



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 04:21 PM EDT

PDB ID : 8VVP / pdb_00008vvp
EMDB ID : EMD-43564
Title : Codon sampling state obtained from Anisomycin-treated mammalian ribosomes
Authors : Loerch, S.; Petrossian, E.; Smith, P.R.; Campbell, Z.T.
Deposited on : 2024-01-31
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

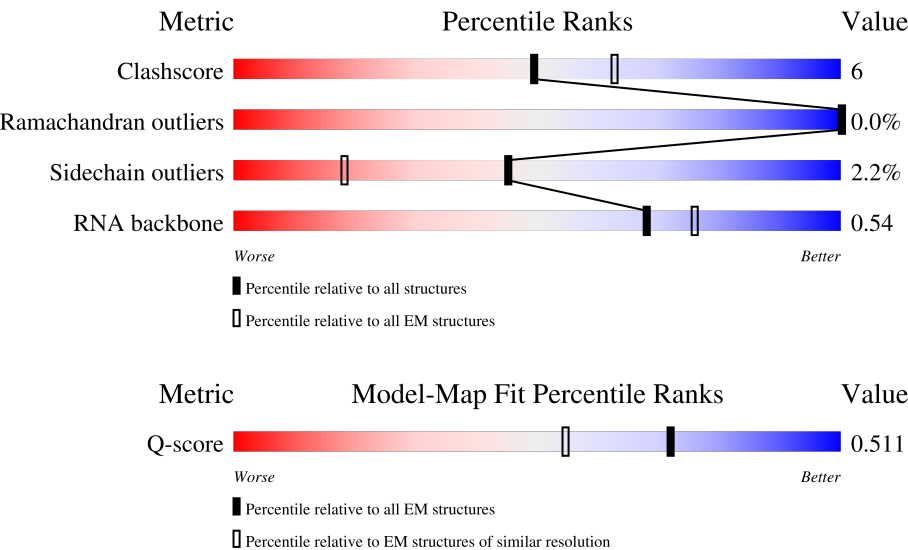
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



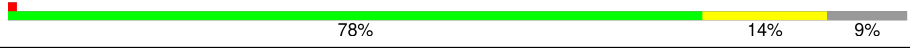
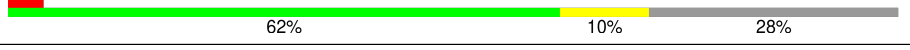
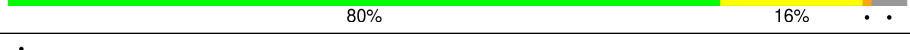
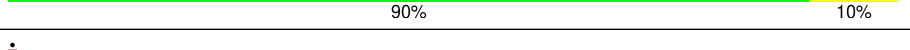
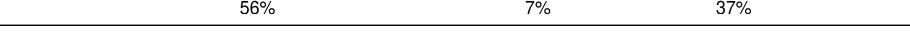
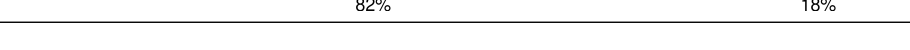
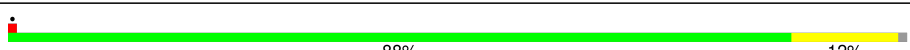
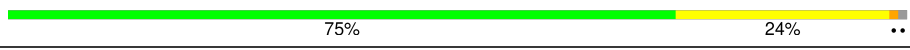
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	403	
3	C	413	

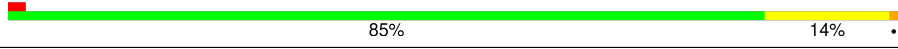
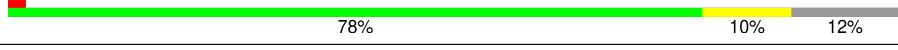
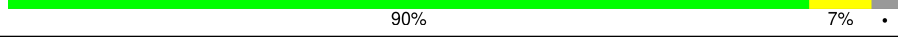
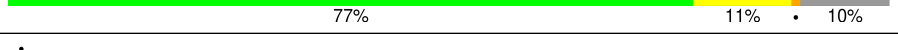
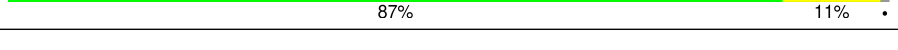
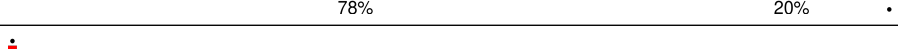
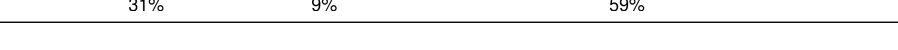
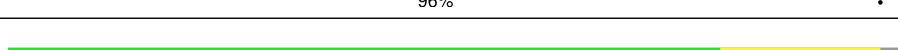
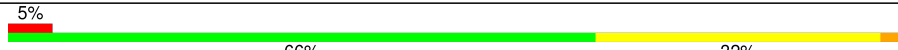
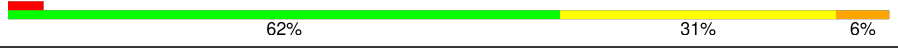
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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	249	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	K	210	
12	L	218	
13	M	204	
14	N	203	
15	O	213	
16	P	188	
17	Q	196	
18	R	224	
19	S	160	
20	T	128	
21	U	140	
22	V	157	
23	W	156	
24	X	145	
25	Y	136	
26	Z	148	
27	AA	245	
28	BA	115	

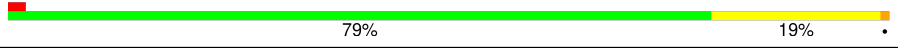
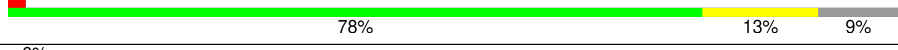
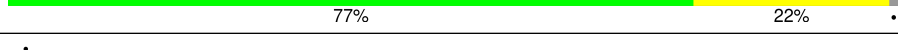
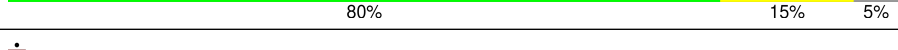
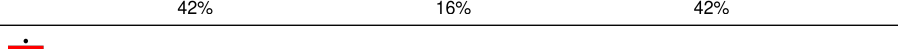
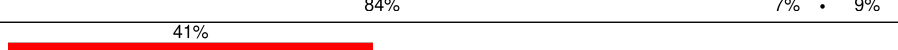
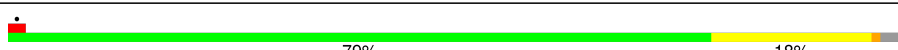
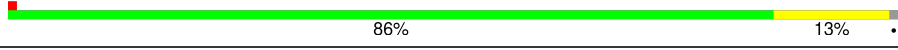
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Mol	Chain	Length	Quality of chain
29	CA	125	
30	DA	135	
31	EA	110	
32	FA	129	
33	GA	123	
34	HA	105	
35	IA	97	
36	JA	70	
37	KA	51	
38	LA	128	
39	MA	25	
40	NA	106	
41	OA	92	
42	PA	137	
43	RA	165	
44	SA	76	
45	TA	76	
46	UA	75	
47	VA	12	
48	WA	3584	
49	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 97 unique types of molecules in this entry. The entry contains 222478 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 uL3.

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 uL2.

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 L13.

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		

- 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		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	38	ARG	CYS	conflict	UNP G1TJR3

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	64	ARG	GLN	conflict	UNP G1TJR3
Q	94	THR	LYS	conflict	UNP G1TJR3

- 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
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		

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ZA	324	U	C	conflict	GB 36162

- 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 1	Mg 1	0
89	I	1	Total 1	Mg 1	0
89	O	1	Total 1	Mg 1	0
89	P	1	Total 1	Mg 1	0
89	U	1	Total 1	Mg 1	0
89	Z	1	Total 1	Mg 1	0
89	DA	1	Total 1	Mg 1	0
89	FA	1	Total 1	Mg 1	0
89	IA	1	Total 1	Mg 1	0
89	SA	2	Total 2	Mg 2	0
89	WA	166	Total 166	Mg 166	0
89	XA	4	Total 4	Mg 4	0
89	YA	2	Total 2	Mg 2	0
89	ZA	74	Total 74	Mg 74	0
89	AC	1	Total 1	Mg 1	0
89	HC	1	Total 1	Mg 1	0
89	b	1	Total 1	Mg 1	0

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

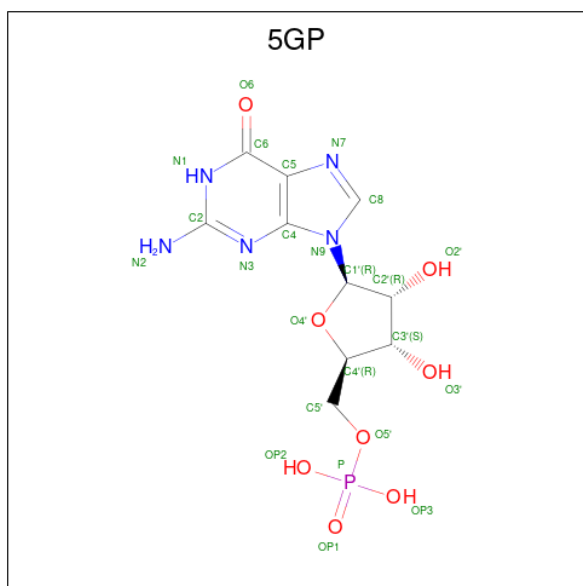
Mol	Chain	Residues	Atoms		AltConf
90	FA	1	Total 1	Zn 1	0
90	IA	1	Total 1	Zn 1	0
90	LA	1	Total 1	Zn 1	0

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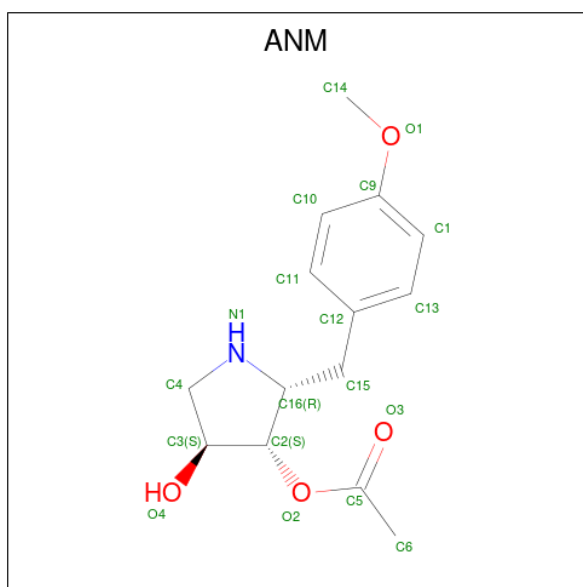
Mol	Chain	Residues	Atoms		AltConf
90	NA	1	Total	Zn	0
			1	1	
90	OA	1	Total	Zn	0
			1	1	
90	AC	1	Total	Zn	0
			1	1	
90	DC	1	Total	Zn	0
			1	1	
90	FC	1	Total	Zn	0
			1	1	

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



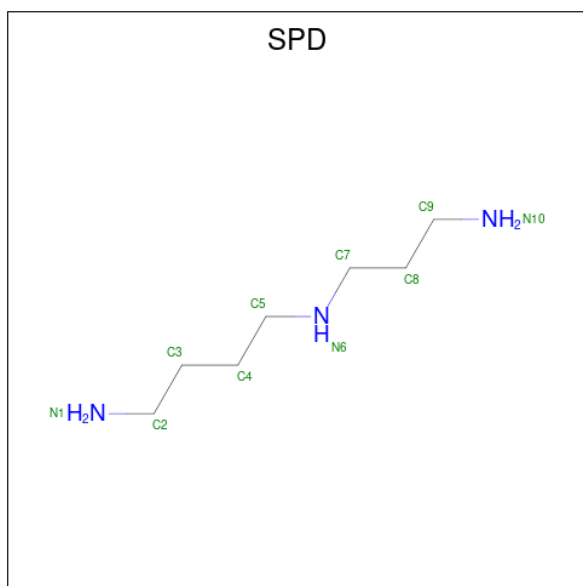
Mol	Chain	Residues	Atoms					AltConf
91	UA	1	Total	C	N	O	P	0
			24	10	5	8	1	

- 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: $C_7H_{19}N_3$).



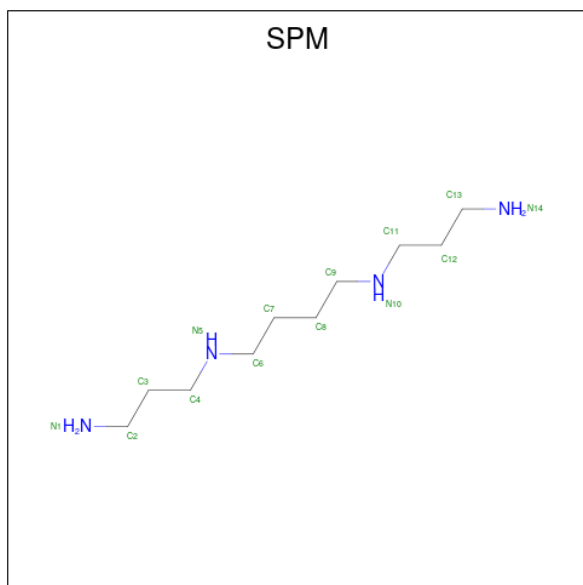
Mol	Chain	Residues	Atoms			AltConf
93	WA	1	Total	C	N	0
			10	7	3	
93	WA	1	Total	C	N	0
			10	7	3	
93	WA	1	Total	C	N	0
			10	7	3	

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

- Molecule 94 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).

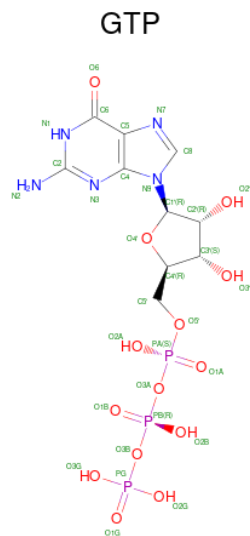


Mol	Chain	Residues	Atoms			AltConf
94	WA	1	Total	C	N	0
			14	10	4	
94	ZA	1	Total	C	N	0
			14	10	4	

- Molecule 95 is POTASSIUM ION (CCD ID: K) (formula: K).

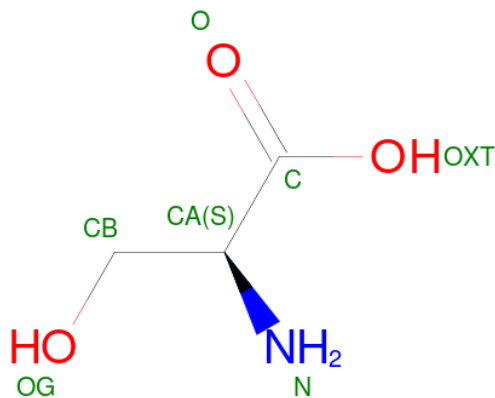
Mol	Chain	Residues	Atoms		AltConf
95	WA	1	Total	K	0
			1	1	

- Molecule 96 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 32	C 10	N 5	O 14	P 3	0

- Molecule 97 is SERINE (CCD ID: SER) (formula: $\text{C}_3\text{H}_7\text{NO}_3$).



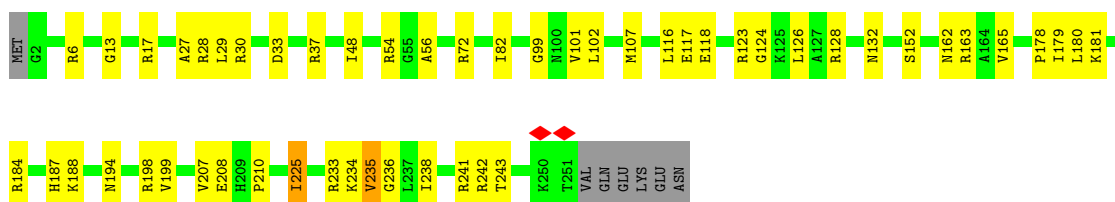
Mol	Chain	Residues	Atoms				AltConf
97	HC	1	Total	C	N	O	0
			6	3	1	2	

3 Residue-property plots [i](#)

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

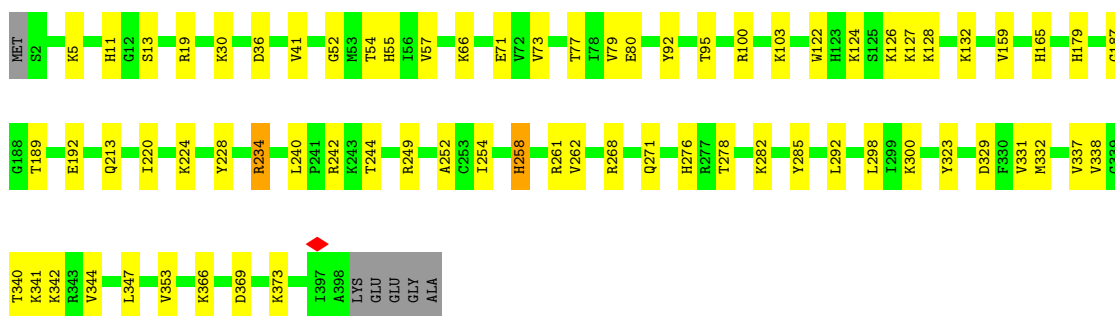
• Molecule 1: uL3

Chain A: 



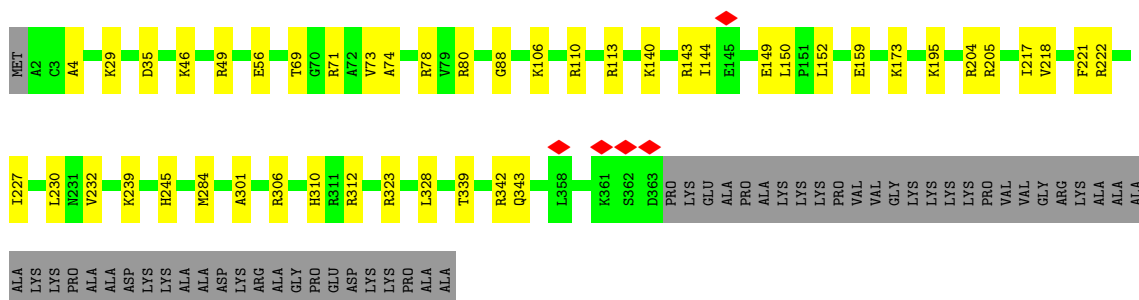
• Molecule 2: uL2

Chain B: 



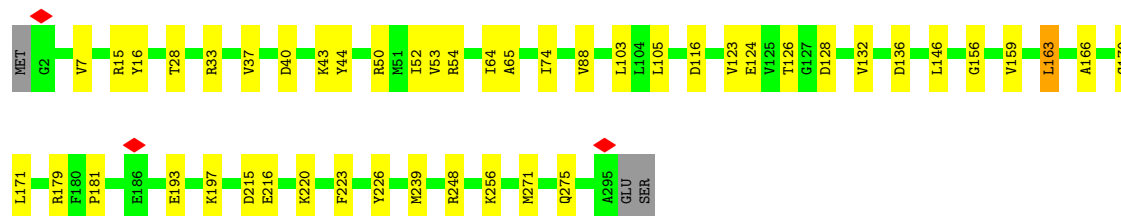
• Molecule 3: uL4

Chain C: 



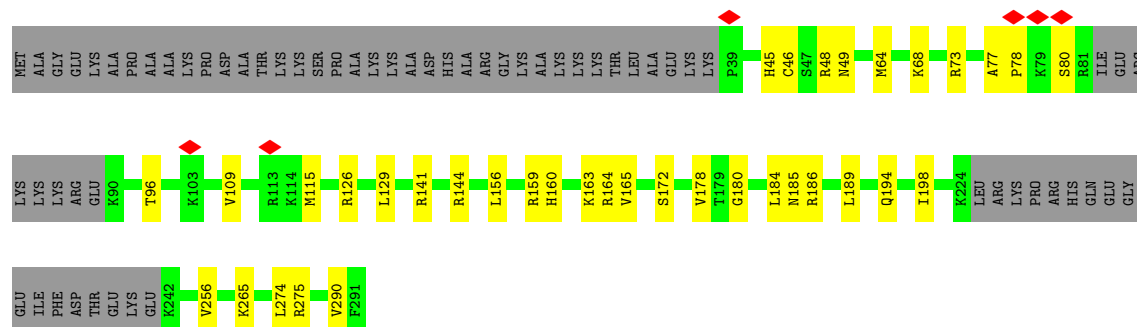
- Molecule 4: uL18

Chain D: 



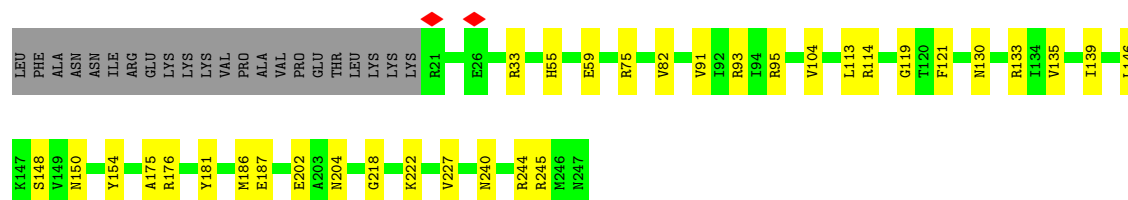
- Molecule 5: L6

Chain E: 



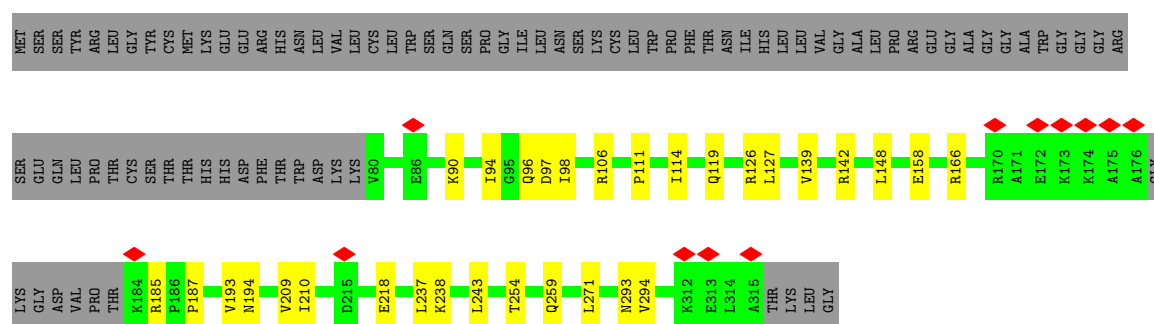
- Molecule 6: uL30

Chain F: 



- Molecule 7: L7A

Chain G: 



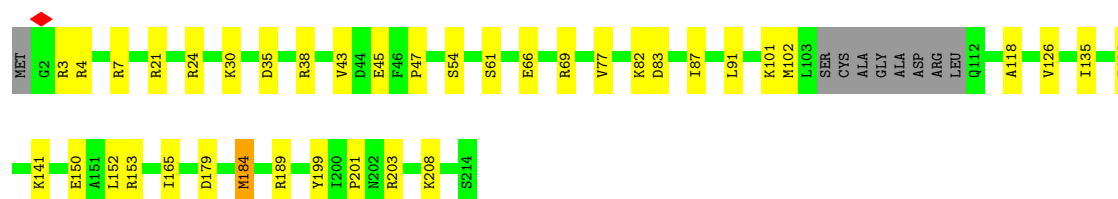
- Molecule 8: L9

Chain H:  83% 15% ..



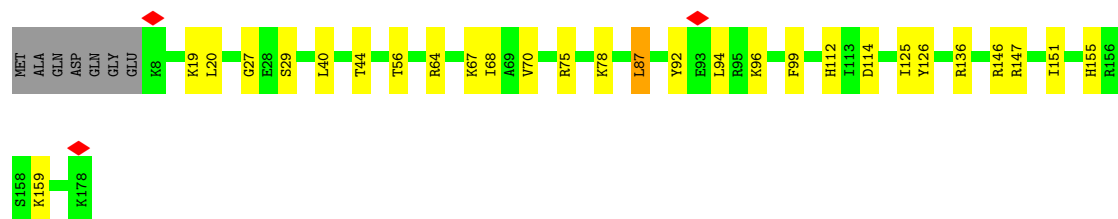
• Molecule 9: L10

Chain I:  78% 17% .



• Molecule 10: uL5

Chain J:  80% 16% ..



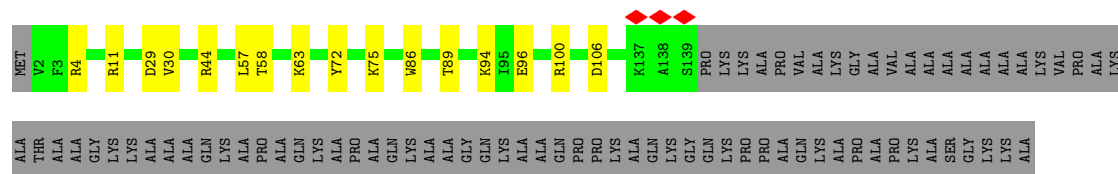
• Molecule 11: L13

Chain K:  90% 10%



• Molecule 12: eL14

Chain L:  56% 7% 37%



• Molecule 13: L15

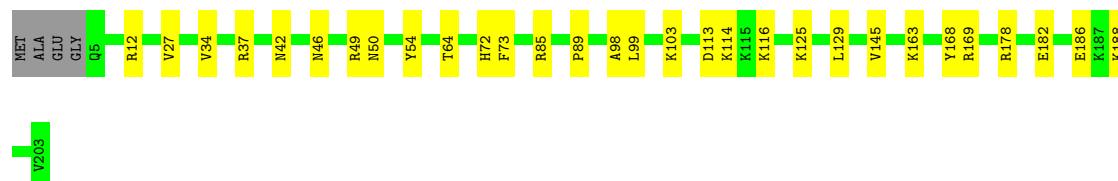
Chain M:  82% 18%





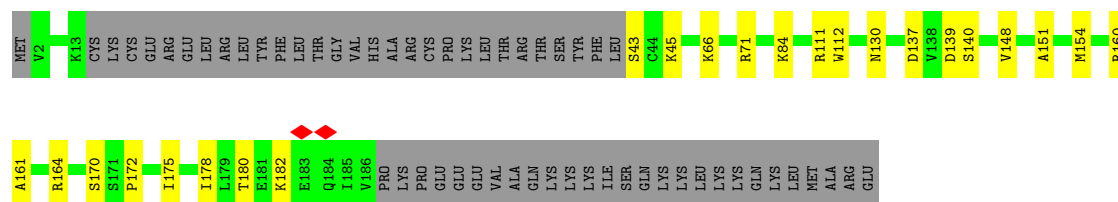
• Molecule 14: uL13

Chain N: 83% 15%



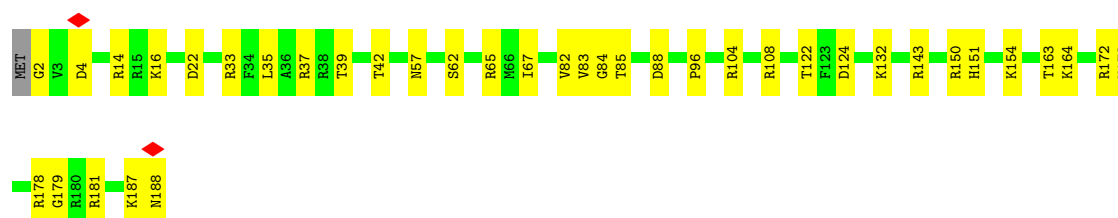
• Molecule 15: uL22

Chain O: 62% 11% 27%



• Molecule 16: eL18

Chain P: 79% 20%



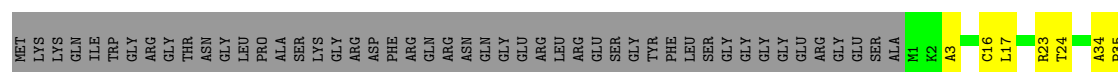
• Molecule 17: eL19

Chain Q: 83% 9% 8%



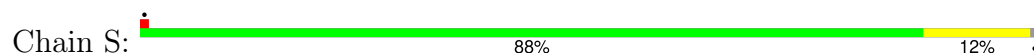
• Molecule 18: L18a

Chain R: 66% 11% 21%





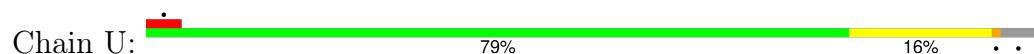
• Molecule 19: eL21



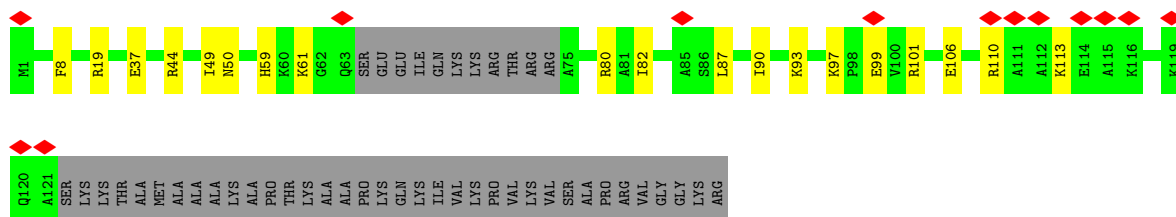
• Molecule 20: eL22



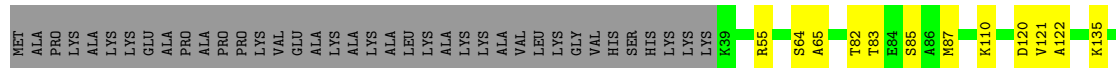
• Molecule 21: L23



• Molecule 22: uL24

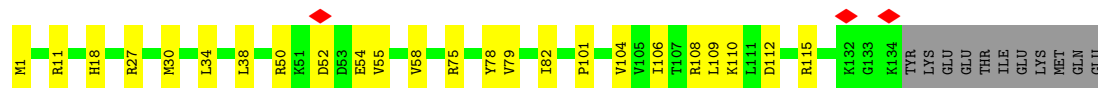


• Molecule 23: uL23



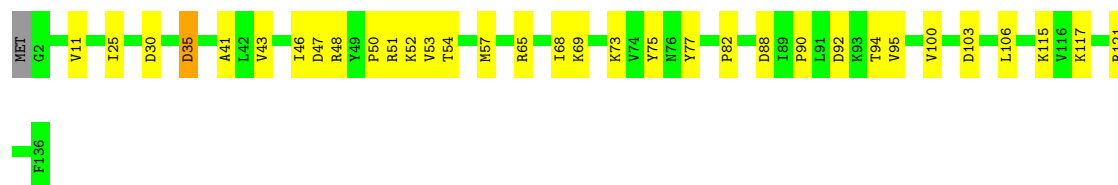
• Molecule 24: L26





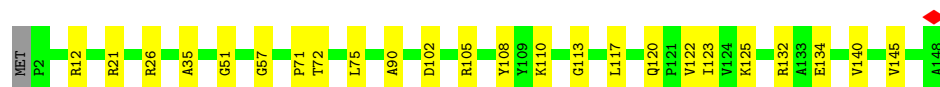
• Molecule 25: L27

Chain Y: 75% 24% ..



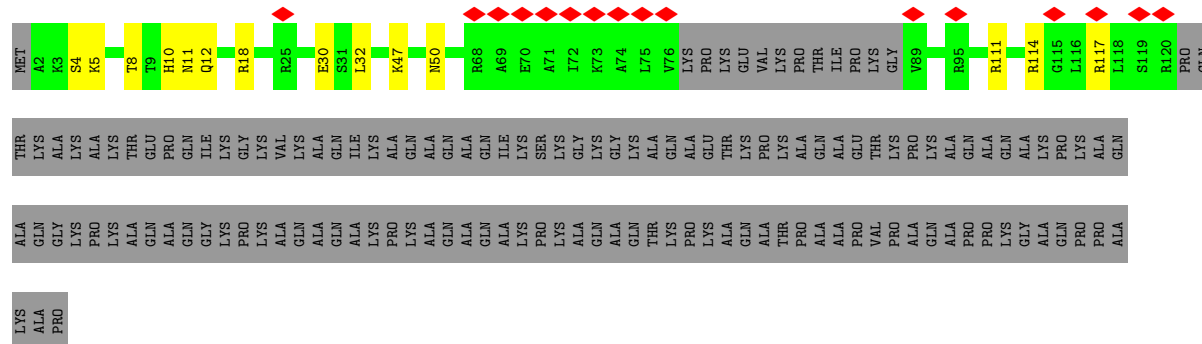
• Molecule 26: L27a

Chain Z: 83% 16% .



• Molecule 27: L29

Chain AA: 7% 38% 6% 56%



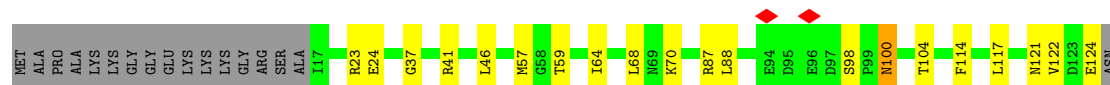
• Molecule 28: eL30

Chain BA: 79% 7% 14%

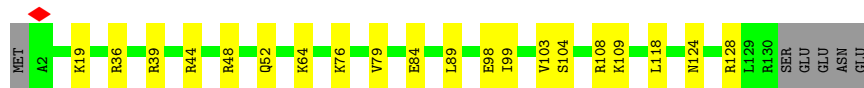


• Molecule 29: L31

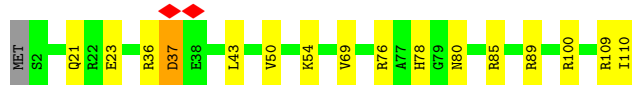
Chain CA: 70% 15% 14%



● Molecule 30: L32

Chain DA:  81% 15%

● Molecule 31: eL33

Chain EA:  85% 14%

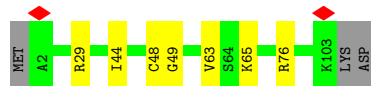
● Molecule 32: L34

Chain FA:  78% 10% 12%

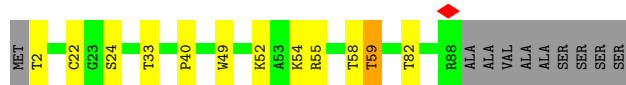
● Molecule 33: L35

Chain GA:  83% 13%

● Molecule 34: L36

Chain HA:  90% 7%

● Molecule 35: L37

Chain IA:  77% 11% 10%

● Molecule 36: eL38

Chain JA:  87% 11%



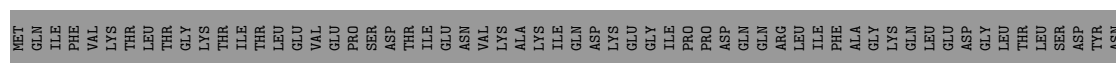
• Molecule 37: eL39

Chain KA: 78% 20%



• Molecule 38: eL40

Chain LA: 31% 9% 59%



• Molecule 39: eL41

Chain MA: 96%



• Molecule 40: eL42

Chain NA: 80% 18%



• Molecule 41: eL43

Chain OA: 88% 11%



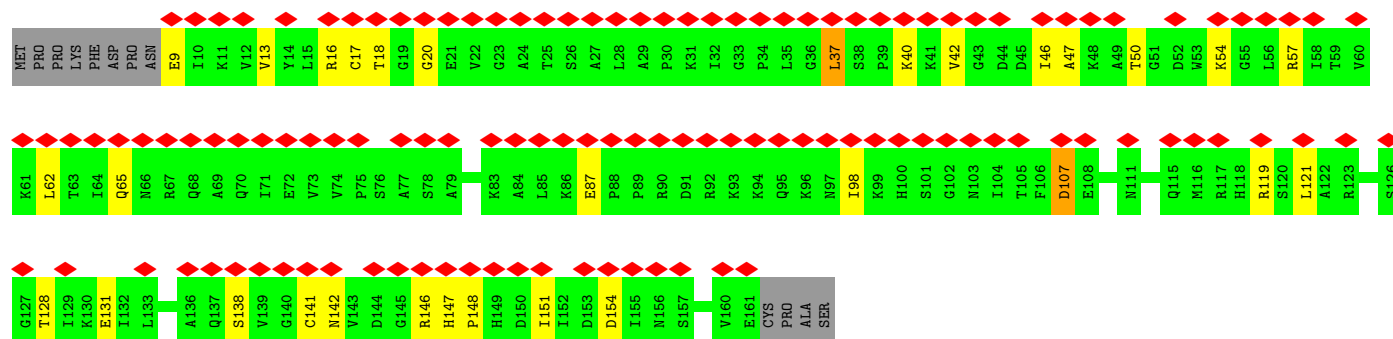
• Molecule 42: L28

Chain PA: 77% 13% 9%



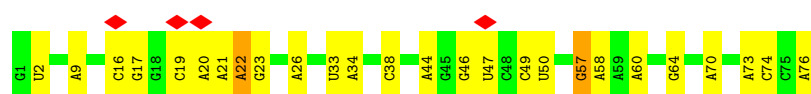
• Molecule 43: L12

Chain RA: 



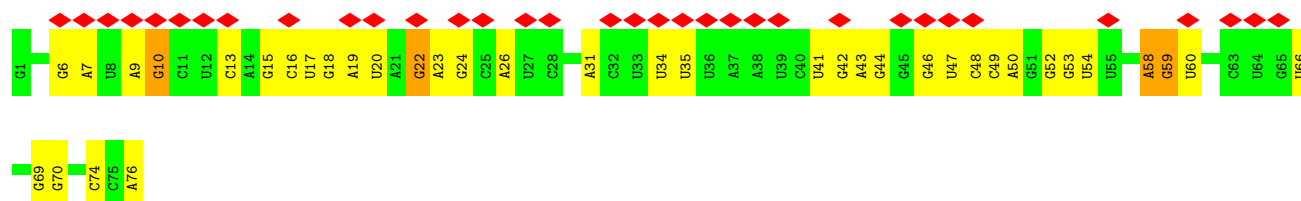
• Molecule 44: P-site tRNA

Chain SA: 



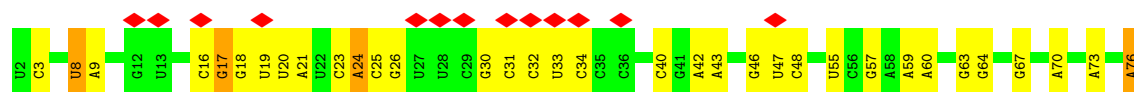
• Molecule 45: E-site tRNA

Chain TA: 



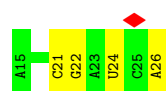
• Molecule 46: A-site tRNA

Chain UA: 



• Molecule 47: mRNA

Chain VA: 

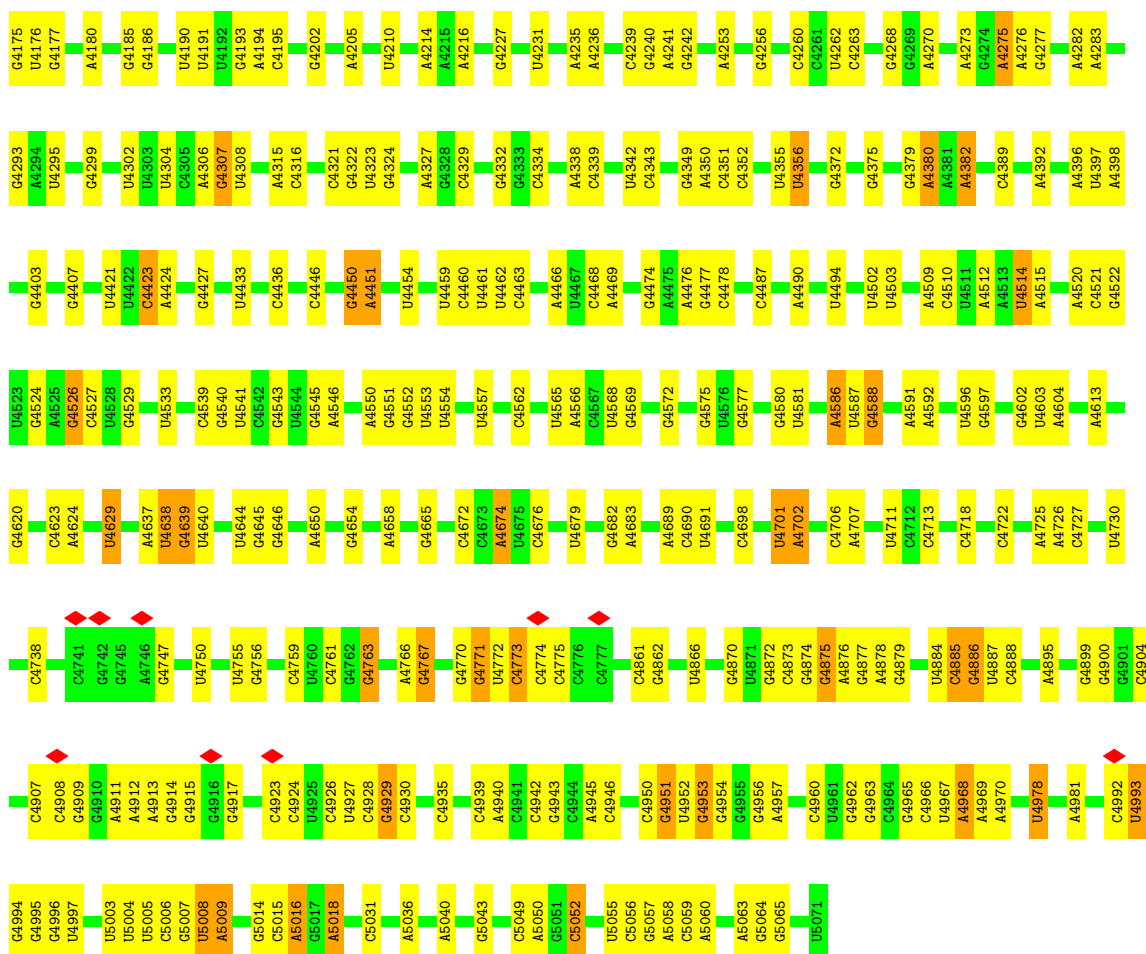


• Molecule 48: 28S rRNA

Chain WA: 



G4078	G3881	A3762	A2845	C2741	U2627	A2531	G2445	U2331	G1987	G1887
A4079	G3882	C3763	A2846	U2742	U2628	C2535	U2446	G2332	G1997	G1897
C4080	G3883	U3775	A2847	A2745	C2629	C2536	G2450	A2333	A1898	A1899
G4086	U3886	A3776	G2848	A2746	G2640	A2540	A2451	A2334	U1999	C1900
C4090	G3891	G3777	G2850	A2747	U2641	U2541	G2452	A2335	A2000	A2001
A4091	A3892	G3778	G2857	A2748	G2642	C2541	G2459	A2336	A2002	G2003
G4092	A3893	G3779	C2858	U2749	A2649	C2542	C2460	C2337	U1908	A1909
U4095	U3894	A3786	G2864	C2750	G2650	G2543	G2461	C2338	G2009	G2010
G4101	G3898	A3787	G2865	G2751	G2651	G2544	C2545	C2339	C2101	A2004
C4102	C3899	U3788	A2866	G2752	G2654	G2546	C2464	G2347	G2102	G2005
C4103	G3902	A3797	G2867	G2760	G2655	U2547	C2467	G2350	A2103	U2006
G4109	A3903	U3798	U2871	G2761	C2659	G2548	G2468	A2351	A2105	U2010
G4110	G3908	G3799	G2878	U2762	G2664	G2549	U2470	U2352	A2106	G1921
C4111	C3909	U3800	A2883	U2763	G2665	G2554	G2473	C2353	U2352	C1922
C4116	A3910	U3804	G2889	A2766	G2666	G2555	G2477	A2362	A2109	G1923
G4117	C3911	G3811	G2900	G2770	C2671	G2557	C2480	G2363	G2112	G1924
C4118	C3912	C3812	G2901	U2771	C2672	G2558	G2481	U2364	U2113	U1929
U4119	U3914	A3813	U2902	G2772	G2673	G2559	G2482	A2365	G2114	U1932
A4120	A3915	G3814	G2903	G2773	C2674	G2564	G2483	A2366	C2023	C1933
C4121	U3916	U3815	G2904	G2779	G2688	C2565	G2484	A2367	G2026	G1835
G4124	U3917	A3819	A3998	G2780	U2689	C2566	G2485	A2368	A2027	A1936
C4125	G3918	G3820	G3599	C2781	G2695	A2567	G2486	A2369	A2028	G1942
U4126	A3919	U3821	C3600	G2782	G2696	G2568	U2487	A2370	A2031	A1943
C4127	A3925	G3825	G3601	G2783	A2697	G2569	G2488	A2371	A2032	A1944
A4129	C3926	U3826	G3602	G2789	U2698	C2570	G2489	A2372	G2036	A1945
G4137	U3930	U3840	U3609	U2790	A2699	U2572	C2490	A2373	G1950	G1951
C4138	U3934	G3841	A3610	U2791	G2704	A2575	C2491	A2374	A2043	U1952
G4141	G3940	U3842	G3611	G2792	G2707	G2576	U2492	A2375	G2048	G1953
C4142	C3941	U3843	A3612	G2793	U2708	G2577	C2493	A2376	A2049	A1962
G4143	A3945	G3724	A3613	G2796	G2709	G2578	G2494	A2377	U2050	G1963
C4144	G3946	A3725	G3617	A2800	U2710	C2585	U2495	A2378	G2054	U1973
A4145	U3949	A3726	G3621	A2808	U2711	G2588	U2497	A2379	G2057	G1974
G4146	C3950	A3727	A3626	G2811	C2712	A2589	G2498	A2380	G2058	G1975
C4147	U3952	A3729	G3627	U2812	G2713	C2590	C2499	A2381	U1976	U1977
U4148	A3953	A3730	G3628	G2813	G2716	C2591	G2505	A2382	C2064	G1977
G4157	G3954	A3731	G3635	C2816	C2721	G2601	C2506	A2383	A2071	U1982
C4158	A4063	A3732	G3636	U2823	G2722	A2602	C2507	A2384	A2074	G1983
A4159	U4064	G3733	A3637	G2828	G2723	A2603	G2508	A2385	C2074	G1984
U4160	C4065	A3734	U3643	U2829	G2728	G2609	A2514	A2386	G2077	A1985
C4161	G4066	A3735	A3644	G2830	G2729	G2610	A2515	A2387	G2078	A1986
U4162	A4067	A3736	A3645	U2831	G2734	G2611	G2518	A2388	G2079	G1987
G4163	U4071	A3737	A3646	G2832	C2735	G2612	A2519	A2389	U1988	C1989
C4164	U4072	A3738	U3647	U2833	U2736	G2613	G2522	A2390	G2081	G1990
U4165	A4073	A3739	A3648	G2834	G2737	G2614	G2523	A2391	U2082	G1991
C4166	U4074	A3740	A3649	U2835	G2738	G2615	G2524	A2392	C2083	A1992
U4167	G4075	G3755	A3650	G2844	G2739	G2616	A2529	A2393	G2085	A1993
G4168	U4076					G2617	G2530	C2325	U2086	U1994
C4169	A4077					G2626		C2326		
U4170	U4078									
A4171	A4172									
C4172	A4173									
U4173	A4174									



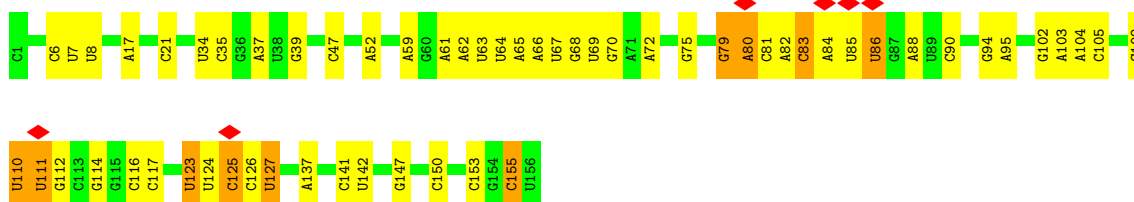
• Molecule 49: 5S rRNA

Chain XA: 78% 19% ..



