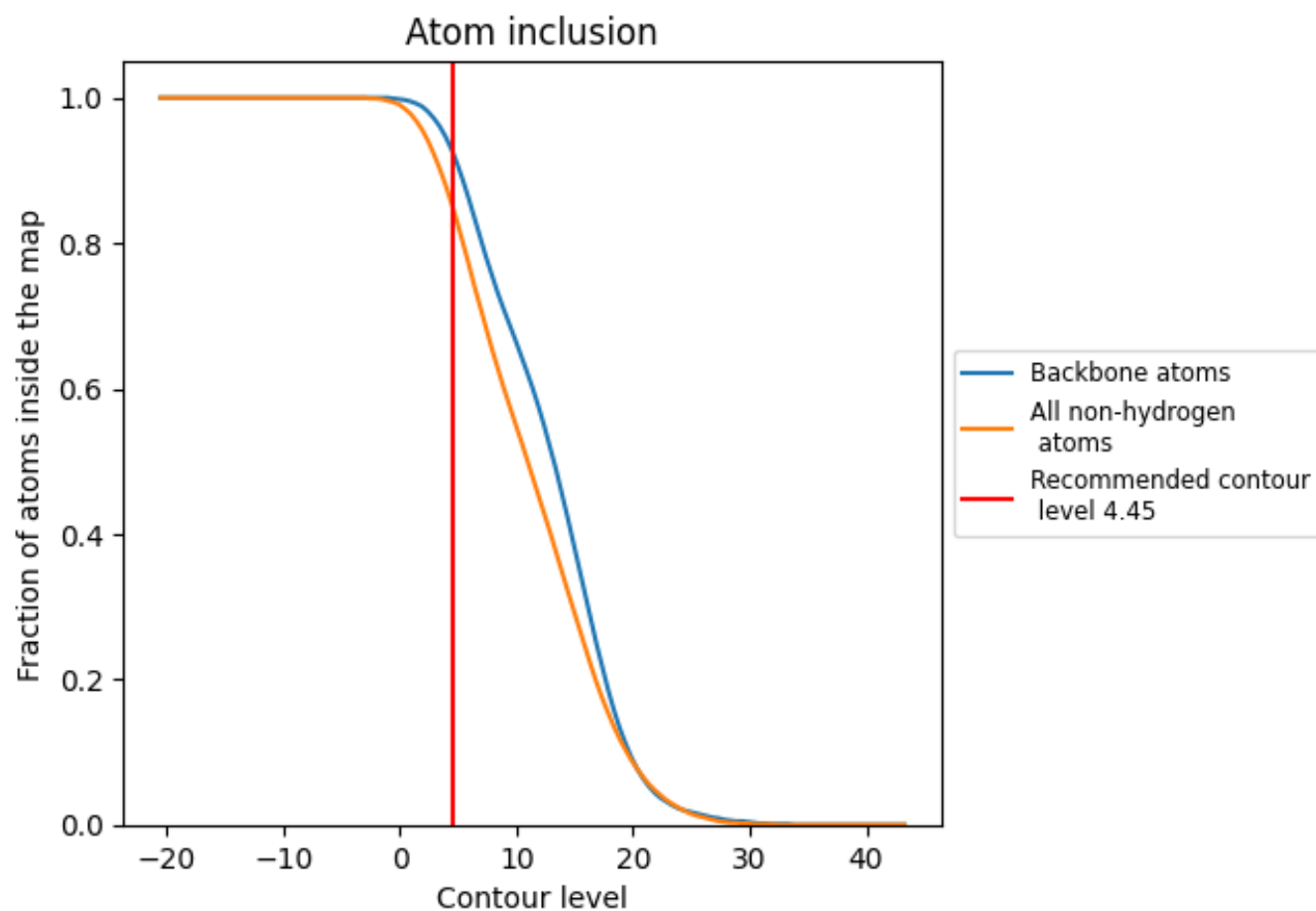
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (4.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.5290
A	 0.8880	 0.5930
AA	 0.7620	 0.5140
AB	 0.8220	 0.5320
AC	 0.8260	 0.5500
B	 0.8820	 0.5730
BA	 0.8540	 0.5550
BB	 0.8130	 0.5430
BC	 0.7930	 0.5350
C	 0.8580	 0.5690
CA	 0.8500	 0.5620
CB	 0.8270	 0.5490
CC	 0.7150	 0.5110
D	 0.8600	 0.5410
DA	 0.8740	 0.5810
DB	 0.7200	 0.4900
DC	 0.8260	 0.5270
E	 0.8230	 0.5350
EA	 0.8860	 0.5920
EB	 0.8200	 0.5400
EC	 0.7020	 0.4920
F	 0.8550	 0.5720
FA	 0.8450	 0.5670
FB	 0.7740	 0.5110
FC	 0.4870	 0.3670
G	 0.8150	 0.5250
GA	 0.8310	 0.5460
GB	 0.7350	 0.4850
GC	 0.6700	 0.4450
H	 0.8280	 0.5520
HA	 0.8330	 0.5330
HB	 0.7220	 0.4850
HC	 0.5500	 0.4120
I	 0.8570	 0.5670
IA	 0.8960	 0.5760



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Chain	Atom inclusion	Q-score
IB	 0.8060	 0.5340
IC	 0.6000	 0.5270
J	 0.8100	 0.5270
JA	 0.7680	 0.5090
JB	 0.8120	 0.5190
K	 0.8370	 0.5470
KA	 0.8690	 0.5610
KB	 0.7240	 0.4750
L	 0.8440	 0.5460
LA	 0.8750	 0.5650
LB	 0.8530	 0.5720
M	 0.9010	 0.5950
MA	 0.8620	 0.5710
MB	 0.4060	 0.2930
N	 0.8740	 0.5720
NA	 0.8720	 0.5840
NB	 0.8470	 0.5550
O	 0.8610	 0.5760
OA	 0.8550	 0.5850
OB	 0.8100	 0.5460
P	 0.8730	 0.5830
PA	 0.8760	 0.5640
PB	 0.6940	 0.4670
Q	 0.8450	 0.5470
QB	 0.7740	 0.5070
R	 0.8810	 0.5710
RA	 0.2760	 0.2790
RB	 0.7380	 0.4880
S	 0.8500	 0.5710
SA	 0.8180	 0.5140
SB	 0.7750	 0.4940
T	 0.7770	 0.4970
TA	 0.4320	 0.3360
TB	 0.7650	 0.4960
U	 0.8380	 0.5760
UA	 0.6010	 0.3440
UB	 0.6800	 0.4790
V	 0.7460	 0.4990
VA	 0.6670	 0.4600
VB	 0.8050	 0.5340
W	 0.8310	 0.5520
WA	 0.9200	 0.5420

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Chain	Atom inclusion	Q-score
WB	 0.8450	 0.5600
X	 0.8500	 0.5570
XA	 0.9740	 0.5740
XB	 0.8330	 0.5660
Y	 0.8670	 0.5560
YA	 0.9100	 0.5460
YB	 0.8050	 0.5120
Z	 0.8900	 0.5830
ZA	 0.8910	 0.5200
ZB	 0.6640	 0.4740
b	 0.3560	 0.2940
c	 0.0460	 0.3160