• Molecule 50: 5.8S rRNA

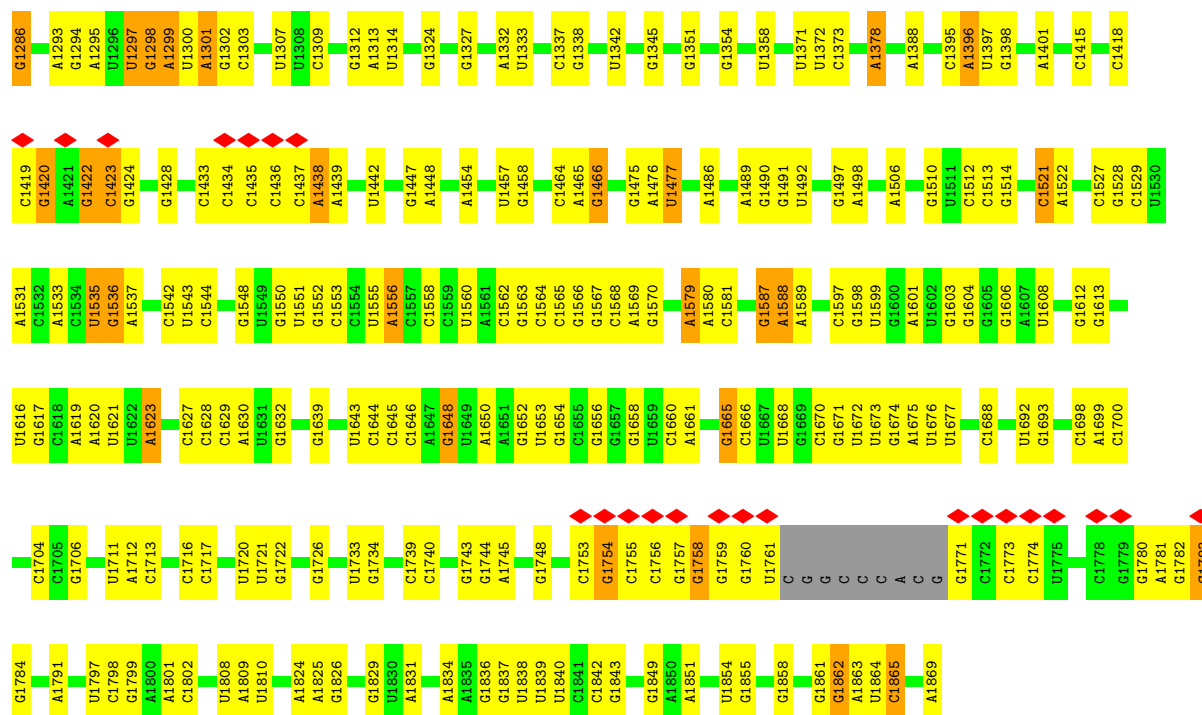
Chain YA: 62% 31% 6%



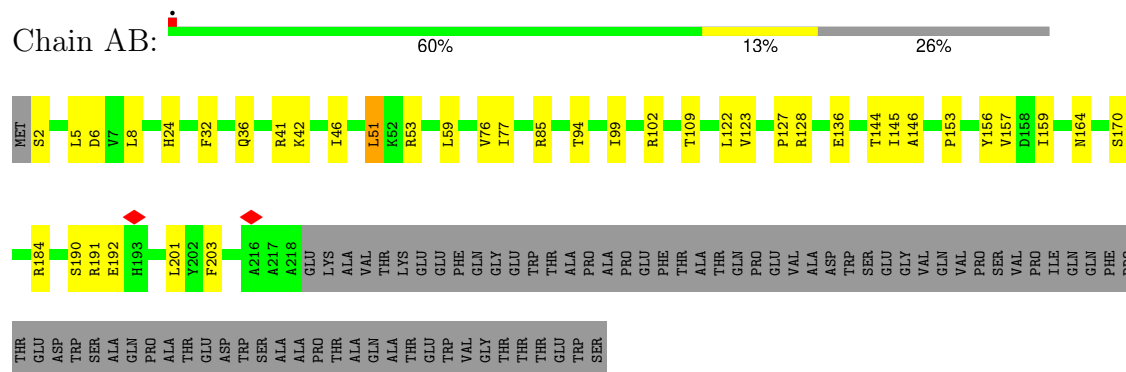
• Molecule 51: 18S rRNA

Chain ZA: 55% 32% 8%

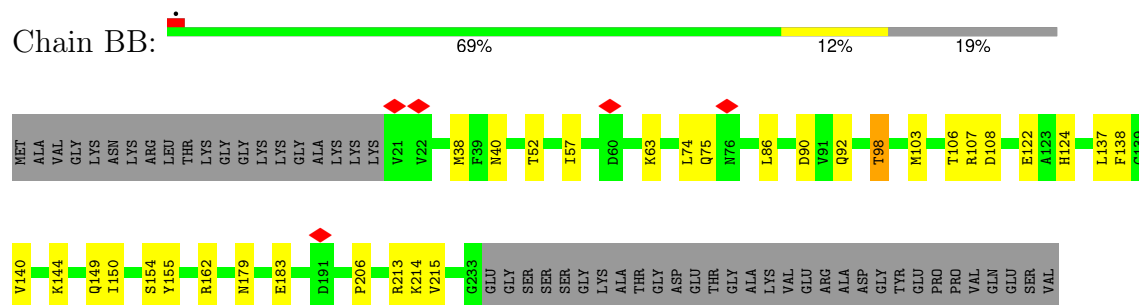




- Molecule 52: RPSA

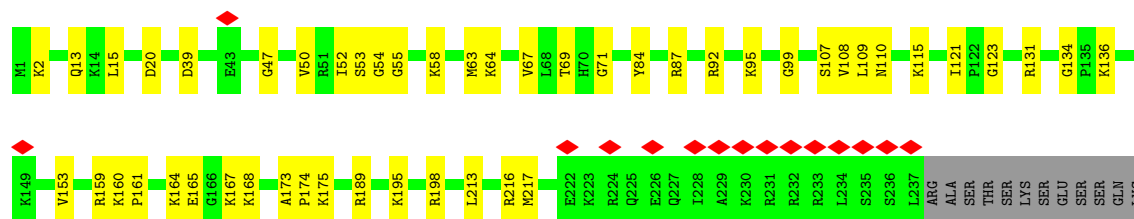


- Molecule 53: S3A

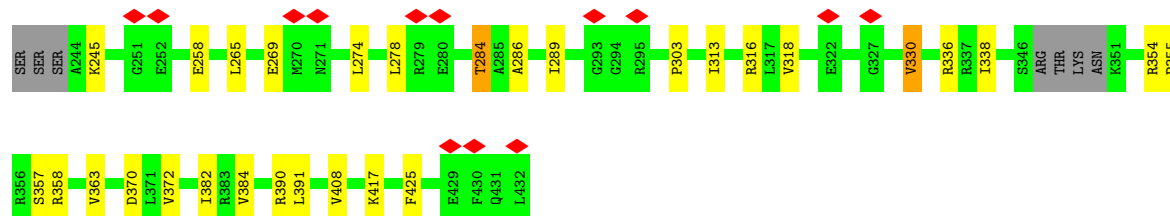
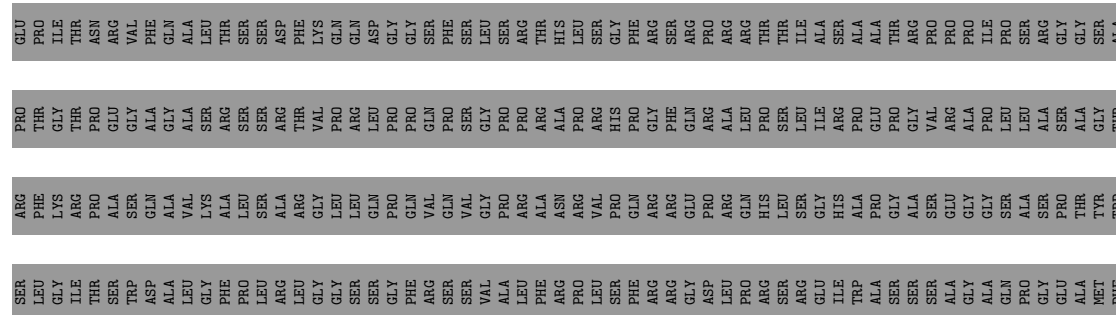
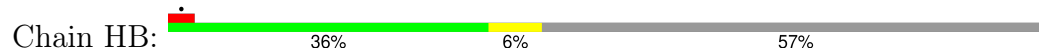


- Molecule 54: S2-like

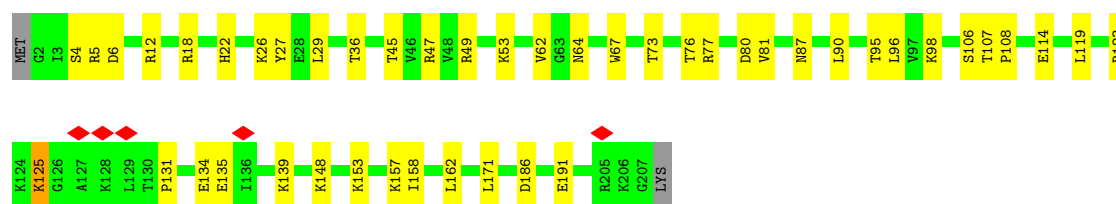
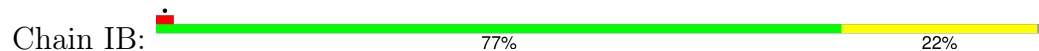




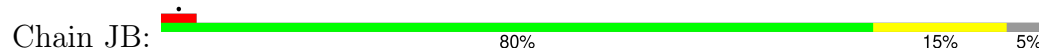
• Molecule 59: eS7



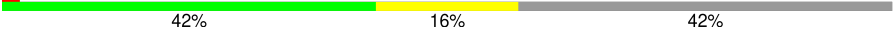
• Molecule 60: S8

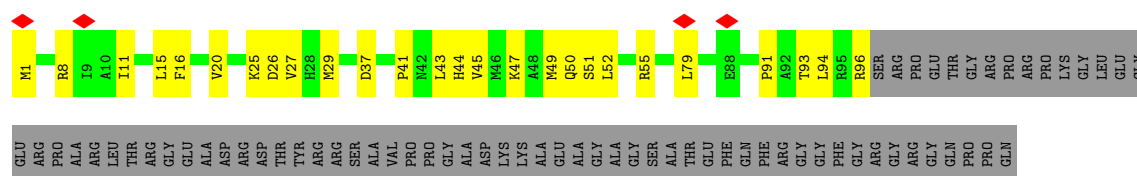


• Molecule 61: S9



• Molecule 62: S10

Chain KB: 



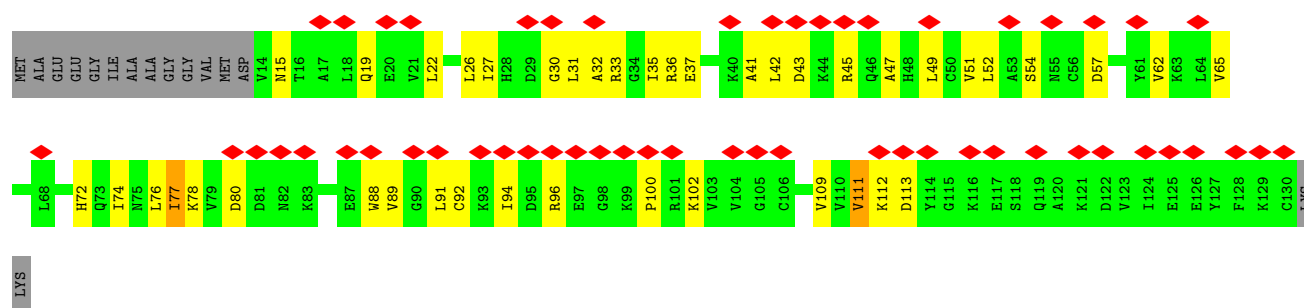
- Molecule 63: S11

Chain LB: 



- Molecule 64: S12

Chain MB: 



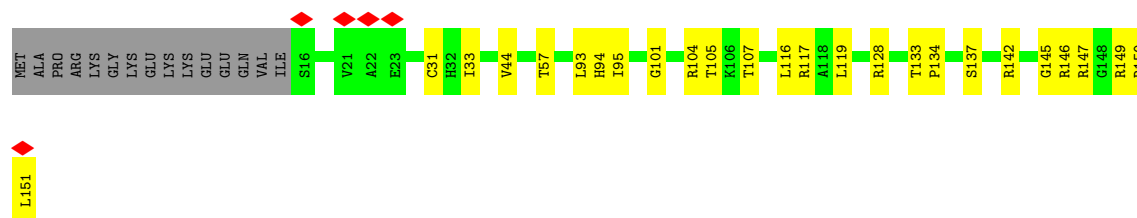
- Molecule 65: uS15

Chain NB: 



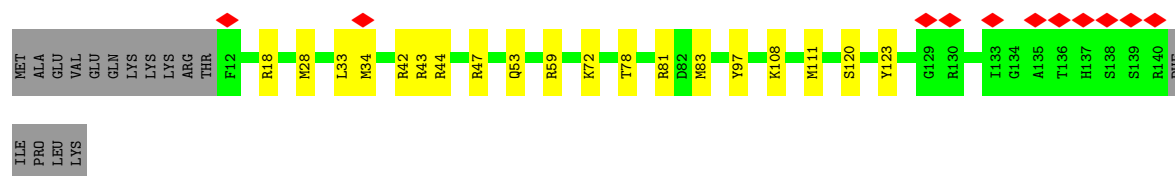
- Molecule 66: S14

Chain OB: 

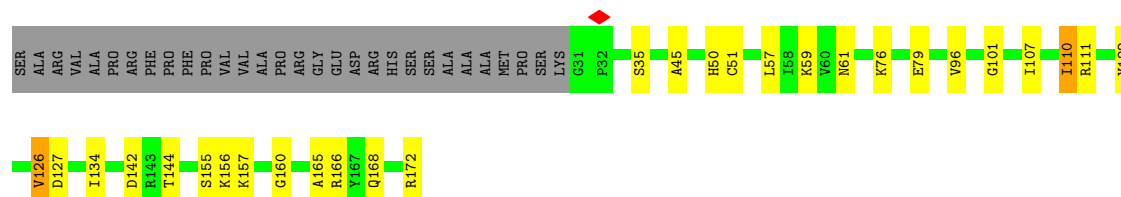


- Molecule 67: S15

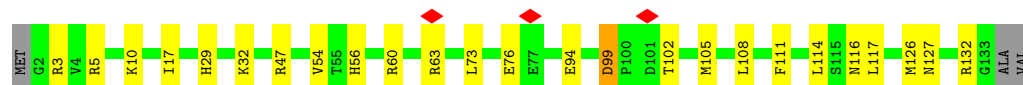
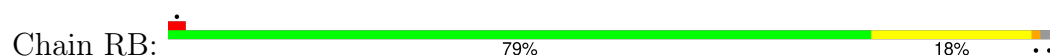
Chain PB: 



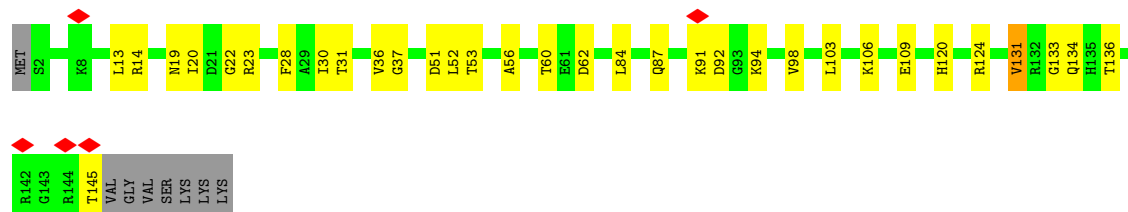
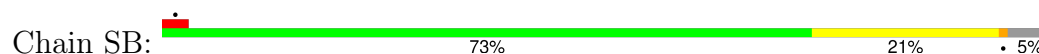
- Molecule 68: uS9



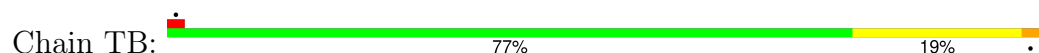
- Molecule 69: eS17



- Molecule 70: S18

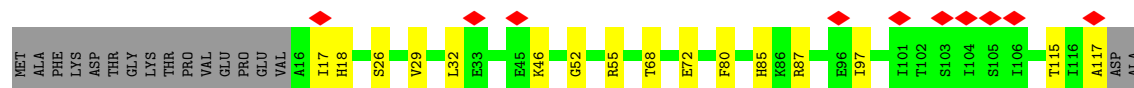


- Molecule 71: S19

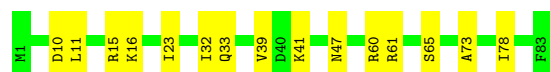
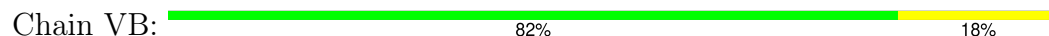


- Molecule 72: uS10

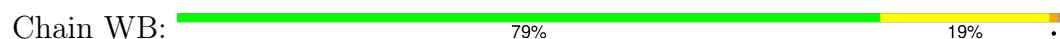




• Molecule 73: S21



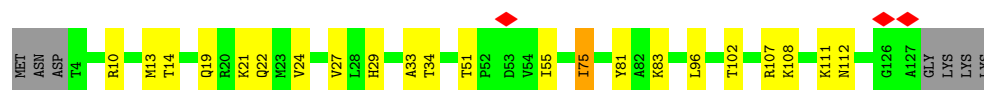
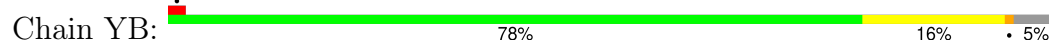
• Molecule 74: S15A



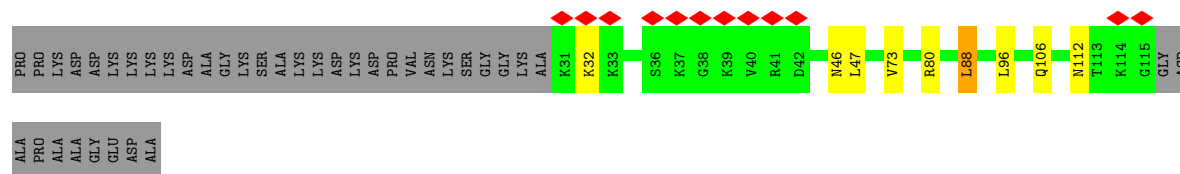
• Molecule 75: S23



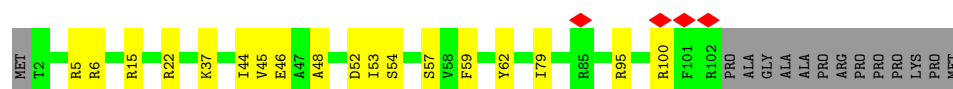
• Molecule 76: S24



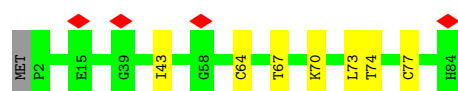
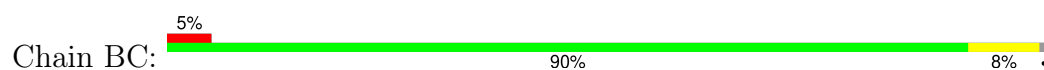
• Molecule 77: eS25



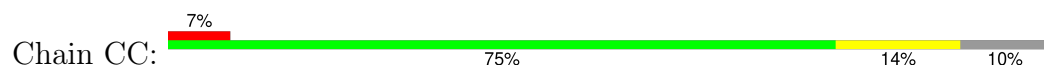
• Molecule 78: S26



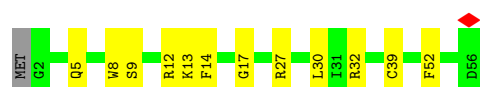
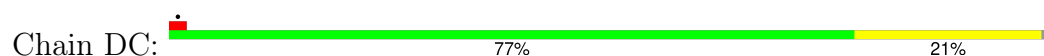
• Molecule 79: S27



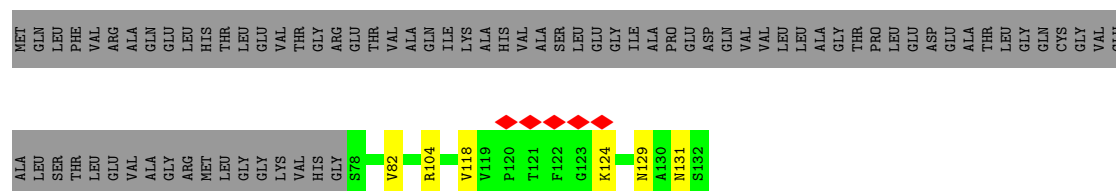
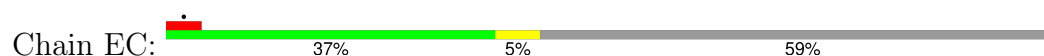
- Molecule 80: S28



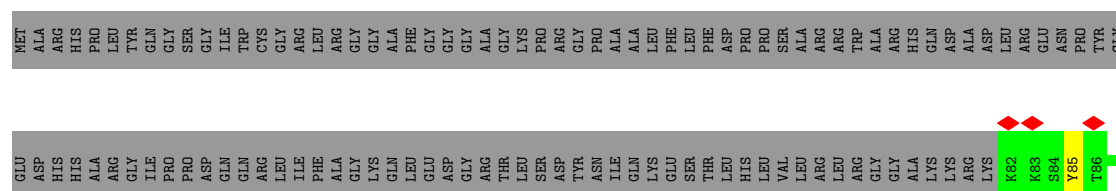
- Molecule 81: uS14



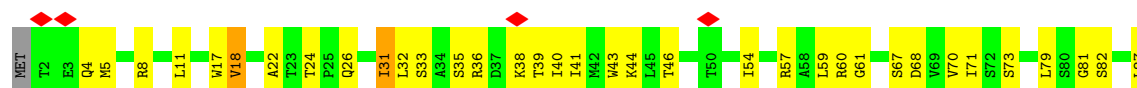
- Molecule 82: S30

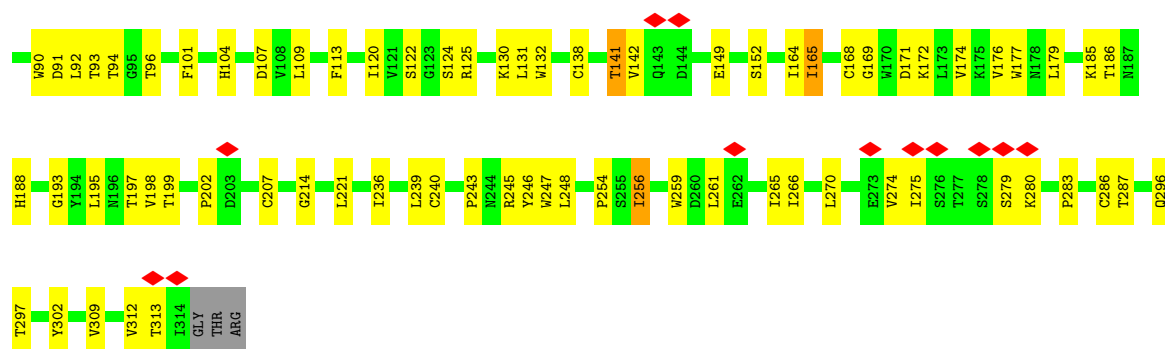


- Molecule 83: S27A

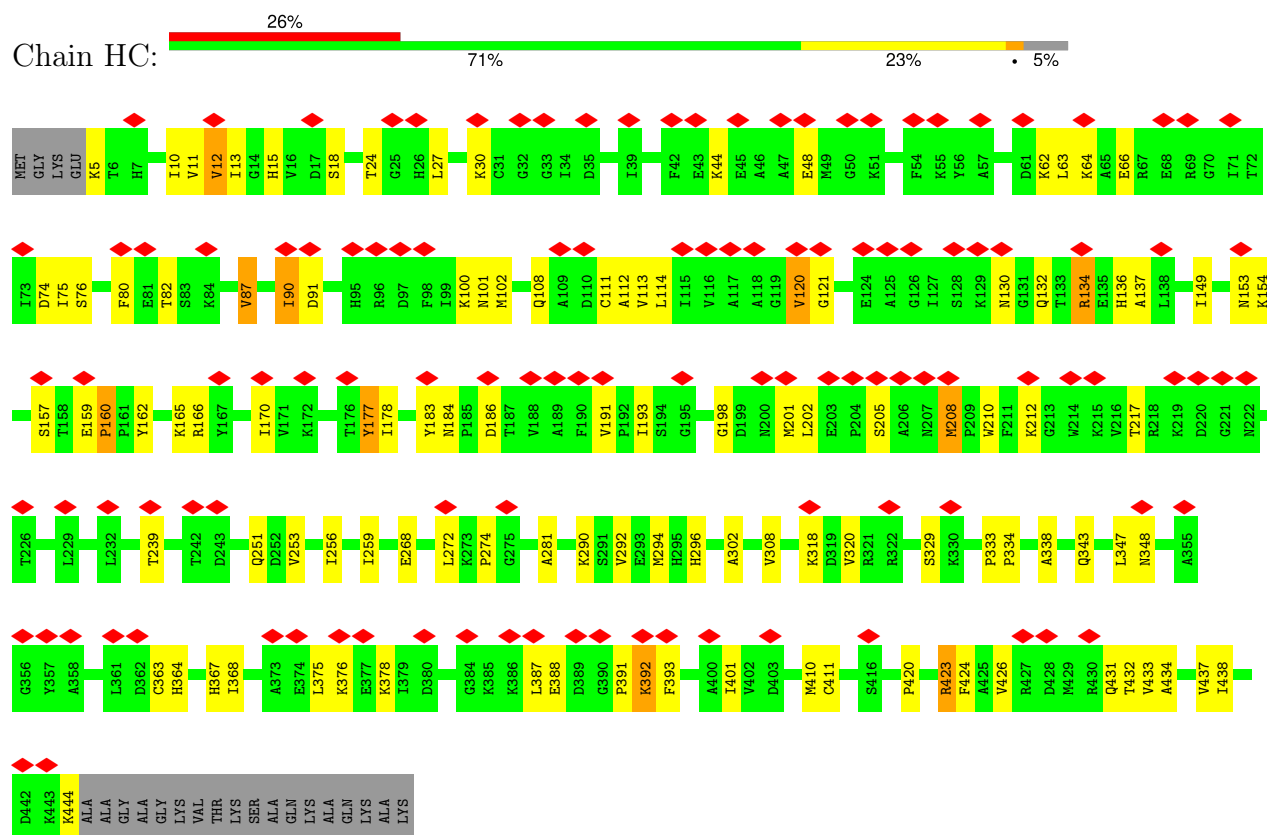


- Molecule 84: RACK1





- Molecule 85: eukaryotic elongation factor 1A

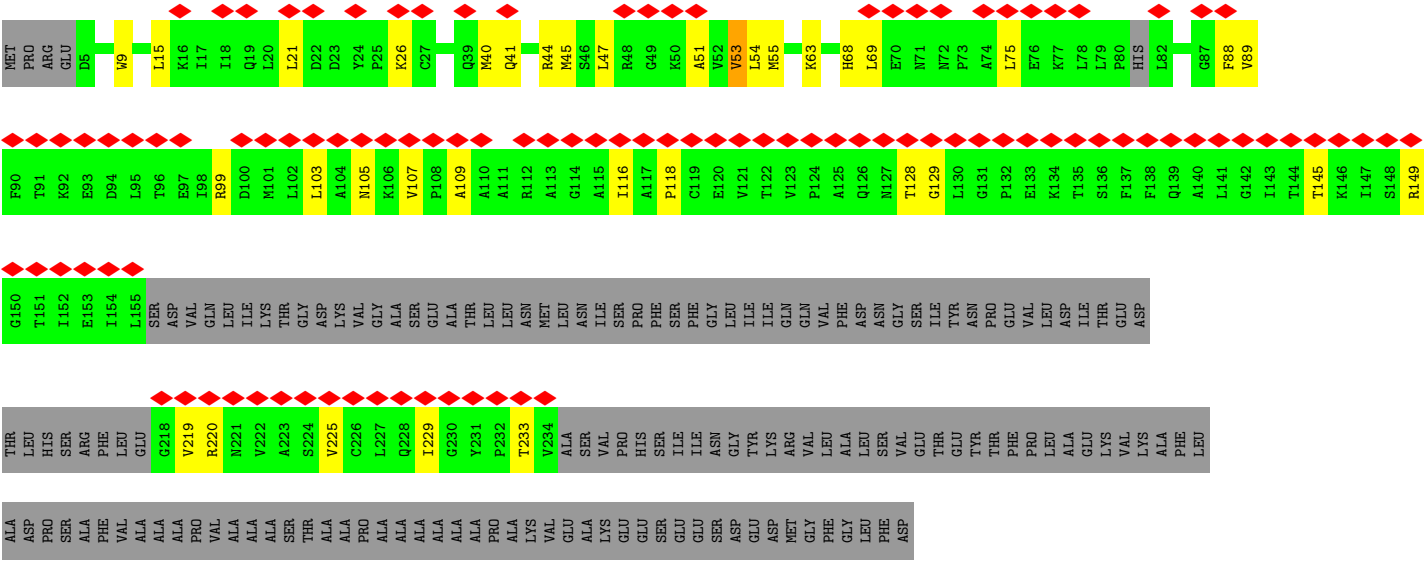


- Molecule 86: peptide

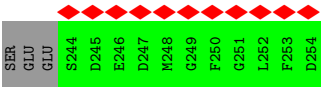
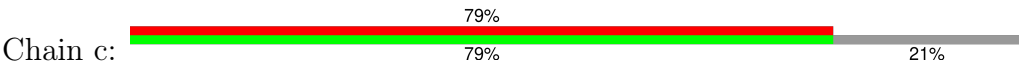


- Molecule 87: RPLP0





● Molecule 88: RPLP peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18090	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	39.640	Depositor
Minimum map value	-21.285	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.322	Depositor
Recommended contour level	4.75	Depositor
Map size ($\text{\AA}$)	686.87994, 686.87994, 686.87994	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, SPD, GTP, ANM, MG, 5GP, SPM, K

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	0.19	0/1952	0.33	0/2617
2	B	0.17	0/3264	0.31	0/4371
3	C	0.16	0/2937	0.29	0/3946
4	D	0.15	0/2441	0.29	0/3269
5	E	0.15	0/1859	0.33	0/2491
6	F	0.16	0/1933	0.29	0/2577
7	G	0.15	0/1881	0.29	0/2532
8	H	0.15	0/1535	0.29	0/2063
9	I	0.16	0/1702	0.26	0/2272
10	J	0.14	0/1395	0.33	0/1863
11	K	0.15	0/1733	0.28	0/2316
12	L	0.15	0/1158	0.29	0/1547
13	M	0.18	0/1746	0.31	0/2338
14	N	0.17	0/1662	0.32	0/2222
15	O	0.16	0/1292	0.32	0/1733
16	P	0.17	0/1539	0.35	0/2054
17	Q	0.14	0/1524	0.27	0/2013
18	R	0.17	0/1501	0.31	0/2012
19	S	0.16	0/1326	0.27	0/1770
20	T	0.14	0/840	0.35	0/1127
21	U	0.17	0/1018	0.31	0/1364
22	V	0.14	0/900	0.28	0/1194
23	W	0.15	0/984	0.29	0/1323
24	X	0.14	0/1132	0.25	0/1504
25	Y	0.15	0/1130	0.31	0/1507
26	Z	0.17	0/1191	0.31	0/1590
27	AA	0.12	0/886	0.22	0/1171
28	BA	0.14	0/779	0.24	0/1044
29	CA	0.17	0/908	0.34	0/1223
30	DA	0.16	0/1082	0.27	0/1443
31	EA	0.18	0/895	0.31	0/1198
32	FA	0.16	0/916	0.30	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	GA	0.13	0/1016	0.25	0/1341
34	HA	0.13	0/841	0.29	0/1112
35	IA	0.17	0/731	0.31	0/966
36	JA	0.14	0/575	0.28	0/761
37	KA	0.16	0/459	0.32	0/608
38	LA	0.15	0/435	0.33	0/575
39	MA	0.15	0/240	0.26	0/305
40	NA	0.15	0/864	0.26	0/1140
41	OA	0.17	0/718	0.29	0/953
42	PA	0.15	0/1010	0.31	0/1354
43	RA	0.13	0/1174	0.33	0/1582
44	SA	0.14	0/1815	0.26	0/2828
45	TA	0.11	0/1804	0.25	0/2810
46	UA	0.11	0/1771	0.28	0/2754
47	VA	0.12	0/278	0.28	0/428
48	WA	0.18	0/85840	0.27	0/133885
49	XA	0.16	0/2836	0.23	0/4421
50	YA	0.17	0/3701	0.24	0/5766
51	ZA	0.16	0/40949	0.27	0/63819
52	AB	0.14	0/1747	0.29	0/2374
53	BB	0.14	0/1756	0.28	0/2350
54	CB	0.15	0/1744	0.31	0/2358
55	DB	0.12	0/1796	0.27	0/2417
56	EB	0.15	0/2118	0.32	0/2849
57	FB	0.14	0/1492	0.31	0/2005
58	GB	0.12	0/1946	0.26	0/2590
59	HB	0.14	0/1511	0.32	0/2022
60	IB	0.15	0/1715	0.30	0/2287
61	JB	0.14	0/1550	0.28	0/2069
62	KB	0.13	0/834	0.29	0/1125
63	LB	0.15	0/1200	0.30	0/1604
64	MB	0.12	0/918	0.33	0/1233
65	NB	0.14	0/1226	0.25	0/1649
66	OB	0.16	0/1029	0.30	0/1380
67	PB	0.12	0/1079	0.27	0/1441
68	QB	0.15	0/1146	0.32	0/1534
69	RB	0.12	0/1082	0.28	0/1452
70	SB	0.12	0/1208	0.30	0/1618
71	TB	0.12	0/1123	0.28	0/1504
72	UB	0.13	0/818	0.31	0/1099
73	VB	0.13	0/643	0.30	0/860
74	WB	0.17	0/1051	0.35	0/1406
75	XB	0.15	0/1116	0.30	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YB	0.13	0/1028	0.30	0/1366
77	ZB	0.11	0/691	0.27	0/922
78	AC	0.16	0/828	0.32	0/1109
79	BC	0.13	0/665	0.26	0/891
80	CC	0.13	0/490	0.29	0/656
81	DC	0.13	0/470	0.29	0/623
82	EC	0.12	0/447	0.28	0/587
83	FC	0.10	0/576	0.25	0/764
84	GC	0.13	0/2493	0.33	0/3394
85	HC	0.13	0/3441	0.33	0/4657
86	IC	0.10	0/19	0.19	0/25
87	b	0.14	0/1298	0.32	0/1752
88	c	0.10	0/87	0.33	0/113
All	All	0.16	0/238479	0.28	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
2	B	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
2	B	258	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1914	0	2013	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3196	0	3339	50	0
3	C	2883	0	3053	32	0
4	D	2395	0	2427	30	0
5	E	1823	0	1995	26	0
6	F	1897	0	2021	25	0
7	G	1850	0	1991	19	0
8	H	1516	0	1597	19	0
9	I	1664	0	1712	24	0
10	J	1372	0	1412	18	0
11	K	1702	0	1820	15	0
12	L	1137	0	1211	12	0
13	M	1701	0	1749	27	0
14	N	1630	0	1778	22	0
15	O	1266	0	1302	16	0
16	P	1515	0	1634	29	0
17	Q	1508	0	1664	15	0
18	R	1462	0	1508	22	0
19	S	1298	0	1366	17	0
20	T	826	0	852	9	0
21	U	1004	0	1063	20	0
22	V	887	0	935	16	0
23	W	967	0	1040	12	0
24	X	1115	0	1205	12	0
25	Y	1107	0	1182	20	0
26	Z	1162	0	1209	18	0
27	AA	873	0	949	11	0
28	BA	769	0	803	4	0
29	CA	893	0	932	10	0
30	DA	1064	0	1160	20	0
31	EA	876	0	912	11	0
32	FA	906	0	998	9	0
33	GA	1008	0	1142	15	0
34	HA	830	0	916	4	0
35	IA	716	0	750	9	0
36	JA	569	0	637	5	0
37	KA	447	0	480	8	0
38	LA	429	0	465	7	0
39	MA	239	0	289	1	0
40	NA	851	0	920	11	0
41	OA	708	0	757	9	0
42	PA	994	0	1051	14	0
43	RA	1160	0	1218	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	SA	1622	0	825	11	0
45	TA	1615	0	820	18	0
46	UA	1586	0	805	7	0
47	VA	249	0	125	2	0
48	WA	76735	0	38759	751	0
49	XA	2538	0	1286	16	0
50	YA	3314	0	1683	30	0
51	ZA	36623	0	18504	386	0
52	AB	1710	0	1711	26	0
53	BB	1729	0	1803	19	0
54	CB	1707	0	1793	25	0
55	DB	1768	0	1863	19	0
56	EB	2076	0	2177	36	0
57	FB	1471	0	1522	18	0
58	GB	1923	0	2089	34	0
59	HB	1489	0	1582	15	0
60	IB	1686	0	1772	28	0
61	JB	1525	0	1640	21	0
62	KB	810	0	836	16	0
63	LB	1180	0	1254	7	0
64	MB	908	0	939	28	0
65	NB	1202	0	1289	17	0
66	OB	1016	0	1039	18	0
67	PB	1058	0	1104	15	0
68	QB	1128	0	1195	17	0
69	RB	1068	0	1121	18	0
70	SB	1190	0	1249	20	0
71	TB	1104	0	1140	24	0
72	UB	808	0	878	8	0
73	VB	636	0	637	10	0
74	WB	1034	0	1080	18	0
75	XB	1098	0	1167	12	0
76	YB	1011	0	1083	13	0
77	ZB	683	0	761	6	0
78	AC	814	0	864	16	0
79	BC	651	0	672	3	0
80	CC	488	0	514	7	0
81	DC	459	0	449	10	0
82	EC	443	0	492	6	0
83	FC	564	0	577	11	0
84	GC	2436	0	2393	55	0
85	HC	3371	0	3425	63	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	15	0
88	c	86	0	66	0	0
89	A	1	0	0	0	0
89	AC	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	O	1	0	0	0	0
89	P	1	0	0	0	0
89	SA	2	0	0	0	0
89	U	1	0	0	0	0
89	WA	166	0	0	0	0
89	XA	4	0	0	0	0
89	YA	2	0	0	0	0
89	Z	1	0	0	0	0
89	ZA	74	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	11	1	0
92	WA	19	0	18	2	0
93	WA	60	0	114	4	0
94	WA	14	0	26	2	0
94	ZA	14	0	26	0	0
95	WA	1	0	0	0	0
96	HC	32	0	12	2	0
97	HC	6	0	4	0	0
All	All	222478	0	166005	2147	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 6.

All (2147) 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)
48:WA:2847:A:H61	48:WA:3845:C:H42	1.10	0.98
48:WA:2487:U:H3	48:WA:2495:G:H1	1.11	0.96
51:ZA:1652:G:H1	51:ZA:1672:U:H3	1.15	0.93
48:WA:1249:U:H3	48:WA:1268:G:H1	1.17	0.92
35:IA:2:THR:N	48:WA:3644:A:HO2'	1.72	0.88
51:ZA:1743:G:H21	51:ZA:1791:A:H62	1.23	0.86
48:WA:1761:G:H1	48:WA:1775:U:H3	1.20	0.85
48:WA:3694:A:H62	48:WA:3825:G:H21	1.23	0.84
48:WA:2847:A:H61	48:WA:3845:C:N4	1.77	0.83
44:SA:50:U:H3	44:SA:64:G:H1	0.87	0.80
48:WA:2847:A:N6	48:WA:3845:C:H42	1.83	0.76
51:ZA:1091:C:HO2'	74:WB:2:VAL:N	1.83	0.76
85:HC:80:PHE:HB2	85:HC:87:VAL:HG22	1.66	0.76
51:ZA:1834:A:H2	51:ZA:1837:G:H1	1.35	0.75
14:N:42:ASN:HD22	14:N:125:LYS:HD3	1.54	0.72
48:WA:995:U:H3	48:WA:1071:G:H1	1.35	0.72
56:EB:185:GLY:H	56:EB:189:LEU:HD13	1.55	0.72
11:K:56:ARG:O	11:K:116:ARG:NH1	2.24	0.71
51:ZA:677:G:H21	51:ZA:1028:A:H62	1.37	0.71
48:WA:4874:G:H4'	48:WA:4875:G:H5'	1.72	0.70
51:ZA:126:G:H1'	51:ZA:181:A:H1'	1.72	0.70
45:TA:15:G:N2	45:TA:48:C:C2	2.58	0.70
5:E:48:ARG:HB2	5:E:64:MET:HE1	1.72	0.70
51:ZA:1396:A:O2'	51:ZA:1398:G:N7	2.23	0.70
58:GB:164:LYS:HG2	58:GB:165:GLU:HG3	1.74	0.70
17:Q:60:ARG:HH12	48:WA:2617:C:H5''	1.56	0.70
48:WA:3643:U:OP2	48:WA:3648:A:N6	2.25	0.70
48:WA:2649:A:H62	48:WA:2688:G:H8	1.39	0.69
48:WA:2522:C:O2	48:WA:2642:G:N2	2.25	0.69
3:C:78:ARG:HB3	3:C:88:GLY:HA2	1.74	0.69
87:b:47:LEU:O	87:b:51:ALA:N	2.22	0.69
53:BB:107:ARG:NH1	66:OB:133:THR:O	2.25	0.68
9:I:184:MET:HG3	9:I:189:ARG:HB2	1.76	0.68
48:WA:1526:A:H62	48:WA:1653:G:H1	1.41	0.68
48:WA:3946:G:H1	48:WA:4071:U:H3	1.42	0.68
59:HB:274:LEU:HD21	59:HB:316:ARG:HD2	1.76	0.68
6:F:176:ARG:NH1	48:WA:2103:A:N7	2.41	0.67
48:WA:1205:G:H2'	48:WA:1206:G:H8	1.60	0.67
72:UB:80:PHE:HB3	81:DC:52:PHE:HB3	1.76	0.67
6:F:218:GLY:O	6:F:245:ARG:NH2	2.28	0.67
56:EB:87:MET:HE2	56:EB:123:LEU:HB2	1.77	0.67
85:HC:208:MET:SD	85:HC:208:MET:N	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XB:68:LYS:HE2	82:EC:82:VAL:HG22	1.77	0.66
51:ZA:1566:G:N7	71:TB:101:ARG:NH2	2.43	0.66
51:ZA:1743:G:N2	51:ZA:1791:A:H62	1.91	0.66
58:GB:69:THR:HG22	58:GB:71:GLY:H	1.60	0.66
69:RB:111:PHE:HB3	69:RB:114:LEU:HD11	1.76	0.66
43:RA:17:CYS:O	43:RA:57:ARG:HA	1.93	0.66
44:SA:33:U:OP2	68:QB:172:ARG:NH2	2.29	0.66
42:PA:31:ASN:ND2	42:PA:40:TYR:O	2.27	0.66
84:GC:87:LEU:HB2	84:GC:101:PHE:HB2	1.77	0.66
51:ZA:1286:G:N2	51:ZA:1312:G:O2'	2.29	0.66
2:B:249:ARG:NH1	48:WA:2839:U:OP1	2.29	0.66
51:ZA:834:C:N3	51:ZA:835:C:N4	2.43	0.66
51:ZA:377:G:H5'	60:IB:98:LYS:HB3	1.78	0.65
1:A:30:ARG:O	1:A:163:ARG:NH2	2.30	0.65
51:ZA:64:A:H2	51:ZA:83:A:H62	1.43	0.65
48:WA:3699:U:H5''	48:WA:3700:G:H5'	1.79	0.65
84:GC:31:ILE:HG23	84:GC:43:TRP:HB2	1.79	0.65
25:Y:50:PRO:HD3	25:Y:68:ILE:HG13	1.79	0.65
48:WA:2000:A:H62	87:b:55:MET:HE3	1.61	0.65
51:ZA:77:A:H2	58:GB:175:LYS:HG3	1.62	0.65
48:WA:169:A:N1	48:WA:267:G:C6	2.65	0.65
34:HA:48:CYS:SG	34:HA:49:GLY:N	2.70	0.65
10:J:56:THR:HG22	10:J:64:ARG:H	1.60	0.64
51:ZA:1864:U:H5'	78:AC:79:ILE:HD11	1.78	0.64
74:WB:11:LEU:HD12	74:WB:74:VAL:HG23	1.79	0.64
4:D:123:VAL:HA	4:D:248:ARG:HH12	1.62	0.64
48:WA:4355:U:H5''	48:WA:4356:U:H5'	1.80	0.64
11:K:35:ARG:NH1	48:WA:105:A:O2'	2.31	0.64
9:I:77:VAL:HG23	9:I:82:LYS:HA	1.79	0.64
16:P:16:LYS:O	16:P:33:ARG:NH2	2.29	0.64
48:WA:2485:G:H2'	48:WA:2486:A:H8	1.61	0.64
46:UA:17:G:O2'	46:UA:57:G:N2	2.31	0.63
36:JA:35:LYS:NZ	48:WA:2695:G:OP1	2.29	0.63
18:R:154:LEU:HB3	18:R:157:ARG:HD3	1.80	0.63
74:WB:52:ILE:HG22	74:WB:61:ILE:HG12	1.81	0.63
48:WA:1256:A:N1	48:WA:1261:G:O6	2.32	0.63
48:WA:1334:C:H2'	48:WA:1335:A:H8	1.64	0.63
6:F:95:ARG:NH2	48:WA:1897:G:OP1	2.31	0.63
10:J:75:ARG:NH1	49:XA:40:U:O2	2.32	0.63
48:WA:986:U:H3	48:WA:1277:G:H1	1.47	0.63
51:ZA:561:A:H5'	61:JB:171:GLY:HA3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1858:G:OP2	66:OB:146:ARG:NH2	2.30	0.63
51:ZA:75:G:H4'	51:ZA:76:U:H5'	1.80	0.63
51:ZA:1298:G:H4'	67:PB:78:THR:HA	1.79	0.63
84:GC:174:VAL:HB	84:GC:188:HIS:HB2	1.79	0.63
26:Z:21:ARG:NH2	48:WA:1319:U:OP1	2.32	0.63
51:ZA:1497:G:N7	62:KB:25:LYS:NZ	2.46	0.63
3:C:143:ARG:NH1	48:WA:2302:A:N7	2.47	0.62
51:ZA:587:A:H5'	51:ZA:592:C:H41	1.62	0.62
51:ZA:1613:G:OP1	67:PB:42:ARG:NH2	2.31	0.62
74:WB:30:CYS:SG	74:WB:31:SER:N	2.72	0.62
48:WA:4637:A:H2	48:WA:4665:G:H21	1.45	0.62
26:Z:72:THR:HG22	26:Z:110:LYS:HB3	1.80	0.62
30:DA:36:ARG:NH2	48:WA:2324:G:OP1	2.33	0.62
45:TA:15:G:N2	45:TA:48:C:O2	2.32	0.62
84:GC:256:ILE:HG23	84:GC:270:LEU:HB2	1.82	0.62
13:M:90:ASN:ND2	48:WA:3930:A:OP1	2.32	0.62
51:ZA:1005:G:OP2	53:BB:162:ARG:NH1	2.32	0.62
51:ZA:1658:G:OP2	51:ZA:1660:C:N4	2.32	0.62
9:I:203:ARG:NH1	49:XA:105:C:OP2	2.33	0.62
66:OB:142:ARG:HB3	78:AC:22:ARG:HD3	1.81	0.62
2:B:95:THR:HG22	48:WA:4912:A:H4'	1.82	0.61
38:LA:74:TYR:O	48:WA:4474:G:O2'	2.18	0.61
51:ZA:126:G:H21	51:ZA:180:G:H21	1.48	0.61
51:ZA:925:G:H1	51:ZA:1017:U:H3	1.46	0.61
65:NB:99:ARG:NH2	65:NB:119:GLU:OE2	2.33	0.61
85:HC:12:VAL:HG23	85:HC:91:ASP:HA	1.81	0.61
11:K:116:ARG:NH2	11:K:155:MET:O	2.33	0.61
30:DA:36:ARG:NH1	48:WA:1663:C:OP1	2.33	0.61
42:PA:107:ARG:NH2	48:WA:2265:A:OP1	2.32	0.61
61:JB:136:ARG:NH1	61:JB:159:PHE:O	2.33	0.61
64:MB:52:LEU:HD11	64:MB:78:LYS:HE3	1.83	0.61
51:ZA:165:G:N2	51:ZA:165:G:OP2	2.34	0.61
1:A:27:ALA:O	1:A:128:ARG:NH2	2.33	0.61
1:A:128:ARG:NH1	48:WA:3683:G:OP2	2.33	0.61
16:P:88:ASP:OD2	16:P:108:ARG:NH1	2.34	0.61
51:ZA:1623:A:H5''	70:SB:133:GLY:HA3	1.82	0.61
48:WA:1092:C:H2'	48:WA:1093:A:H8	1.64	0.61
5:E:115:MET:O	42:PA:87:ARG:NH1	2.33	0.61
23:W:110:LYS:NZ	23:W:121:VAL:O	2.34	0.61
54:CB:123:ARG:NH1	54:CB:143:CYS:SG	2.73	0.61
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:111:GLU:OE1	20:T:113:ARG:NH1	2.34	0.61
59:HB:289:ILE:HD12	59:HB:417:LYS:HG2	1.81	0.61
51:ZA:495:U:O2'	56:EB:27:PHE:O	2.19	0.60
4:D:166:ALA:HB1	4:D:171:LEU:HD12	1.83	0.60
4:D:256:LYS:HD2	49:XA:117:G:H5'	1.83	0.60
48:WA:1200:G:N2	48:WA:1201:G:O6	2.34	0.60
3:C:301:ALA:HB1	16:P:132:LYS:HE3	1.83	0.60
5:E:159:ARG:NH1	48:WA:4942:C:OP1	2.33	0.60
30:DA:103:VAL:O	30:DA:128:ARG:NH1	2.34	0.60
48:WA:2485:G:N1	48:WA:2497:U:N3	2.49	0.60
5:E:164:ARG:NH1	12:L:106:ASP:OD2	2.34	0.60
48:WA:4324:G:N2	48:WA:4327:A:OP2	2.31	0.60
51:ZA:3:C:O2	61:JB:18:ARG:NH1	2.31	0.60
59:HB:408:VAL:HG13	59:HB:425:PHE:HB2	1.84	0.60
1:A:225:ILE:HD11	1:A:233:ARG:HG3	1.83	0.60
2:B:213:GLN:NE2	2:B:285:TYR:O	2.35	0.60
51:ZA:1616:U:HO2'	51:ZA:1661:A:HO2'	1.43	0.60
66:OB:105:THR:HG22	66:OB:107:THR:H	1.66	0.60
18:R:160:ARG:HB3	48:WA:1923:C:H1'	1.83	0.60
48:WA:1554:G:O2'	48:WA:1576:G:N2	2.29	0.60
48:WA:2505:G:N2	48:WA:4086:G:O4'	2.35	0.60
5:E:144:ARG:NH1	31:EA:110:ILE:OXT	2.33	0.60
53:BB:122:GLU:HG2	53:BB:140:VAL:HG12	1.83	0.60
4:D:223:PHE:HB3	4:D:226:TYR:HB2	1.84	0.60
51:ZA:1535:U:O2	57:FB:82:ASN:ND2	2.35	0.60
16:P:67:ILE:HD12	16:P:96:PRO:HD2	1.83	0.60
58:GB:2:LYS:HB3	58:GB:15:LEU:HD11	1.84	0.60
60:IB:131:PRO:HD2	60:IB:134:GLU:HB2	1.82	0.60
5:E:265:LYS:NZ	48:WA:4935:C:OP2	2.34	0.60
48:WA:4451:A:H8	92:WA:5250:ANM:H61	1.66	0.60
51:ZA:851:C:H5''	51:ZA:852:G:H5'	1.84	0.60
51:ZA:1556:A:N6	81:DC:13:LYS:O	2.34	0.60
58:GB:2:LYS:HD3	58:GB:15:LEU:HD21	1.82	0.60
14:N:72:HIS:N	48:WA:4588:G:OP1	2.35	0.59
19:S:127:GLN:NE2	19:S:129:LYS:O	2.35	0.59
42:PA:6:GLN:HG3	42:PA:44:ILE:HD12	1.83	0.59
51:ZA:538:U:O4	51:ZA:546:G:N1	2.35	0.59
51:ZA:846:G:OP2	56:EB:108:ARG:NH1	2.35	0.59
55:DB:144:ARG:HG3	55:DB:213:VAL:HG22	1.84	0.59
58:GB:165:GLU:OE1	58:GB:167:LYS:NZ	2.34	0.59
17:Q:172:ARG:HH12	51:ZA:908:A:H5''	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SA:34:A:H61	47:VA:21:C:H42	1.50	0.59
48:WA:1671:A:N3	48:WA:1854:U:O2'	2.33	0.59
19:S:70:HIS:NE2	48:WA:4329:C:OP1	2.35	0.59
51:ZA:1259:A:H1'	51:ZA:1264:C:H42	1.66	0.59
22:V:8:PHE:HZ	22:V:49:ILE:HD12	1.66	0.59
48:WA:62:A:N3	48:WA:77:U:O2'	2.31	0.59
48:WA:2380:G:N2	48:WA:2383:A:OP2	2.33	0.59
48:WA:2603:A:N6	48:WA:2746:A:OP2	2.35	0.59
48:WA:332:C:OP2	93:WA:5253:SPD:N10	2.36	0.59
48:WA:970:G:N2	48:WA:2098:G:O2'	2.35	0.59
48:WA:2377:A:H2'	48:WA:2378:A:H8	1.66	0.59
51:ZA:1016:U:H5''	65:NB:14:SER:HB2	1.85	0.59
51:ZA:1513:C:OP1	81:DC:12:ARG:NH1	2.36	0.59
8:H:43:VAL:HG12	8:H:59:LYS:HD3	1.84	0.59
29:CA:59:THR:HG1	29:CA:104:THR:HG1	1.46	0.59
5:E:186:ARG:HG3	48:WA:4940:A:H5'	1.84	0.59
25:Y:52:LYS:O	25:Y:65:ARG:NH2	2.35	0.59
48:WA:1977:G:N2	48:WA:1985:A:OP1	2.36	0.59
51:ZA:1556:A:H61	81:DC:14:PHE:HB3	1.68	0.59
54:CB:187:ARG:HE	54:CB:192:LEU:HD12	1.67	0.59
48:WA:2494:C:H2'	48:WA:2495:G:C8	2.38	0.59
48:WA:4908:C:H2'	48:WA:4909:G:H8	1.68	0.59
51:ZA:1654:G:OP1	71:TB:90:SER:OG	2.19	0.59
58:GB:55:GLY:H	58:GB:63:MET:HE2	1.68	0.59
1:A:179:ILE:HG23	1:A:184:ARG:HB2	1.85	0.58
5:E:141:ARG:NH1	5:E:172:SER:O	2.36	0.58
15:O:164:ARG:NH2	48:WA:1598:U:O2'	2.36	0.58
18:R:160:ARG:HH11	18:R:160:ARG:HA	1.67	0.58
51:ZA:1130:G:N2	51:ZA:1130:G:OP2	2.36	0.58
44:SA:50:U:O2	44:SA:64:G:N2	2.29	0.58
51:ZA:1761:U:O2	51:ZA:1771:G:O6	2.21	0.58
53:BB:149:GLN:HE22	53:BB:154:SER:HB3	1.68	0.58
1:A:102:LEU:HB2	1:A:107:MET:HE3	1.86	0.58
10:J:44:THR:O	10:J:78:LYS:NZ	2.37	0.58
51:ZA:940:U:H3	51:ZA:1002:U:H3	1.51	0.58
57:FB:199:VAL:O	57:FB:203:ASN:ND2	2.36	0.58
8:H:85:THR:HG23	8:H:86:LEU:HG	1.85	0.58
48:WA:2850:G:O2'	48:WA:3840:U:O4	2.20	0.58
48:WA:3762:A:N6	51:ZA:1826:G:OP2	2.36	0.58
21:U:35:LYS:HB2	21:U:67:LYS:HG3	1.86	0.58
74:WB:18:GLU:HG3	74:WB:69:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:IB:114:GLU:OE2	60:IB:123:ARG:NH1	2.36	0.58
83:FC:121:CYS:CB	83:FC:126:CYS:SG	2.91	0.58
1:A:30:ARG:NH1	1:A:33:ASP:OD2	2.36	0.58
2:B:52:GLY:HA2	2:B:341:LYS:HE3	1.86	0.58
9:I:3:ARG:NH2	48:WA:4433:U:OP2	2.36	0.58
48:WA:1678:C:H41	48:WA:4380:A:H2'	1.67	0.58
51:ZA:379:C:O2	60:IB:5:ARG:NH1	2.36	0.58
48:WA:916:U:H4'	48:WA:917:A:H5'	1.86	0.58
48:WA:1392:G:N2	48:WA:1395:G:OP2	2.33	0.58
51:ZA:847:A:OP1	56:EB:108:ARG:NH2	2.37	0.58
51:ZA:1228:A:H2'	51:ZA:1229:G:C8	2.39	0.58
51:ZA:1521:C:OP2	70:SB:136:THR:OG1	2.18	0.58
68:QB:79:GLU:OE1	68:QB:111:ARG:NH1	2.37	0.58
71:TB:126:GLN:OE1	71:TB:129:ARG:NH2	2.37	0.58
14:N:89:PRO:HD3	48:WA:1916:C:H4'	1.84	0.58
32:FA:61:PRO:HA	32:FA:64:LEU:HD13	1.86	0.58
48:WA:308:G:OP2	48:WA:308:G:N2	2.32	0.58
1:A:101:VAL:HG22	1:A:165:VAL:HG22	1.84	0.58
2:B:329:ASP:OD1	2:B:329:ASP:N	2.36	0.58
15:O:161:ALA:HB2	48:WA:1599:G:H5'	1.86	0.58
17:Q:70:ARG:NH2	48:WA:2813:G:OP1	2.37	0.58
40:NA:15:CYS:SG	40:NA:19:GLN:NE2	2.77	0.58
41:OA:4:ARG:NH1	48:WA:1556:A:OP2	2.33	0.58
48:WA:126:C:H2'	48:WA:127:G:H8	1.69	0.58
51:ZA:1513:C:H2'	51:ZA:1514:G:H8	1.68	0.58
12:L:11:ARG:NH1	12:L:58:THR:O	2.34	0.57
53:BB:40:ASN:OD1	53:BB:75:GLN:NE2	2.36	0.57
75:XB:91:LEU:HB3	82:EC:82:VAL:HG11	1.85	0.57
48:WA:4539:C:H2'	48:WA:4540:G:H8	1.68	0.57
30:DA:89:LEU:HD13	30:DA:118:LEU:HD22	1.86	0.57
80:CC:17:VAL:HA	80:CC:30:VAL:HG23	1.85	0.57
43:RA:16:ARG:NH1	48:WA:1977:G:O2'	2.37	0.57
51:ZA:5:U:H2'	51:ZA:6:G:H8	1.70	0.57
51:ZA:1228:A:H2'	51:ZA:1229:G:H8	1.69	0.57
51:ZA:1617:G:N1	51:ZA:1620:A:OP2	2.38	0.57
16:P:2:GLY:N	48:WA:2074:C:OP1	2.37	0.57
68:QB:155:SER:O	68:QB:157:LYS:NZ	2.36	0.57
7:G:142:ARG:NH1	50:YA:155:C:OP1	2.37	0.57
22:V:93:LYS:O	22:V:101:ARG:NH2	2.37	0.57
48:WA:2411:U:H4'	48:WA:2430:A:H4'	1.86	0.57
51:ZA:148:U:H2'	51:ZA:149:A:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:PB:123:TYR:OH	70:SB:124:ARG:NH1	2.37	0.57
7:G:96:GLN:O	48:WA:4126:G:N2	2.37	0.57
18:R:69:GLU:OE2	18:R:76:LYS:NZ	2.38	0.57
48:WA:3666:G:H2'	48:WA:3667:G:H8	1.69	0.57
51:ZA:1297:U:O4	67:PB:59:ARG:NH2	2.37	0.57
8:H:113:GLU:HG2	8:H:125:ARG:HG2	1.87	0.57
29:CA:114:PHE:HA	29:CA:117:LEU:HD22	1.87	0.57
51:ZA:581:U:OP1	61:JB:133:ARG:NH2	2.38	0.57
85:HC:157:SER:OG	96:HC:601:GTP:N2	2.38	0.57
44:SA:17:G:O2'	44:SA:57:G:N2	2.29	0.57
45:TA:42:G:H2'	45:TA:43:A:H8	1.69	0.57
10:J:87:LEU:HD12	10:J:92:TYR:HA	1.87	0.56
51:ZA:183:G:O2'	51:ZA:184:G:O4'	2.22	0.56
19:S:43:LYS:NZ	48:WA:1735:G:OP1	2.38	0.56
31:EA:50:VAL:HG22	31:EA:69:VAL:HG22	1.87	0.56
31:EA:100:ARG:NH1	48:WA:4755:U:OP1	2.37	0.56
40:NA:81:ARG:NH2	48:WA:4295:U:O2'	2.39	0.56
48:WA:4276:A:H2'	48:WA:4277:G:H8	1.69	0.56
48:WA:4596:U:H2'	48:WA:4597:G:H8	1.70	0.56
52:AB:156:TYR:OH	73:VB:61:ARG:NH1	2.37	0.56
56:EB:137:PRO:HB2	56:EB:150:PRO:HD2	1.87	0.56
84:GC:26:GLN:NE2	84:GC:73:SER:O	2.38	0.56
3:C:339:THR:HG22	3:C:342:ARG:HH22	1.70	0.56
18:R:3:ALA:O	18:R:111:ARG:NH2	2.38	0.56
19:S:87:LYS:NZ	48:WA:4302:U:OP1	2.38	0.56
25:Y:88:ASP:O	25:Y:121:ARG:NH1	2.38	0.56
35:IA:49:TRP:O	48:WA:1648:A:O2'	2.23	0.56
48:WA:4:G:H2'	48:WA:5:A:H8	1.70	0.56
51:ZA:1309:C:OP1	83:FC:104:LYS:NZ	2.36	0.56
69:RB:94:GLU:O	69:RB:116:ASN:ND2	2.38	0.56
5:E:156:LEU:HD11	5:E:198:ILE:HG13	1.86	0.56
48:WA:2546:G:N1	50:YA:123:U:O2	2.39	0.56
53:BB:138:PHE:O	53:BB:213:ARG:N	2.38	0.56
64:MB:22:LEU:HD13	64:MB:89:VAL:HA	1.87	0.56
2:B:57:VAL:HG22	2:B:73:VAL:HG22	1.86	0.56
3:C:4:ALA:O	3:C:29:LYS:NZ	2.37	0.56
11:K:31:ARG:HD2	11:K:35:ARG:HH21	1.70	0.56
48:WA:1334:C:H2'	48:WA:1335:A:C8	2.41	0.56
48:WA:3598:A:H61	63:LB:2:ALA:HA	1.70	0.56
57:FB:114:ASN:OD1	57:FB:118:ASN:ND2	2.39	0.56
71:TB:113:VAL:HG12	71:TB:123:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:3621:G:H22	48:WA:3626:A:H1'	1.71	0.56
52:AB:8:LEU:HD11	73:VB:39:VAL:HG11	1.86	0.56
54:CB:196:ILE:HB	54:CB:223:TYR:HB2	1.88	0.56
58:GB:58:LYS:HA	58:GB:107:SER:HB2	1.86	0.56
84:GC:67:SER:H	84:GC:82:SER:HA	1.71	0.56
1:A:207:VAL:HG13	1:A:208:GLU:HG3	1.86	0.56
14:N:27:VAL:HG13	14:N:98:ALA:HB1	1.86	0.56
45:TA:22:G:H2'	45:TA:23:A:H8	1.70	0.56
48:WA:1249:U:O2	48:WA:1268:G:N2	2.37	0.56
48:WA:2467:C:H1'	48:WA:3674:G:H1	1.71	0.56
52:AB:77:ILE:HG12	52:AB:99:ILE:HB	1.86	0.56
61:JB:173:VAL:O	61:JB:177:ASN:ND2	2.39	0.56
76:YB:108:LYS:O	76:YB:112:ASN:ND2	2.38	0.56
2:B:249:ARG:NH2	48:WA:3847:A:OP2	2.39	0.56
5:E:96:THR:HG22	5:E:109:VAL:HG22	1.87	0.56
17:Q:44:LEU:HD22	17:Q:49:LEU:HD12	1.87	0.56
37:KA:20:ASN:O	37:KA:41:ARG:NH1	2.38	0.56
48:WA:4276:A:H2'	48:WA:4277:G:C8	2.41	0.56
48:WA:5059:C:H2'	48:WA:5060:A:C8	2.41	0.56
68:QB:156:LYS:NZ	68:QB:160:GLY:O	2.38	0.56
2:B:369:ASP:OD2	2:B:373:LYS:NZ	2.38	0.56
13:M:116:LEU:HD22	13:M:135:ILE:HD11	1.88	0.56
48:WA:169:A:C2	48:WA:267:G:C2	2.93	0.56
51:ZA:1458:G:OP1	84:GC:279:SER:OG	2.21	0.56
52:AB:51:LEU:HD23	69:RB:105:MET:HE1	1.87	0.56
53:BB:90:ASP:OD2	53:BB:92:GLN:NE2	2.39	0.56
33:GA:66:LYS:NZ	33:GA:82:ASP:OD2	2.34	0.56
48:WA:4090:C:H2'	48:WA:4091:G:H8	1.70	0.56
51:ZA:1203:G:H2'	51:ZA:1204:A:C8	2.41	0.56
51:ZA:1465:A:OP1	69:RB:56:HIS:NE2	2.39	0.56
84:GC:24:THR:HB	84:GC:71:ILE:HG12	1.87	0.56
26:Z:132:ARG:NH1	48:WA:1470:C:OP1	2.40	0.55
51:ZA:981:A:H2'	51:ZA:982:G:C8	2.42	0.55
51:ZA:1285:G:H4'	64:MB:35:ILE:HD11	1.87	0.55
51:ZA:1373:C:O2'	69:RB:10:LYS:NZ	2.32	0.55
32:FA:29:ARG:NH1	48:WA:2524:G:OP1	2.39	0.55
48:WA:470:A:H62	48:WA:685:G:H21	1.55	0.55
48:WA:759:G:H2'	48:WA:760:G:H8	1.72	0.55
6:F:146:LEU:O	6:F:150:ASN:ND2	2.31	0.55
51:ZA:496:C:OP1	56:EB:49:ARG:NH2	2.36	0.55
56:EB:251:GLU:OE2	56:EB:255:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JB:127:ARG:HD3	82:EC:104:ARG:HD3	1.88	0.55
62:KB:27:VAL:HG13	62:KB:43:LEU:HD13	1.88	0.55
13:M:114:ARG:HE	13:M:137:PRO:HG3	1.70	0.55
48:WA:20:U:H3'	48:WA:21:G:H8	1.71	0.55
48:WA:4929:G:H5''	48:WA:4930:C:H5	1.70	0.55
78:AC:59:PHE:HB2	78:AC:62:TYR:HB2	1.87	0.55
13:M:35:ALA:HA	13:M:65:ARG:HG2	1.89	0.55
37:KA:37:TYR:O	48:WA:362:A:N6	2.39	0.55
48:WA:982:G:N2	48:WA:982:G:OP2	2.39	0.55
48:WA:1975:G:H2'	48:WA:1976:U:H2'	1.87	0.55
48:WA:4176:U:H2'	48:WA:4177:G:H8	1.71	0.55
51:ZA:928:G:H2'	51:ZA:929:G:C8	2.41	0.55
51:ZA:1401:A:H4'	72:UB:52:GLY:HA3	1.89	0.55
51:ZA:1743:G:H21	51:ZA:1791:A:N6	2.00	0.55
2:B:234:ARG:NH1	2:B:271:GLN:O	2.34	0.55
48:WA:408:A:O2'	48:WA:411:G:OP2	2.24	0.55
48:WA:4080:C:O2'	48:WA:4174:A:N6	2.39	0.55
51:ZA:332:G:O6	58:GB:189:ARG:NH2	2.39	0.55
51:ZA:640:A:H2'	51:ZA:641:A:C8	2.41	0.55
51:ZA:1758:G:H2'	51:ZA:1759:G:C8	2.41	0.55
51:ZA:1855:G:OP2	66:OB:147:ARG:NH1	2.39	0.55
64:MB:36:ARG:NH2	83:FC:129:GLY:O	2.40	0.55
81:DC:17:GLY:O	81:DC:27:ARG:NH1	2.40	0.55
31:EA:43:LEU:O	31:EA:109:ARG:NH1	2.40	0.55
48:WA:1247:C:H2'	48:WA:1248:G:H8	1.72	0.55
59:HB:245:LYS:NZ	59:HB:269:GLU:OE2	2.38	0.55
76:YB:102:THR:O	76:YB:107:ARG:NH2	2.40	0.55
33:GA:31:LEU:HB3	33:GA:47:ILE:HG22	1.88	0.55
37:KA:21:ARG:NH1	50:YA:52:A:OP1	2.40	0.55
48:WA:484:G:H5'	48:WA:485:U:H5''	1.87	0.55
48:WA:1973:U:O2	87:b:41:GLN:NE2	2.40	0.55
48:WA:2485:G:O6	48:WA:2497:U:O4	2.24	0.55
48:WA:2747:A:H2'	48:WA:2748:A:H8	1.72	0.55
51:ZA:1677:U:OP1	57:FB:71:ARG:NH2	2.39	0.55
16:P:65:ARG:NH1	48:WA:1504:G:OP1	2.40	0.55
23:W:55:ARG:NH2	50:YA:116:C:O2'	2.40	0.55
25:Y:103:ASP:HB3	25:Y:106:LEU:HB2	1.89	0.55
43:RA:9:GLU:O	43:RA:65:GLN:NE2	2.40	0.55
48:WA:2488:G:O2'	50:YA:125:C:N4	2.39	0.55
51:ZA:809:A:OP1	56:EB:187:ALA:N	2.40	0.55
59:HB:355:PRO:HG2	59:HB:358:ARG:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:TB:13:GLU:OE1	71:TB:16:ARG:NH1	2.40	0.55
71:TB:104:LEU:HB3	71:TB:121:ARG:HE	1.72	0.55
79:BC:74:THR:OG1	79:BC:77:CYS:SG	2.65	0.55
7:G:194:ASN:ND2	48:WA:151:G:N7	2.52	0.55
48:WA:2737:G:H2'	48:WA:2738:G:H8	1.72	0.55
51:ZA:1477:U:OP2	69:RB:3:ARG:NH2	2.40	0.55
14:N:116:LYS:HE3	18:R:169:THR:HG21	1.89	0.54
27:AA:18:ARG:NH1	48:WA:1688:C:O2'	2.40	0.54
30:DA:39:ARG:NH2	48:WA:1664:C:OP2	2.39	0.54
48:WA:4147:C:N4	48:WA:4148:G:O6	2.40	0.54
87:b:99:ARG:HD2	87:b:103:LEU:HD23	1.89	0.54
6:F:227:VAL:HA	18:R:39:VAL:HG12	1.89	0.54
7:G:106:ARG:NH2	48:WA:4165:U:OP2	2.39	0.54
12:L:94:LYS:NZ	48:WA:4874:G:OP2	2.40	0.54
21:U:50:ASN:ND2	48:WA:4459:U:OP1	2.40	0.54
22:V:61:LYS:NZ	48:WA:5040:A:OP1	2.41	0.54
37:KA:2:SER:N	48:WA:2408:G:N7	2.55	0.54
48:WA:1812:G:H1	48:WA:1830:C:H42	1.53	0.54
48:WA:4476:A:OP2	48:WA:4478:C:N4	2.40	0.54
71:TB:76:THR:HB	71:TB:94:ARG:HB3	1.88	0.54
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.89	0.54
5:E:184:LEU:O	48:WA:4885:C:N4	2.41	0.54
48:WA:1335:A:H2'	48:WA:1336:A:H8	1.73	0.54
48:WA:2000:A:H2'	48:WA:2001:A:C8	2.42	0.54
50:YA:67:U:H2'	50:YA:68:G:H8	1.71	0.54
51:ZA:1126:G:OP1	52:AB:41:ARG:NH1	2.41	0.54
55:DB:70:ASP:OD2	55:DB:103:ARG:NH1	2.40	0.54
58:GB:159:ARG:HG2	58:GB:173:ALA:HB2	1.89	0.54
60:IB:157:LYS:NZ	60:IB:158:ILE:O	2.40	0.54
84:GC:109:LEU:HD23	84:GC:152:SER:HA	1.89	0.54
48:WA:300:A:H2'	48:WA:301:G:H8	1.72	0.54
48:WA:3811:G:OP2	48:WA:3811:G:N2	2.30	0.54
48:WA:4774:C:N4	48:WA:4866:U:O2	2.41	0.54
51:ZA:551:U:H2'	51:ZA:552:G:H8	1.72	0.54
61:JB:113:GLN:OE1	61:JB:154:GLN:NE2	2.40	0.54
87:b:116:ILE:HG22	87:b:118:PRO:HD2	1.89	0.54
12:L:86:TRP:O	12:L:89:THR:OG1	2.25	0.54
23:W:65:ALA:HB2	33:GA:69:LEU:HD11	1.89	0.54
48:WA:2487:U:O2	48:WA:2495:G:N2	2.32	0.54
52:AB:145:ILE:HG12	52:AB:159:ILE:HB	1.88	0.54
61:JB:131:ARG:NH1	61:JB:143:ASN:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:111:CYS:SG	85:HC:112:ALA:N	2.80	0.54
85:HC:162:TYR:O	85:HC:210:TRP:NE1	2.36	0.54
9:I:7:ARG:NH2	48:WA:4407:G:OP1	2.40	0.54
26:Z:75:LEU:HG	26:Z:113:GLY:HA2	1.90	0.54
40:NA:63:THR:O	40:NA:87:ARG:NH1	2.40	0.54
48:WA:1804:A:H5''	48:WA:1805:G:H5'	1.89	0.54
8:H:94:SER:HB3	8:H:142:ASP:HB3	1.89	0.54
38:LA:92:THR:HG22	38:LA:94:ASN:H	1.72	0.54
43:RA:119:ARG:NH1	48:WA:1976:U:OP1	2.41	0.54
48:WA:4240:G:H2'	48:WA:4241:A:H8	1.73	0.54
48:WA:4603:U:H2'	48:WA:4604:A:H8	1.72	0.54
51:ZA:1528:G:O2'	51:ZA:1666:C:OP1	2.24	0.54
85:HC:205:SER:HB2	85:HC:208:MET:HE1	1.90	0.54
10:J:112:HIS:HE1	10:J:125:ILE:HA	1.72	0.54
84:GC:254:PRO:HB3	84:GC:283:PRO:HB2	1.88	0.54
2:B:224:LYS:HG2	2:B:340:THR:HB	1.89	0.54
40:NA:19:GLN:NE2	40:NA:72:CYS:SG	2.81	0.54
46:UA:3:C:H42	46:UA:70:A:H61	1.54	0.54
85:HC:74:ASP:HA	85:HC:101:ASN:HD22	1.73	0.54
85:HC:272:LEU:HB3	85:HC:302:ALA:HB3	1.90	0.54
87:b:53:VAL:HG12	87:b:89:VAL:HG12	1.90	0.54
14:N:49:ARG:NH1	48:WA:1932:U:OP2	2.35	0.54
23:W:139:ARG:NH1	48:WA:2535:C:OP1	2.41	0.54
51:ZA:629:A:O2'	51:ZA:631:U:OP1	2.26	0.54
51:ZA:1160:U:O4	75:XB:3:LYS:NZ	2.37	0.54
2:B:71:GLU:OE2	2:B:366:LYS:NZ	2.40	0.53
22:V:80:ARG:HH21	58:GB:131:ARG:HG2	1.73	0.53
22:V:97:LYS:HG3	22:V:99:GLU:H	1.73	0.53
48:WA:2522:C:H2'	48:WA:2523:G:H8	1.72	0.53
48:WA:2545:A:H5'	50:YA:127:U:H1'	1.90	0.53
48:WA:4524:G:O2'	48:WA:4527:C:OP2	2.25	0.53
51:ZA:681:U:H4'	75:XB:9:THR:HG22	1.89	0.53
51:ZA:1307:U:H1'	83:FC:135:HIS:HE1	1.73	0.53
70:SB:23:ARG:NH2	77:ZB:46:ASN:O	2.41	0.53
85:HC:62:LYS:NZ	85:HC:76:SER:OG	2.39	0.53
85:HC:63:LEU:HD23	85:HC:66:GLU:HG3	1.90	0.53
46:UA:64:G:N2	46:UA:64:G:OP2	2.41	0.53
51:ZA:1606:G:O2'	51:ZA:1632:G:N2	2.40	0.53
56:EB:11:ARG:HA	56:EB:28:ALA:HB2	1.90	0.53
5:E:275:ARG:NH2	48:WA:4886:G:N7	2.55	0.53
6:F:104:VAL:HG13	6:F:135:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DA:98:GLU:OE1	48:WA:2326:C:O2'	2.25	0.53
37:KA:5:LYS:NZ	48:WA:2409:G:N7	2.56	0.53
48:WA:1074:G:N2	48:WA:1075:G:O6	2.40	0.53
51:ZA:1617:G:N7	67:PB:47:ARG:NH1	2.55	0.53
52:AB:36:GLN:O	52:AB:53:ARG:NH1	2.41	0.53
64:MB:26:LEU:HD22	64:MB:33:ARG:HH22	1.73	0.53
67:PB:81:ARG:NH2	67:PB:120:SER:O	2.34	0.53
7:G:158:GLU:OE2	7:G:166:ARG:NH2	2.36	0.53
25:Y:35:ASP:N	25:Y:35:ASP:OD1	2.41	0.53
31:EA:37:ASP:N	31:EA:37:ASP:OD1	2.42	0.53
32:FA:24:ARG:HD3	48:WA:2640:G:H4'	1.90	0.53
51:ZA:85:A:HO2'	51:ZA:149:A:HO2'	1.51	0.53
83:FC:141:CYS:SG	83:FC:142:GLY:N	2.81	0.53
84:GC:132:TRP:CD1	84:GC:138:CYS:HA	2.43	0.53
6:F:33:ARG:NH1	48:WA:1274:C:OP2	2.41	0.53
17:Q:13:SER:OG	17:Q:38:ARG:NH2	2.41	0.53
18:R:127:MET:HG2	19:S:153:PRO:HB2	1.89	0.53
51:ZA:1017:U:OP1	65:NB:62:GLN:NE2	2.42	0.53
56:EB:216:ASN:OD1	56:EB:216:ASN:N	2.42	0.53
60:IB:4:SER:OG	60:IB:6:ASP:OD2	2.26	0.53
87:b:107:VAL:HG12	87:b:109:ALA:H	1.74	0.53
1:A:117:GLU:O	1:A:162:ASN:ND2	2.42	0.53
2:B:298:LEU:HD23	2:B:300:LYS:HE2	1.90	0.53
11:K:18:TRP:NE1	48:WA:1518:G:O2'	2.37	0.53
15:O:154:MET:HB2	15:O:170:SER:HB3	1.91	0.53
29:CA:24:GLU:OE2	29:CA:87:ARG:NH1	2.41	0.53
48:WA:1963:G:O2'	48:WA:2026:G:N2	2.42	0.53
51:ZA:1550:G:H3'	51:ZA:1579:A:H61	1.73	0.53
79:BC:64:CYS:HB3	79:BC:73:LEU:HD23	1.91	0.53
84:GC:94:THR:HG23	84:GC:96:THR:H	1.73	0.53
14:N:12:ARG:O	18:R:171:ARG:NH2	2.40	0.53
21:U:43:LYS:HD2	48:WA:4510:C:H5''	1.90	0.53
25:Y:100:VAL:HG13	25:Y:106:LEU:HB3	1.91	0.53
48:WA:39:A:OP1	93:WA:5255:SPD:N10	2.40	0.53
48:WA:961:A:H1'	48:WA:2078:G:H5''	1.91	0.53
48:WA:4063:C:H2'	48:WA:4064:A:H8	1.74	0.53
51:ZA:520:A:O2'	51:ZA:825:A:N3	2.38	0.53
51:ZA:980:A:H2'	51:ZA:981:A:C8	2.44	0.53
65:NB:19:ARG:HH21	65:NB:21:SER:HB2	1.74	0.53
85:HC:113:VAL:HA	85:HC:149:ILE:O	2.09	0.53
4:D:126:THR:HG22	4:D:128:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:140:SER:OG	11:K:143:GLU:OE1	2.26	0.53
40:NA:99:ARG:HE	40:NA:102:GLN:HG3	1.73	0.53
43:RA:18:THR:HA	43:RA:57:ARG:HG2	1.91	0.53
43:RA:47:ALA:O	43:RA:50:THR:OG1	2.27	0.53
44:SA:50:U:O4	44:SA:64:G:O6	2.27	0.53
52:AB:109:THR:OG1	52:AB:136:GLU:OE1	2.27	0.53
56:EB:112:HIS:NE2	56:EB:237:SER:O	2.42	0.53
64:MB:92:CYS:SG	64:MB:102:LYS:NZ	2.79	0.53
65:NB:136:PRO:HG2	65:NB:139:TRP:HB2	1.91	0.53
85:HC:154:LYS:HE2	96:HC:601:GTP:H1'	1.89	0.53
2:B:124:LYS:NZ	48:WA:5065:G:O6	2.38	0.53
16:P:22:ASP:OD1	16:P:22:ASP:N	2.41	0.53
48:WA:2413:C:H2'	48:WA:2414:A:C8	2.44	0.53
51:ZA:311:C:H5''	51:ZA:312:G:H5''	1.91	0.53
51:ZA:1332:A:O2'	55:DB:183:GLN:O	2.27	0.53
80:CC:44:ARG:NH2	80:CC:63:ARG:O	2.41	0.53
30:DA:48:ARG:O	48:WA:1885:G:O2'	2.23	0.53
48:WA:1962:A:H1'	87:b:63:LYS:HG2	1.90	0.53
51:ZA:990:A:OP2	78:AC:37:LYS:NZ	2.38	0.53
51:ZA:1612:G:OP1	67:PB:18:ARG:NH2	2.42	0.53
85:HC:108:GLN:NE2	85:HC:251:GLN:OE1	2.38	0.53
16:P:150:ARG:NH2	48:WA:1501:C:OP1	2.42	0.52
25:Y:46:ILE:HG23	25:Y:68:ILE:HG23	1.91	0.52
41:OA:4:ARG:NH2	48:WA:1557:G:O6	2.41	0.52
48:WA:382:G:N1	48:WA:385:A:OP2	2.40	0.52
51:ZA:1092:G:OP1	65:NB:2:GLY:N	2.43	0.52
62:KB:16:PHE:HB2	62:KB:79:LEU:HD23	1.91	0.52
65:NB:33:VAL:HG21	65:NB:66:VAL:HG11	1.90	0.52
85:HC:12:VAL:HG21	85:HC:24:THR:HG21	1.91	0.52
11:K:48:PRO:HG3	33:GA:118:LYS:HE3	1.91	0.52
13:M:123:GLU:OE1	13:M:128:LYS:NZ	2.42	0.52
28:BA:50:ASN:ND2	28:BA:75:SER:O	2.42	0.52
51:ZA:307:G:H1'	60:IB:45:THR:HG22	1.91	0.52
51:ZA:1568:C:OP1	71:TB:96:SER:OG	2.25	0.52
67:PB:81:ARG:NH1	67:PB:97:TYR:O	2.42	0.52
84:GC:107:ASP:N	84:GC:107:ASP:OD1	2.41	0.52
2:B:103:LYS:NZ	48:WA:4727:C:OP1	2.42	0.52
17:Q:38:ARG:NH1	48:WA:2529:A:OP1	2.42	0.52
19:S:28:ALA:HA	19:S:31:MET:HG2	1.92	0.52
48:WA:2022:U:H2'	48:WA:2023:G:H8	1.74	0.52
48:WA:4539:C:H2'	48:WA:4540:G:C8	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1156:U:O4	54:CB:194:ARG:NH1	2.43	0.52
51:ZA:1565:C:OP2	71:TB:101:ARG:NH1	2.42	0.52
55:DB:69:GLU:O	55:DB:92:ARG:NH2	2.43	0.52
83:FC:133:ALA:N	83:FC:140:TYR:O	2.34	0.52
13:M:172:ARG:NH1	48:WA:62:A:OP1	2.39	0.52
29:CA:64:ILE:HG23	29:CA:68:LEU:HD23	1.91	0.52
43:RA:20:GLY:N	43:RA:54:LYS:O	2.39	0.52
48:WA:1183:U:H2'	48:WA:1184:G:C8	2.45	0.52
51:ZA:1781:A:H2'	51:ZA:1782:G:C8	2.45	0.52
85:HC:348:ASN:ND2	85:HC:431:GLN:OE1	2.43	0.52
11:K:59:VAL:HB	48:WA:74:G:H5'	1.92	0.52
21:U:74:LYS:NZ	48:WA:3800:U:OP2	2.40	0.52
22:V:80:ARG:NH2	51:ZA:167:G:O2'	2.43	0.52
91:UA:101:5GP:OP2	85:HC:100:LYS:NZ	2.40	0.52
48:WA:85:G:O2'	48:WA:97:G:O6	2.26	0.52
48:WA:3665:A:N6	48:WA:4170:G:O2'	2.43	0.52
48:WA:3691:G:O2'	48:WA:3820:U:OP2	2.25	0.52
48:WA:4190:U:H2'	48:WA:4191:U:C6	2.45	0.52
51:ZA:957:A:H3'	51:ZA:958:G:H21	1.73	0.52
51:ZA:1617:G:O6	67:PB:43:ARG:NH1	2.43	0.52
57:FB:27:ASP:OD1	57:FB:107:ASN:ND2	2.40	0.52
16:P:187:LYS:NZ	16:P:188:ASN:O	2.43	0.52
45:TA:26:A:H2	45:TA:44:G:H22	1.57	0.52
48:WA:4969:A:H2'	48:WA:4970:A:H8	1.74	0.52
55:DB:70:ASP:OD1	55:DB:95:ASN:ND2	2.43	0.52
58:GB:67:VAL:HB	58:GB:99:GLY:HA2	1.91	0.52
59:HB:258:GLU:HG3	59:HB:286:ALA:HB3	1.92	0.52
70:SB:124:ARG:HB2	70:SB:131:VAL:HG13	1.92	0.52
14:N:54:TYR:OH	14:N:73:PHE:O	2.27	0.52
14:N:125:LYS:HG3	14:N:129:LEU:HD12	1.90	0.52
48:WA:4899:G:H2'	48:WA:4900:G:H8	1.75	0.52
50:YA:102:G:OP2	50:YA:104:A:O2'	2.25	0.52
52:AB:164:ASN:O	52:AB:170:SER:OG	2.21	0.52
56:EB:87:MET:HE1	56:EB:236:ILE:HG21	1.90	0.52
60:IB:135:GLU:O	60:IB:139:LYS:HB2	2.09	0.52
27:AA:10:HIS:NE2	48:WA:1879:G:O6	2.42	0.52
40:NA:4:VAL:O	40:NA:94:GLY:N	2.42	0.52
48:WA:3734:A:H2'	48:WA:3735:A:C8	2.45	0.52
51:ZA:1276:A:H1'	62:KB:50:GLN:HE22	1.74	0.52
51:ZA:1608:U:OP1	70:SB:134:GLN:NE2	2.43	0.52
51:ZA:1865:C:O2'	78:AC:95:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:MB:33:ARG:NH2	64:MB:89:VAL:O	2.43	0.52
1:A:28:ARG:HE	1:A:123:ARG:HD3	1.75	0.52
4:D:103:LEU:HD11	4:D:248:ARG:HE	1.75	0.52
9:I:38:ARG:HD3	9:I:83:ASP:HB3	1.90	0.52
11:K:178:ALA:N	26:Z:134:GLU:OE2	2.38	0.52
21:U:92:ASP:OD1	21:U:92:ASP:N	2.37	0.52
27:AA:12:GLN:NE2	48:WA:1672:G:OP1	2.42	0.52
48:WA:1215:U:O2'	48:WA:1217:G:O4'	2.28	0.52
71:TB:116:ASP:OD1	71:TB:117:GLN:N	2.41	0.52
84:GC:91:ASP:OD2	84:GC:93:THR:OG1	2.24	0.52
1:A:181:LYS:HB2	48:WA:1579:G:C5	2.45	0.52
33:GA:87:LYS:HD3	33:GA:91:MET:HE2	1.92	0.52
48:WA:2413:C:H2'	48:WA:2414:A:H8	1.74	0.52
51:ZA:453:C:O2'	58:GB:92:ARG:O	2.28	0.52
51:ZA:649:U:H2'	51:ZA:650:A:H8	1.74	0.52
51:ZA:677:G:N2	51:ZA:1028:A:H62	2.05	0.52
51:ZA:913:A:N6	59:HB:357:SER:O	2.42	0.52
62:KB:15:LEU:HD22	62:KB:49:MET:HE1	1.91	0.52
65:NB:4:MET:SD	65:NB:124:ARG:NH1	2.83	0.52
84:GC:132:TRP:HD1	84:GC:138:CYS:HA	1.75	0.52
21:U:13:LYS:NZ	21:U:59:ASP:OD1	2.43	0.51
51:ZA:107:A:H2'	51:ZA:108:G:C8	2.44	0.51
51:ZA:570:C:O2'	76:YB:34:THR:O	2.28	0.51
51:ZA:1275:G:N2	51:ZA:1506:A:OP2	2.33	0.51
84:GC:202:PRO:HG2	84:GC:243:PRO:HA	1.91	0.51
3:C:204:ARG:NH1	3:C:205:ARG:O	2.42	0.51
35:IA:22:CYS:SG	35:IA:24:SER:OG	2.65	0.51
48:WA:4637:A:H8	48:WA:5050:A:H61	1.58	0.51
48:WA:4899:G:H2'	48:WA:4900:G:C8	2.46	0.51
51:ZA:183:G:O2'	51:ZA:184:G:O5'	2.29	0.51
51:ZA:866:U:H2'	51:ZA:867:G:C8	2.46	0.51
57:FB:40:ALA:HB1	57:FB:45:TYR:CG	2.46	0.51
73:VB:10:ASP:N	73:VB:10:ASP:OD1	2.42	0.51
84:GC:165:ILE:HG13	84:GC:177:TRP:HB2	1.92	0.51
4:D:52:ILE:HD13	49:XA:6:C:H4'	1.93	0.51
4:D:53:VAL:HG11	4:D:159:VAL:HA	1.92	0.51
7:G:218:GLU:OE2	13:M:26:ARG:NH1	2.43	0.51
24:X:109:LEU:HD22	24:X:115:ARG:HH12	1.76	0.51
48:WA:2782:C:H2'	48:WA:2783:G:H8	1.74	0.51
48:WA:4090:C:H2'	48:WA:4091:G:C8	2.45	0.51
48:WA:4770:G:H2'	48:WA:4771:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:375:U:OP2	63:LB:59:LYS:NZ	2.44	0.51
54:CB:192:LEU:HB3	54:CB:227:ARG:HB3	1.92	0.51
56:EB:45:ILE:HA	56:EB:61:VAL:HG11	1.91	0.51
64:MB:32:ALA:HB1	64:MB:37:GLU:HB3	1.92	0.51
17:Q:105:LEU:HD23	17:Q:138:LEU:HD23	1.91	0.51
19:S:122:LYS:HB3	19:S:124:THR:HG22	1.91	0.51
27:AA:111:ARG:NH2	48:WA:1270:G:N7	2.58	0.51
48:WA:1335:A:H2'	48:WA:1336:A:C8	2.45	0.51
48:WA:1727:U:H2'	48:WA:1728:U:H6	1.76	0.51
9:I:152:LEU:HB3	9:I:165:ILE:HD12	1.93	0.51
24:X:18:HIS:O	24:X:78:TYR:OH	2.24	0.51
24:X:52:ASP:OD2	24:X:110:LYS:NZ	2.43	0.51
48:WA:478:G:H2'	48:WA:479:G:H8	1.75	0.51
48:WA:1183:U:H2'	48:WA:1184:G:H8	1.75	0.51
48:WA:1560:A:H2'	48:WA:1561:G:H8	1.74	0.51
48:WA:2557:G:H2'	48:WA:2558:G:H8	1.76	0.51
48:WA:5014:G:O2'	48:WA:5016:A:OP1	2.27	0.51
51:ZA:921:G:C5	74:WB:28:ARG:HD3	2.46	0.51
60:IB:106:SER:HB3	60:IB:171:LEU:HG	1.92	0.51
85:HC:368:ILE:HD11	85:HC:410:MET:HB2	1.92	0.51
14:N:163:LYS:NZ	48:WA:4911:A:OP1	2.43	0.51
43:RA:119:ARG:NH1	48:WA:1975:G:O2'	2.44	0.51
48:WA:132:G:O6	48:WA:137:G:N2	2.33	0.51
48:WA:1194:C:H2'	48:WA:1195:G:H8	1.75	0.51
51:ZA:70:G:N2	51:ZA:71:G:O6	2.42	0.51
51:ZA:608:C:O4'	82:EC:131:ASN:ND2	2.44	0.51
51:ZA:807:G:H2'	51:ZA:808:A:H8	1.76	0.51
51:ZA:916:A:C5	65:NB:73:ARG:HD3	2.45	0.51
3:C:71:ARG:HB2	3:C:73:VAL:HG22	1.93	0.51
16:P:14:ARG:NH2	48:WA:2085:C:OP2	2.43	0.51
24:X:112:ASP:H	24:X:115:ARG:HB2	1.76	0.51
31:EA:89:ARG:NH2	48:WA:710:C:OP1	2.44	0.51
35:IA:52:LYS:HG2	35:IA:55:ARG:HH22	1.76	0.51
43:RA:121:LEU:H	87:b:45:MET:HE3	1.76	0.51
44:SA:26:A:H61	44:SA:44:A:H61	1.59	0.51
48:WA:153:G:H2'	48:WA:154:G:H8	1.75	0.51
48:WA:4994:G:H2'	48:WA:4995:G:C8	2.46	0.51
51:ZA:5:U:H2'	51:ZA:6:G:C8	2.45	0.51
51:ZA:641:A:OP1	61:JB:40:LYS:NZ	2.39	0.51
51:ZA:1232:U:H2'	51:ZA:1233:G:H8	1.75	0.51
51:ZA:1255:G:OP1	51:ZA:1256:G:O2'	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:18:SER:O	85:HC:153:ASN:ND2	2.44	0.51
2:B:276:HIS:ND1	48:WA:4718:C:OP1	2.44	0.51
51:ZA:1422:G:H2'	51:ZA:1423:C:H4'	1.93	0.51
9:I:47:PRO:HD2	9:I:141:LYS:HA	1.93	0.51
43:RA:131:GLU:OE1	48:WA:1975:G:N2	2.37	0.51
48:WA:369:G:N2	48:WA:372:A:OP2	2.35	0.51
48:WA:3738:A:H2'	48:WA:3739:A:C8	2.46	0.51
48:WA:4241:A:H2'	48:WA:4242:G:C8	2.45	0.51
51:ZA:1023:A:OP2	65:NB:124:ARG:NH1	2.44	0.51
65:NB:29:THR:OG1	65:NB:31:ASP:OD1	2.26	0.51
8:H:120:GLU:HG2	48:WA:4613:A:H2	1.76	0.51
17:Q:84:THR:HG22	48:WA:2866:A:H5''	1.92	0.51
24:X:30:MET:HB3	24:X:101:PRO:HG2	1.93	0.51
26:Z:12:ARG:NH1	48:WA:2347:G:OP2	2.44	0.51
33:GA:97:LYS:HD3	48:WA:135:G:C6	2.46	0.51
48:WA:1434:G:O2'	48:WA:1454:A:N6	2.44	0.51
48:WA:2523:G:H2'	48:WA:2524:G:H8	1.75	0.51
48:WA:2640:G:H1	48:WA:2699:A:H61	1.59	0.51
51:ZA:943:U:OP1	53:BB:214:LYS:NZ	2.39	0.51
51:ZA:1711:U:H2'	51:ZA:1712:A:H8	1.76	0.51
60:IB:162:LEU:HD11	60:IB:191:GLU:HG2	1.93	0.51
66:OB:101:GLY:HA3	66:OB:134:PRO:HG2	1.93	0.51
74:WB:42:MET:HE2	74:WB:49:GLU:HA	1.92	0.51
2:B:54:THR:OG1	2:B:55:HIS:N	2.44	0.50
16:P:85:THR:HG22	16:P:104:ARG:HB2	1.92	0.50
20:T:25:CYS:HB3	20:T:112:LEU:HD13	1.92	0.50
42:PA:19:LYS:HB2	48:WA:2339:C:H4'	1.94	0.50
48:WA:1249:U:O4	48:WA:1268:G:O6	2.28	0.50
48:WA:1826:G:H2'	48:WA:1827:A:C8	2.46	0.50
48:WA:1908:U:H2'	48:WA:1909:A:H8	1.76	0.50
48:WA:1929:U:OP1	48:WA:1951:U:O2'	2.26	0.50
48:WA:4701:U:H1'	48:WA:4702:A:H5''	1.92	0.50
51:ZA:43:U:OP2	51:ZA:485:A:N6	2.42	0.50
52:AB:85:ARG:NH1	52:AB:203:PHE:O	2.44	0.50
54:CB:104:ASP:HB3	54:CB:130:ILE:HG13	1.93	0.50
70:SB:22:GLY:HA2	70:SB:56:ALA:HB3	1.93	0.50
87:b:229:ILE:O	87:b:233:THR:OG1	2.28	0.50
1:A:152:SER:OG	48:WA:3663:G:N7	2.43	0.50
1:A:242:ARG:NH2	1:A:243:THR:O	2.44	0.50
11:K:91:ALA:HB1	11:K:96:ILE:HB	1.92	0.50
30:DA:64:LYS:NZ	48:WA:2081:G:OP2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:PA:67:ARG:NH1	48:WA:667:G:OP2	2.45	0.50
48:WA:1935:G:H2'	48:WA:1936:A:C8	2.46	0.50
51:ZA:1245:G:N2	72:UB:72:GLU:OE2	2.45	0.50
53:BB:52:THR:HG23	53:BB:57:ILE:HG22	1.93	0.50
2:B:11:HIS:NE2	48:WA:4460:C:OP1	2.42	0.50
13:M:178:HIS:ND1	48:WA:68:U:OP1	2.33	0.50
17:Q:176:ARG:NH2	51:ZA:910:G:OP1	2.44	0.50
48:WA:756:U:H3	48:WA:911:G:H1	1.59	0.50
48:WA:3850:U:H2'	48:WA:3851:A:H8	1.76	0.50
48:WA:4240:G:H2'	48:WA:4241:A:C8	2.46	0.50
48:WA:4241:A:H2'	48:WA:4242:G:H8	1.77	0.50
48:WA:4993:U:H2'	48:WA:4994:G:C8	2.46	0.50
57:FB:34:SER:HA	80:CC:55:VAL:HB	1.93	0.50
1:A:28:ARG:HB3	1:A:123:ARG:HB3	1.93	0.50
5:E:73:ARG:HH11	48:WA:989:C:H5	1.60	0.50
5:E:80:SER:OG	48:WA:1272:A:N1	2.44	0.50
10:J:151:ILE:HG22	10:J:155:HIS:HB3	1.94	0.50
21:U:21:PRO:HA	21:U:54:ALA:HA	1.94	0.50
42:PA:35:ARG:NH2	48:WA:2267:G:OP1	2.41	0.50
43:RA:46:ILE:HD11	43:RA:62:LEU:HD21	1.92	0.50
48:WA:2337:C:H2'	48:WA:2338:G:H8	1.76	0.50
51:ZA:28:U:H2'	51:ZA:29:G:H8	1.76	0.50
51:ZA:65:C:N4	58:GB:134:GLY:O	2.41	0.50
51:ZA:1113:A:H2'	51:ZA:1114:U:C6	2.47	0.50
51:ZA:1415:C:O2'	71:TB:132:ASP:OD2	2.27	0.50
62:KB:37:ASP:N	62:KB:37:ASP:OD1	2.44	0.50
85:HC:5:LYS:NZ	85:HC:82:THR:O	2.44	0.50
85:HC:184:ASN:ND2	85:HC:186:ASP:OD1	2.45	0.50
85:HC:426:VAL:HB	85:HC:434:ALA:HB3	1.94	0.50
2:B:13:SER:HB2	48:WA:4624:A:H4'	1.94	0.50
48:WA:3719:A:H2'	48:WA:3720:A:C8	2.46	0.50
51:ZA:319:C:OP1	51:ZA:319:C:H4'	2.10	0.50
51:ZA:919:A:OP2	65:NB:64:ARG:NH2	2.40	0.50
51:ZA:1018:U:O2'	65:NB:86:GLU:OE2	2.28	0.50
62:KB:11:ILE:HD11	62:KB:45:VAL:HG22	1.93	0.50
83:FC:107:LYS:HD2	83:FC:115:SER:HB3	1.94	0.50
83:FC:121:CYS:HB3	83:FC:126:CYS:SG	2.51	0.50
1:A:188:LYS:NZ	48:WA:2741:C:O2	2.44	0.50
40:NA:26:TYR:HB3	40:NA:67:VAL:HB	1.94	0.50
48:WA:3724:G:H2'	48:WA:3725:A:H8	1.76	0.50
48:WA:4342:U:O2	93:WA:5255:SPD:N1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:5008:U:H4'	48:WA:5009:A:H5'	1.92	0.50
51:ZA:912:C:H3'	51:ZA:913:A:H3'	1.93	0.50
54:CB:176:LYS:O	54:CB:200:ARG:NH2	2.44	0.50
56:EB:122:LYS:NZ	56:EB:123:LEU:O	2.45	0.50
59:HB:318:VAL:HG23	59:HB:330:VAL:HG13	1.92	0.50
60:IB:80:ASP:OD1	60:IB:81:VAL:N	2.44	0.50
72:UB:46:LYS:NZ	72:UB:97:ILE:O	2.38	0.50
4:D:40:ASP:HB2	4:D:43:LYS:HG2	1.94	0.50
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.92	0.50
7:G:210:ILE:HA	7:G:254:THR:HG22	1.94	0.50
9:I:21:ARG:O	9:I:24:ARG:NH2	2.44	0.50
15:O:71:ARG:NH2	15:O:139:ASP:OD1	2.44	0.50
48:WA:1256:A:H2	48:WA:1261:G:H1	1.59	0.50
48:WA:2485:G:H2'	48:WA:2486:A:C8	2.46	0.50
48:WA:2485:G:O6	48:WA:2497:U:C4	2.65	0.50
48:WA:2795:G:H5'	48:WA:2796:C:H5''	1.93	0.50
51:ZA:1098:C:H2'	51:ZA:1099:G:C8	2.46	0.50
54:CB:199:PRO:HG3	61:JB:58:ARG:HD3	1.93	0.50
76:YB:83:LYS:NZ	76:YB:96:LEU:O	2.44	0.50
1:A:13:GLY:O	1:A:17:ARG:NE	2.43	0.50
3:C:312:ARG:NH2	48:WA:2077:G:OP1	2.44	0.50
30:DA:48:ARG:NH2	48:WA:2281:A:O2'	2.45	0.50
37:KA:23:ILE:HG23	37:KA:38:ASN:HB2	1.94	0.50
48:WA:164:G:H2'	48:WA:165:A:H8	1.77	0.50
48:WA:3719:A:OP2	48:WA:3737:G:N2	2.44	0.50
51:ZA:1562:C:H2'	51:ZA:1563:G:H8	1.77	0.50
54:CB:72:ASP:OD2	54:CB:272:HIS:NE2	2.40	0.50
54:CB:81:ILE:HG23	54:CB:86:LEU:HB2	1.93	0.50
61:JB:42:GLU:OE1	61:JB:45:ARG:NH2	2.45	0.50
84:GC:199:THR:HG21	84:GC:240:CYS:HA	1.94	0.50
2:B:234:ARG:NH2	48:WA:4568:U:O2'	2.44	0.50
6:F:91:VAL:O	6:F:119:GLY:HA2	2.12	0.50
43:RA:142:ASN:HB3	43:RA:146:ARG:HD3	1.93	0.50
48:WA:1505:A:H4'	48:WA:1506:G:H5'	1.94	0.50
48:WA:4926:C:O2'	48:WA:4927:U:O4'	2.26	0.50
48:WA:4950:C:OP2	48:WA:4951:G:O2'	2.23	0.50
49:XA:92:C:H2'	49:XA:93:G:H8	1.75	0.50
51:ZA:1527:C:OP1	68:QB:168:GLN:NE2	2.45	0.50
64:MB:41:ALA:HA	64:MB:45:ARG:HB2	1.94	0.50
76:YB:55:ILE:HG12	76:YB:75:ILE:HG23	1.93	0.50
1:A:179:ILE:O	48:WA:3655:A:O2'	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:2813:G:N1	48:WA:2816:C:OP2	2.29	0.49
48:WA:5049:C:O2'	48:WA:5052:C:OP2	2.28	0.49
67:PB:108:LYS:HB3	67:PB:111:MET:HG3	1.93	0.49
68:QB:57:LEU:HD11	68:QB:59:LYS:HE3	1.94	0.49
84:GC:130:LYS:HG2	84:GC:141:THR:HB	1.93	0.49
84:GC:286:CYS:HA	84:GC:302:TYR:HA	1.94	0.49
85:HC:364:HIS:NE2	85:HC:411:CYS:O	2.44	0.49
26:Z:35:ALA:HB1	48:WA:39:A:H5''	1.94	0.49
29:CA:70:LYS:HG3	48:WA:2391:A:H4'	1.94	0.49
48:WA:456:C:H2'	48:WA:457:G:C8	2.47	0.49
48:WA:2031:A:H2'	48:WA:2032:A:C8	2.46	0.49
48:WA:3738:A:H2'	48:WA:3739:A:H8	1.77	0.49
48:WA:3872:C:H2'	48:WA:3873:A:H8	1.77	0.49
52:AB:2:SER:HB3	52:AB:59:LEU:HG	1.93	0.49
87:b:128:THR:OG1	87:b:129:GLY:N	2.41	0.49
13:M:49:ARG:HH12	48:WA:152:U:P	2.35	0.49
22:V:106:GLU:OE2	22:V:110:ARG:NH1	2.46	0.49
30:DA:104:SER:HB2	48:WA:2305:C:H5''	1.94	0.49
48:WA:2846:A:N6	48:WA:3841:G:O2'	2.45	0.49
48:WA:4494:U:O2'	48:WA:4514:U:O2	2.26	0.49
51:ZA:158:A:H2'	51:ZA:159:A:O4'	2.12	0.49
51:ZA:1013:U:OP1	51:ZA:1129:G:O2'	2.29	0.49
56:EB:43:PRO:HD2	56:EB:46:ILE:HD11	1.95	0.49
3:C:306:ARG:HG2	48:WA:2101:C:H3'	1.94	0.49
51:ZA:692:G:H2'	51:ZA:693:A:H8	1.76	0.49
56:EB:18:TRP:HB3	56:EB:20:LEU:HD13	1.94	0.49
71:TB:22:LEU:HG	71:TB:28:LEU:HD21	1.94	0.49
84:GC:22:ALA:HB1	84:GC:71:ILE:HG22	1.93	0.49
85:HC:281:ALA:HB2	85:HC:334:PRO:HB2	1.94	0.49
2:B:66:LYS:NZ	21:U:127:ASP:OD2	2.42	0.49
3:C:323:ARG:HB2	48:WA:1283:G:H5'	1.93	0.49
13:M:9:GLU:HB2	34:HA:44:ILE:HG13	1.94	0.49
19:S:63:ARG:NH2	27:AA:30:GLU:OE1	2.45	0.49
48:WA:35:U:O2'	48:WA:1527:A:N1	2.43	0.49
51:ZA:563:G:O2'	51:ZA:564:A:H8	1.96	0.49
51:ZA:931:C:H2'	51:ZA:932:G:C8	2.47	0.49
51:ZA:1619:A:O3'	67:PB:44:ARG:NH1	2.45	0.49
60:IB:64:ASN:O	60:IB:186:ASP:HA	2.12	0.49
62:KB:91:PRO:HD2	62:KB:94:LEU:HD12	1.94	0.49
72:UB:115:THR:HG22	72:UB:117:ALA:H	1.76	0.49
74:WB:55:ASP:OD1	74:WB:56:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:256:ILE:HB	85:HC:259:ILE:HB	1.94	0.49
2:B:80:GLU:OE1	2:B:323:TYR:OH	2.27	0.49
14:N:188:LYS:NZ	48:WA:4895:A:OP1	2.46	0.49
17:Q:21:LYS:NZ	48:WA:2823:U:OP1	2.33	0.49
20:T:35:ASP:HB2	20:T:38:ASN:HB3	1.93	0.49
21:U:87:SER:HA	21:U:97:TYR:HB3	1.94	0.49
30:DA:44:ARG:NH2	48:WA:1314:A:O2'	2.45	0.49
33:GA:96:ASN:N	33:GA:96:ASN:OD1	2.45	0.49
48:WA:262:G:H2'	48:WA:263:G:H8	1.77	0.49
51:ZA:433:A:H5''	60:IB:22:HIS:HB3	1.94	0.49
58:GB:160:LYS:HD2	58:GB:161:PRO:HD2	1.95	0.49
67:PB:43:ARG:HH12	67:PB:47:ARG:HH11	1.60	0.49
9:I:201:PRO:HB2	9:I:203:ARG:HG3	1.94	0.49
35:IA:52:LYS:NZ	48:WA:364:G:O6	2.35	0.49
48:WA:1560:A:H2'	48:WA:1561:G:C8	2.47	0.49
48:WA:2409:G:OP2	48:WA:2409:G:N2	2.39	0.49
51:ZA:1204:A:O2'	51:ZA:1700:C:OP2	2.26	0.49
51:ZA:1650:A:H5''	68:QB:165:ALA:HB2	1.94	0.49
54:CB:168:GLY:N	54:CB:179:THR:O	2.42	0.49
84:GC:214:GLY:HA2	84:GC:236:ILE:HG13	1.94	0.49
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.95	0.49
40:NA:58:LYS:NZ	48:WA:4382:A:OP1	2.41	0.49
48:WA:2000:A:H4'	87:b:9:TRP:HZ2	1.78	0.49
51:ZA:1760:G:H1	51:ZA:1773:C:H42	1.60	0.49
57:FB:81:ARG:HG3	57:FB:82:ASN:HD22	1.78	0.49
60:IB:27:TYR:HB3	60:IB:49:ARG:HH12	1.78	0.49
65:NB:4:MET:HE3	65:NB:121:ARG:HG2	1.95	0.49
68:QB:45:ALA:HB2	68:QB:101:GLY:HA3	1.94	0.49
75:XB:54:LYS:HE3	75:XB:91:LEU:HG	1.95	0.49
3:C:46:LYS:HB3	3:C:49:ARG:HH21	1.78	0.49
3:C:218:VAL:O	3:C:222:ARG:HB3	2.12	0.49
25:Y:92:ASP:OD2	25:Y:94:THR:OG1	2.26	0.49
43:RA:107:ASP:N	43:RA:107:ASP:OD1	2.44	0.49
48:WA:1384:G:H2'	48:WA:1385:G:H8	1.78	0.49
48:WA:1768:A:H3'	48:WA:1769:A:H8	1.77	0.49
48:WA:3656:G:O2'	48:WA:3695:U:OP1	2.29	0.49
50:YA:111:U:H4'	50:YA:112:G:H5'	1.95	0.49
70:SB:98:VAL:HG11	70:SB:106:LYS:HG3	1.95	0.49
85:HC:274:PRO:HG3	85:HC:292:VAL:HG22	1.94	0.49
1:A:198:ARG:NH2	48:WA:3690:U:OP2	2.46	0.49
1:A:243:THR:HB	48:WA:3750:A:H5''	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:39:ARG:NH2	48:WA:1364:G:OP1	2.45	0.49
44:SA:22:A:H2'	44:SA:23:G:C8	2.47	0.49
48:WA:1944:A:H2'	48:WA:1945:A:C8	2.47	0.49
48:WA:2523:G:H2'	48:WA:2524:G:C8	2.47	0.49
51:ZA:1232:U:H2'	51:ZA:1233:G:C8	2.48	0.49
51:ZA:1783:C:H4'	51:ZA:1784:G:H5'	1.95	0.49
57:FB:142:SER:HB3	80:CC:50:VAL:HG22	1.94	0.49
64:MB:42:LEU:HD22	64:MB:74:ILE:HG13	1.93	0.49
8:H:92:MET:HG2	8:H:181:VAL:HG22	1.95	0.48
8:H:92:MET:HE2	8:H:179:ILE:HG22	1.95	0.48
16:P:151:HIS:ND1	16:P:164:LYS:O	2.42	0.48
41:OA:30:GLU:HA	41:OA:33:GLN:HG2	1.94	0.48
48:WA:2488:G:H2'	48:WA:2489:G:C8	2.48	0.48
51:ZA:959:G:OP1	66:OB:104:ARG:NH2	2.33	0.48
51:ZA:1588:A:H2'	51:ZA:1589:A:C8	2.48	0.48
55:DB:210:VAL:O	55:DB:211:ARG:NH1	2.40	0.48
56:EB:31:PRO:HG3	56:EB:43:PRO:HG3	1.94	0.48
56:EB:122:LYS:NZ	56:EB:124:CYS:SG	2.74	0.48
60:IB:90:LEU:HD22	60:IB:95:THR:HG21	1.95	0.48
67:PB:28:MET:HG3	67:PB:33:LEU:HD22	1.94	0.48
68:QB:157:LYS:HB2	68:QB:166:ARG:HH22	1.77	0.48
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.94	0.48
3:C:159:GLU:HA	3:C:217:ILE:HB	1.95	0.48
8:H:177:ASP:OD1	8:H:177:ASP:N	2.46	0.48
10:J:99:PHE:O	10:J:159:LYS:NZ	2.40	0.48
13:M:96:ARG:NH2	13:M:104:GLU:OE1	2.43	0.48
16:P:172:ARG:HD2	26:Z:57:GLY:HA3	1.94	0.48
21:U:15:ARG:NH2	48:WA:4674:A:OP1	2.45	0.48
29:CA:57:MET:HG2	29:CA:88:LEU:HD23	1.95	0.48
48:WA:162:A:H2'	48:WA:163:A:H8	1.78	0.48
48:WA:4956:G:H2'	48:WA:4957:A:H8	1.78	0.48
51:ZA:472:C:O2'	51:ZA:474:G:OP1	2.22	0.48
85:HC:132:GLN:HB3	85:HC:136:HIS:CE1	2.48	0.48
5:E:126:ARG:O	48:WA:963:G:O2'	2.28	0.48
6:F:148:SER:OG	6:F:244:ARG:NH2	2.43	0.48
13:M:68:ARG:HA	13:M:98:LEU:HD21	1.94	0.48
18:R:95:ARG:NH2	48:WA:1953:G:O2'	2.46	0.48
51:ZA:106:C:H2'	51:ZA:107:A:H8	1.78	0.48
51:ZA:1447:G:OP1	72:UB:85:HIS:ND1	2.37	0.48
51:ZA:1599:U:OP2	77:ZB:46:ASN:ND2	2.46	0.48
51:ZA:1797:U:H2'	51:ZA:1798:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EB:66:MET:SD	56:EB:78:THR:OG1	2.71	0.48
84:GC:18:VAL:O	84:GC:287:THR:OG1	2.30	0.48
85:HC:11:VAL:HA	85:HC:90:ILE:HG23	1.94	0.48
3:C:56:GLU:OE1	3:C:106:LYS:NZ	2.46	0.48
5:E:185:ASN:ND2	5:E:274:LEU:O	2.38	0.48
12:L:96:GLU:OE2	12:L:100:ARG:NH2	2.46	0.48
13:M:157:LYS:O	13:M:162:ARG:NH1	2.45	0.48
26:Z:35:ALA:HB2	48:WA:38:A:H5'	1.95	0.48
48:WA:4772:U:H2'	48:WA:4773:C:C4	2.48	0.48
76:YB:10:ARG:HH21	76:YB:24:VAL:HG11	1.78	0.48
1:A:117:GLU:OE2	1:A:163:ARG:NH1	2.47	0.48
4:D:16:TYR:O	49:XA:11:A:N6	2.47	0.48
6:F:154:TYR:OH	6:F:187:GLU:OE2	2.30	0.48
16:P:104:ARG:NH2	48:WA:1355:G:N7	2.61	0.48
34:HA:63:VAL:HG23	34:HA:65:LYS:HG3	1.95	0.48
48:WA:699:G:H2'	48:WA:700:C:C6	2.48	0.48
48:WA:2555:A:H2	48:WA:2767:A:H62	1.61	0.48
48:WA:2811:G:O2'	48:WA:4646:G:OP1	2.30	0.48
73:VB:32:ILE:HG12	73:VB:60:ARG:HD2	1.96	0.48
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.96	0.48
14:N:85:ARG:HG3	14:N:99:LEU:HD11	1.94	0.48
15:O:148:VAL:HG22	15:O:175:ILE:HG23	1.95	0.48
24:X:54:GLU:HB2	24:X:108:ARG:HB3	1.95	0.48
46:UA:76:A:H62	85:HC:259:ILE:HD12	1.78	0.48
48:WA:175:C:H2'	48:WA:176:G:C8	2.49	0.48
48:WA:291:U:OP1	94:WA:5252:SPM:N14	2.46	0.48
48:WA:4908:C:H2'	48:WA:4909:G:C8	2.49	0.48
51:ZA:1464:C:OP2	69:RB:63:ARG:NH2	2.47	0.48
51:ZA:1665:G:OP1	71:TB:91:HIS:NE2	2.45	0.48
51:ZA:1798:C:H2'	51:ZA:1799:G:O4'	2.14	0.48
67:PB:34:MET:HG2	67:PB:42:ARG:HG3	1.95	0.48
70:SB:51:ASP:OD2	70:SB:53:THR:OG1	2.30	0.48
79:BC:67:THR:OG1	79:BC:70:LYS:O	2.32	0.48
1:A:37:ARG:NH1	48:WA:4090:C:OP1	2.47	0.48
4:D:88:VAL:HA	4:D:239:MET:HE3	1.95	0.48
4:D:132:VAL:HG21	4:D:170:GLY:HA2	1.94	0.48
10:J:151:ILE:O	49:XA:55:A:O2'	2.25	0.48
13:M:8:GLN:NE2	48:WA:279:A:OP2	2.44	0.48
16:P:181:ARG:NH2	48:WA:1393:A:OP1	2.44	0.48
17:Q:108:ARG:NH2	48:WA:2901:C:OP1	2.39	0.48
48:WA:1745:A:N1	48:WA:1791:C:O2'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:86:LEU:HB3	53:BB:98:THR:HB	1.95	0.48
8:H:128:MET:HE2	8:H:134:CYS:HB2	1.95	0.48
24:X:11:ARG:HG3	48:WA:229:G:H5''	1.95	0.48
31:EA:36:ARG:HG3	31:EA:80:ASN:HA	1.95	0.48
48:WA:1330:G:O2'	48:WA:2351:A:OP1	2.30	0.48
48:WA:2416:G:H2'	48:WA:2417:U:H6	1.78	0.48
48:WA:2445:G:OP2	48:WA:2518:G:N2	2.40	0.48
66:OB:31:CYS:HB3	66:OB:44:VAL:HG22	1.96	0.48
11:K:195:ARG:NH2	48:WA:1486:G:O2'	2.45	0.48
17:Q:121:HIS:ND1	48:WA:2666:G:OP2	2.42	0.48
21:U:19:GLY:O	48:WA:2848:G:O2'	2.32	0.48
26:Z:125:LYS:HG2	26:Z:145:VAL:HB	1.95	0.48
38:LA:80:ARG:HH21	48:WA:4698:C:H4'	1.79	0.48
48:WA:158:A:H5''	48:WA:159:C:H2'	1.96	0.48
48:WA:3613:A:O2'	48:WA:5018:A:O2'	2.23	0.48
51:ZA:1486:A:O3'	54:CB:121:ARG:NH2	2.47	0.48
63:LB:113:LEU:HD21	63:LB:120:VAL:HG11	1.96	0.48
64:MB:49:LEU:HB3	64:MB:111:VAL:HG13	1.95	0.48
68:QB:96:VAL:HG11	68:QB:110:ILE:HG12	1.95	0.48
73:VB:11:LEU:HD23	73:VB:11:LEU:H	1.79	0.48
12:L:29:ASP:OD1	12:L:30:VAL:N	2.46	0.48
16:P:178:ARG:N	26:Z:51:GLY:HA2	2.29	0.48
48:WA:2446:U:O2'	50:YA:112:G:O2'	2.24	0.48
48:WA:2495:G:O2'	50:YA:127:U:OP1	2.20	0.48
51:ZA:637:U:O2	82:EC:129:ASN:ND2	2.45	0.48
51:ZA:860:G:H21	74:WB:107:SER:HB2	1.77	0.48
51:ZA:1536:G:H2'	51:ZA:1537:A:C8	2.49	0.48
51:ZA:1587:G:C8	71:TB:78:ILE:HD11	2.48	0.48
54:CB:169:TYR:OH	54:CB:175:GLY:O	2.31	0.48
63:LB:126:VAL:HG22	63:LB:145:VAL:HG22	1.96	0.48
9:I:54:SER:HB2	9:I:135:ILE:HD11	1.96	0.47
35:IA:33:THR:HG22	35:IA:40:PRO:HG2	1.96	0.47
48:WA:137:G:H2'	48:WA:138:G:H8	1.78	0.47
48:WA:417:G:OP1	48:WA:2331:U:O2'	2.32	0.47
48:WA:4591:A:N1	48:WA:4623:C:O2'	2.47	0.47
48:WA:4682:G:H2'	48:WA:4683:A:C8	2.48	0.47
51:ZA:419:G:N2	51:ZA:661:U:O2	2.47	0.47
51:ZA:1089:G:O6	75:XB:3:LYS:NZ	2.46	0.47
53:BB:106:THR:HG22	53:BB:108:ASP:H	1.77	0.47
69:RB:60:ARG:HD2	69:RB:63:ARG:HH21	1.79	0.47
70:SB:28:PHE:O	70:SB:31:THR:OG1	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:378:LYS:HB3	85:HC:388:GLU:HB2	1.96	0.47
1:A:132:ASN:ND2	48:WA:3685:C:OP1	2.45	0.47
5:E:160:HIS:HB3	5:E:163:LYS:HD2	1.96	0.47
10:J:96:LYS:O	10:J:159:LYS:NZ	2.43	0.47
10:J:146:ARG:HG2	10:J:147:ARG:HG3	1.96	0.47
25:Y:54:THR:H	25:Y:57:MET:HE2	1.78	0.47
25:Y:68:ILE:O	25:Y:115:LYS:NZ	2.44	0.47
28:BA:38:ILE:HG21	28:BA:63:TYR:HB3	1.96	0.47
30:DA:104:SER:HG	48:WA:2307:U:HO2'	1.57	0.47
51:ZA:952:G:H2'	51:ZA:953:C:C6	2.49	0.47
51:ZA:1692:U:H2'	51:ZA:1693:G:C8	2.48	0.47
51:ZA:1693:G:N2	51:ZA:1834:A:H8	2.12	0.47
51:ZA:1862:G:O2'	78:AC:5:ARG:NH2	2.47	0.47
56:EB:162:ILE:HG22	56:EB:169:ILE:HA	1.96	0.47
1:A:72:ARG:NH2	48:WA:4086:G:O6	2.47	0.47
9:I:118:ALA:O	48:WA:1866:G:O2'	2.25	0.47
17:Q:12:SER:OG	17:Q:17:CYS:O	2.29	0.47
18:R:34:ALA:HB1	18:R:39:VAL:HG23	1.96	0.47
48:WA:462:G:H2'	48:WA:463:A:C8	2.49	0.47
48:WA:760:G:H2'	48:WA:761:G:H8	1.79	0.47
48:WA:3912:C:H2'	48:WA:3913:C:H6	1.78	0.47
48:WA:3912:C:H2'	48:WA:3913:C:C6	2.49	0.47
49:XA:110:G:H2'	49:XA:111:C:C6	2.48	0.47
51:ZA:163:U:OP2	58:GB:87:ARG:NH2	2.38	0.47
1:A:242:ARG:NH1	48:WA:3660:C:OP1	2.45	0.47
2:B:331:VAL:HG21	2:B:347:LEU:HD21	1.96	0.47
9:I:101:LYS:NZ	9:I:102:MET:O	2.45	0.47
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.97	0.47
19:S:71:ALA:HB3	48:WA:4315:A:H4'	1.96	0.47
23:W:55:ARG:HH22	50:YA:117:C:H5'	1.79	0.47
48:WA:955:G:H2'	48:WA:956:G:H8	1.79	0.47
48:WA:3882:G:H2'	48:WA:3883:G:C8	2.49	0.47
48:WA:4262:U:H2'	48:WA:4263:C:H6	1.79	0.47
48:WA:4637:A:O2'	48:WA:4639:G:OP1	2.30	0.47
51:ZA:1801:A:H2'	51:ZA:1802:C:C6	2.50	0.47
2:B:122:TRP:CH2	2:B:127:LYS:HG2	2.50	0.47
2:B:189:THR:HG23	2:B:192:GLU:H	1.79	0.47
13:M:73:ARG:NH1	48:WA:32:G:OP1	2.48	0.47
16:P:108:ARG:NH2	48:WA:1357:G:OP1	2.48	0.47
25:Y:48:ARG:NH2	48:WA:2578:G:OP1	2.47	0.47
47:VA:21:C:OP1	51:ZA:1704:C:N4	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1144:A:H2'	51:ZA:1145:A:C8	2.50	0.47
4:D:53:VAL:O	4:D:54:ARG:NH1	2.42	0.47
8:H:66:GLU:O	8:H:69:THR:OG1	2.30	0.47
9:I:189:ARG:NH2	9:I:199:TYR:OH	2.46	0.47
14:N:169:ARG:NH2	48:WA:4862:G:O3'	2.47	0.47
17:Q:62:ARG:NH2	48:WA:4650:A:OP1	2.47	0.47
21:U:41:SER:OG	48:WA:4509:A:O2'	2.29	0.47
43:RA:138:SER:HB3	48:WA:2004:A:H62	1.80	0.47
48:WA:262:G:H2'	48:WA:263:G:C8	2.50	0.47
48:WA:692:C:H2'	48:WA:693:A:C8	2.50	0.47
48:WA:2377:A:H2'	48:WA:2378:A:C8	2.48	0.47
48:WA:4165:U:H5'	48:WA:4166:C:H5''	1.96	0.47
51:ZA:220:U:H2'	51:ZA:221:A:H8	1.79	0.47
56:EB:212:ASP:OD1	56:EB:213:ALA:N	2.47	0.47
66:OB:117:ARG:NE	78:AC:52:ASP:OD2	2.47	0.47
2:B:77:THR:HG21	2:B:337:VAL:HG22	1.96	0.47
6:F:130:ASN:ND2	48:WA:1729:U:OP1	2.48	0.47
7:G:185:ARG:NH2	48:WA:119:G:O4'	2.44	0.47
8:H:129:ARG:NH1	8:H:156:ASN:OD1	2.45	0.47
9:I:4:ARG:NH1	48:WA:1868:U:OP1	2.42	0.47
10:J:40:LEU:HD12	10:J:70:VAL:HG22	1.95	0.47
15:O:151:ALA:HB3	15:O:172:PRO:HG2	1.96	0.47
19:S:130:ARG:NH2	48:WA:1730:U:O2	2.48	0.47
25:Y:48:ARG:HB3	25:Y:69:LYS:HB3	1.97	0.47
33:GA:17:LEU:HD12	33:GA:17:LEU:HA	1.78	0.47
36:JA:26:LYS:HE2	48:WA:2698:A:H5'	1.96	0.47
42:PA:103:HIS:ND1	42:PA:105:ASP:OD1	2.41	0.47
43:RA:37:LEU:HD12	43:RA:42:VAL:HB	1.96	0.47
48:WA:416:U:H4'	48:WA:2332:G:H4'	1.96	0.47
48:WA:422:C:H2'	48:WA:423:G:H8	1.79	0.47
48:WA:1664:C:H2'	48:WA:1665:C:C6	2.50	0.47
48:WA:3612:A:H2'	48:WA:3613:A:H8	1.80	0.47
48:WA:3734:A:H2'	48:WA:3735:A:H8	1.79	0.47
48:WA:4450:G:H5''	48:WA:4451:A:H5'	1.96	0.47
50:YA:47:C:H1'	50:YA:61:A:H2'	1.96	0.47
51:ZA:126:G:OP2	58:GB:198:ARG:NH1	2.47	0.47
51:ZA:1010:G:H2'	51:ZA:1011:A:H8	1.77	0.47
52:AB:24:HIS:HB3	52:AB:51:LEU:HD21	1.97	0.47
52:AB:85:ARG:HH21	52:AB:201:LEU:HD12	1.79	0.47
58:GB:121:ILE:HG22	58:GB:123:GLY:H	1.79	0.47
64:MB:33:ARG:HG2	64:MB:109:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:MB:51:VAL:HG22	64:MB:77:ILE:HG13	1.97	0.47
68:QB:35:SER:OG	68:QB:50:HIS:NE2	2.41	0.47
84:GC:57:ARG:NH1	84:GC:94:THR:O	2.47	0.47
2:B:36:ASP:OD1	2:B:36:ASP:N	2.48	0.47
13:M:184:ILE:HG23	13:M:194:ARG:HH22	1.80	0.47
39:MA:1:MET:HB2	51:ZA:1706:G:H5'	1.97	0.47
48:WA:2260:C:H5'	48:WA:2261:G:C8	2.49	0.47
51:ZA:527:C:H2'	51:ZA:528:A:H8	1.80	0.47
70:SB:120:HIS:CE1	70:SB:124:ARG:HD2	2.49	0.47
74:WB:55:ASP:OD1	74:WB:57:ARG:NH1	2.48	0.47
84:GC:18:VAL:HA	84:GC:35:SER:HA	1.96	0.47
2:B:128:LYS:HG3	48:WA:4968:A:H5'	1.97	0.47
6:F:114:ARG:NH1	16:P:4:ASP:O	2.46	0.47
13:M:65:ARG:NH2	48:WA:2459:G:OP1	2.43	0.47
14:N:113:ASP:OD1	14:N:114:LYS:N	2.48	0.47
16:P:154:LYS:O	16:P:163:THR:OG1	2.28	0.47
30:DA:76:LYS:NZ	30:DA:98:GLU:OE2	2.36	0.47
48:WA:2762:G:H4'	48:WA:2763:U:H5'	1.97	0.47
48:WA:3857:C:H2'	48:WA:3858:A:H8	1.80	0.47
51:ZA:1115:U:H1'	51:ZA:1116:C:H2'	1.96	0.47
51:ZA:1277:C:H2'	51:ZA:1278:A:H8	1.80	0.47
51:ZA:1808:U:H2'	51:ZA:1809:A:H8	1.79	0.47
54:CB:60:TRP:O	54:CB:71:LYS:NZ	2.35	0.47
56:EB:141:THR:OG1	56:EB:143:ASP:OD1	2.25	0.47
57:FB:125:SER:HB3	57:FB:203:ASN:HD21	1.80	0.47
60:IB:12:ARG:HE	60:IB:18:ARG:HG3	1.80	0.47
84:GC:5:MET:HB2	84:GC:270:LEU:HD21	1.97	0.47
84:GC:124:SER:OG	84:GC:125:ARG:N	2.47	0.47
7:G:237:LEU:HD23	7:G:243:LEU:HD13	1.97	0.47
43:RA:146:ARG:HB3	43:RA:148:PRO:HD2	1.96	0.47
48:WA:2006:U:C2	48:WA:2018:C:H1'	2.50	0.47
48:WA:2081:G:H2'	48:WA:2082:U:C6	2.50	0.47
48:WA:2297:C:H2'	48:WA:2298:G:H8	1.80	0.47
51:ZA:880:G:H2'	51:ZA:881:G:H8	1.80	0.47
64:MB:19:GLN:OE1	64:MB:88:TRP:HB3	2.15	0.47
76:YB:14:THR:HG22	76:YB:21:LYS:HD2	1.97	0.47
4:D:28:THR:O	48:WA:4282:A:N6	2.42	0.46
6:F:181:TYR:CZ	6:F:202:GLU:HG2	2.50	0.46
7:G:127:LEU:O	7:G:293:ASN:N	2.43	0.46
20:T:28:PRO:HB2	20:T:34:MET:HG2	1.97	0.46
30:DA:124:ASN:OD1	30:DA:124:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:TA:58:A:O2'	45:TA:60:U:OP2	2.24	0.46
48:WA:4461:U:H2'	48:WA:4462:U:C6	2.50	0.46
48:WA:4738:C:H42	48:WA:4966:C:H42	1.62	0.46
51:ZA:375:U:H2'	51:ZA:376:A:C8	2.50	0.46
51:ZA:551:U:H2'	51:ZA:552:G:C8	2.49	0.46
64:MB:52:LEU:HD23	64:MB:76:LEU:HD11	1.96	0.46
70:SB:30:ILE:HG22	70:SB:36:VAL:HG11	1.97	0.46
2:B:261:ARG:HB2	14:N:64:THR:HG21	1.97	0.46
3:C:80:ARG:NH2	48:WA:1647:C:OP1	2.45	0.46
14:N:46:ASN:O	14:N:50:ASN:ND2	2.48	0.46
30:DA:99:ILE:HG21	30:DA:108:ARG:HG2	1.98	0.46
48:WA:137:G:H2'	48:WA:138:G:C8	2.50	0.46
48:WA:3850:U:H2'	48:WA:3851:A:C8	2.50	0.46
48:WA:3863:A:H2'	48:WA:3864:A:H8	1.79	0.46
51:ZA:948:C:H2'	51:ZA:949:G:H8	1.80	0.46
54:CB:78:LEU:HD23	54:CB:81:ILE:HD12	1.97	0.46
57:FB:49:LEU:HD13	68:QB:76:LYS:HE2	1.98	0.46
63:LB:76:VAL:HG22	63:LB:125:ILE:HD13	1.98	0.46
2:B:220:ILE:HG12	2:B:278:THR:HG23	1.97	0.46
2:B:373:LYS:HD2	48:WA:4629:U:H4'	1.98	0.46
3:C:140:LYS:HE3	3:C:245:HIS:HB2	1.98	0.46
48:WA:44:A:H5'	94:WA:5252:SPM:H81	1.97	0.46
48:WA:478:G:H2'	48:WA:479:G:C8	2.50	0.46
48:WA:4706:C:H2'	48:WA:4707:A:H8	1.80	0.46
51:ZA:309:G:OP2	60:IB:53:LYS:NZ	2.44	0.46
51:ZA:476:A:N3	51:ZA:488:U:O2'	2.40	0.46
51:ZA:639:C:H2'	51:ZA:640:A:H8	1.79	0.46
51:ZA:1568:C:O2	51:ZA:1627:C:O2'	2.32	0.46
56:EB:126:VAL:HA	56:EB:141:THR:HA	1.97	0.46
85:HC:44:LYS:NZ	85:HC:48:GLU:OE2	2.45	0.46
24:X:27:ARG:HB2	24:X:75:ARG:CZ	2.45	0.46
48:WA:162:A:H2'	48:WA:163:A:C8	2.51	0.46
48:WA:3713:A:O2'	48:WA:3715:U:OP2	2.22	0.46
48:WA:4969:A:H2'	48:WA:4970:A:C8	2.50	0.46
51:ZA:1513:C:H2'	51:ZA:1514:G:C8	2.50	0.46
51:ZA:1550:G:O2'	51:ZA:1558:C:O2	2.27	0.46
53:BB:124:HIS:HA	53:BB:137:LEU:O	2.16	0.46
68:QB:122:TYR:HA	68:QB:126:VAL:HG23	1.97	0.46
8:H:91:LYS:HD3	8:H:183:GLU:HB3	1.97	0.46
11:K:87:HIS:HB3	11:K:90:VAL:HG23	1.97	0.46
25:Y:30:ASP:OD1	25:Y:30:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:1741:G:N3	48:WA:1744:A:N6	2.64	0.46
48:WA:2541:C:H2'	48:WA:2542:C:C6	2.50	0.46
48:WA:4899:G:H1'	48:WA:4929:G:H22	1.79	0.46
51:ZA:674:C:H2'	51:ZA:675:U:C6	2.50	0.46
51:ZA:929:G:H2'	51:ZA:930:C:O4'	2.16	0.46
54:CB:94:ILE:HD12	54:CB:162:ILE:HD11	1.97	0.46
55:DB:105:ARG:NE	62:KB:93:THR:O	2.42	0.46
73:VB:73:ALA:HB1	73:VB:78:ILE:HB	1.98	0.46
74:WB:80:ASP:OD1	74:WB:124:LYS:NZ	2.37	0.46
85:HC:130:ASN:HB3	85:HC:431:GLN:HE22	1.81	0.46
2:B:268:ARG:NH1	48:WA:3898:C:O2'	2.34	0.46
30:DA:44:ARG:NH2	30:DA:52:GLN:OE1	2.49	0.46
30:DA:84:GLU:OE1	42:PA:20:ARG:NH2	2.49	0.46
33:GA:89:ARG:NH1	50:YA:37:A:OP2	2.44	0.46
41:OA:59:SER:HA	48:WA:2654:G:H1	1.80	0.46
48:WA:164:G:H2'	48:WA:165:A:C8	2.50	0.46
48:WA:4460:C:H2'	48:WA:4461:U:C6	2.51	0.46
57:FB:140:ASP:OD2	80:CC:44:ARG:NH1	2.45	0.46
80:CC:36:ASP:OD1	80:CC:36:ASP:N	2.48	0.46
9:I:38:ARG:NH2	9:I:45:GLU:OE1	2.48	0.46
14:N:178:ARG:NH1	14:N:182:GLU:OE2	2.49	0.46
20:T:27:HIS:HB3	20:T:114:TYR:HE1	1.81	0.46
48:WA:520:C:H2'	48:WA:521:U:H5	1.80	0.46
48:WA:712:A:H2'	48:WA:713:C:C6	2.51	0.46
48:WA:1664:C:H2'	48:WA:1665:C:H6	1.80	0.46
48:WA:2461:G:N2	48:WA:2464:C:OP2	2.47	0.46
48:WA:2482:G:H2'	48:WA:2483:G:H8	1.80	0.46
48:WA:2555:A:OP2	48:WA:2576:G:O2'	2.33	0.46
51:ZA:28:U:H2'	51:ZA:29:G:C8	2.51	0.46
51:ZA:562:U:H2'	51:ZA:563:G:C8	2.51	0.46
58:GB:39:ASP:N	58:GB:39:ASP:OD1	2.47	0.46
33:GA:10:ARG:NH2	50:YA:65:A:O2'	2.49	0.46
44:SA:73:A:H5'	44:SA:74:C:H5'	1.96	0.46
48:WA:1300:C:H2'	48:WA:1301:G:C8	2.51	0.46
48:WA:1827:A:H2'	48:WA:1828:G:C8	2.51	0.46
48:WA:2626:G:H2'	48:WA:2627:U:H6	1.80	0.46
48:WA:2772:C:H2'	48:WA:2773:G:H8	1.81	0.46
48:WA:3949:A:N6	48:WA:3951:A:H61	2.14	0.46
51:ZA:189:U:OP1	60:IB:148:LYS:NZ	2.38	0.46
54:CB:68:ARG:NH1	54:CB:72:ASP:OD1	2.49	0.46
59:HB:245:LYS:NZ	59:HB:278:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SB:60:THR:OG1	70:SB:62:ASP:OD1	2.28	0.46
84:GC:39:THR:HG22	84:GC:60:ARG:HG2	1.96	0.46
13:M:46:ASP:OD1	13:M:46:ASP:N	2.49	0.46
19:S:4:THR:OG1	48:WA:4210:U:OP2	2.30	0.46
43:RA:128:THR:O	43:RA:131:GLU:HG2	2.16	0.46
48:WA:1751:A:H2'	48:WA:1752:G:C8	2.51	0.46
48:WA:3762:A:N6	51:ZA:1824:A:O2'	2.48	0.46
49:XA:58:A:H2'	49:XA:59:G:H8	1.81	0.46
51:ZA:65:C:OP1	58:GB:136:LYS:NZ	2.44	0.46
51:ZA:1203:G:H2'	51:ZA:1204:A:H8	1.80	0.46
53:BB:38:MET:HE2	53:BB:38:MET:HB3	1.87	0.46
60:IB:119:LEU:HD11	60:IB:153:LYS:HG3	1.96	0.46
67:PB:53:GLN:HB3	67:PB:83:MET:HE1	1.98	0.46
73:VB:15:ARG:NH1	73:VB:33:GLN:OE1	2.42	0.46
77:ZB:73:VAL:HG21	77:ZB:88:LEU:HD11	1.98	0.46
1:A:118:GLU:OE2	48:WA:3664:A:O2'	2.30	0.46
4:D:215:ASP:OD1	4:D:215:ASP:N	2.49	0.46
5:E:129:LEU:O	48:WA:965:A:N6	2.46	0.46
6:F:244:ARG:HA	6:F:244:ARG:HD3	1.85	0.46
8:H:155:SER:OG	48:WA:4690:C:O2'	2.33	0.46
48:WA:1341:U:H2'	48:WA:1342:C:C6	2.50	0.46
48:WA:3870:G:H22	48:WA:3902:G:H1'	1.79	0.46
48:WA:3880:C:N4	48:WA:4520:A:O4'	2.49	0.46
51:ZA:1221:G:O2'	51:ZA:1676:U:O2	2.29	0.46
51:ZA:1854:U:H2'	51:ZA:1855:G:H8	1.81	0.46
52:AB:102:ARG:HA	52:AB:102:ARG:HD2	1.70	0.46
56:EB:100:ARG:HB2	56:EB:114:ILE:HD13	1.98	0.46
66:OB:33:ILE:HD11	66:OB:119:LEU:HD21	1.97	0.46
84:GC:4:GLN:HB3	84:GC:313:THR:HB	1.98	0.46
84:GC:197:THR:HG21	84:GC:239:LEU:H	1.81	0.46
85:HC:27:LEU:HD13	85:HC:201:MET:HG2	1.98	0.46
1:A:243:THR:H	48:WA:3747:U:HO2'	1.64	0.45
13:M:193:ARG:O	13:M:197:THR:OG1	2.30	0.45
23:W:122:ALA:HB3	23:W:139:ARG:HG3	1.96	0.45
27:AA:5:LYS:HE3	27:AA:8:THR:HB	1.98	0.45
48:WA:760:G:H2'	48:WA:761:G:C8	2.51	0.45
48:WA:1516:U:H2'	48:WA:1517:A:C8	2.50	0.45
48:WA:1872:C:H2'	48:WA:1873:A:H8	1.81	0.45
48:WA:1994:U:H1'	48:WA:2004:A:H2	1.81	0.45
48:WA:2364:U:H2'	48:WA:2365:A:H8	1.81	0.45
48:WA:2482:G:H2'	48:WA:2483:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:2559:G:H1	48:WA:2572:U:H3	1.63	0.45
51:ZA:689:U:H2'	51:ZA:690:G:C8	2.51	0.45
51:ZA:1529:C:O2'	71:TB:87:VAL:O	2.29	0.45
55:DB:80:THR:OG1	55:DB:83:ARG:O	2.26	0.45
55:DB:234:GLY:HA3	55:DB:239:LYS:HG2	1.97	0.45
58:GB:52:ILE:HG23	58:GB:109:LEU:HD11	1.98	0.45
78:AC:54:SER:O	78:AC:57:SER:OG	2.32	0.45
42:PA:39:ARG:NH1	48:WA:2268:C:O2'	2.50	0.45
45:TA:15:G:H2'	45:TA:59:G:H1	1.80	0.45
48:WA:3925:A:H2'	48:WA:3926:C:C6	2.50	0.45
48:WA:4994:G:H2'	48:WA:4995:G:H8	1.81	0.45
51:ZA:1564:C:OP1	71:TB:121:ARG:NH2	2.49	0.45
78:AC:45:VAL:HG11	78:AC:53:ILE:HG13	1.98	0.45
78:AC:46:GLU:HG3	78:AC:48:ALA:H	1.80	0.45
85:HC:114:LEU:HD22	85:HC:137:ALA:HB2	1.97	0.45
9:I:179:ASP:OD1	9:I:179:ASP:N	2.41	0.45
14:N:145:VAL:O	48:WA:4713:C:O2'	2.32	0.45
16:P:179:GLY:H	26:Z:51:GLY:HA2	1.80	0.45
45:TA:41:U:H2'	45:TA:42:G:C8	2.51	0.45
46:UA:76:A:OP2	85:HC:296:HIS:NE2	2.38	0.45
48:WA:759:G:H2'	48:WA:760:G:C8	2.50	0.45
48:WA:2603:A:N6	48:WA:2745:A:H3'	2.31	0.45
48:WA:3725:A:H2'	48:WA:3726:A:H8	1.82	0.45
48:WA:3798:U:HO2'	51:ZA:1720:U:HO2'	1.56	0.45
48:WA:5004:U:H2'	48:WA:5005:U:C6	2.51	0.45
51:ZA:941:C:H2'	51:ZA:942:G:C8	2.52	0.45
51:ZA:1324:G:O2'	51:ZA:1510:G:O2'	2.34	0.45
51:ZA:1351:G:O2'	51:ZA:1378:A:N1	2.47	0.45
2:B:92:TYR:HB2	2:B:159:VAL:HB	1.97	0.45
2:B:252:ALA:HB1	48:WA:4526:G:C2	2.52	0.45
14:N:34:VAL:HG22	14:N:103:LYS:HB3	1.98	0.45
18:R:99:ASP:OD1	18:R:100:LEU:N	2.44	0.45
23:W:110:LYS:HG3	23:W:121:VAL:HB	1.98	0.45
24:X:1:MET:HE2	48:WA:1370:A:H1'	1.98	0.45
48:WA:215:C:H5''	48:WA:216:C:H5'	1.99	0.45
50:YA:67:U:H2'	50:YA:68:G:C8	2.50	0.45
51:ZA:996:A:H2'	51:ZA:997:A:C8	2.51	0.45
51:ZA:1358:U:OP2	54:CB:123:ARG:NH2	2.50	0.45
65:NB:24:THR:O	65:NB:27:LYS:NZ	2.41	0.45
77:ZB:96:LEU:O	77:ZB:112:ASN:ND2	2.49	0.45
81:DC:17:GLY:HA2	81:DC:27:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:222:LYS:HE3	48:WA:1909:A:H4'	1.97	0.45
15:O:66:LYS:NZ	48:WA:425:U:OP1	2.46	0.45
32:FA:66:ARG:NH2	48:WA:2519:A:O3'	2.49	0.45
48:WA:177:G:H2'	48:WA:178:C:C6	2.52	0.45
48:WA:3940:G:N2	48:WA:4173:C:OP2	2.46	0.45
48:WA:4580:G:H2'	48:WA:4581:U:C6	2.52	0.45
51:ZA:98:C:OP2	51:ZA:426:A:O2'	2.26	0.45
51:ZA:688:U:OP1	59:HB:354:ARG:NH2	2.50	0.45
51:ZA:1093:A:H2'	51:ZA:1094:C:C6	2.52	0.45
52:AB:42:LYS:HE2	52:AB:46:ILE:HB	1.99	0.45
53:BB:144:LYS:HE2	53:BB:206:PRO:HB2	1.98	0.45
54:CB:109:ILE:HD11	54:CB:151:ILE:HD11	1.99	0.45
4:D:156:GLY:HA2	4:D:181:PRO:HD3	1.98	0.45
21:U:31:ASN:OD1	21:U:31:ASN:N	2.49	0.45
32:FA:24:ARG:NH2	48:WA:2615:C:OP1	2.49	0.45
40:NA:64:LYS:HD2	48:WA:4372:G:H5''	1.98	0.45
48:WA:4:G:H2'	48:WA:5:A:C8	2.50	0.45
48:WA:1346:C:H2'	48:WA:1347:A:H8	1.81	0.45
48:WA:1657:C:O2	48:WA:4392:A:O2'	2.35	0.45
48:WA:1808:G:H2'	48:WA:1809:C:H6	1.82	0.45
48:WA:2650:G:H2'	48:WA:2651:G:H8	1.82	0.45
51:ZA:564:A:H2'	51:ZA:565:G:O4'	2.16	0.45
51:ZA:1217:A:H2'	51:ZA:1218:C:C6	2.51	0.45
52:AB:190:SER:OG	52:AB:192:GLU:OE1	2.34	0.45
71:TB:102:ARG:HA	71:TB:102:ARG:HD2	1.83	0.45
2:B:282:LYS:NZ	48:WA:4676:C:O2'	2.46	0.45
38:LA:85:ARG:HG3	38:LA:86:LYS:HD2	1.99	0.45
48:WA:1505:A:H1'	48:WA:1506:G:C8	2.52	0.45
48:WA:1619:G:H1'	48:WA:2515:A:N6	2.32	0.45
48:WA:1852:A:N3	48:WA:2285:G:O2'	2.49	0.45
48:WA:2051:G:HO2'	48:WA:3886:U:HO2'	1.59	0.45
48:WA:3877:G:N1	48:WA:3881:G:OP1	2.40	0.45
48:WA:4323:U:H2'	48:WA:4324:G:C8	2.52	0.45
51:ZA:942:G:N2	66:OB:137:SER:OG	2.49	0.45
51:ZA:1157:G:O2'	74:WB:74:VAL:O	2.24	0.45
51:ZA:1263:U:H4'	81:DC:27:ARG:HD2	1.98	0.45
51:ZA:1294:G:H2'	51:ZA:1295:A:H8	1.81	0.45
51:ZA:1447:G:H2'	51:ZA:1448:A:C8	2.51	0.45
54:CB:201:GLY:O	61:JB:54:ARG:NH1	2.50	0.45
55:DB:175:VAL:HG22	55:DB:189:LYS:HG3	1.99	0.45
61:JB:107:GLU:HA	61:JB:112:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:GC:296:GLN:HG3	84:GC:312:VAL:HB	1.97	0.45
4:D:37:VAL:HG12	4:D:50:ARG:HD3	1.98	0.45
7:G:148:LEU:HA	7:G:271:LEU:HD21	1.98	0.45
23:W:82:THR:HA	23:W:87:MET:HE3	1.99	0.45
38:LA:88:LYS:NZ	48:WA:4487:C:O2'	2.50	0.45
42:PA:90:LEU:HG	42:PA:111:ILE:HG23	1.99	0.45
43:RA:141:CYS:SG	43:RA:142:ASN:N	2.90	0.45
48:WA:912:G:H2'	48:WA:913:U:H6	1.81	0.45
48:WA:4262:U:H2'	48:WA:4263:C:C6	2.52	0.45
48:WA:4690:C:H2'	48:WA:4691:U:C6	2.52	0.45
48:WA:5004:U:H2'	48:WA:5005:U:H6	1.82	0.45
51:ZA:17:C:H2'	51:ZA:18:C:C6	2.51	0.45
51:ZA:671:A:H4'	51:ZA:672:A:H5''	1.99	0.45
51:ZA:1711:U:H2'	51:ZA:1712:A:C8	2.51	0.45
51:ZA:1761:U:O2	51:ZA:1771:G:C6	2.70	0.45
52:AB:76:VAL:HG12	52:AB:123:VAL:HB	1.98	0.45
56:EB:79:ASP:HB2	56:EB:82:TYR:HB2	1.99	0.45
60:IB:26:LYS:O	60:IB:29:LEU:HB2	2.16	0.45
1:A:116:LEU:HB3	1:A:126:LEU:HB2	1.98	0.45
1:A:241:ARG:NH1	48:WA:3661:G:OP1	2.50	0.45
4:D:124:GLU:OE1	4:D:126:THR:OG1	2.34	0.45
14:N:37:ARG:NH1	48:WA:4763:G:OP2	2.50	0.45
19:S:108:ARG:NH1	48:WA:1839:A:OP1	2.50	0.45
48:WA:1346:C:H2'	48:WA:1347:A:C8	2.51	0.45
48:WA:1447:U:O2	48:WA:2112:G:N2	2.50	0.45
48:WA:4962:G:H2'	48:WA:4963:G:H8	1.82	0.45
51:ZA:15:U:H2'	51:ZA:16:G:O4'	2.17	0.45
51:ZA:56:G:OP1	76:YB:111:LYS:NZ	2.46	0.45
51:ZA:65:C:C6	58:GB:174:PRO:HB3	2.51	0.45
51:ZA:107:A:H2'	51:ZA:108:G:H8	1.80	0.45
51:ZA:211:G:H2'	51:ZA:212:C:C6	2.51	0.45
51:ZA:436:G:OP2	51:ZA:471:G:O2'	2.34	0.45
84:GC:70:VAL:HG23	84:GC:79:LEU:HB3	1.98	0.45
4:D:146:LEU:HD22	4:D:163:LEU:HD13	1.98	0.45
12:L:11:ARG:HD3	12:L:57:LEU:HB3	1.98	0.45
22:V:80:ARG:HH12	51:ZA:167:G:H4'	1.82	0.45
23:W:64:SER:HB2	33:GA:69:LEU:HD13	1.99	0.45
41:OA:44:LYS:NZ	48:WA:2674:C:OP1	2.40	0.45
51:ZA:1004:U:H2'	51:ZA:1005:G:H8	1.82	0.45
51:ZA:1378:A:N6	52:AB:136:GLU:OE2	2.50	0.45
84:GC:8:ARG:HB3	84:GC:309:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:b:26:LYS:HD2	87:b:88:PHE:CG	2.51	0.45
1:A:210:PRO:HG2	1:A:235:VAL:HG11	1.98	0.44
15:O:137:ASP:OD1	15:O:137:ASP:N	2.45	0.44
16:P:173:LYS:NZ	48:WA:88:A:N7	2.63	0.44
25:Y:90:PRO:O	25:Y:117:LYS:NZ	2.50	0.44
48:WA:991:C:H2'	48:WA:992:C:C6	2.53	0.44
48:WA:2488:G:H2'	48:WA:2489:G:H8	1.82	0.44
50:YA:83:C:OP1	50:YA:86:U:O2'	2.31	0.44
51:ZA:527:C:H4'	61:JB:121:LYS:HD2	1.98	0.44
51:ZA:788:G:H2'	51:ZA:789:G:C8	2.53	0.44
51:ZA:1245:G:O2'	51:ZA:1492:U:OP1	2.32	0.44
51:ZA:1568:C:H2'	51:ZA:1569:A:C8	2.52	0.44
51:ZA:1630:A:H5''	70:SB:37:GLY:H	1.83	0.44
76:YB:29:HIS:ND1	76:YB:29:HIS:O	2.50	0.44
85:HC:30:LYS:NZ	85:HC:198:GLY:O	2.50	0.44
9:I:150:GLU:OE2	9:I:153:ARG:NH2	2.36	0.44
18:R:16:CYS:SG	18:R:17:LEU:N	2.90	0.44
25:Y:51:ARG:HB2	25:Y:65:ARG:HE	1.82	0.44
48:WA:1481:G:H2'	48:WA:1482:C:C6	2.52	0.44
48:WA:3918:G:H2'	48:WA:3919:A:C8	2.52	0.44
48:WA:4451:A:C8	92:WA:5250:ANM:H61	2.49	0.44
48:WA:4509:A:H2'	48:WA:4510:C:C6	2.52	0.44
51:ZA:14:C:H2'	51:ZA:15:U:C6	2.53	0.44
51:ZA:126:G:N2	51:ZA:180:G:H21	2.12	0.44
51:ZA:852:G:H1'	63:LB:97:ARG:HH21	1.81	0.44
61:JB:114:VAL:HG13	61:JB:119:LEU:HB2	1.98	0.44
64:MB:57:ASP:OD1	64:MB:57:ASP:N	2.50	0.44
71:TB:65:TYR:HE1	71:TB:128:GLN:HG3	1.82	0.44
84:GC:87:LEU:HD22	84:GC:132:TRP:HZ3	1.83	0.44
84:GC:152:SER:H	84:GC:169:GLY:HA2	1.81	0.44
85:HC:375:LEU:HB2	85:HC:391:PRO:HD2	2.00	0.44
1:A:194:ASN:HB2	48:WA:1541:G:H4'	2.00	0.44
3:C:149:GLU:OE2	42:PA:71:ARG:NE	2.43	0.44
25:Y:47:ASP:N	25:Y:69:LYS:O	2.50	0.44
48:WA:1204:G:H2'	48:WA:1205:G:C8	2.51	0.44
51:ZA:1388:A:H61	55:DB:199:GLY:HA3	1.83	0.44
2:B:240:LEU:HB3	2:B:244:THR:HG21	1.98	0.44
21:U:107:ASN:HD21	21:U:111:GLU:HB2	1.83	0.44
31:EA:21:GLN:NE2	31:EA:23:GLU:OE2	2.49	0.44
36:JA:23:VAL:HA	36:JA:35:LYS:O	2.17	0.44
48:WA:2546:G:H1	50:YA:123:U:H1'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:2609:C:H2'	48:WA:2610:G:H8	1.82	0.44
48:WA:2779:G:H5''	48:WA:2780:G:H5'	1.99	0.44
48:WA:4128:C:H5''	48:WA:4129:A:H5''	1.99	0.44
51:ZA:639:C:H2'	51:ZA:640:A:C8	2.52	0.44
51:ZA:942:G:H2'	51:ZA:943:U:C6	2.53	0.44
51:ZA:1221:G:H2'	51:ZA:1222:G:C8	2.52	0.44
51:ZA:1661:A:OP2	81:DC:32:ARG:NH2	2.42	0.44
52:AB:5:LEU:HD21	73:VB:41:LYS:HA	1.99	0.44
64:MB:42:LEU:O	64:MB:72:HIS:ND1	2.42	0.44
70:SB:91:LYS:NZ	70:SB:109:GLU:OE1	2.50	0.44
3:C:144:ILE:HG21	3:C:150:LEU:HD13	1.99	0.44
10:J:19:LYS:HD3	10:J:75:ARG:HH22	1.82	0.44
15:O:160:ARG:NH2	48:WA:1599:G:OP1	2.49	0.44
29:CA:37:GLY:O	29:CA:41:ARG:HG3	2.18	0.44
33:GA:112:ARG:NH2	48:WA:265:C:O2'	2.51	0.44
48:WA:36:U:OP1	48:WA:1653:G:N2	2.40	0.44
48:WA:470:A:H62	48:WA:685:G:N2	2.16	0.44
48:WA:1496:U:H2'	48:WA:1497:G:C8	2.52	0.44
48:WA:3600:C:H2'	48:WA:3601:A:H8	1.82	0.44
48:WA:3660:C:H2'	48:WA:3661:G:H8	1.83	0.44
50:YA:64:U:H2'	50:YA:65:A:H8	1.81	0.44
51:ZA:106:C:H2'	51:ZA:107:A:C8	2.53	0.44
51:ZA:1025:U:H2'	51:ZA:1026:C:O4'	2.18	0.44
59:HB:338:ILE:HG12	59:HB:363:VAL:HG11	1.99	0.44
64:MB:15:ASN:O	64:MB:19:GLN:HG2	2.18	0.44
64:MB:43:ASP:OD1	83:FC:116:ARG:NH2	2.51	0.44
85:HC:363:CYS:HB3	85:HC:424:PHE:HB3	2.00	0.44
4:D:44:TYR:O	48:WA:1825:G:O2'	2.35	0.44
4:D:136:ASP:OD1	4:D:136:ASP:N	2.46	0.44
4:D:193:GLU:HG3	4:D:197:LYS:HE2	2.00	0.44
48:WA:175:C:H2'	48:WA:176:G:H8	1.82	0.44
48:WA:970:G:O2'	48:WA:973:C:N3	2.51	0.44
48:WA:1192:U:H2'	48:WA:1193:G:N3	2.33	0.44
48:WA:1343:U:H2'	48:WA:1344:A:H8	1.82	0.44
48:WA:1394:A:H2'	48:WA:1395:G:C8	2.53	0.44
48:WA:3709:U:H2'	48:WA:3710:C:C6	2.53	0.44
48:WA:4275:A:H2'	48:WA:4276:A:C8	2.52	0.44
48:WA:4993:U:H2'	48:WA:4994:G:H8	1.83	0.44
51:ZA:1179:G:N2	51:ZA:1182:A:OP2	2.49	0.44
51:ZA:1466:G:OP2	69:RB:5:ARG:NH1	2.51	0.44
51:ZA:1670:C:H2'	51:ZA:1671:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1712:A:H2'	51:ZA:1713:C:C6	2.53	0.44
56:EB:72:ILE:HG21	56:EB:82:TYR:HE2	1.81	0.44
57:FB:71:ARG:NH2	57:FB:148:ASN:OD1	2.37	0.44
59:HB:336:ARG:NH2	59:HB:370:ASP:OD2	2.40	0.44
66:OB:149:ARG:HH12	66:OB:151:LEU:HD13	1.82	0.44
16:P:122:THR:OG1	16:P:124:ASP:OD1	2.28	0.44
22:V:110:ARG:HA	22:V:113:LYS:HG2	1.99	0.44
46:UA:8:U:H2'	46:UA:46:G:H21	1.83	0.44
48:WA:1506:G:H2'	48:WA:1507:C:C6	2.52	0.44
48:WA:2505:G:H2'	48:WA:2506:C:O4'	2.17	0.44
48:WA:3635:C:H2'	48:WA:3636:G:C8	2.53	0.44
51:ZA:992:A:N7	78:AC:15:ARG:NH2	2.65	0.44
51:ZA:1010:G:H2'	51:ZA:1011:A:C8	2.52	0.44
51:ZA:1198:G:H2'	51:ZA:1199:A:C8	2.53	0.44
55:DB:100:LYS:HE2	62:KB:96:ARG:HH21	1.82	0.44
55:DB:206:VAL:HA	55:DB:226:ILE:O	2.16	0.44
57:FB:176:GLU:OE2	57:FB:187:SER:OG	2.33	0.44
17:Q:108:ARG:HH22	48:WA:2901:C:P	2.41	0.44
25:Y:41:ALA:HB2	25:Y:77:TYR:HE1	1.82	0.44
48:WA:2747:A:H2'	48:WA:2748:A:C8	2.52	0.44
48:WA:3643:U:H5	48:WA:3648:A:N7	2.15	0.44
51:ZA:1128:C:H2'	51:ZA:1129:G:C8	2.53	0.44
61:JB:136:ARG:HD2	61:JB:139:LYS:HA	1.99	0.44
64:MB:30:GLY:HA3	64:MB:113:ASP:HB3	2.00	0.44
64:MB:54:SER:HB2	64:MB:80:ASP:HA	1.99	0.44
1:A:48:ILE:HD13	41:OA:65:ALA:HB2	1.99	0.44
20:T:84:LYS:HB2	20:T:110:TYR:CZ	2.53	0.44
24:X:50:ARG:HB2	24:X:115:ARG:NH2	2.33	0.44
48:WA:169:A:C2	48:WA:267:G:N1	2.86	0.44
48:WA:197:A:N1	48:WA:225:G:O2'	2.43	0.44
48:WA:1482:C:O2'	48:WA:1484:G:OP2	2.34	0.44
48:WA:3913:C:H2'	48:WA:3914:U:H6	1.82	0.44
48:WA:4861:C:H2'	48:WA:4862:G:H8	1.83	0.44
51:ZA:165:G:H4'	58:GB:53:SER:HB2	2.00	0.44
56:EB:100:ARG:HH21	56:EB:118:GLU:HG2	1.83	0.44
70:SB:84:LEU:O	70:SB:87:GLN:NE2	2.41	0.44
6:F:75:ARG:NE	48:WA:731:G:OP2	2.47	0.43
6:F:121:PHE:O	6:F:204:ASN:ND2	2.51	0.43
8:H:43:VAL:O	48:WA:4766:A:O2'	2.30	0.43
48:WA:652:C:H2'	48:WA:653:G:C8	2.53	0.43
48:WA:752:U:H1'	48:WA:919:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:4063:C:H2'	48:WA:4064:A:C8	2.52	0.43
48:WA:4321:C:H2'	48:WA:4322:G:H8	1.82	0.43
51:ZA:544:G:H2'	51:ZA:545:A:H8	1.83	0.43
51:ZA:553:U:O2'	51:ZA:554:A:H8	2.01	0.43
51:ZA:824:C:C2	61:JB:144:ILE:HG12	2.53	0.43
51:ZA:1015:U:O2'	65:NB:55:ARG:NH1	2.51	0.43
51:ZA:1858:G:N7	66:OB:146:ARG:NH1	2.66	0.43
75:XB:46:HIS:HB3	75:XB:101:LEU:HD11	2.00	0.43
84:GC:107:ASP:OD2	84:GC:125:ARG:NH1	2.49	0.43
15:O:45:LYS:HB3	15:O:178:ILE:HG12	2.00	0.43
19:S:91:VAL:HB	19:S:96:ILE:HD11	2.00	0.43
48:WA:173:C:H2'	48:WA:174:C:C6	2.54	0.43
48:WA:968:G:H2'	48:WA:969:A:C8	2.53	0.43
48:WA:2902:U:H2'	48:WA:2903:G:C8	2.53	0.43
49:XA:57:C:H2'	49:XA:58:A:H8	1.83	0.43
50:YA:79:G:H3'	50:YA:80:A:H4'	2.00	0.43
51:ZA:84:A:N3	51:ZA:150:A:O2'	2.49	0.43
51:ZA:1277:C:H2'	51:ZA:1278:A:C8	2.53	0.43
61:JB:107:GLU:O	61:JB:113:GLN:NE2	2.50	0.43
64:MB:94:ILE:HB	64:MB:102:LYS:HE3	1.99	0.43
81:DC:5:GLN:O	81:DC:9:SER:OG	2.33	0.43
48:WA:260:C:H2'	48:WA:261:G:C8	2.53	0.43
48:WA:1452:C:O2'	48:WA:2106:A:O2'	2.21	0.43
48:WA:1593:U:N3	48:WA:4557:U:OP1	2.34	0.43
48:WA:3863:A:H2'	48:WA:3864:A:C8	2.54	0.43
48:WA:3892:A:N6	48:WA:4572:G:O2'	2.49	0.43
48:WA:4543:G:N2	48:WA:4546:A:OP2	2.38	0.43
51:ZA:85:A:H2'	51:ZA:86:C:H6	1.83	0.43
51:ZA:388:U:H2'	51:ZA:389:A:C8	2.53	0.43
51:ZA:583:A:OP1	61:JB:162:ARG:NH2	2.51	0.43
51:ZA:880:G:H2'	51:ZA:881:G:C8	2.53	0.43
51:ZA:1189:A:H2'	51:ZA:1190:A:H8	1.82	0.43
75:XB:39:ASN:OD1	75:XB:42:GLY:N	2.51	0.43
85:HC:329:SER:HA	85:HC:333:PRO:HB3	2.01	0.43
22:V:87:LEU:HA	22:V:90:ILE:HG12	1.99	0.43
27:AA:114:ARG:HG3	27:AA:117:ARG:HH22	1.83	0.43
48:WA:6:C:H2'	48:WA:7:C:H6	1.83	0.43
48:WA:494:G:H2'	48:WA:495:C:C6	2.53	0.43
48:WA:1095:G:H2'	48:WA:1096:G:H8	1.83	0.43
51:ZA:388:U:H2'	51:ZA:389:A:H8	1.83	0.43
74:WB:66:THR:HG21	74:WB:68:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:ALA:HB2	4:D:74:ILE:HD13	2.00	0.43
11:K:169:ILE:HG12	26:Z:123:ILE:HD11	1.99	0.43
48:WA:424:U:H2'	48:WA:425:U:C6	2.53	0.43
48:WA:680:C:H2'	48:WA:681:G:C8	2.54	0.43
48:WA:1307:C:OP1	50:YA:7:U:O2'	2.36	0.43
48:WA:1568:C:H2'	48:WA:1569:U:H6	1.83	0.43
48:WA:4091:G:H2'	48:WA:4092:G:C8	2.54	0.43
48:WA:4171:G:H4'	48:WA:4173:C:C2	2.53	0.43
48:WA:4190:U:H2'	48:WA:4191:U:H6	1.83	0.43
51:ZA:496:C:H2'	51:ZA:497:C:H6	1.84	0.43
51:ZA:1438:A:H2'	51:ZA:1439:A:C8	2.53	0.43
51:ZA:1808:U:H2'	51:ZA:1809:A:C8	2.54	0.43
59:HB:382:ILE:HB	74:WB:52:ILE:HG13	1.99	0.43
84:GC:32:LEU:HD11	84:GC:92:LEU:HD21	2.00	0.43
3:C:284:MET:HE3	16:P:124:ASP:HB3	2.00	0.43
8:H:103:VAL:HG21	8:H:144:LEU:HD11	2.00	0.43
16:P:57:ASN:O	16:P:143:ARG:NE	2.51	0.43
18:R:36:ASN:OD1	18:R:36:ASN:N	2.50	0.43
37:KA:2:SER:OG	48:WA:2406:A:OP2	2.36	0.43
48:WA:253:G:H2'	48:WA:254:G:C8	2.53	0.43
48:WA:2100:G:H2'	48:WA:2101:C:C6	2.54	0.43
48:WA:3872:C:H2'	48:WA:3873:A:C8	2.53	0.43
48:WA:4644:U:H2'	48:WA:4645:G:H8	1.82	0.43
51:ZA:902:G:H2'	51:ZA:903:A:H8	1.84	0.43
51:ZA:1124:C:O2'	69:RB:126:MET:O	2.37	0.43
51:ZA:1617:G:N2	51:ZA:1619:A:H3'	2.34	0.43
51:ZA:1839:U:H2'	51:ZA:1840:U:C6	2.53	0.43
58:GB:54:GLY:O	58:GB:110:ASN:ND2	2.51	0.43
7:G:97:ASP:OD1	7:G:98:ILE:N	2.49	0.43
7:G:187:PRO:HB3	7:G:259:GLN:HG3	2.00	0.43
13:M:68:ARG:NH1	13:M:124:ASP:O	2.43	0.43
24:X:55:VAL:HG12	24:X:106:ILE:HA	2.00	0.43
32:FA:25:THR:OG1	48:WA:2523:G:O3'	2.36	0.43
40:NA:75:PRO:O	40:NA:78:ARG:NE	2.46	0.43
45:TA:53:G:H2'	45:TA:54:U:H6	1.84	0.43
48:WA:2494:C:H2'	48:WA:2495:G:H8	1.84	0.43
48:WA:2564:G:N2	48:WA:2567:A:OP2	2.40	0.43
48:WA:3788:U:OP1	48:WA:4552:G:O2'	2.34	0.43
48:WA:3813:G:O2'	48:WA:3816:U:OP2	2.36	0.43
48:WA:4091:G:H2'	48:WA:4092:G:H8	1.84	0.43
48:WA:4462:U:H2'	48:WA:4463:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:126:G:H5''	58:GB:195:LYS:HD3	2.01	0.43
51:ZA:1221:G:H2'	51:ZA:1222:G:H8	1.83	0.43
51:ZA:1562:C:H2'	51:ZA:1563:G:C8	2.54	0.43
55:DB:179:LYS:NZ	55:DB:217:GLN:O	2.48	0.43
70:SB:13:LEU:HB2	70:SB:20:ILE:HB	2.00	0.43
78:AC:44:ILE:HG23	78:AC:45:VAL:HG23	2.01	0.43
84:GC:33:SER:HB2	84:GC:41:ILE:HG22	2.01	0.43
84:GC:168:CYS:HB2	84:GC:195:LEU:HD13	2.00	0.43
84:GC:172:LYS:HE3	84:GC:193:GLY:H	1.83	0.43
1:A:178:PRO:HD2	41:OA:26:VAL:HG22	2.01	0.43
5:E:144:ARG:NH2	5:E:194:GLN:O	2.51	0.43
22:V:82:ILE:HG12	58:GB:131:ARG:HB2	2.01	0.43
24:X:34:LEU:HD23	24:X:38:LEU:HB3	2.00	0.43
27:AA:47:LYS:NZ	48:WA:1466:C:O3'	2.46	0.43
46:UA:23:C:H2'	46:UA:24:A:C8	2.53	0.43
48:WA:176:G:H2'	48:WA:177:G:C8	2.54	0.43
48:WA:176:G:H2'	48:WA:177:G:H8	1.82	0.43
48:WA:1565:A:N6	51:ZA:1028:A:N1	2.67	0.43
48:WA:2519:A:N3	48:WA:2541:C:O2'	2.48	0.43
49:XA:92:C:H2'	49:XA:93:G:C8	2.54	0.43
51:ZA:616:A:OP1	75:XB:68:LYS:NZ	2.51	0.43
51:ZA:1733:U:H2'	51:ZA:1734:G:O4'	2.19	0.43
52:AB:127:PRO:HG3	52:AB:146:ALA:HB1	2.01	0.43
64:MB:96:ARG:HG3	64:MB:100:PRO:HG3	1.99	0.43
1:A:29:LEU:O	1:A:123:ARG:NH1	2.51	0.43
3:C:69:THR:HG21	48:WA:3908:A:H2'	1.99	0.43
3:C:110:ARG:O	3:C:113:ARG:NH1	2.36	0.43
4:D:271:MET:HE3	4:D:275:GLN:HB3	2.01	0.43
9:I:35:ASP:HA	9:I:87:ILE:O	2.18	0.43
10:J:112:HIS:HD1	10:J:126:TYR:H	1.67	0.43
10:J:136:ARG:HG3	10:J:157:ILE:HD11	2.00	0.43
27:AA:32:LEU:HD12	48:WA:1466:C:H5''	2.01	0.43
48:WA:1826:G:H2'	48:WA:1827:A:H8	1.83	0.43
48:WA:2751:C:H2'	48:WA:2752:G:C8	2.54	0.43
48:WA:3724:G:H2'	48:WA:3725:A:C8	2.53	0.43
48:WA:4423:C:H42	48:WA:4477:G:H22	1.66	0.43
49:XA:4:U:H2'	49:XA:5:A:H8	1.84	0.43
51:ZA:17:C:O2'	51:ZA:1194:A:N1	2.49	0.43
51:ZA:649:U:H2'	51:ZA:650:A:C8	2.54	0.43
51:ZA:788:G:H2'	51:ZA:789:G:H8	1.83	0.43
51:ZA:1299:A:O2'	51:ZA:1301:A:OP1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:1314:U:O2'	62:KB:8:ARG:NH2	2.52	0.43
62:KB:47:LYS:HD3	62:KB:47:LYS:HA	1.69	0.43
66:OB:145:GLY:O	78:AC:22:ARG:NH2	2.52	0.43
69:RB:32:LYS:HG3	69:RB:47:ARG:HD3	2.00	0.43
85:HC:134:ARG:NH1	85:HC:177:TYR:OH	2.52	0.43
2:B:100:ARG:NE	48:WA:4913:A:OP2	2.52	0.43
2:B:242:ARG:NH2	48:WA:2858:C:O2	2.43	0.43
2:B:254:ILE:HG21	2:B:262:VAL:HG22	2.01	0.43
5:E:165:VAL:HG12	5:E:180:GLY:HA3	2.01	0.43
13:M:185:GLY:HA2	48:WA:78:U:H5'	2.01	0.43
25:Y:25:ILE:HA	25:Y:43:VAL:HG12	2.01	0.43
26:Z:117:LEU:HB3	26:Z:140:VAL:HG21	2.01	0.43
45:TA:52:G:H2'	45:TA:53:G:H8	1.84	0.43
48:WA:128:C:H2'	48:WA:129:C:C6	2.54	0.43
48:WA:1736:G:N2	48:WA:1737:U:O4	2.39	0.43
48:WA:1944:A:H2'	48:WA:1945:A:H8	1.83	0.43
48:WA:3612:A:H2'	48:WA:3613:A:C8	2.54	0.43
48:WA:3879:A:N3	48:WA:4403:G:O2'	2.35	0.43
48:WA:4639:G:H2'	48:WA:4640:U:C6	2.54	0.43
51:ZA:145:G:H2'	51:ZA:146:G:C8	2.54	0.43
51:ZA:219:U:H2'	51:ZA:220:U:C6	2.54	0.43
51:ZA:1226:G:N1	51:ZA:1639:G:OP2	2.40	0.43
52:AB:122:LEU:HB3	52:AB:144:THR:HG22	2.00	0.43
54:CB:191:VAL:HG11	54:CB:236:PHE:HA	2.01	0.43
62:KB:41:PRO:HD2	62:KB:44:HIS:CD2	2.54	0.43
63:LB:135:SER:O	63:LB:139:ARG:NH1	2.42	0.43
2:B:165:HIS:HA	2:B:179:HIS:O	2.19	0.42
2:B:285:TYR:N	2:B:332:MET:O	2.49	0.42
23:W:120:ASP:OD1	23:W:120:ASP:N	2.49	0.42
26:Z:102:ASP:HB3	26:Z:105:ARG:HB3	2.00	0.42
27:AA:11:ASN:ND2	48:WA:1671:A:OP1	2.50	0.42
48:WA:1343:U:H2'	48:WA:1344:A:C8	2.54	0.42
48:WA:3725:A:H2'	48:WA:3726:A:C8	2.54	0.42
48:WA:4110:G:H2'	48:WA:4111:G:H8	1.83	0.42
48:WA:4529:G:OP2	48:WA:4529:G:N2	2.47	0.42
48:WA:4596:U:H2'	48:WA:4597:G:C8	2.52	0.42
51:ZA:866:U:H2'	51:ZA:867:G:H8	1.84	0.42
66:OB:93:LEU:HD23	66:OB:119:LEU:HD13	2.01	0.42
76:YB:27:VAL:HG12	76:YB:29:HIS:HD2	1.83	0.42
84:GC:87:LEU:HD21	84:GC:122:SER:HB3	2.00	0.42
19:S:87:LYS:HZ3	48:WA:4307:G:N2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:15:ARG:HB2	48:WA:4620:G:H5''	2.00	0.42
21:U:87:SER:HB3	22:V:19:ARG:HH21	1.84	0.42
26:Z:71:PRO:HG2	26:Z:108:TYR:HA	2.01	0.42
28:BA:36:LYS:NZ	48:WA:2659:G:OP2	2.40	0.42
28:BA:79:ILE:HG12	28:BA:90:ARG:HG2	2.01	0.42
29:CA:23:ARG:HG2	29:CA:121:ASN:HA	2.00	0.42
35:IA:54:LYS:O	35:IA:58:THR:HB	2.19	0.42
48:WA:4706:C:H2'	48:WA:4707:A:C8	2.55	0.42
50:YA:6:C:H2'	50:YA:7:U:C6	2.54	0.42
51:ZA:319:C:H2'	51:ZA:320:G:C8	2.54	0.42
51:ZA:527:C:H2'	51:ZA:528:A:C8	2.54	0.42
57:FB:35:LEU:HD13	57:FB:146:ARG:HH21	1.84	0.42
75:XB:84:PHE:CE2	75:XB:86:PRO:HA	2.54	0.42
83:FC:121:CYS:SG	83:FC:126:CYS:HB3	2.58	0.42
84:GC:259:TRP:HD1	84:GC:266:ILE:HA	1.84	0.42
85:HC:120:VAL:HG13	85:HC:121:GLY:H	1.84	0.42
6:F:82:VAL:HG22	18:R:62:VAL:HA	2.01	0.42
12:L:44:ARG:HD3	48:WA:939:A:H4'	2.00	0.42
13:M:49:ARG:HH21	48:WA:114:G:P	2.42	0.42
13:M:53:TYR:HB2	13:M:133:ILE:HD13	2.01	0.42
13:M:113:LEU:HD11	50:YA:141:C:H5'	2.01	0.42
20:T:66:SER:OG	20:T:67:LYS:N	2.52	0.42
48:WA:1317:C:N4	48:WA:1318:G:O6	2.52	0.42
48:WA:2081:G:H2'	48:WA:2082:U:H6	1.83	0.42
48:WA:2469:U:H4'	48:WA:2470:U:H5'	2.01	0.42
48:WA:2575:A:H62	48:WA:2763:U:H3	1.66	0.42
51:ZA:223:C:H2'	51:ZA:224:A:C8	2.54	0.42
51:ZA:1147:C:OP1	78:AC:6:ARG:NH1	2.40	0.42
51:ZA:1628:C:H2'	51:ZA:1629:C:C6	2.55	0.42
56:EB:126:VAL:HG12	56:EB:158:ASP:O	2.20	0.42
60:IB:36:THR:O	60:IB:96:LEU:N	2.51	0.42
68:QB:126:VAL:HG12	68:QB:127:ASP:H	1.83	0.42
84:GC:67:SER:N	84:GC:81:GLY:O	2.52	0.42
7:G:90:LYS:NZ	48:WA:4128:C:OP1	2.53	0.42
9:I:61:SER:HA	9:I:126:VAL:HG23	2.00	0.42
12:L:72:TYR:HD1	12:L:75:LYS:HE2	1.85	0.42
14:N:168:TYR:OH	48:WA:4770:G:OP1	2.34	0.42
48:WA:158:A:N1	48:WA:276:C:O2'	2.42	0.42
48:WA:212:A:H2'	48:WA:213:G:H8	1.84	0.42
48:WA:691:C:H2'	48:WA:692:C:C6	2.54	0.42
48:WA:2021:C:H2'	48:WA:2022:U:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:3600:C:H2'	48:WA:3601:A:C8	2.54	0.42
48:WA:3729:A:H2'	48:WA:3730:A:C8	2.55	0.42
48:WA:3934:U:H2'	48:WA:3935:G:H8	1.83	0.42
51:ZA:1755:C:H2'	51:ZA:1756:C:C6	2.54	0.42
56:EB:248:ILE:H	56:EB:248:ILE:HG12	1.65	0.42
85:HC:102:MET:HE3	85:HC:102:MET:HB3	1.82	0.42
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.79	0.42
16:P:82:VAL:HG12	16:P:84:GLY:H	1.84	0.42
31:EA:43:LEU:HD22	31:EA:76:ARG:HA	2.02	0.42
45:TA:23:A:H2'	45:TA:24:G:C8	2.55	0.42
45:TA:49:C:H2'	45:TA:50:A:H8	1.84	0.42
48:WA:19:G:H2'	48:WA:20:U:C6	2.55	0.42
48:WA:254:G:H2'	48:WA:255:C:C6	2.55	0.42
48:WA:3951:A:H2	48:WA:4067:G:H22	1.68	0.42
48:WA:4996:G:H2'	48:WA:4997:U:C6	2.54	0.42
51:ZA:634:A:H2'	51:ZA:635:G:H8	1.83	0.42
51:ZA:807:G:H2'	51:ZA:808:A:C8	2.53	0.42
51:ZA:1101:U:H2'	51:ZA:1102:G:C8	2.55	0.42
51:ZA:1124:C:H5''	53:BB:150:ILE:HG12	2.01	0.42
51:ZA:1199:A:H2'	51:ZA:1200:A:C8	2.55	0.42
51:ZA:1801:A:H2'	51:ZA:1802:C:H6	1.83	0.42
56:EB:185:GLY:N	56:EB:189:LEU:HD13	2.30	0.42
59:HB:284:THR:HG23	59:HB:303:PRO:HG3	2.02	0.42
74:WB:3:ARG:NH2	74:WB:28:ARG:HH21	2.17	0.42
75:XB:89:GLY:HA2	82:EC:82:VAL:HG12	2.01	0.42
84:GC:246:TYR:HB3	84:GC:261:LEU:HB2	2.01	0.42
85:HC:338:ALA:HB2	85:HC:444:LYS:HG3	2.01	0.42
1:A:117:GLU:HG2	1:A:124:GLY:H	1.83	0.42
3:C:35:ASP:OD1	3:C:35:ASP:N	2.53	0.42
3:C:221:PHE:HB3	3:C:227:ILE:HG21	2.01	0.42
6:F:133:ARG:NH1	49:XA:97:G:O5'	2.53	0.42
6:F:175:ALA:HB1	48:WA:2104:G:C8	2.54	0.42
15:O:43:SER:HB3	15:O:180:THR:HG22	2.02	0.42
20:T:113:ARG:NH2	48:WA:2704:C:O3'	2.51	0.42
33:GA:89:ARG:O	33:GA:93:ARG:HG2	2.19	0.42
41:OA:83:ILE:HD13	41:OA:83:ILE:HA	1.87	0.42
48:WA:93:G:H2'	48:WA:94:A:C8	2.54	0.42
48:WA:1763:G:O6	48:WA:1774:C:N4	2.53	0.42
48:WA:2498:G:H2'	48:WA:2499:C:C6	2.53	0.42
48:WA:2864:G:N3	48:WA:3626:A:H2'	2.35	0.42
48:WA:4194:A:H2'	48:WA:4195:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:4586:A:H2'	48:WA:4587:U:O4'	2.19	0.42
49:XA:58:A:H2'	49:XA:59:G:C8	2.55	0.42
51:ZA:1189:A:H2'	51:ZA:1190:A:C8	2.55	0.42
51:ZA:1674:G:OP1	57:FB:51:HIS:NE2	2.29	0.42
54:CB:244:ILE:O	54:CB:247:THR:OG1	2.30	0.42
55:DB:173:GLU:HG2	55:DB:191:VAL:HG13	2.02	0.42
68:QB:61:ASN:O	71:TB:7:LYS:NZ	2.40	0.42
84:GC:40:ILE:HB	84:GC:59:LEU:HB2	2.01	0.42
84:GC:207:CYS:HB2	84:GC:221:LEU:HD21	2.02	0.42
2:B:342:LYS:O	48:WA:4978:U:N3	2.53	0.42
3:C:230:LEU:HD21	3:C:239:LYS:HD2	2.02	0.42
4:D:116:ASP:OD1	4:D:116:ASP:N	2.53	0.42
9:I:66:GLU:OE1	9:I:69:ARG:NH1	2.53	0.42
18:R:80:ILE:HG23	18:R:129:VAL:HG22	2.02	0.42
32:FA:33:LEU:HD12	32:FA:33:LEU:HA	1.89	0.42
36:JA:47:ILE:HG22	36:JA:49:ASP:H	1.84	0.42
45:TA:43:A:H2'	45:TA:44:G:H8	1.84	0.42
48:WA:649:G:H2'	48:WA:650:A:H8	1.84	0.42
48:WA:1540:U:H2'	48:WA:1541:G:H8	1.85	0.42
48:WA:1606:G:H2'	48:WA:1607:G:C8	2.54	0.42
48:WA:2415:U:H2'	48:WA:2416:G:H8	1.84	0.42
48:WA:2568:G:H2'	48:WA:2569:G:C8	2.54	0.42
48:WA:4349:G:H2'	48:WA:4350:A:C8	2.55	0.42
48:WA:4637:A:OP1	48:WA:4638:U:O2'	2.33	0.42
51:ZA:1093:A:H2'	51:ZA:1094:C:H6	1.85	0.42
52:AB:6:ASP:OD1	52:AB:6:ASP:N	2.52	0.42
60:IB:62:VAL:HG12	60:IB:77:ARG:HA	2.01	0.42
60:IB:125:LYS:HE2	60:IB:125:LYS:HB3	1.91	0.42
72:UB:55:ARG:HA	72:UB:87:ARG:HD3	2.01	0.42
84:GC:35:SER:OG	84:GC:36:ARG:N	2.53	0.42
1:A:54:ARG:HG2	1:A:56:ALA:H	1.84	0.42
3:C:74:ALA:H	3:C:78:ARG:HH21	1.68	0.42
7:G:148:LEU:HD21	7:G:209:VAL:HG21	2.02	0.42
12:L:63:LYS:HB2	12:L:63:LYS:HE2	1.71	0.42
48:WA:715:G:H2'	48:WA:716:G:H8	1.84	0.42
48:WA:1099:C:H2'	48:WA:1100:G:H8	1.85	0.42
48:WA:2001:A:H2'	48:WA:2002:G:C5	2.55	0.42
48:WA:2745:A:H2'	48:WA:2746:A:C8	2.54	0.42
48:WA:3719:A:N3	48:WA:4180:A:O2'	2.49	0.42
50:YA:109:C:H4'	50:YA:110:U:H5	1.84	0.42
51:ZA:1420:G:O2'	51:ZA:1422:G:OP1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:179:ASN:HB3	53:BB:183:GLU:HB2	2.01	0.42
55:DB:253:ASP:OD1	55:DB:253:ASP:N	2.50	0.42
66:OB:94:HIS:CE1	66:OB:128:ARG:HG3	2.54	0.42
84:GC:104:HIS:NE2	84:GC:122:SER:OG	2.47	0.42
85:HC:75:ILE:HG23	85:HC:101:ASN:HB3	2.02	0.42
85:HC:178:ILE:HB	85:HC:183:TYR:HB2	2.01	0.42
2:B:41:VAL:HA	2:B:187:GLY:HA3	2.01	0.42
2:B:132:LYS:NZ	48:WA:4730:U:OP1	2.52	0.42
16:P:37:ARG:NH1	48:WA:2089:C:OP2	2.47	0.42
16:P:181:ARG:HH12	48:WA:1393:A:P	2.42	0.42
25:Y:11:VAL:HG12	25:Y:82:PRO:HA	2.01	0.42
26:Z:26:ARG:HD3	26:Z:26:ARG:HA	1.90	0.42
38:LA:60:ALA:O	38:LA:64:ASN:HB2	2.20	0.42
48:WA:287:U:H2'	48:WA:288:G:C8	2.55	0.42
48:WA:1496:U:H2'	48:WA:1497:G:H8	1.84	0.42
48:WA:1806:A:H4'	48:WA:1807:A:O5'	2.20	0.42
48:WA:2485:G:C6	48:WA:2497:U:N3	2.88	0.42
48:WA:2871:U:O2'	48:WA:2883:A:N7	2.48	0.42
48:WA:3797:A:H2'	48:WA:3798:U:C6	2.54	0.42
51:ZA:223:C:H2'	51:ZA:224:A:H8	1.85	0.42
51:ZA:1171:G:O2'	51:ZA:1187:G:O6	2.33	0.42
52:AB:184:ARG:HD3	52:AB:191:ARG:HG2	2.02	0.42
57:FB:99:ILE:HD11	77:ZB:106:GLN:HE22	1.84	0.42
58:GB:64:LYS:HB3	58:GB:67:VAL:HG23	2.01	0.42
71:TB:96:SER:HB3	71:TB:99:VAL:HG22	2.01	0.42
85:HC:364:HIS:O	85:HC:364:HIS:ND1	2.52	0.42
4:D:216:GLU:HG3	4:D:220:LYS:HE2	2.02	0.42
5:E:48:ARG:HG2	48:WA:986:U:OP1	2.20	0.42
8:H:59:LYS:HE2	8:H:66:GLU:HB3	2.02	0.42
18:R:23:ARG:HH12	48:WA:1206:G:H5'	1.85	0.42
37:KA:13:LEU:HD22	48:WA:2409:G:H2'	2.01	0.42
48:WA:4942:C:H5'	48:WA:4943:G:H5''	2.02	0.42
51:ZA:71:G:N1	51:ZA:79:A:N7	2.68	0.42
51:ZA:1284:A:C6	64:MB:91:LEU:HD11	2.55	0.42
51:ZA:1457:U:H2'	51:ZA:1458:G:H8	1.84	0.42
51:ZA:1491:G:H2'	51:ZA:1492:U:C6	2.55	0.42
51:ZA:1512:C:H5''	81:DC:8:TRP:HZ3	1.85	0.42
51:ZA:1542:C:OP1	71:TB:62:ARG:NH1	2.52	0.42
57:FB:192:LYS:HA	57:FB:192:LYS:HD3	1.76	0.42
69:RB:102:THR:O	69:RB:105:MET:HG3	2.20	0.42
85:HC:100:LYS:HG3	85:HC:367:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:TYR:O	48:WA:2837:A:O2'	2.35	0.41
3:C:195:LYS:NZ	50:YA:21:C:OP1	2.50	0.41
3:C:328:LEU:HD13	6:F:186:MET:HE2	2.02	0.41
3:C:343:GLN:HG2	48:WA:725:C:H1'	2.02	0.41
4:D:146:LEU:HD21	4:D:159:VAL:HG22	2.01	0.41
4:D:179:ARG:HD3	4:D:179:ARG:HA	1.79	0.41
15:O:140:SER:OG	15:O:182:LYS:O	2.25	0.41
23:W:135:LYS:NZ	48:WA:2438:U:OP2	2.49	0.41
35:IA:58:THR:OG1	35:IA:59:THR:N	2.52	0.41
48:WA:86:U:H2'	48:WA:87:A:C8	2.55	0.41
48:WA:1474:C:H2'	48:WA:1475:U:C6	2.54	0.41
48:WA:2899:G:H2'	48:WA:2900:G:H8	1.85	0.41
48:WA:4545:G:H2'	48:WA:4546:A:C8	2.55	0.41
48:WA:4953:G:H2'	48:WA:4954:G:H8	1.85	0.41
48:WA:4996:G:H2'	48:WA:4997:U:H6	1.84	0.41
51:ZA:220:U:H2'	51:ZA:221:A:C8	2.55	0.41
51:ZA:432:G:H2'	51:ZA:433:A:C8	2.55	0.41
51:ZA:446:G:P	60:IB:47:ARG:HH22	2.43	0.41
51:ZA:498:C:H2'	51:ZA:499:G:C8	2.55	0.41
51:ZA:677:G:N1	51:ZA:1027:A:OP2	2.39	0.41
51:ZA:989:C:OP2	53:BB:155:TYR:OH	2.36	0.41
51:ZA:1265:A:H4'	51:ZA:1327:G:P	2.60	0.41
51:ZA:1579:A:H4'	51:ZA:1581:C:H5	1.85	0.41
71:TB:123:LEU:HD23	71:TB:123:LEU:HA	1.88	0.41
74:WB:11:LEU:HA	74:WB:14:ILE:HG12	2.02	0.41
84:GC:265:ILE:HD12	84:GC:265:ILE:HA	1.95	0.41
85:HC:343:GLN:HG3	85:HC:401:ILE:HG12	2.02	0.41
6:F:240:ASN:O	6:F:244:ARG:HG2	2.20	0.41
14:N:12:ARG:HB2	14:N:37:ARG:HD2	2.01	0.41
16:P:35:LEU:O	16:P:39:THR:OG1	2.28	0.41
32:FA:56:VAL:HG13	32:FA:72:LYS:HA	2.02	0.41
48:WA:649:G:H2'	48:WA:650:A:C8	2.56	0.41
48:WA:1292:G:H2'	48:WA:1293:G:H8	1.85	0.41
48:WA:1886:C:H2'	48:WA:1887:G:H8	1.84	0.41
48:WA:2555:A:N6	48:WA:2767:A:OP2	2.53	0.41
48:WA:2601:G:N2	48:WA:2749:U:O4	2.53	0.41
48:WA:4565:U:H2'	48:WA:4566:A:H8	1.84	0.41
50:YA:66:A:H2'	50:YA:67:U:C6	2.55	0.41
51:ZA:115:U:H2'	51:ZA:116:U:C6	2.55	0.41
69:RB:29:HIS:HA	69:RB:32:LYS:HE2	2.01	0.41
69:RB:99:ASP:OD1	69:RB:102:THR:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:HC:159:GLU:HB3	85:HC:160:PRO:HD2	2.02	0.41
85:HC:423:ARG:H	85:HC:423:ARG:HD2	1.85	0.41
22:V:44:ARG:NH1	48:WA:3617:G:O3'	2.54	0.41
29:CA:98:SER:OG	29:CA:100:ASN:OD1	2.34	0.41
38:LA:74:TYR:OH	48:WA:4427:G:OP1	2.31	0.41
44:SA:38:C:O2'	51:ZA:1058:A:OP1	2.35	0.41
45:TA:43:A:H2'	45:TA:44:G:C8	2.55	0.41
48:WA:1293:G:H2'	48:WA:1294:C:C6	2.56	0.41
48:WA:4770:G:C6	48:WA:4771:G:O6	2.73	0.41
51:ZA:4:C:H4'	54:CB:207:ALA:HB2	2.02	0.41
51:ZA:29:G:H2'	51:ZA:30:C:C6	2.54	0.41
51:ZA:1865:C:OP2	78:AC:5:ARG:NH1	2.52	0.41
71:TB:115:LYS:HE2	71:TB:121:ARG:HH12	1.85	0.41
73:VB:16:LYS:HG2	73:VB:23:ILE:HG22	2.02	0.41
85:HC:62:LYS:HE2	85:HC:62:LYS:HB2	1.90	0.41
4:D:33:ARG:HH21	49:XA:7:G:H4'	1.86	0.41
5:E:77:ALA:HA	5:E:78:PRO:HD3	1.88	0.41
7:G:126:ARG:NH1	7:G:294:VAL:O	2.50	0.41
23:W:83:THR:HG22	23:W:85:SER:H	1.85	0.41
36:JA:61:PRO:HA	36:JA:62:PRO:HD3	1.94	0.41
45:TA:69:G:H2'	45:TA:70:G:H8	1.84	0.41
48:WA:1761:G:O6	48:WA:1775:U:O4	2.38	0.41
48:WA:3602:G:H2'	48:WA:3603:C:C6	2.56	0.41
48:WA:4462:U:H2'	48:WA:4463:C:H6	1.84	0.41
48:WA:4469:A:O2'	48:WA:4512:A:N3	2.37	0.41
48:WA:4565:U:C2	48:WA:4566:A:C8	3.08	0.41
48:WA:4907:C:H2'	48:WA:4908:C:C6	2.56	0.41
51:ZA:73:C:H2'	51:ZA:74:G:O4'	2.20	0.41
51:ZA:1543:U:P	71:TB:62:ARG:HH22	2.42	0.41
51:ZA:1809:A:H2'	51:ZA:1810:U:C6	2.56	0.41
52:AB:157:VAL:O	73:VB:65:SER:OG	2.39	0.41
62:KB:26:ASP:HB3	62:KB:29:MET:HE3	2.02	0.41
64:MB:42:LEU:HD23	64:MB:47:ALA:HB3	2.01	0.41
85:HC:423:ARG:HA	85:HC:437:VAL:HG12	2.02	0.41
8:H:128:MET:HE3	8:H:157:SER:HB2	2.01	0.41
16:P:62:SER:OG	48:WA:1504:G:OP2	2.27	0.41
19:S:5:LYS:HD2	48:WA:4304:U:H4'	2.02	0.41
29:CA:122:VAL:HG12	29:CA:124:GLU:H	1.85	0.41
31:EA:78:HIS:HB2	31:EA:85:ARG:HG3	2.01	0.41
45:TA:22:G:H2'	45:TA:23:A:C8	2.54	0.41
48:WA:286:U:H2'	48:WA:287:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:417:G:H1'	50:YA:17:A:H61	1.85	0.41
48:WA:1292:G:H2'	48:WA:1293:G:C8	2.56	0.41
48:WA:1848:G:H2'	48:WA:1849:C:H6	1.84	0.41
48:WA:2266:C:H2'	48:WA:2267:G:O4'	2.20	0.41
48:WA:4095:G:H1	48:WA:4117:G:H1	1.67	0.41
48:WA:4109:G:H2'	48:WA:4110:G:C8	2.56	0.41
48:WA:4116:C:H2'	48:WA:4117:G:C8	2.55	0.41
48:WA:4540:G:H2'	48:WA:4541:U:C6	2.56	0.41
48:WA:4580:G:H2'	48:WA:4581:U:H6	1.85	0.41
51:ZA:161:U:O2'	58:GB:87:ARG:NH1	2.54	0.41
51:ZA:675:U:H2'	51:ZA:676:C:H6	1.85	0.41
51:ZA:857:U:H4'	56:EB:201:HIS:CE1	2.55	0.41
51:ZA:1230:C:H2'	51:ZA:1231:C:H6	1.85	0.41
51:ZA:1598:G:H3'	77:ZB:80:ARG:HD2	2.02	0.41
51:ZA:1616:U:H2'	51:ZA:1617:G:C8	2.55	0.41
51:ZA:1673:U:H2'	51:ZA:1674:G:O4'	2.20	0.41
54:CB:82:TYR:CZ	54:CB:164:PRO:HD3	2.55	0.41
55:DB:113:LYS:HE2	55:DB:113:LYS:HB3	1.82	0.41
58:GB:84:TYR:HD1	58:GB:95:LYS:HD2	1.86	0.41
66:OB:150:ARG:H	66:OB:150:ARG:HG2	1.68	0.41
69:RB:17:ILE:HD11	69:RB:54:VAL:HA	2.01	0.41
70:SB:14:ARG:NH1	70:SB:19:ASN:OD1	2.45	0.41
85:HC:13:ILE:HD12	85:HC:136:HIS:HB3	2.02	0.41
85:HC:198:GLY:HA2	85:HC:201:MET:HE3	2.02	0.41
2:B:19:ARG:NH2	2:B:234:ARG:O	2.53	0.41
3:C:173:LYS:HD3	3:C:173:LYS:HA	1.89	0.41
45:TA:53:G:H2'	45:TA:54:U:C6	2.55	0.41
48:WA:163:A:H2'	48:WA:164:G:H8	1.86	0.41
48:WA:1281:A:O2'	48:WA:1283:G:N7	2.53	0.41
48:WA:1347:A:H2'	48:WA:1348:C:C6	2.56	0.41
51:ZA:582:U:H1'	76:YB:33:ALA:HB2	2.03	0.41
51:ZA:1097:G:H4'	52:AB:32:PHE:CD1	2.56	0.41
51:ZA:1277:C:OP1	62:KB:51:SER:OG	2.35	0.41
80:CC:12:ALA:HB1	80:CC:32:VAL:HB	2.01	0.41
84:GC:17:TRP:HB2	84:GC:36:ARG:HG3	2.01	0.41
84:GC:149:GLU:H	84:GC:171:ASP:HB3	1.85	0.41
84:GC:245:ARG:HG3	84:GC:247:TRP:CG	2.56	0.41
1:A:117:GLU:HG2	1:A:124:GLY:N	2.35	0.41
1:A:236:GLY:N	48:WA:3689:A:O2'	2.54	0.41
2:B:5:LYS:NZ	48:WA:4503:U:OP1	2.53	0.41
32:FA:70:THR:HA	32:FA:73:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:6:C:H2'	48:WA:7:C:C6	2.56	0.41
48:WA:1264:G:H2'	48:WA:1265:A:C8	2.56	0.41
48:WA:1474:C:H2'	48:WA:1475:U:H6	1.85	0.41
48:WA:2082:U:H2'	48:WA:2083:C:C6	2.56	0.41
48:WA:2734:G:H2'	48:WA:2735:C:C6	2.56	0.41
48:WA:3609:U:H2'	48:WA:3610:A:C8	2.56	0.41
48:WA:4725:A:H2'	48:WA:4726:A:C8	2.54	0.41
51:ZA:212:C:H2'	51:ZA:213:G:C8	2.56	0.41
51:ZA:391:C:H2'	51:ZA:392:A:H8	1.86	0.41
51:ZA:529:A:H2'	51:ZA:530:U:C6	2.56	0.41
51:ZA:969:U:OP1	51:ZA:970:G:O2'	2.33	0.41
51:ZA:1293:A:N6	51:ZA:1294:G:O6	2.54	0.41
51:ZA:1628:C:H2'	51:ZA:1629:C:H6	1.85	0.41
51:ZA:1643:U:H2'	51:ZA:1644:C:C6	2.56	0.41
51:ZA:1842:C:H2'	51:ZA:1843:G:C8	2.56	0.41
56:EB:192:ILE:HG12	56:EB:243:GLY:HA3	2.03	0.41
60:IB:76:THR:HG22	60:IB:108:PRO:HG2	2.01	0.41
64:MB:47:ALA:HA	64:MB:112:LYS:HB3	2.03	0.41
66:OB:95:ILE:HG21	66:OB:116:LEU:HD13	2.02	0.41
69:RB:108:LEU:HD23	69:RB:108:LEU:HA	1.93	0.41
85:HC:15:HIS:CE1	85:HC:132:GLN:H	2.38	0.41
85:HC:268:GLU:HB3	85:HC:420:PRO:HG2	2.01	0.41
5:E:189:LEU:HD21	5:E:256:VAL:HG21	2.03	0.41
15:O:112:TRP:O	48:WA:3858:A:H5''	2.20	0.41
20:T:83:LEU:HD23	20:T:83:LEU:HA	1.87	0.41
30:DA:19:LYS:HB3	30:DA:19:LYS:HE2	1.91	0.41
30:DA:79:VAL:N	30:DA:98:GLU:O	2.50	0.41
30:DA:109:LYS:NZ	30:DA:128:ARG:O	2.51	0.41
31:EA:54:LYS:HE3	48:WA:4750:U:H5''	2.01	0.41
33:GA:34:ALA:HA	33:GA:37:THR:HG22	2.02	0.41
33:GA:52:LYS:HA	33:GA:52:LYS:HD3	1.82	0.41
44:SA:2:U:HO2'	48:WA:4202:G:HO2'	1.60	0.41
48:WA:146:G:H2'	48:WA:147:A:H8	1.86	0.41
48:WA:652:C:H2'	48:WA:653:G:H8	1.86	0.41
48:WA:1082:C:H2'	48:WA:1083:C:C6	2.56	0.41
48:WA:1348:C:H2'	48:WA:1349:G:C8	2.55	0.41
48:WA:1671:A:H4'	48:WA:1687:G:N2	2.36	0.41
48:WA:1848:G:H2'	48:WA:1849:C:C6	2.56	0.41
48:WA:4137:G:H2'	48:WA:4138:G:H8	1.86	0.41
48:WA:4322:G:H2'	48:WA:4323:U:C6	2.56	0.41
48:WA:5006:C:H2'	48:WA:5007:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:196:C:H2'	51:ZA:197:U:C6	2.56	0.41
51:ZA:1259:A:H1'	51:ZA:1264:C:N4	2.34	0.41
51:ZA:1656:G:H1	51:ZA:1668:U:H3	1.69	0.41
53:BB:63:LYS:HZ3	53:BB:90:ASP:HA	1.85	0.41
56:EB:61:VAL:HG12	56:EB:80:ILE:HG22	2.02	0.41
68:QB:35:SER:HA	68:QB:51:CYS:O	2.20	0.41
74:WB:106:THR:OG1	74:WB:109:GLY:O	2.36	0.41
84:GC:61:GLY:HA3	84:GC:90:TRP:HZ2	1.85	0.41
85:HC:294:MET:HB2	85:HC:308:VAL:HG12	2.02	0.41
1:A:187:HIS:NE2	48:WA:1615:A:OP2	2.52	0.41
8:H:111:LEU:HB2	8:H:127:ARG:HH21	1.86	0.41
9:I:208:LYS:HB2	9:I:208:LYS:HE3	1.87	0.41
10:J:94:LEU:HD23	10:J:94:LEU:HA	1.95	0.41
10:J:114:ASP:OD1	70:SB:14:ARG:NE	2.53	0.41
13:M:54:LYS:NZ	48:WA:153:G:OP2	2.50	0.41
13:M:181:HIS:CD2	48:WA:99:A:H4'	2.56	0.41
21:U:112:MET:HE2	21:U:112:MET:HB3	1.91	0.41
27:AA:4:SER:HB2	48:WA:1857:G:OP1	2.20	0.41
34:HA:76:ARG:HA	34:HA:76:ARG:HD2	1.80	0.41
48:WA:64:A:H1'	48:WA:76:A:H1'	2.03	0.41
48:WA:129:C:H2'	48:WA:130:C:C6	2.56	0.41
48:WA:272:U:H2'	48:WA:273:U:C6	2.56	0.41
48:WA:307:A:N3	48:WA:310:G:O2'	2.54	0.41
48:WA:753:G:H3'	48:WA:754:G:H8	1.86	0.41
48:WA:1079:G:H22	48:WA:1244:A:H2	1.69	0.41
48:WA:1176:G:H2'	48:WA:1177:G:C8	2.56	0.41
48:WA:1348:C:H2'	48:WA:1349:G:H8	1.85	0.41
48:WA:1507:C:H2'	48:WA:1508:G:C8	2.55	0.41
48:WA:1727:U:H2'	48:WA:1728:U:C6	2.56	0.41
48:WA:2043:A:N7	48:WA:4436:C:O2'	2.49	0.41
48:WA:2450:G:H2'	48:WA:2451:A:C8	2.56	0.41
48:WA:2612:G:H2'	48:WA:2613:A:H8	1.86	0.41
48:WA:3873:A:H2'	48:WA:3874:A:C8	2.56	0.41
51:ZA:656:G:H5'	51:ZA:662:G:N2	2.36	0.41
51:ZA:883:U:H2'	51:ZA:884:C:C6	2.55	0.41
51:ZA:941:C:H2'	51:ZA:942:G:H8	1.86	0.41
51:ZA:1158:G:H5''	74:WB:76:SER:HB2	2.02	0.41
51:ZA:1345:G:OP1	51:ZA:1688:C:O2'	2.38	0.41
51:ZA:1395:C:O2'	51:ZA:1396:A:H5''	2.21	0.41
51:ZA:1648:G:H22	51:ZA:1675:A:P	2.43	0.41
52:AB:128:ARG:NH1	52:AB:153:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:103:MET:HE3	53:BB:215:VAL:HG23	2.02	0.41
54:CB:157:LEU:HD23	54:CB:157:LEU:HA	1.92	0.41
55:DB:201:PRO:O	55:DB:205:TYR:HB2	2.21	0.41
59:HB:384:VAL:HG22	59:HB:390:ARG:HG2	2.02	0.41
61:JB:152:ASP:OD1	61:JB:152:ASP:N	2.53	0.41
68:QB:142:ASP:OD2	68:QB:144:THR:OG1	2.37	0.41
69:RB:73:LEU:O	69:RB:76:GLU:HG3	2.20	0.41
69:RB:117:LEU:HD23	69:RB:117:LEU:HA	1.93	0.41
76:YB:13:MET:SD	76:YB:22:GLN:NE2	2.93	0.41
85:HC:134:ARG:H	85:HC:134:ARG:HG3	1.65	0.41
85:HC:191:VAL:HG12	85:HC:193:ILE:HG13	2.02	0.41
1:A:208:GLU:HG2	48:WA:1631:G:H1	1.87	0.41
2:B:30:LYS:HG3	48:WA:4718:C:OP2	2.21	0.41
6:F:93:ARG:HB2	6:F:113:LEU:HB3	2.02	0.41
11:K:46:ILE:HB	11:K:49:ARG:HB2	2.02	0.41
12:L:4:ARG:NH2	48:WA:4767:G:O6	2.50	0.41
15:O:111:ARG:NH2	48:WA:2364:U:OP1	2.53	0.41
18:R:35:PRO:HD2	18:R:39:VAL:HG21	2.03	0.41
19:S:87:LYS:HD2	48:WA:4307:G:H1	1.85	0.41
22:V:59:HIS:HB3	22:V:61:LYS:HZ3	1.86	0.41
45:TA:9:A:O2'	45:TA:10:G:N7	2.46	0.41
48:WA:711:G:H2'	48:WA:712:A:C8	2.56	0.41
48:WA:1647:C:H2'	48:WA:1648:A:C8	2.56	0.41
48:WA:1689:U:H2'	48:WA:1690:G:C8	2.56	0.41
48:WA:3719:A:H2'	48:WA:3720:A:H8	1.82	0.41
48:WA:4157:C:H2'	48:WA:4158:G:O4'	2.21	0.41
48:WA:4929:G:H5''	48:WA:4930:C:C5	2.53	0.41
48:WA:5057:G:H2'	48:WA:5058:A:C8	2.56	0.41
51:ZA:1716:C:H2'	51:ZA:1717:C:H6	1.85	0.41
51:ZA:1754:G:H2'	51:ZA:1755:C:C6	2.55	0.41
58:GB:216:ARG:HA	58:GB:216:ARG:HD3	1.83	0.41
64:MB:33:ARG:HH11	64:MB:91:LEU:HD13	1.85	0.41
70:SB:92:ASP:HB3	70:SB:94:LYS:HG3	2.02	0.41
75:XB:46:HIS:CD2	75:XB:103:ALA:HB2	2.56	0.41
83:FC:141:CYS:HB3	83:FC:146:LEU:H	1.85	0.41
1:A:6:ARG:HH12	1:A:199:VAL:H	1.69	0.40
2:B:252:ALA:HB1	48:WA:4526:G:N3	2.36	0.40
3:C:310:HIS:NE2	48:WA:2102:G:H2'	2.36	0.40
6:F:55:HIS:NE2	6:F:59:GLU:OE2	2.54	0.40
35:IA:2:THR:HG23	93:WA:5257:SPD:H22	2.03	0.40
40:NA:69:ARG:HG3	40:NA:82:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:PA:105:ASP:OD1	42:PA:105:ASP:N	2.53	0.40
48:WA:460:C:N3	48:WA:698:G:N1	2.69	0.40
48:WA:1208:C:H2'	48:WA:1209:G:C8	2.56	0.40
48:WA:1735:G:N3	48:WA:4216:A:H2'	2.36	0.40
50:YA:141:C:H2'	50:YA:142:U:C6	2.56	0.40
51:ZA:1030:A:H2'	51:ZA:1031:A:H8	1.86	0.40
60:IB:87:ASN:HB3	60:IB:90:LEU:HG	2.02	0.40
64:MB:62:VAL:HA	64:MB:65:VAL:HG12	2.03	0.40
85:HC:392:LYS:HG3	85:HC:393:PHE:CD2	2.56	0.40
2:B:79:VAL:HB	2:B:331:VAL:HG23	2.03	0.40
6:F:135:VAL:HG23	6:F:139:ILE:HD13	2.02	0.40
7:G:119:GLN:HG3	13:M:28:TRP:CH2	2.56	0.40
12:L:30:VAL:O	18:R:98:ARG:NH1	2.53	0.40
18:R:87:ARG:HH21	48:WA:2036:G:H5'	1.86	0.40
21:U:27:ASN:O	21:U:102:ALA:HA	2.20	0.40
21:U:43:LYS:HD3	21:U:62:MET:HE2	2.03	0.40
48:WA:92:C:OP2	48:WA:4343:C:O2'	2.30	0.40
48:WA:270:U:H2'	48:WA:271:C:C6	2.56	0.40
48:WA:461:G:H2'	48:WA:462:G:C8	2.56	0.40
48:WA:2364:U:H2'	48:WA:2365:A:C8	2.57	0.40
48:WA:2542:C:H2'	48:WA:2543:G:H8	1.86	0.40
48:WA:3934:U:H2'	48:WA:3935:G:C8	2.56	0.40
48:WA:4072:U:H2'	48:WA:4073:U:C6	2.57	0.40
48:WA:4239:C:O2'	48:WA:4323:U:O2	2.40	0.40
49:XA:3:C:H2'	49:XA:4:U:C6	2.56	0.40
51:ZA:149:A:N6	51:ZA:169:U:C2	2.90	0.40
51:ZA:993:G:O6	78:AC:15:ARG:HG2	2.22	0.40
51:ZA:1215:C:O2'	51:ZA:1645:C:OP2	2.30	0.40
51:ZA:1294:G:H2'	51:ZA:1295:A:C8	2.57	0.40
85:HC:75:ILE:HB	85:HC:90:ILE:HD11	2.04	0.40
3:C:150:LEU:O	3:C:152:LEU:N	2.55	0.40
5:E:49:ASN:OD1	5:E:49:ASN:N	2.55	0.40
10:J:29:SER:OG	10:J:67:LYS:O	2.27	0.40
15:O:130:ASN:OD1	48:WA:399:G:N2	2.53	0.40
18:R:23:ARG:HG3	18:R:24:THR:HG23	2.02	0.40
21:U:97:TYR:OH	22:V:37:GLU:OE2	2.29	0.40
41:OA:6:LYS:H	48:WA:2878:G:P	2.45	0.40
48:WA:680:C:H2'	48:WA:681:G:H8	1.85	0.40
48:WA:711:G:H2'	48:WA:712:A:H8	1.87	0.40
48:WA:1869:A:H2'	48:WA:1870:A:C8	2.56	0.40
48:WA:2590:C:OP1	48:WA:2770:C:O2'	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:4553:U:H2'	48:WA:4554:U:C6	2.57	0.40
48:WA:5015:C:H41	48:WA:5031:C:P	2.45	0.40
50:YA:69:U:H2'	50:YA:70:G:O4'	2.21	0.40
51:ZA:153:G:N2	58:GB:13:GLN:OE1	2.43	0.40
51:ZA:414:A:H2'	51:ZA:415:A:H8	1.86	0.40
51:ZA:1033:G:N1	51:ZA:1080:A:O2'	2.38	0.40
51:ZA:1261:C:H41	51:ZA:1661:A:H62	1.68	0.40
51:ZA:1337:C:H2'	51:ZA:1338:G:H8	1.86	0.40
51:ZA:1739:C:H2'	51:ZA:1740:C:H6	1.85	0.40
55:DB:51:ALA:HA	55:DB:54:ILE:HG22	2.03	0.40
56:EB:155:LYS:HA	56:EB:155:LYS:HD3	1.82	0.40
56:EB:181:CYS:SG	56:EB:182:MET:N	2.93	0.40
60:IB:67:TRP:NE1	60:IB:191:GLU:OE2	2.48	0.40
85:HC:166:ARG:HE	85:HC:170:ILE:HD11	1.86	0.40
3:C:49:ARG:HD3	48:WA:349:A:N7	2.36	0.40
5:E:68:LYS:HD3	48:WA:986:U:OP2	2.22	0.40
42:PA:65:LYS:O	42:PA:102:TYR:OH	2.27	0.40
48:WA:1492:G:H2'	48:WA:1493:A:C8	2.57	0.40
48:WA:3913:C:H2'	48:WA:3914:U:C6	2.56	0.40
48:WA:4176:U:H2'	48:WA:4177:G:C8	2.55	0.40
51:ZA:1277:C:H5''	62:KB:55:ARG:HH11	1.87	0.40
51:ZA:1589:A:N3	51:ZA:1653:U:O2'	2.46	0.40
51:ZA:1597:C:H4'	51:ZA:1603:G:O6	2.21	0.40
58:GB:20:ASP:N	58:GB:20:ASP:OD1	2.53	0.40
58:GB:47:GLY:O	58:GB:115:LYS:NZ	2.37	0.40
58:GB:168:LYS:HE3	58:GB:168:LYS:HB3	1.94	0.40
65:NB:4:MET:HG2	65:NB:5:HIS:CD2	2.57	0.40
72:UB:26:SER:HB3	72:UB:32:LEU:HD13	2.02	0.40
76:YB:19:GLN:HG3	76:YB:81:TYR:CD2	2.56	0.40
84:GC:248:LEU:HB2	84:GC:261:LEU:HD21	2.02	0.40
85:HC:253:VAL:HG11	85:HC:320:VAL:HG23	2.03	0.40
2:B:126:LYS:O	2:B:128:LYS:N	2.54	0.40
5:E:45:HIS:ND1	5:E:46:CYS:O	2.53	0.40
8:H:41:ILE:HG22	8:H:43:VAL:HG13	2.04	0.40
9:I:91:LEU:HD12	9:I:135:ILE:HG23	2.04	0.40
15:O:84:LYS:HD3	15:O:84:LYS:HA	1.84	0.40
18:R:127:MET:HA	19:S:153:PRO:HD2	2.04	0.40
22:V:50:ASN:OD1	22:V:50:ASN:N	2.55	0.40
25:Y:73:LYS:HD3	25:Y:75:TYR:CZ	2.57	0.40
26:Z:90:ALA:HB3	26:Z:120:GLN:HE21	1.86	0.40
48:WA:223:G:H4'	48:WA:225:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:WA:269:G:H2'	48:WA:270:U:C6	2.56	0.40
48:WA:378:A:O2'	48:WA:413:G:N2	2.48	0.40
48:WA:1309:A:H2'	48:WA:1310:C:C6	2.56	0.40
48:WA:1521:C:H2'	48:WA:1522:C:H6	1.86	0.40
48:WA:4510:C:N3	48:WA:4514:U:H5	2.20	0.40
48:WA:5003:U:H2'	48:WA:5004:U:O4'	2.21	0.40
50:YA:7:U:H2'	50:YA:8:U:C6	2.56	0.40
51:ZA:381:C:H41	60:IB:27:TYR:HB2	1.86	0.40
51:ZA:545:A:H2'	51:ZA:546:G:C8	2.57	0.40
51:ZA:991:G:C6	51:ZA:1134:G:H4'	2.57	0.40
61:JB:131:ARG:HD2	61:JB:131:ARG:HA	1.87	0.40
84:GC:164:ILE:HG23	84:GC:176:VAL:HG13	2.04	0.40
87:b:44:ARG:NH2	87:b:53:VAL:O	2.54	0.40
87:b:220:ARG:HA	87:b:220:ARG:HD3	1.82	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%)	237 (96%)	11 (4%)	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%)	286 (98%)	6 (2%)	0	100	100
5	E	222/291 (76%)	214 (96%)	8 (4%)	0	100	100
6	F	225/249 (90%)	220 (98%)	5 (2%)	0	100	100
7	G	225/319 (70%)	221 (98%)	4 (2%)	0	100	100
8	H	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
9	I	201/214 (94%)	195 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	169/178 (95%)	167 (99%)	2 (1%)	0	100	100
11	K	208/210 (99%)	203 (98%)	5 (2%)	0	100	100
12	L	136/218 (62%)	130 (96%)	6 (4%)	0	100	100
13	M	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
14	N	197/203 (97%)	193 (98%)	4 (2%)	0	100	100
15	O	154/213 (72%)	152 (99%)	2 (1%)	0	100	100
16	P	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
17	Q	178/196 (91%)	175 (98%)	3 (2%)	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%)	94 (95%)	5 (5%)	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%)	114 (98%)	2 (2%)	0	100	100
24	X	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
25	Y	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
26	Z	145/148 (98%)	139 (96%)	6 (4%)	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%)	104 (98%)	2 (2%)	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%)	117 (98%)	2 (2%)	0	100	100
34	HA	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
35	IA	85/97 (88%)	82 (96%)	3 (4%)	0	100	100
36	JA	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	KA	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
38	LA	50/128 (39%)	48 (96%)	2 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	OA	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
42	PA	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
43	RA	151/165 (92%)	141 (93%)	10 (7%)	0	100	100
52	AB	215/295 (73%)	208 (97%)	7 (3%)	0	100	100
53	BB	211/264 (80%)	204 (97%)	7 (3%)	0	100	100
54	CB	218/293 (74%)	215 (99%)	3 (1%)	0	100	100
55	DB	226/281 (80%)	223 (99%)	3 (1%)	0	100	100
56	EB	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
57	FB	181/204 (89%)	175 (97%)	6 (3%)	0	100	100
58	GB	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
59	HB	181/432 (42%)	177 (98%)	4 (2%)	0	100	100
60	IB	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
61	JB	183/194 (94%)	182 (100%)	1 (0%)	0	100	100
62	KB	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
63	LB	140/158 (89%)	137 (98%)	3 (2%)	0	100	100
64	MB	115/132 (87%)	110 (96%)	5 (4%)	0	100	100
65	NB	147/151 (97%)	147 (100%)	0	0	100	100
66	OB	134/151 (89%)	129 (96%)	5 (4%)	0	100	100
67	PB	127/145 (88%)	126 (99%)	1 (1%)	0	100	100
68	QB	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
69	RB	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
70	SB	142/152 (93%)	140 (99%)	2 (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%)	79 (98%)	2 (2%)	0	100	100
74	WB	127/130 (98%)	122 (96%)	5 (4%)	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%)	96 (97%)	3 (3%)	0	100	100
79	BC	81/84 (96%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	51 (96%)	2 (4%)	0	100	100
83	FC	67/188 (36%)	63 (94%)	4 (6%)	0	100	100
84	GC	311/317 (98%)	299 (96%)	12 (4%)	0	100	100
85	HC	438/462 (95%)	416 (95%)	21 (5%)	1 (0%)	43	72
86	IC	2/4 (50%)	2 (100%)	0	0	100	100
87	b	165/318 (52%)	150 (91%)	14 (8%)	1 (1%)	21	51
88	c	9/14 (64%)	9 (100%)	0	0	100	100
All	All	12000/14276 (84%)	11650 (97%)	348 (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%)	190 (99%)	2 (1%)	68	89
2	B	344/348 (99%)	338 (98%)	6 (2%)	53	82
3	C	302/337 (90%)	301 (100%)	1 (0%)	86	96
4	D	247/250 (99%)	244 (99%)	3 (1%)	63	86
5	E	201/251 (80%)	199 (99%)	2 (1%)	68	89
6	F	198/218 (91%)	198 (100%)	0	100	100
7	G	197/273 (72%)	195 (99%)	2 (1%)	68	89
8	H	169/171 (99%)	164 (97%)	5 (3%)	36	70
9	I	175/181 (97%)	172 (98%)	3 (2%)	53	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	144/149 (97%)	142 (99%)	2 (1%)	59	85
11	K	175/175 (100%)	173 (99%)	2 (1%)	65	88
12	L	117/161 (73%)	117 (100%)	0	100	100
13	M	171/172 (99%)	170 (99%)	1 (1%)	78	93
14	N	171/173 (99%)	170 (99%)	1 (1%)	78	93
15	O	137/190 (72%)	137 (100%)	0	100	100
16	P	164/165 (99%)	162 (99%)	2 (1%)	63	86
17	Q	159/175 (91%)	159 (100%)	0	100	100
18	R	157/192 (82%)	152 (97%)	5 (3%)	34	68
19	S	139/140 (99%)	138 (99%)	1 (1%)	76	92
20	T	91/114 (80%)	91 (100%)	0	100	100
21	U	103/107 (96%)	101 (98%)	2 (2%)	50	79
22	V	89/126 (71%)	89 (100%)	0	100	100
23	W	106/134 (79%)	105 (99%)	1 (1%)	70	90
24	X	124/135 (92%)	120 (97%)	4 (3%)	34	68
25	Y	117/118 (99%)	114 (97%)	3 (3%)	40	73
26	Z	119/120 (99%)	118 (99%)	1 (1%)	73	90
27	AA	87/184 (47%)	86 (99%)	1 (1%)	65	88
28	BA	85/98 (87%)	84 (99%)	1 (1%)	63	86
29	CA	98/110 (89%)	96 (98%)	2 (2%)	48	78
30	DA	115/121 (95%)	115 (100%)	0	100	100
31	EA	88/89 (99%)	87 (99%)	1 (1%)	65	88
32	FA	98/109 (90%)	96 (98%)	2 (2%)	48	78
33	GA	109/110 (99%)	105 (96%)	4 (4%)	30	64
34	HA	86/89 (97%)	85 (99%)	1 (1%)	63	86
35	IA	74/80 (92%)	72 (97%)	2 (3%)	39	73
36	JA	64/65 (98%)	63 (98%)	1 (2%)	55	83
37	KA	47/48 (98%)	46 (98%)	1 (2%)	47	77
38	LA	48/116 (41%)	45 (94%)	3 (6%)	16	45
39	MA	24/24 (100%)	24 (100%)	0	100	100
40	NA	92/94 (98%)	91 (99%)	1 (1%)	65	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	OA	74/75 (99%)	73 (99%)	1 (1%)	59	85
42	PA	108/121 (89%)	106 (98%)	2 (2%)	50	79
43	RA	126/137 (92%)	117 (93%)	9 (7%)	13	40
52	AB	180/244 (74%)	178 (99%)	2 (1%)	65	88
53	BB	194/231 (84%)	192 (99%)	2 (1%)	68	89
54	CB	186/225 (83%)	184 (99%)	2 (1%)	65	88
55	DB	190/232 (82%)	185 (97%)	5 (3%)	40	73
56	EB	224/225 (100%)	220 (98%)	4 (2%)	51	80
57	FB	158/170 (93%)	156 (99%)	2 (1%)	61	86
58	GB	207/218 (95%)	202 (98%)	5 (2%)	43	75
59	HB	165/360 (46%)	159 (96%)	6 (4%)	31	65
60	IB	178/180 (99%)	175 (98%)	3 (2%)	53	82
61	JB	161/168 (96%)	158 (98%)	3 (2%)	50	79
62	KB	87/136 (64%)	84 (97%)	3 (3%)	32	66
63	LB	130/142 (92%)	128 (98%)	2 (2%)	57	84
64	MB	99/108 (92%)	95 (96%)	4 (4%)	28	62
65	NB	130/131 (99%)	129 (99%)	1 (1%)	73	90
66	OB	106/119 (89%)	105 (99%)	1 (1%)	70	90
67	PB	115/130 (88%)	114 (99%)	1 (1%)	70	90
68	QB	117/140 (84%)	113 (97%)	4 (3%)	32	66
69	RB	119/121 (98%)	116 (98%)	3 (2%)	42	74
70	SB	125/132 (95%)	121 (97%)	4 (3%)	34	68
71	TB	112/115 (97%)	107 (96%)	5 (4%)	24	58
72	UB	93/107 (87%)	89 (96%)	4 (4%)	26	60
73	VB	67/67 (100%)	66 (98%)	1 (2%)	57	84
74	WB	112/113 (99%)	110 (98%)	2 (2%)	51	80
75	XB	113/115 (98%)	108 (96%)	5 (4%)	25	59
76	YB	107/113 (95%)	105 (98%)	2 (2%)	50	79
77	ZB	75/102 (74%)	72 (96%)	3 (4%)	28	62
78	AC	88/98 (90%)	87 (99%)	1 (1%)	65	88
79	BC	75/76 (99%)	74 (99%)	1 (1%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	CC	55/62 (89%)	54 (98%)	1 (2%)	51	80
81	DC	48/49 (98%)	46 (96%)	2 (4%)	26	60
82	EC	46/106 (43%)	44 (96%)	2 (4%)	26	60
83	FC	62/154 (40%)	59 (95%)	3 (5%)	23	55
84	GC	272/275 (99%)	249 (92%)	23 (8%)	10	31
85	HC	366/379 (97%)	342 (93%)	24 (7%)	15	43
87	b	138/258 (54%)	126 (91%)	12 (9%)	9	30
88	c	9/12 (75%)	9 (100%)	0	100	100
All	All	10440/12057 (87%)	10211 (98%)	229 (2%)	45	77

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ILE
1	A	235	VAL
2	B	234	ARG
2	B	258	HIS
2	B	292	LEU
2	B	338	VAL
2	B	344	VAL
2	B	353	VAL
3	C	232	VAL
4	D	7	VAL
4	D	15	ARG
4	D	163	LEU
5	E	178	VAL
5	E	290	VAL
7	G	94	ILE
7	G	193	VAL
8	H	47	LEU
8	H	66	GLU
8	H	95	VAL
8	H	177	ASP
8	H	188	GLN
9	I	30	LYS
9	I	43	VAL
9	I	184	MET
10	J	20	LEU
10	J	87	LEU

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Mol	Chain	Res	Type
11	K	70	VAL
11	K	90	VAL
13	M	142	ILE
14	N	186	GLU
16	P	42	THR
16	P	83	VAL
18	R	39	VAL
18	R	84	TYR
18	R	154	LEU
18	R	160	ARG
18	R	173	ASN
19	S	80	VAL
21	U	92	ASP
21	U	108	ASN
23	W	155	ILE
24	X	58	VAL
24	X	79	VAL
24	X	82	ILE
24	X	104	VAL
25	Y	35	ASP
25	Y	53	VAL
25	Y	95	VAL
26	Z	122	VAL
27	AA	50	ASN
28	BA	14	ILE
29	CA	46	LEU
29	CA	100	ASN
31	EA	37	ASP
32	FA	20	THR
32	FA	38	VAL
33	GA	13	LYS
33	GA	17	LEU
33	GA	47	ILE
33	GA	96	ASN
34	HA	29	ARG
35	IA	59	THR
35	IA	82	THR
36	JA	56	LEU
37	KA	51	LEU
38	LA	58	GLN
38	LA	100	LYS
38	LA	101	VAL

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Mol	Chain	Res	Type
40	NA	77	CYS
41	OA	52	VAL
42	PA	103	HIS
42	PA	124	VAL
43	RA	13	VAL
43	RA	37	LEU
43	RA	40	LYS
43	RA	87	GLU
43	RA	98	ILE
43	RA	107	ASP
43	RA	147	HIS
43	RA	151	ILE
43	RA	154	ASP
52	AB	51	LEU
52	AB	94	THR
53	BB	74	LEU
53	BB	98	THR
54	CB	59	GLU
54	CB	248	TYR
55	DB	42	GLN
55	DB	79	VAL
55	DB	110	VAL
55	DB	123	GLU
55	DB	253	ASP
56	EB	216	ASN
56	EB	220	THR
56	EB	222	LEU
56	EB	248	ILE
57	FB	69	VAL
57	FB	102	LEU
58	GB	50	VAL
58	GB	108	VAL
58	GB	153	VAL
58	GB	213	LEU
58	GB	217	MET
59	HB	265	LEU
59	HB	284	THR
59	HB	313	ILE
59	HB	330	VAL
59	HB	372	VAL
59	HB	391	LEU
60	IB	73	THR

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Mol	Chain	Res	Type
60	IB	107	THR
60	IB	125	LYS
61	JB	66	LYS
61	JB	95	ASP
61	JB	123	ILE
62	KB	1	MET
62	KB	20	VAL
62	KB	52	LEU
63	LB	48	LYS
63	LB	126	VAL
64	MB	27	ILE
64	MB	31	LEU
64	MB	77	ILE
64	MB	111	VAL
65	NB	134	VAL
66	OB	57	THR
67	PB	72	LYS
68	QB	107	ILE
68	QB	110	ILE
68	QB	126	VAL
68	QB	134	ILE
69	RB	99	ASP
69	RB	127	ASN
69	RB	132	ARG
70	SB	52	LEU
70	SB	103	LEU
70	SB	131	VAL
70	SB	145	THR
71	TB	4	VAL
71	TB	24	LYS
71	TB	62	ARG
71	TB	78	ILE
71	TB	99	VAL
72	UB	17	ILE
72	UB	18	HIS
72	UB	29	VAL
72	UB	68	THR
73	VB	47	ASN
74	WB	52	ILE
74	WB	105	THR
75	XB	17	ARG
75	XB	61	GLN

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Mol	Chain	Res	Type
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
80	CC	38	THR
81	DC	30	LEU
81	DC	39	CYS
82	EC	118	VAL
82	EC	124	LYS
83	FC	85	TYR
83	FC	108	VAL
83	FC	135	HIS
84	GC	11	LEU
84	GC	18	VAL
84	GC	31	ILE
84	GC	38	LYS
84	GC	44	LYS
84	GC	46	THR
84	GC	54	ILE
84	GC	68	ASP
84	GC	113	PHE
84	GC	120	ILE
84	GC	131	LEU
84	GC	141	THR
84	GC	142	VAL
84	GC	165	ILE
84	GC	179	LEU
84	GC	185	LYS
84	GC	186	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
85	HC	10	ILE

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Mol	Chain	Res	Type
85	HC	12	VAL
85	HC	64	LYS
85	HC	87	VAL
85	HC	90	ILE
85	HC	120	VAL
85	HC	134	ARG
85	HC	165	LYS
85	HC	177	TYR
85	HC	202	LEU
85	HC	208	MET
85	HC	212	LYS
85	HC	217	THR
85	HC	239	THR
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	423	ARG
85	HC	432	THR
85	HC	433	VAL
85	HC	438	ILE
87	b	15	LEU
87	b	21	LEU
87	b	40	MET
87	b	53	VAL
87	b	54	LEU
87	b	68	HIS
87	b	69	LEU
87	b	75	LEU
87	b	105	ASN
87	b	145	THR
87	b	149	ARG
87	b	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	205	ASN
2	B	184	GLN

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Mol	Chain	Res	Type
2	B	203	GLN
2	B	236	HIS
3	C	38	ASN
3	C	187	GLN
3	C	329	ASN
5	E	248	GLN
5	E	269	GLN
6	F	79	ASN
6	F	98	ASN
7	G	99	GLN
8	H	63	ASN
9	I	73	ASN
11	K	115	GLN
12	L	48	GLN
13	M	32	GLN
13	M	86	HIS
13	M	117	ASN
14	N	42	ASN
14	N	167	HIS
15	O	10	ASN
15	O	93	ASN
15	O	145	HIS
16	P	188	ASN
17	Q	34	ASN
17	Q	143	HIS
19	S	127	GLN
21	U	36	ASN
24	X	14	ASN
24	X	96	HIS
26	Z	60	HIS
26	Z	66	ASN
27	AA	6	ASN
27	AA	12	GLN
30	DA	80	HIS
31	EA	55	ASN
33	GA	65	GLN
34	HA	80	HIS
36	JA	31	ASN
42	PA	21	ASN
42	PA	31	ASN
42	PA	36	ASN
43	RA	142	ASN

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Mol	Chain	Res	Type
43	RA	156	ASN
53	BB	75	GLN
53	BB	186	ASN
54	CB	136	HIS
54	CB	172	ASN
55	DB	139	GLN
55	DB	197	HIS
55	DB	245	HIS
57	FB	82	ASN
57	FB	203	ASN
58	GB	65	GLN
59	HB	271	ASN
59	HB	277	GLN
60	IB	146	GLN
61	JB	140	GLN
62	KB	42	ASN
62	KB	44	HIS
63	LB	11	GLN
63	LB	39	ASN
63	LB	108	ASN
63	LB	141	ASN
64	MB	55	ASN
65	NB	13	GLN
65	NB	58	HIS
65	NB	90	HIS
71	TB	85	ASN
74	WB	24	GLN
75	XB	77	ASN
75	XB	92	ASN
77	ZB	112	ASN
78	AC	8	ASN
80	CC	29	GLN
80	CC	45	ASN
82	EC	95	GLN
83	FC	93	HIS
84	GC	119	GLN
84	GC	178	ASN
84	GC	222	ASN
84	GC	305	ASN
85	HC	136	HIS
85	HC	197	ASN
85	HC	200	ASN

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Mol	Chain	Res	Type
85	HC	348	ASN
87	b	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	SA	75/76 (98%)	13 (17%)	3 (4%)
45	TA	75/76 (98%)	20 (26%)	0
46	UA	74/75 (98%)	28 (37%)	1 (1%)
47	VA	11/12 (91%)	3 (27%)	0
48	WA	3558/3584 (99%)	583 (16%)	21 (0%)
49	XA	118/120 (98%)	11 (9%)	0
50	YA	155/156 (99%)	35 (22%)	0
51	ZA	1707/1869 (91%)	304 (17%)	9 (0%)
All	All	5773/5968 (96%)	997 (17%)	34 (0%)

All (997) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	SA	9	A
44	SA	16	C
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	49	C
44	SA	58	A
44	SA	60	A
44	SA	70	A
44	SA	76	A
45	TA	6	G
45	TA	7	A
45	TA	10	G
45	TA	13	C
45	TA	16	C
45	TA	17	U
45	TA	18	G
45	TA	19	A
45	TA	20	U

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Mol	Chain	Res	Type
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	59	G
45	TA	66	U
45	TA	74	C
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
46	UA	30	G
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	67	G
46	UA	73	A
46	UA	76	A
47	VA	22	G
47	VA	24	U
47	VA	26	A

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Mol	Chain	Res	Type
48	WA	12	A
48	WA	13	U
48	WA	25	A
48	WA	39	A
48	WA	42	A
48	WA	48	G
48	WA	59	A
48	WA	64	A
48	WA	65	A
48	WA	91	G
48	WA	108	A
48	WA	110	C
48	WA	117	C
48	WA	119	G
48	WA	120	A
48	WA	132	G
48	WA	134	G
48	WA	135	G
48	WA	136	C
48	WA	143	C
48	WA	144	G
48	WA	157	U
48	WA	159	C
48	WA	171	U
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	217	C
48	WA	218	A
48	WA	219	G
48	WA	224	U
48	WA	233	U
48	WA	234	G
48	WA	258	G
48	WA	266	C
48	WA	267	G
48	WA	280	G
48	WA	297	U
48	WA	306	A

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Mol	Chain	Res	Type
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	363	A
48	WA	386	A
48	WA	387	G
48	WA	409	G
48	WA	410	A
48	WA	412	G
48	WA	417	G
48	WA	428	G
48	WA	449	C
48	WA	450	G
48	WA	452	A
48	WA	454	U
48	WA	455	C
48	WA	467	U
48	WA	468	U
48	WA	482	C
48	WA	483	G
48	WA	484	G
48	WA	485	U
48	WA	487	C
48	WA	488	G
48	WA	493	U
48	WA	494	G
48	WA	499	C
48	WA	506	G
48	WA	511	U
48	WA	521	U
48	WA	643	G
48	WA	662	C
48	WA	667	G
48	WA	686	C
48	WA	689	U
48	WA	698	G
48	WA	705	C
48	WA	720	C
48	WA	732	G

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Mol	Chain	Res	Type
48	WA	739	C
48	WA	741	G
48	WA	751	G
48	WA	758	G
48	WA	763	G
48	WA	905	U
48	WA	909	C
48	WA	910	G
48	WA	915	U
48	WA	917	A
48	WA	919	A
48	WA	929	C
48	WA	930	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	944	G
48	WA	946	C
48	WA	948	A
48	WA	950	U
48	WA	964	G
48	WA	965	A
48	WA	966	G
48	WA	971	A
48	WA	972	C
48	WA	974	C
48	WA	978	C
48	WA	984	C
48	WA	989	C
48	WA	1078	C
48	WA	1085	C
48	WA	1101	A
48	WA	1102	C
48	WA	1104	G
48	WA	1186	C
48	WA	1201	G
48	WA	1202	G
48	WA	1216	C
48	WA	1217	G

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Mol	Chain	Res	Type
48	WA	1220	C
48	WA	1221	C
48	WA	1222	C
48	WA	1243	C
48	WA	1244	A
48	WA	1246	G
48	WA	1250	C
48	WA	1253	C
48	WA	1255	G
48	WA	1258	A
48	WA	1259	A
48	WA	1265	A
48	WA	1268	G
48	WA	1271	G
48	WA	1272	A
48	WA	1274	C
48	WA	1275	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	1414	G
48	WA	1416	C
48	WA	1421	G

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Mol	Chain	Res	Type
48	WA	1422	A
48	WA	1437	G
48	WA	1448	C
48	WA	1467	G
48	WA	1485	C
48	WA	1499	A
48	WA	1500	G
48	WA	1504	G
48	WA	1520	A
48	WA	1525	A
48	WA	1527	A
48	WA	1536	A
48	WA	1549	A
48	WA	1566	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	1643	G
48	WA	1656	G
48	WA	1663	C
48	WA	1678	C
48	WA	1679	U
48	WA	1736	G
48	WA	1743	G
48	WA	1744	A
48	WA	1756	U
48	WA	1757	C
48	WA	1758	U
48	WA	1763	G
48	WA	1766	G
48	WA	1768	A
48	WA	1770	C

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Mol	Chain	Res	Type
48	WA	1772	A
48	WA	1774	C
48	WA	1783	U
48	WA	1789	A
48	WA	1806	A
48	WA	1807	A
48	WA	1817	G
48	WA	1821	G
48	WA	1823	G
48	WA	1830	C
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	1950	G
48	WA	1963	G
48	WA	1975	G
48	WA	1976	U
48	WA	1977	G
48	WA	1984	G
48	WA	1986	A
48	WA	1987	G
48	WA	1988	U
48	WA	1989	C
48	WA	1992	A
48	WA	1993	A
48	WA	1996	C
48	WA	1998	C
48	WA	1999	U
48	WA	2000	A
48	WA	2001	A

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Mol	Chain	Res	Type
48	WA	2002	G
48	WA	2003	G
48	WA	2004	A
48	WA	2005	G
48	WA	2006	U
48	WA	2010	U
48	WA	2013	C
48	WA	2014	A
48	WA	2023	G
48	WA	2027	A
48	WA	2028	A
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	2100	G
48	WA	2102	G
48	WA	2104	G
48	WA	2106	A
48	WA	2107	A
48	WA	2108	G
48	WA	2109	A
48	WA	2114	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	2272	G
48	WA	2277	G
48	WA	2291	C
48	WA	2302	A

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Mol	Chain	Res	Type
48	WA	2303	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	2423	G
48	WA	2424	C
48	WA	2427	U
48	WA	2435	G
48	WA	2443	C
48	WA	2452	G
48	WA	2473	G
48	WA	2477	G
48	WA	2485	G
48	WA	2490	C
48	WA	2492	U
48	WA	2493	C
48	WA	2494	C
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
48	WA	2554	G
48	WA	2555	A
48	WA	2570	C
48	WA	2585	C
48	WA	2588	G
48	WA	2591	C
48	WA	2603	A
48	WA	2629	C

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Mol	Chain	Res	Type
48	WA	2640	G
48	WA	2642	G
48	WA	2655	C
48	WA	2664	G
48	WA	2671	C
48	WA	2672	C
48	WA	2688	G
48	WA	2689	U
48	WA	2696	G
48	WA	2697	A
48	WA	2698	A
48	WA	2707	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	2716	G
48	WA	2721	C
48	WA	2723	G
48	WA	2727	A
48	WA	2728	G
48	WA	2742	U
48	WA	2745	A
48	WA	2746	A
48	WA	2760	G
48	WA	2766	A
48	WA	2771	U
48	WA	2789	A
48	WA	2790	U
48	WA	2792	U
48	WA	2796	C
48	WA	2800	A
48	WA	2808	A
48	WA	2828	U
48	WA	2829	G
48	WA	2830	U
48	WA	2844	G
48	WA	2857	G
48	WA	2904	G
48	WA	3599	G

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Mol	Chain	Res	Type
48	WA	3600	C
48	WA	3627	G
48	WA	3628	G
48	WA	3637	A
48	WA	3645	A
48	WA	3646	U
48	WA	3650	A
48	WA	3664	A
48	WA	3674	G
48	WA	3675	C
48	WA	3714	A
48	WA	3716	G
48	WA	3750	A
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	3800	U
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
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	3903	A
48	WA	3908	A

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Mol	Chain	Res	Type
48	WA	3909	G
48	WA	3910	A
48	WA	3916	U
48	WA	3917	U
48	WA	3919	A
48	WA	3940	G
48	WA	3941	G
48	WA	3945	A
48	WA	3949	A
48	WA	3950	C
48	WA	3952	U
48	WA	4066	C
48	WA	4067	G
48	WA	4078	G
48	WA	4090	C
48	WA	4101	G
48	WA	4102	C
48	WA	4118	C
48	WA	4120	U
48	WA	4121	C
48	WA	4124	G
48	WA	4129	A
48	WA	4141	G
48	WA	4144	C
48	WA	4145	C
48	WA	4146	G
48	WA	4160	C
48	WA	4165	U
48	WA	4168	G
48	WA	4172	A
48	WA	4174	A
48	WA	4175	G
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

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Mol	Chain	Res	Type
48	WA	4256	G
48	WA	4260	C
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	4299	G
48	WA	4306	A
48	WA	4307	G
48	WA	4308	U
48	WA	4316	C
48	WA	4332	G
48	WA	4334	C
48	WA	4338	A
48	WA	4339	C
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	4382	A
48	WA	4389	C
48	WA	4396	A
48	WA	4397	U
48	WA	4398	A
48	WA	4421	U
48	WA	4423	C
48	WA	4424	A
48	WA	4446	C
48	WA	4450	G
48	WA	4451	A
48	WA	4454	U
48	WA	4466	A
48	WA	4468	C
48	WA	4490	A
48	WA	4502	U
48	WA	4514	U
48	WA	4515	A
48	WA	4521	C

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Mol	Chain	Res	Type
48	WA	4522	G
48	WA	4526	G
48	WA	4533	U
48	WA	4550	A
48	WA	4551	G
48	WA	4562	C
48	WA	4569	G
48	WA	4575	G
48	WA	4577	G
48	WA	4586	A
48	WA	4588	G
48	WA	4592	A
48	WA	4602	G
48	WA	4629	U
48	WA	4638	U
48	WA	4639	G
48	WA	4654	G
48	WA	4658	A
48	WA	4672	C
48	WA	4674	A
48	WA	4679	U
48	WA	4689	A
48	WA	4702	A
48	WA	4711	U
48	WA	4722	C
48	WA	4747	G
48	WA	4756	G
48	WA	4759	C
48	WA	4761	C
48	WA	4763	G
48	WA	4767	G
48	WA	4771	G
48	WA	4773	C
48	WA	4775	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

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Mol	Chain	Res	Type
48	WA	4884	U
48	WA	4885	C
48	WA	4887	U
48	WA	4888	C
48	WA	4904	C
48	WA	4914	G
48	WA	4915	G
48	WA	4917	G
48	WA	4923	C
48	WA	4924	C
48	WA	4928	C
48	WA	4929	G
48	WA	4939	C
48	WA	4945	A
48	WA	4946	C
48	WA	4951	G
48	WA	4952	U
48	WA	4953	G
48	WA	4960	C
48	WA	4965	G
48	WA	4967	U
48	WA	4968	A
48	WA	4978	U
48	WA	4981	A
48	WA	4992	C
48	WA	4993	U
48	WA	5008	U
48	WA	5009	A
48	WA	5016	A
48	WA	5018	A
48	WA	5036	A
48	WA	5043	G
48	WA	5052	C
48	WA	5055	U
48	WA	5056	C
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

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Mol	Chain	Res	Type
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	79	G
50	YA	80	A
50	YA	81	C
50	YA	82	A
50	YA	83	C
50	YA	84	A
50	YA	85	U
50	YA	86	U
50	YA	88	A
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	114	G
50	YA	123	U
50	YA	124	U
50	YA	125	C
50	YA	126	C
50	YA	127	U
50	YA	137	A
50	YA	147	G
50	YA	150	C
50	YA	153	C
50	YA	155	C
51	ZA	3	C

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Mol	Chain	Res	Type
51	ZA	4	C
51	ZA	25	A
51	ZA	33	G
51	ZA	41	G
51	ZA	42	A
51	ZA	46	A
51	ZA	56	G
51	ZA	58	C
51	ZA	59	U
51	ZA	62	G
51	ZA	67	C
51	ZA	68	A
51	ZA	70	G
51	ZA	71	G
51	ZA	73	C
51	ZA	76	U
51	ZA	79	A
51	ZA	103	A
51	ZA	113	G
51	ZA	115	U
51	ZA	116	U
51	ZA	126	G
51	ZA	130	G
51	ZA	143	U
51	ZA	147	A
51	ZA	155	G
51	ZA	160	U
51	ZA	162	C
51	ZA	163	U
51	ZA	170	A
51	ZA	173	A
51	ZA	178	C
51	ZA	181	A
51	ZA	182	C
51	ZA	183	G
51	ZA	184	G
51	ZA	188	C
51	ZA	196	C
51	ZA	198	U
51	ZA	199	C
51	ZA	200	G
51	ZA	202	G

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Mol	Chain	Res	Type
51	ZA	204	G
51	ZA	292	A
51	ZA	307	G
51	ZA	308	G
51	ZA	309	G
51	ZA	319	C
51	ZA	320	G
51	ZA	323	C
51	ZA	325	C
51	ZA	326	C
51	ZA	328	U
51	ZA	330	G
51	ZA	335	G
51	ZA	347	G
51	ZA	351	G
51	ZA	362	C
51	ZA	364	A
51	ZA	368	U
51	ZA	369	C
51	ZA	370	G
51	ZA	381	C
51	ZA	383	G
51	ZA	384	U
51	ZA	385	G
51	ZA	386	C
51	ZA	398	A
51	ZA	400	C
51	ZA	409	C
51	ZA	438	G
51	ZA	448	A
51	ZA	449	A
51	ZA	450	C
51	ZA	464	A
51	ZA	472	C
51	ZA	473	A
51	ZA	474	G
51	ZA	476	A
51	ZA	482	G
51	ZA	487	U
51	ZA	492	C
51	ZA	493	A
51	ZA	502	C

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Mol	Chain	Res	Type
51	ZA	508	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	563	G
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	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

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Mol	Chain	Res	Type
51	ZA	752	G
51	ZA	753	C
51	ZA	754	G
51	ZA	799	U
51	ZA	811	A
51	ZA	821	G
51	ZA	822	U
51	ZA	827	A
51	ZA	834	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	874	G
51	ZA	875	A
51	ZA	878	G
51	ZA	884	C
51	ZA	888	U
51	ZA	889	U
51	ZA	890	U
51	ZA	891	G
51	ZA	892	U
51	ZA	893	U
51	ZA	894	G
51	ZA	895	G
51	ZA	897	U
51	ZA	898	U
51	ZA	901	G
51	ZA	902	G
51	ZA	905	C
51	ZA	909	G
51	ZA	913	A
51	ZA	914	U
51	ZA	920	A
51	ZA	922	A
51	ZA	933	G

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Mol	Chain	Res	Type
51	ZA	934	G
51	ZA	943	U
51	ZA	971	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	1060	A
51	ZA	1061	U
51	ZA	1062	A
51	ZA	1080	A
51	ZA	1083	A
51	ZA	1085	C
51	ZA	1100	A
51	ZA	1115	U
51	ZA	1116	C
51	ZA	1117	C
51	ZA	1118	C
51	ZA	1121	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
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	1285	G

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Mol	Chain	Res	Type
51	ZA	1286	G
51	ZA	1297	U
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	1313	A
51	ZA	1333	U
51	ZA	1342	U
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	1418	C
51	ZA	1419	C
51	ZA	1420	G
51	ZA	1422	G
51	ZA	1423	C
51	ZA	1424	G
51	ZA	1428	G
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	1442	U
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	1498	A
51	ZA	1521	C
51	ZA	1522	A
51	ZA	1531	A

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Mol	Chain	Res	Type
51	ZA	1533	A
51	ZA	1535	U
51	ZA	1536	G
51	ZA	1544	C
51	ZA	1548	G
51	ZA	1551	U
51	ZA	1552	G
51	ZA	1553	C
51	ZA	1555	U
51	ZA	1556	A
51	ZA	1560	U
51	ZA	1567	G
51	ZA	1570	G
51	ZA	1579	A
51	ZA	1580	A
51	ZA	1587	G
51	ZA	1588	A
51	ZA	1601	A
51	ZA	1604	G
51	ZA	1621	U
51	ZA	1623	A
51	ZA	1646	C
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	1754	G
51	ZA	1757	G
51	ZA	1758	G
51	ZA	1774	C
51	ZA	1780	G
51	ZA	1783	C
51	ZA	1825	A
51	ZA	1829	G
51	ZA	1831	A

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Mol	Chain	Res	Type
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 (34) 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
48	WA	1293	G
48	WA	1635	G
48	WA	1677	C
48	WA	1806	A
48	WA	1820	G
48	WA	2048	G
48	WA	2095	G
48	WA	2101	C
48	WA	2268	C
48	WA	2641	U
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
51	ZA	24	C
51	ZA	553	U
51	ZA	561	A
51	ZA	752	G

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Mol	Chain	Res	Type
51	ZA	870	A
51	ZA	874	G
51	ZA	890	U
51	ZA	1137	U
51	ZA	1433	C

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 281 ligands modelled in this entry, 269 are monoatomic - leaving 12 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	GTP	HC	601	89	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
94	SPM	ZA	1955	-	13,13,13	0.36	0	12,12,12	1.00	0
91	5GP	UA	101	46	26,26,26	1.00	2 (7%)	39,40,40	1.73	7 (17%)
93	SPD	WA	5253	-	9,9,9	0.28	0	8,8,8	0.34	0
93	SPD	WA	5257	-	9,9,9	0.27	0	8,8,8	0.32	0
93	SPD	WA	5256	-	9,9,9	0.28	0	8,8,8	0.30	0
93	SPD	WA	5255	-	9,9,9	0.29	0	8,8,8	0.43	0
93	SPD	WA	5254	-	9,9,9	0.28	0	8,8,8	0.25	0
94	SPM	WA	5252	-	13,13,13	0.34	0	12,12,12	0.92	0
93	SPD	WA	5251	-	9,9,9	0.27	0	8,8,8	0.32	0
97	SER	HC	603	-	4,5,6	0.57	0	1,5,7	0.55	0
92	ANM	WA	5250	95	20,20,20	4.08	7 (35%)	24,27,27	1.44	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	GTP	HC	601	89	-	6/22/38/38	0/3/3/3
94	SPM	ZA	1955	-	-	4/11/11/11	-
91	5GP	UA	101	46	-	1/10/26/26	0/3/3/3
93	SPD	WA	5253	-	-	0/7/7/7	-
93	SPD	WA	5257	-	-	0/7/7/7	-
93	SPD	WA	5256	-	-	2/7/7/7	-
93	SPD	WA	5255	-	-	0/7/7/7	-
93	SPD	WA	5254	-	-	4/7/7/7	-
94	SPM	WA	5252	-	-	3/11/11/11	-
93	SPD	WA	5251	-	-	1/7/7/7	-
97	SER	HC	603	-	-	0/2/4/6	-
92	ANM	WA	5250	95	-	6/10/23/23	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	WA	5250	ANM	C3-C2	-11.91	1.32	1.53
92	WA	5250	ANM	C16-N1	-8.91	1.30	1.47
92	WA	5250	ANM	C2-C16	7.36	1.67	1.53
92	WA	5250	ANM	C4-C3	3.86	1.58	1.53
92	WA	5250	ANM	C4-N1	3.81	1.60	1.47
92	WA	5250	ANM	O2-C5	3.53	1.43	1.35
91	UA	101	5GP	C6-N1	-2.55	1.34	1.38
92	WA	5250	ANM	C6-C5	2.41	1.57	1.49
96	HC	601	GTP	C2-N3	2.14	1.38	1.33
91	UA	101	5GP	C5-N7	-2.03	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	UA	101	5GP	C5-C4-N3	-5.84	119.10	128.39
92	WA	5250	ANM	O2-C5-C6	5.36	120.65	111.09
96	HC	601	GTP	C5-C4-N3	-5.34	119.89	128.39
96	HC	601	GTP	C2-N3-C4	4.76	120.49	112.30
91	UA	101	5GP	C2-N3-C4	4.51	120.06	112.30
91	UA	101	5GP	N9-C4-N3	3.73	133.40	125.95
96	HC	601	GTP	N9-C4-N3	3.48	132.91	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
96	HC	601	GTP	C2-N1-C6	-2.97	119.72	125.11
96	HC	601	GTP	C5-C6-N1	2.51	119.64	113.25
91	UA	101	5GP	O6-C6-C5	-2.46	120.05	126.53
96	HC	601	GTP	O6-C6-C5	-2.45	120.06	126.53
91	UA	101	5GP	C5-C6-N1	2.45	119.48	113.25
91	UA	101	5GP	C2-N1-C6	-2.42	120.72	125.11
96	HC	601	GTP	C8-N7-C5	2.35	108.44	104.26
96	HC	601	GTP	N9-C8-N7	-2.32	109.09	113.40
91	UA	101	5GP	N9-C8-N7	-2.30	109.14	113.40
96	HC	601	GTP	C3'-C2'-C1'	2.23	105.67	101.46
92	WA	5250	ANM	C12-C15-C16	-2.04	109.95	113.40

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	WA	5250	ANM	O3-C5-O2-C2
92	WA	5250	ANM	C6-C5-O2-C2
92	WA	5250	ANM	C1-C9-O1-C14
92	WA	5250	ANM	C10-C9-O1-C14
94	ZA	1955	SPM	C2-C3-C4-N5
96	HC	601	GTP	C3'-C4'-C5'-O5'
96	HC	601	GTP	O4'-C4'-C5'-O5'
94	WA	5252	SPM	C12-C11-N10-C9
93	WA	5251	SPD	C2-C3-C4-C5
94	WA	5252	SPM	N10-C11-C12-C13
94	ZA	1955	SPM	C12-C11-N10-C9
93	WA	5256	SPD	C3-C4-C5-N6
94	WA	5252	SPM	N1-C2-C3-C4
93	WA	5254	SPD	C2-C3-C4-C5
94	ZA	1955	SPM	N5-C6-C7-C8
96	HC	601	GTP	PA-O3A-PB-O2B
93	WA	5254	SPD	C8-C7-N6-C5
94	ZA	1955	SPM	C6-C7-C8-C9
96	HC	601	GTP	C5'-O5'-PA-O1A
93	WA	5254	SPD	C7-C8-C9-N10
93	WA	5254	SPD	C4-C5-N6-C7
93	WA	5256	SPD	C8-C7-N6-C5
96	HC	601	GTP	PA-O3A-PB-O1B
92	WA	5250	ANM	C11-C12-C15-C16
96	HC	601	GTP	C4'-C5'-O5'-PA
92	WA	5250	ANM	C13-C12-C15-C16

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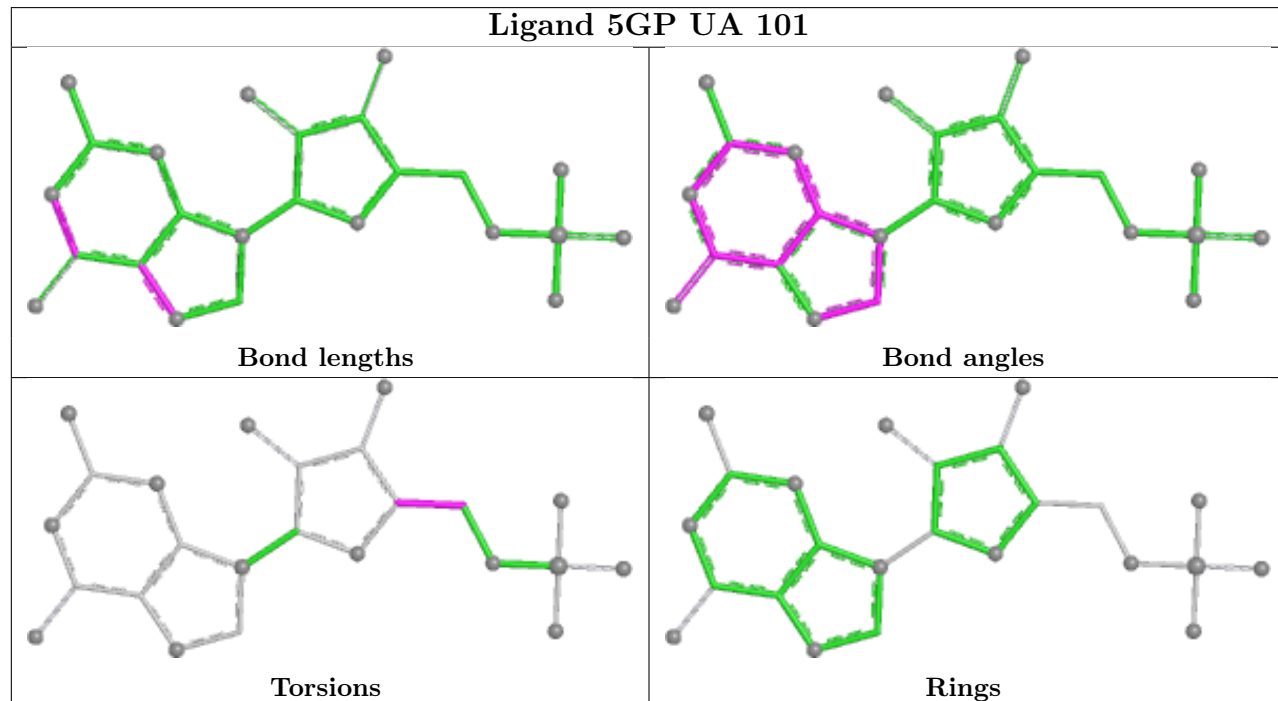
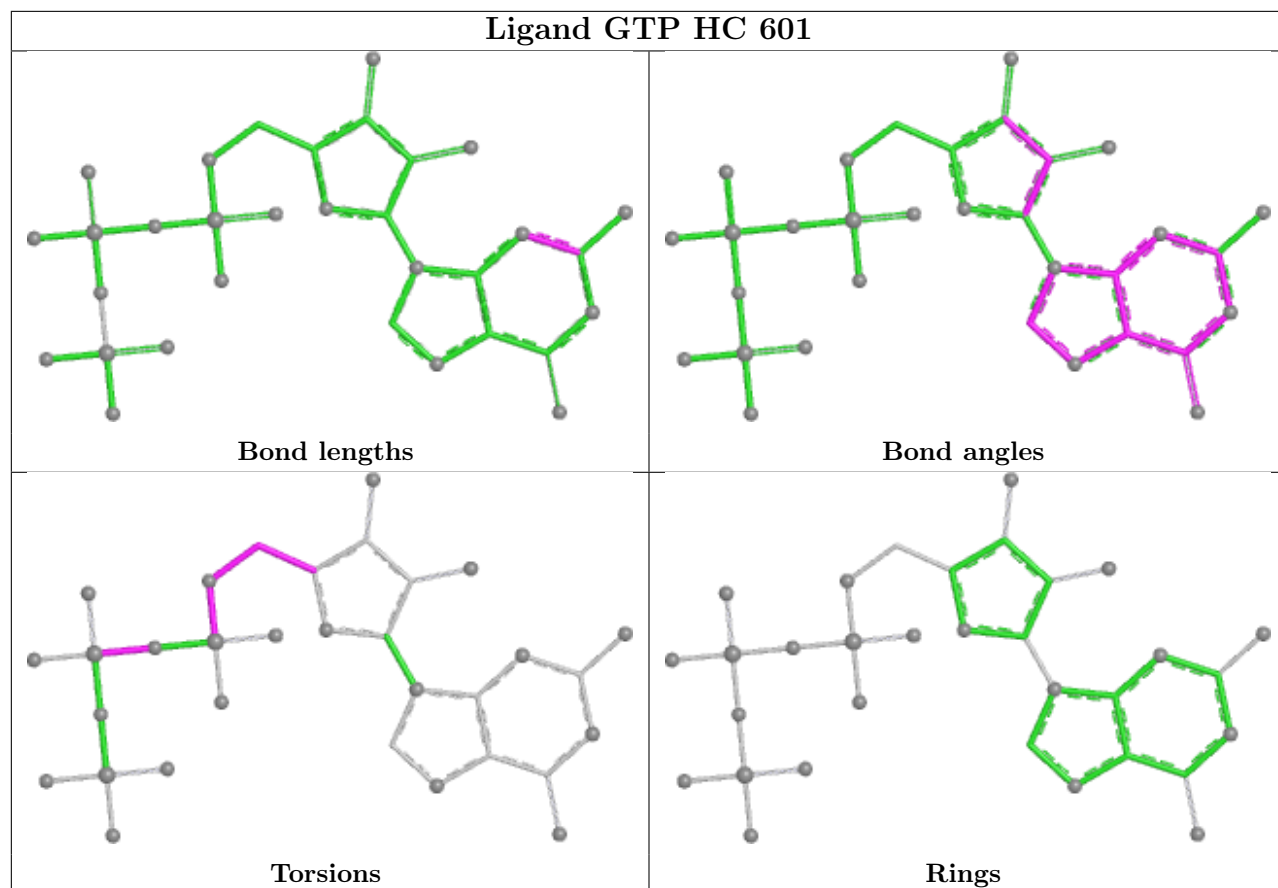
Mol	Chain	Res	Type	Atoms
91	UA	101	5GP	O4'-C4'-C5'-O5'

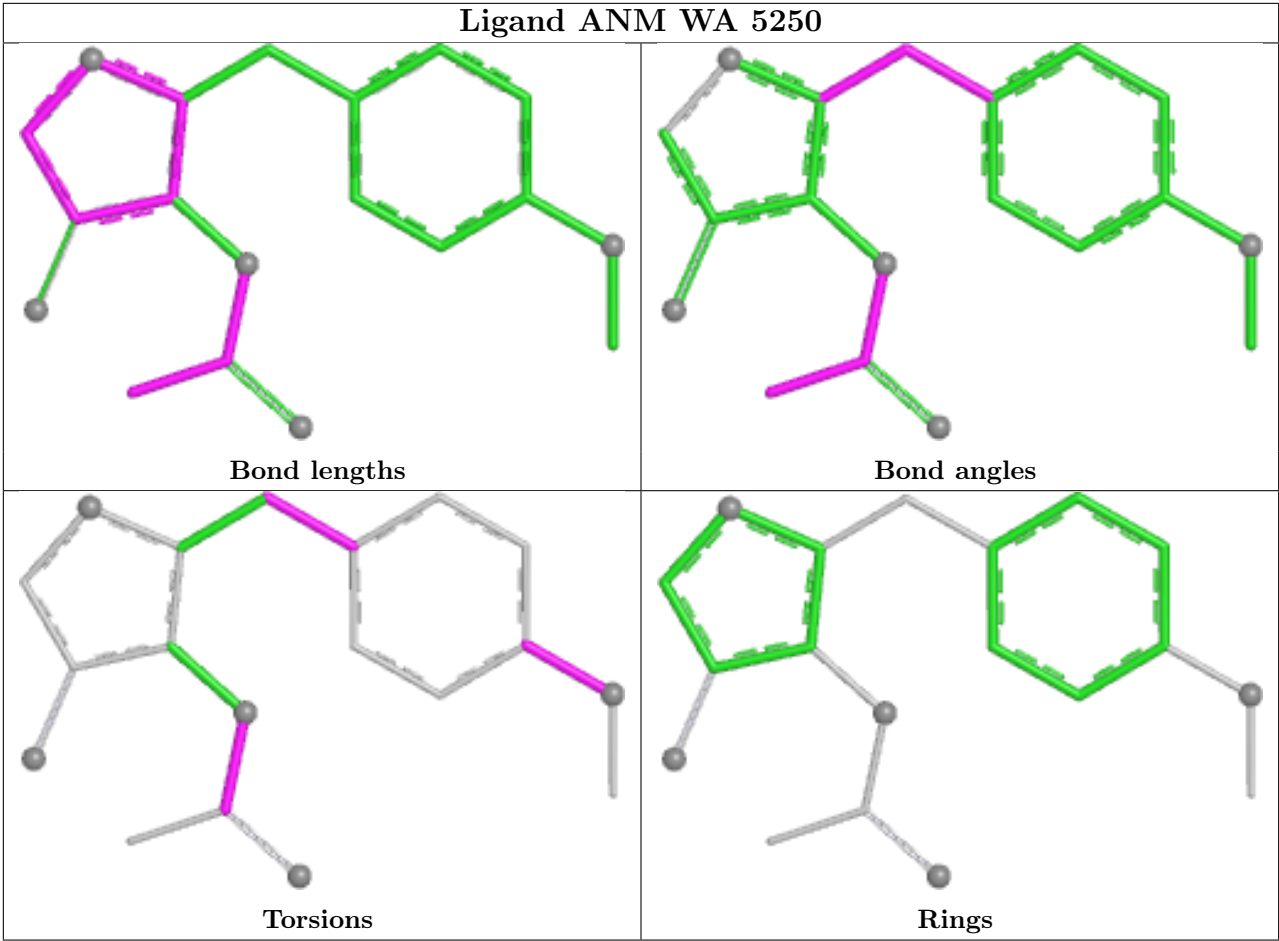
There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
96	HC	601	GTP	2	0
91	UA	101	5GP	1	0
93	WA	5253	SPD	1	0
93	WA	5257	SPD	1	0
93	WA	5255	SPD	2	0
94	WA	5252	SPM	2	0
92	WA	5250	ANM	2	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	36.45
1	WA	1225:G	O3'	1239:G	P	21.34
1	WA	763:G	O3'	904:C	P	17.81
1	WA	996:C	O3'	1070:G	P	17.79
1	WA	524:C	O3'	639:G	P	16.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	WA	4103:C	O3'	4109:G	P	16.64
1	WA	4779:C	O3'	4861:C	P	15.15
1	WA	1698:C	O3'	1722:C	P	14.45
1	WA	5024:U	O3'	5030:G	P	13.77
1	WA	2904:G	O3'	3598:A	P	13.47
1	WA	1366:U	O3'	1370:A	P	13.33
1	WA	182:G	O3'	189:G	P	10.93
1	WA	1186:C	O3'	1189:C	P	10.82
1	WA	4731:A	O3'	4737:G	P	10.29
1	WA	3954:A	O3'	4063:C	P	9.98
1	WA	513:U	O3'	516:C	P	6.82
1	WA	4742:G	O3'	4745:G	P	6.22
1	WA	501:G	O3'	505:G	P	5.98
1	WA	1106:U	O3'	1174:G	P	5.72
1	WA	4901:G	O3'	4904:C	P	3.26

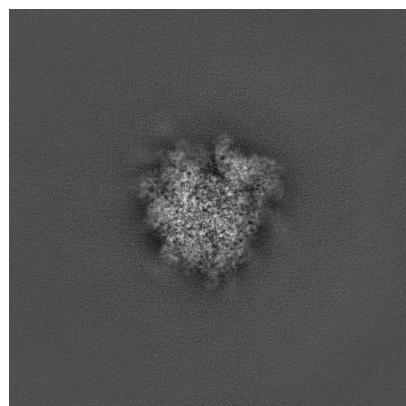
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43564. These allow visual inspection of the internal detail of the map and identification of artifacts.

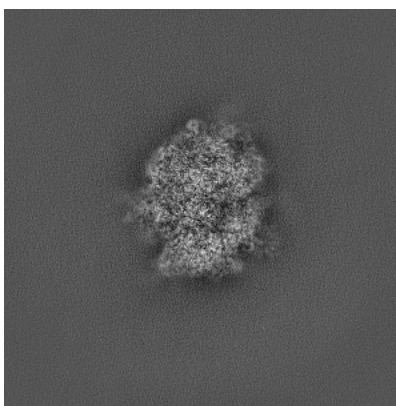
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

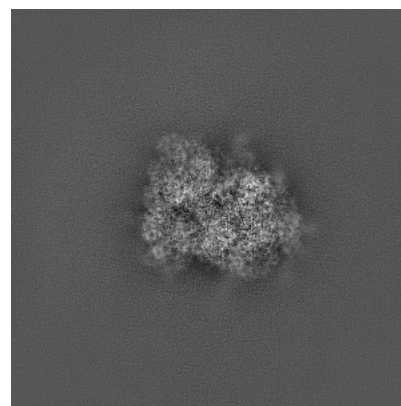
6.1.1 Primary map



X

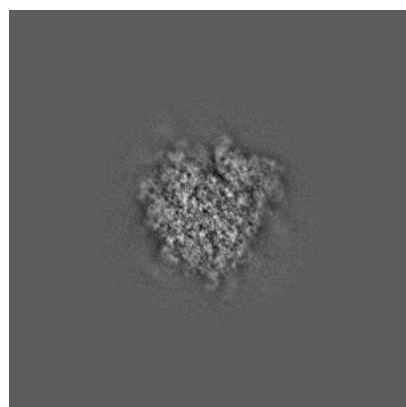


Y

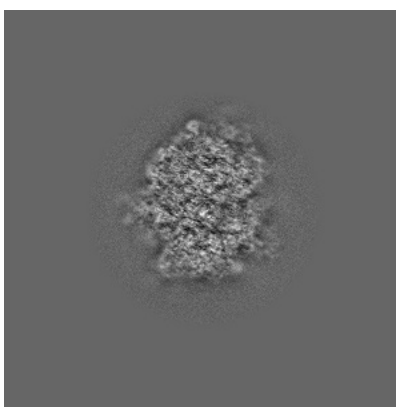


Z

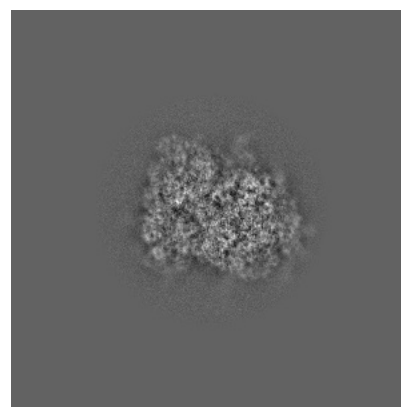
6.1.2 Raw map



X



Y

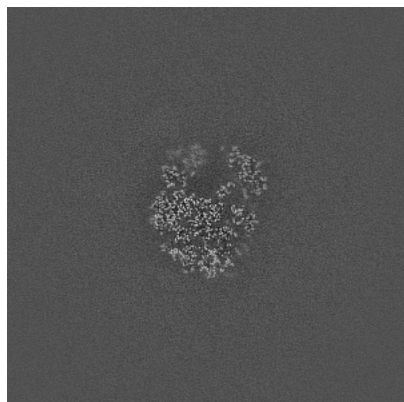


Z

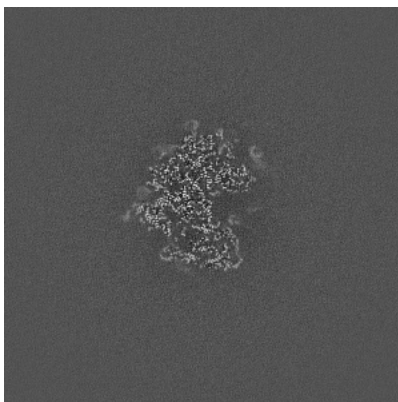
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

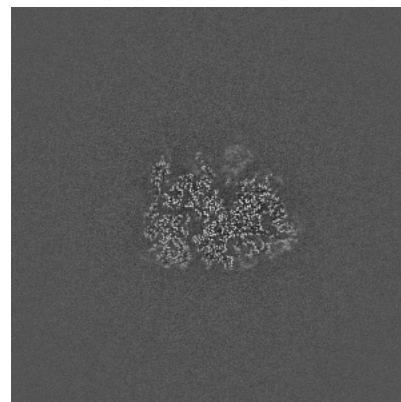
6.2.1 Primary map



X Index: 324

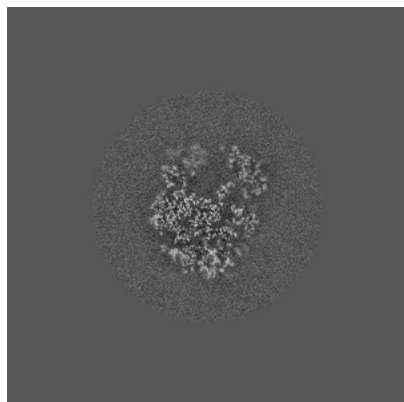


Y Index: 324

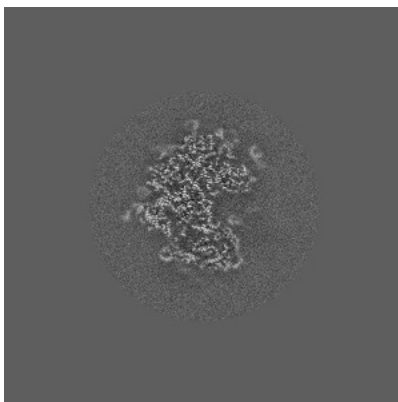


Z Index: 324

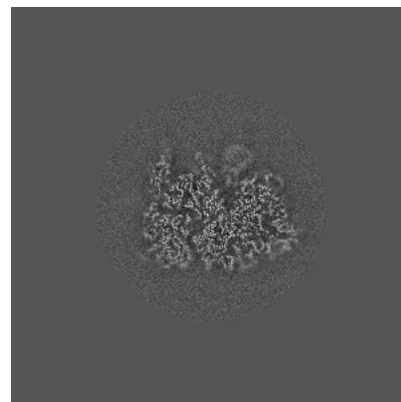
6.2.2 Raw map



X Index: 324



Y Index: 324

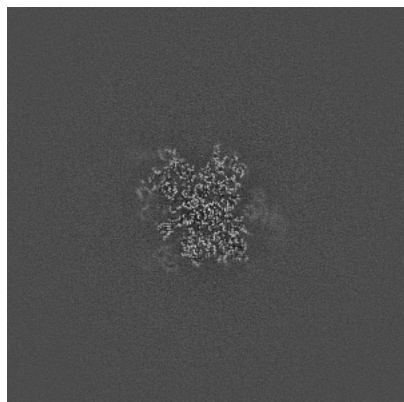


Z Index: 324

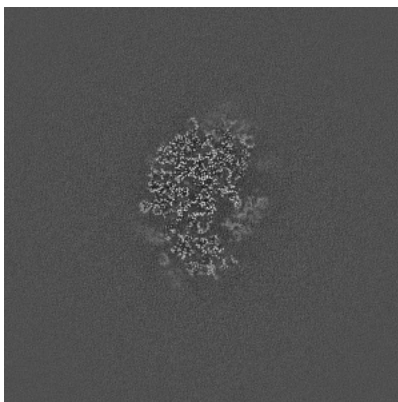
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

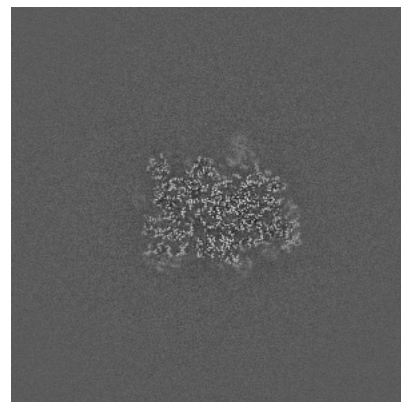
6.3.1 Primary map



X Index: 378

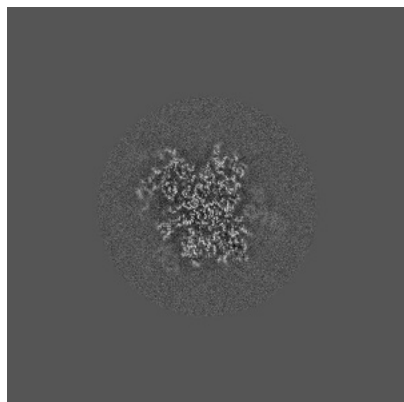


Y Index: 299

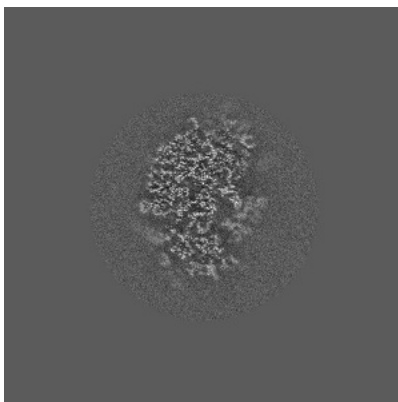


Z Index: 312

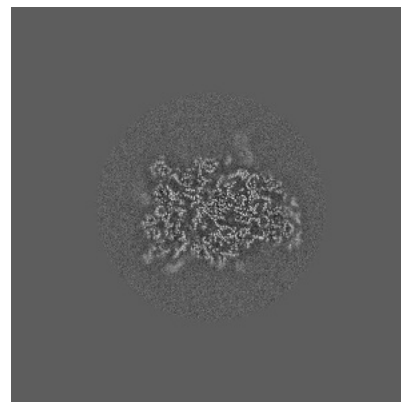
6.3.2 Raw map



X Index: 378



Y Index: 299

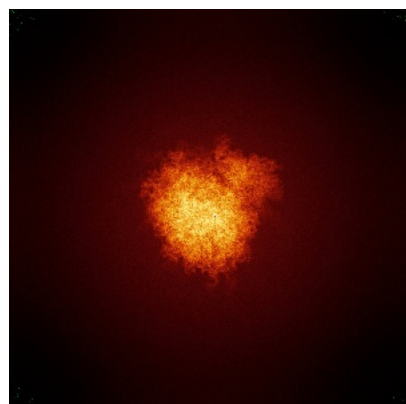


Z Index: 305

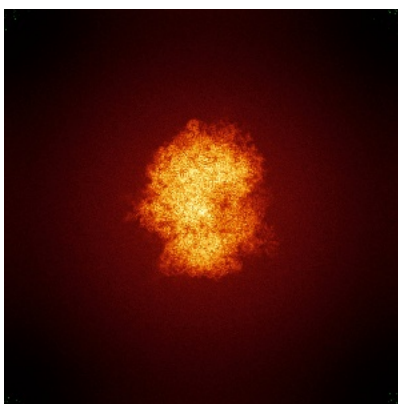
The images above show the largest variance slices of the map in three orthogonal directions.

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

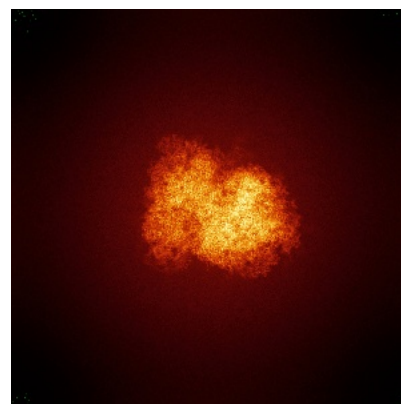
6.4.1 Primary map



X

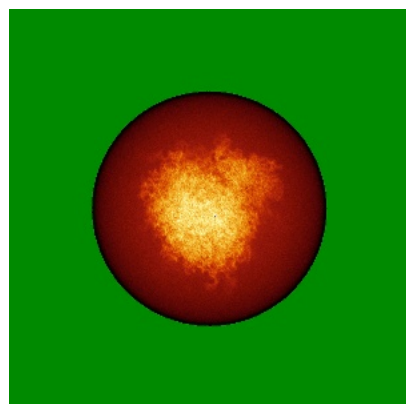


Y

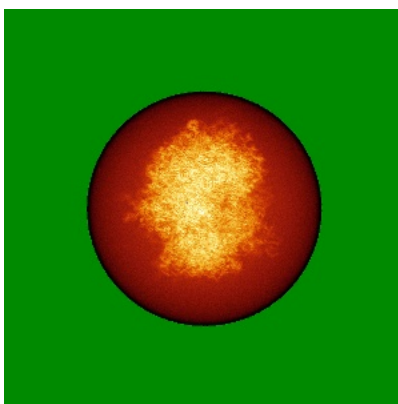


Z

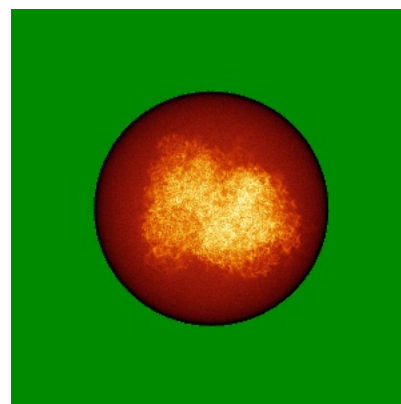
6.4.2 Raw map



X



Y



Z

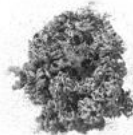
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



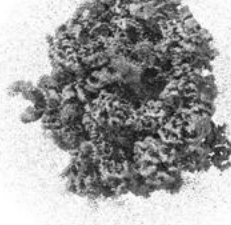
Z

The images above show the 3D surface view of the map at the recommended contour level 4.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

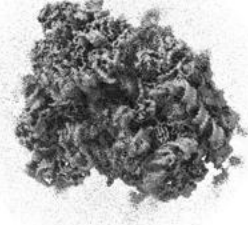
6.5.2 Raw map



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.

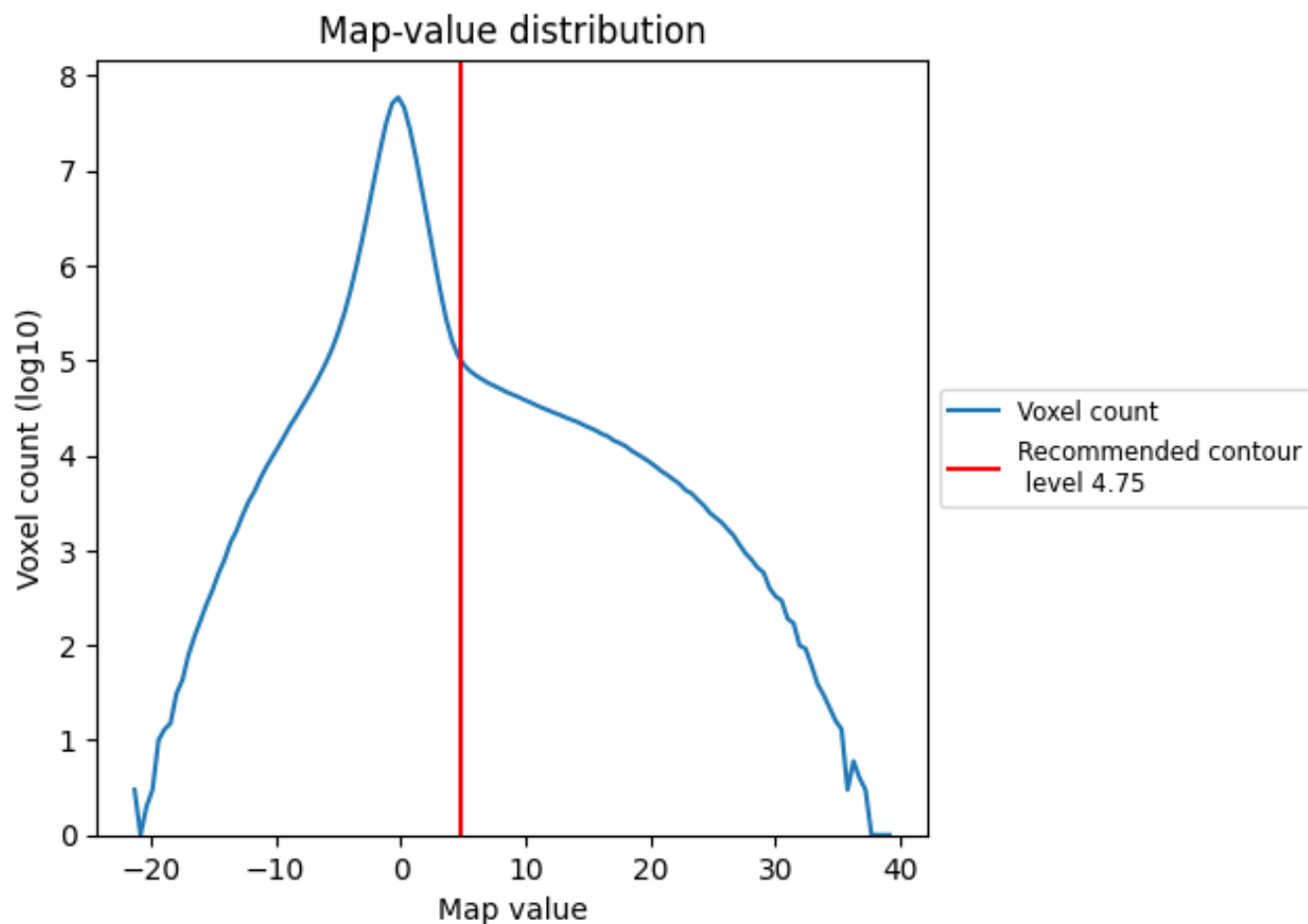
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

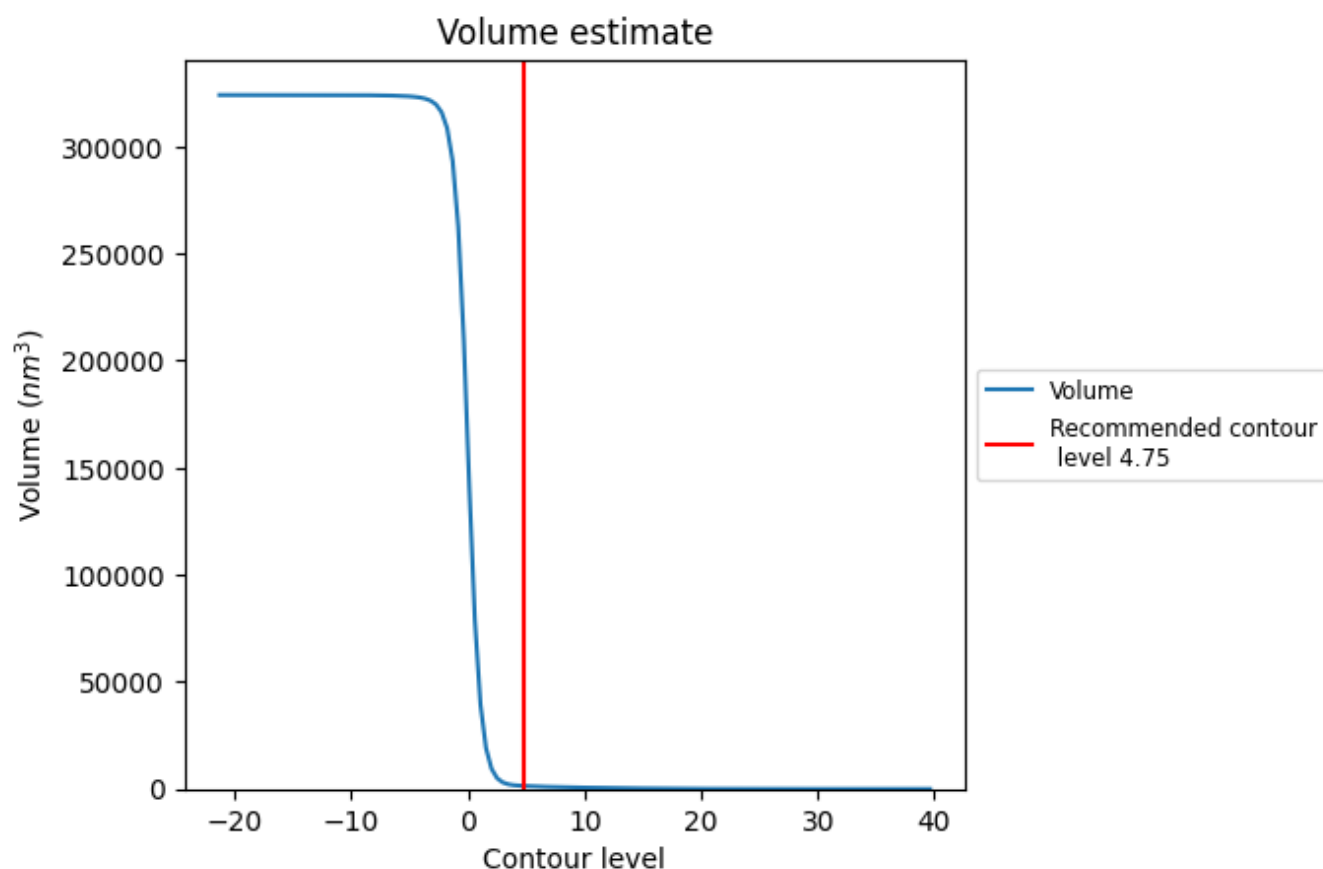
This section contains the results of statistical analysis of the map.

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.

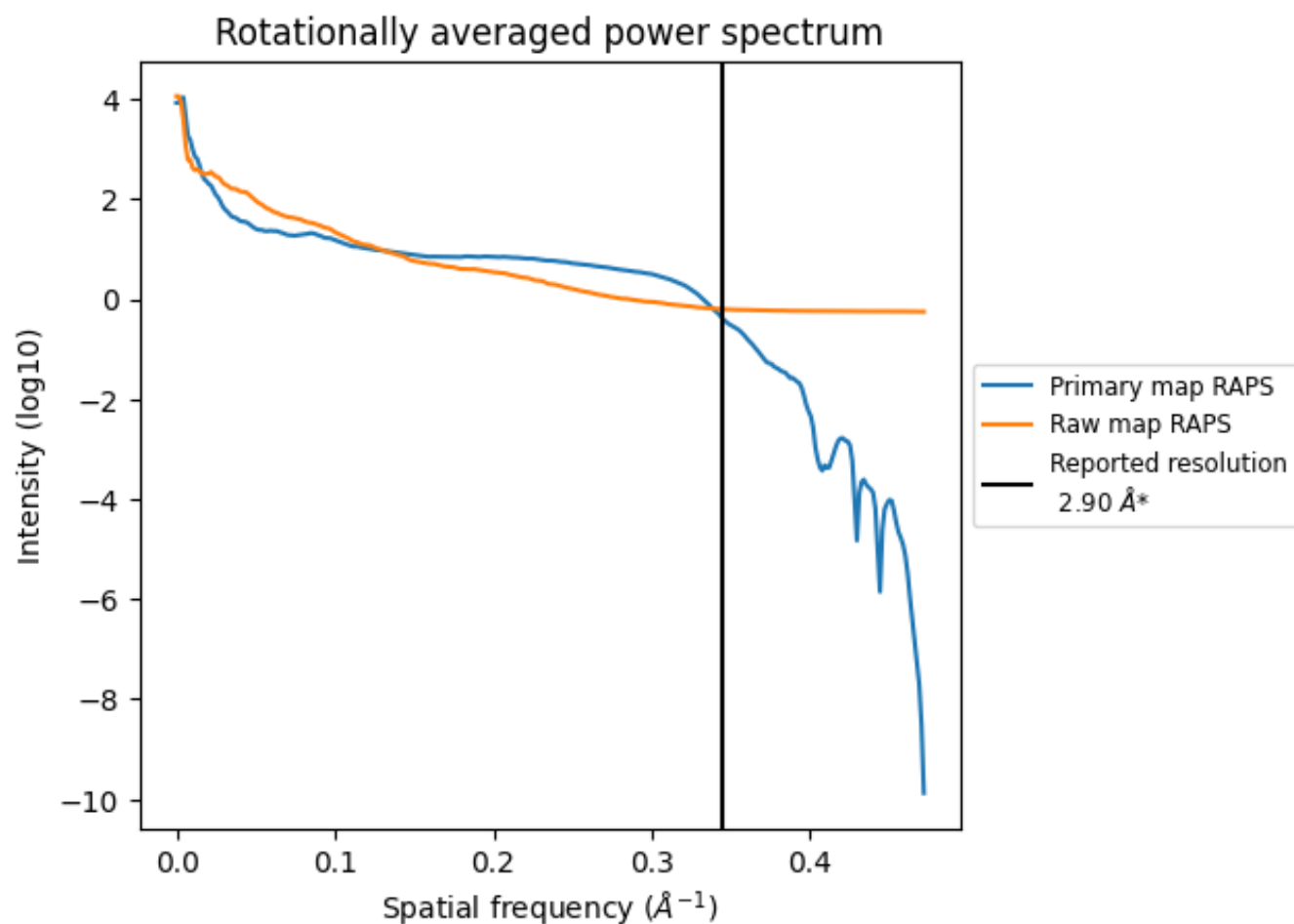
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1431 nm^3 ; this corresponds to an approximate mass of 1293 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 ⓘ

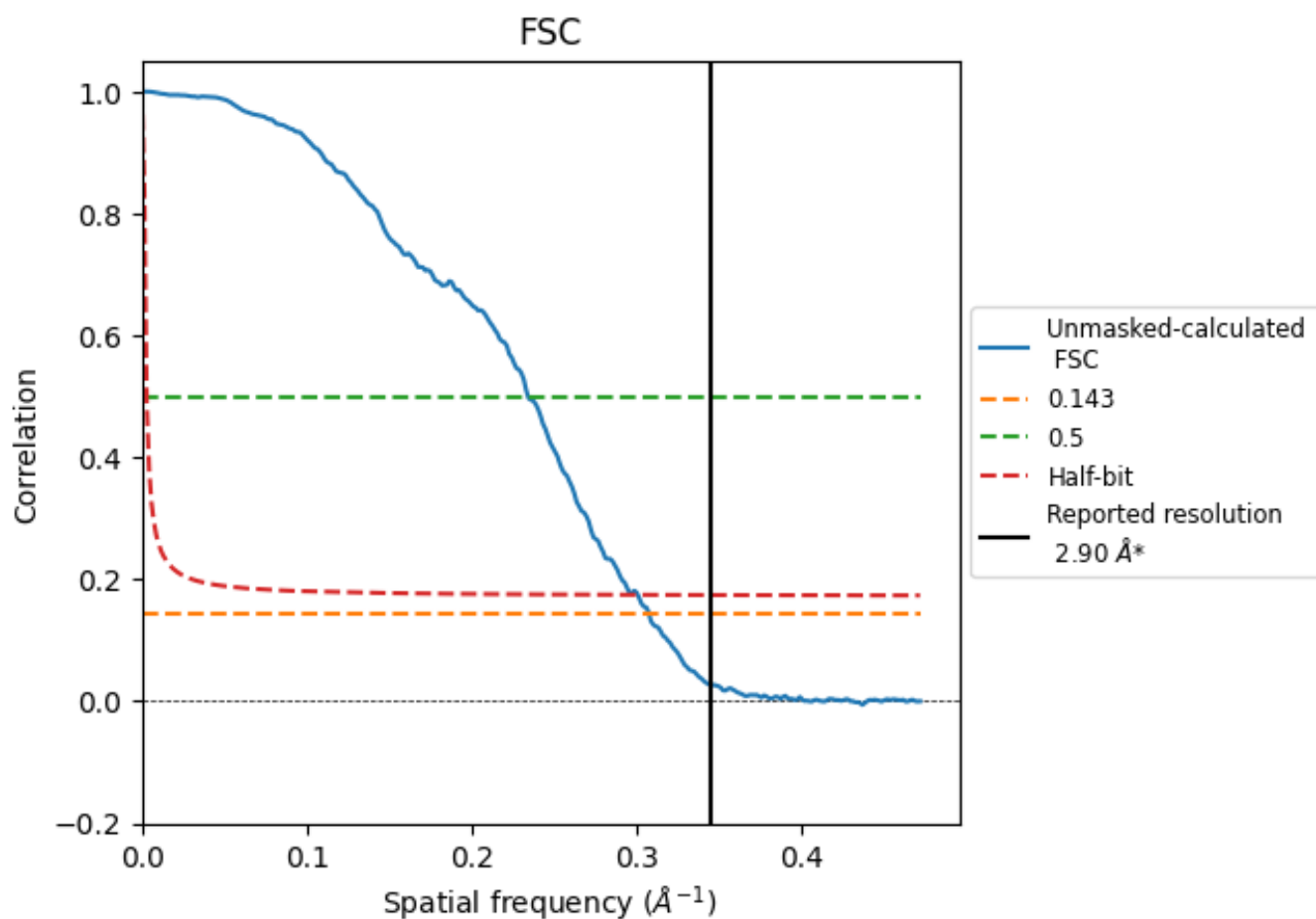


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

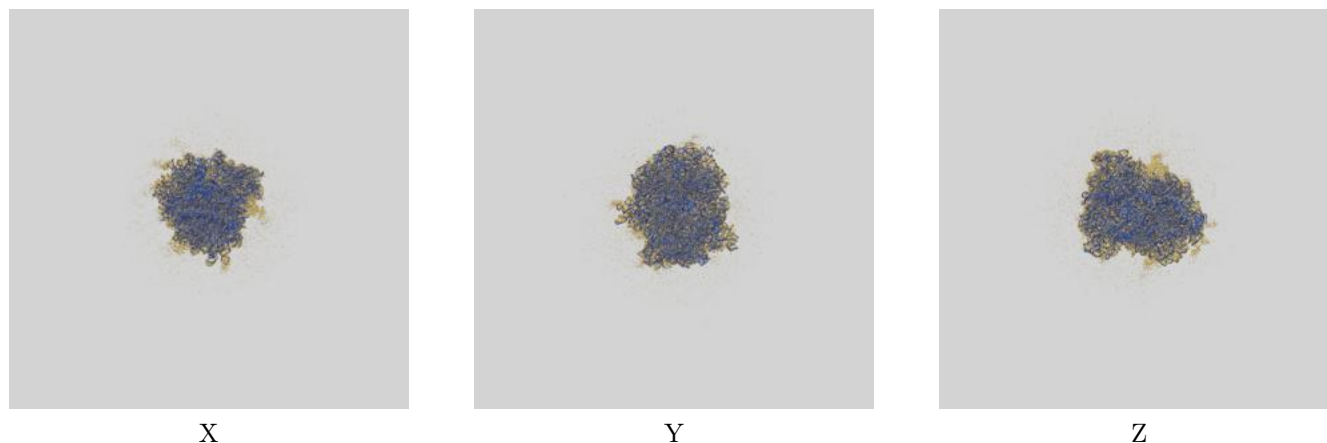
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.25	4.27	3.33

*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 3.25 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

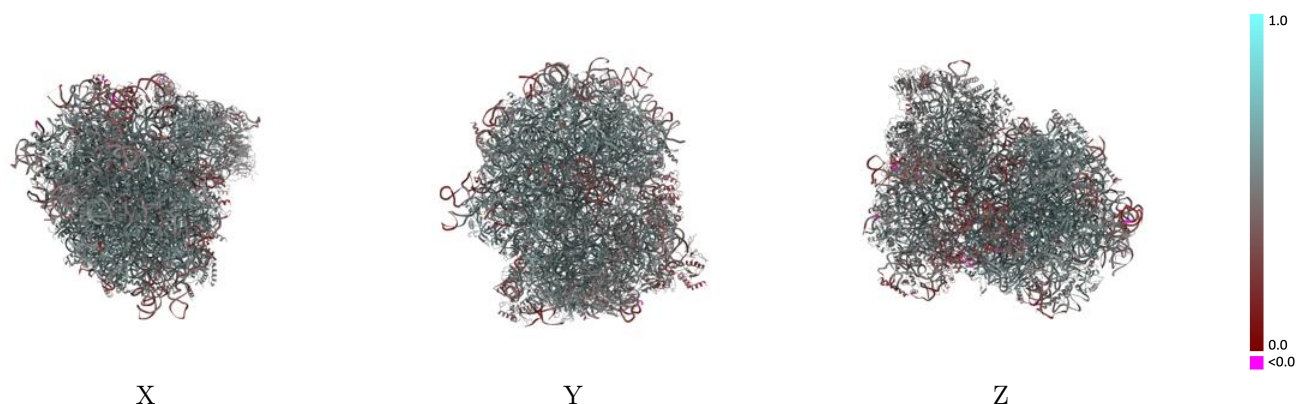
This section contains information regarding the fit between EMDB map EMD-43564 and PDB model 8VVP. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



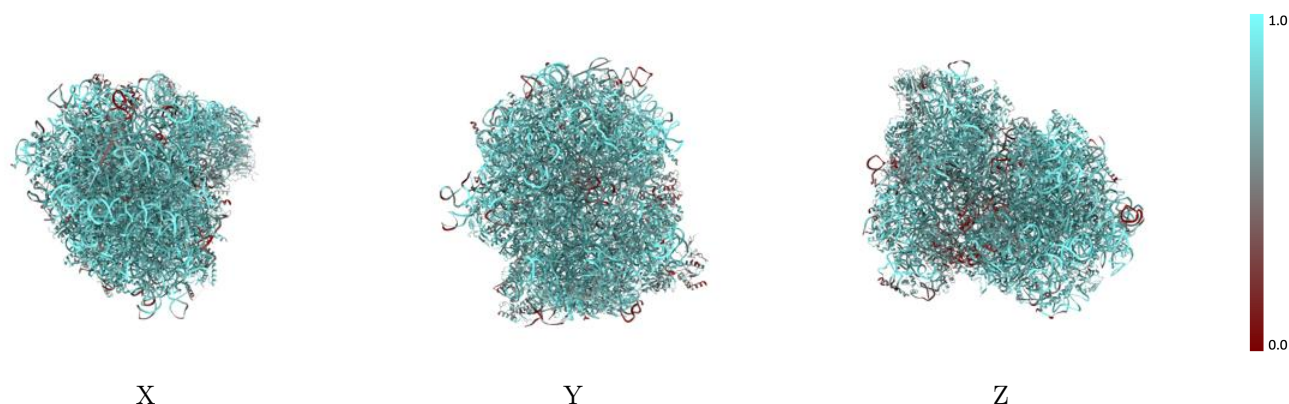
The images above show the 3D surface view of the map at the recommended contour level 4.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



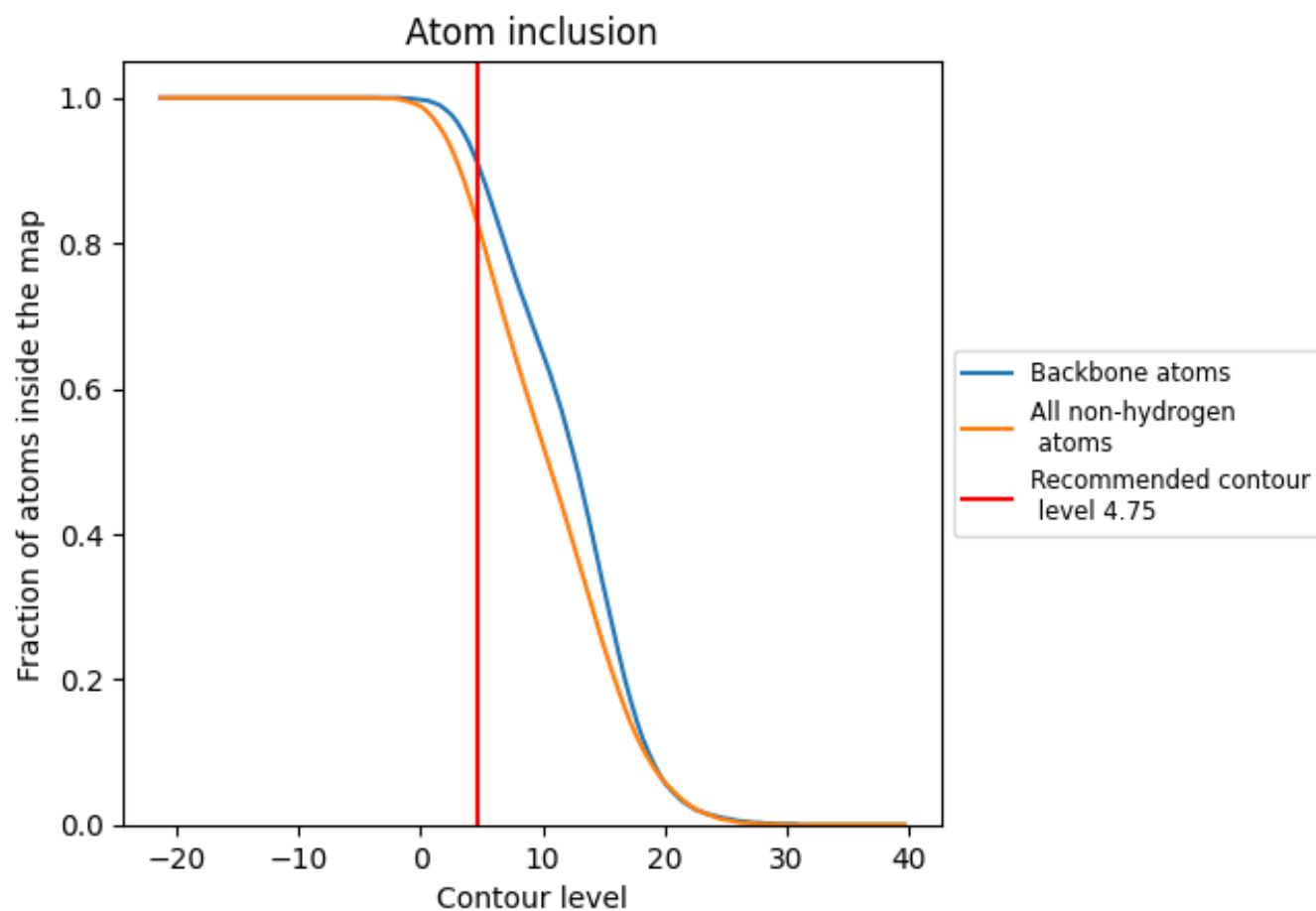
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (4.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8230	 0.5110
A	 0.8460	 0.5740
AA	 0.7100	 0.4950
AB	 0.7810	 0.5150
AC	 0.7830	 0.5340
B	 0.8420	 0.5580
BA	 0.8100	 0.5410
BB	 0.7760	 0.5300
BC	 0.7420	 0.5140
C	 0.8220	 0.5550
CA	 0.8190	 0.5460
CB	 0.7930	 0.5350
CC	 0.7090	 0.5030
D	 0.8300	 0.5230
DA	 0.8300	 0.5640
DB	 0.6960	 0.4790
DC	 0.8010	 0.5130
E	 0.7830	 0.5140
EA	 0.8350	 0.5720
EB	 0.7780	 0.5250
EC	 0.6780	 0.4940
F	 0.8130	 0.5530
FA	 0.8220	 0.5530
FB	 0.7390	 0.4970
FC	 0.5070	 0.3750
G	 0.7750	 0.5110
GA	 0.7980	 0.5320
GB	 0.7050	 0.4660
GC	 0.6630	 0.4380
H	 0.7940	 0.5370
HA	 0.8080	 0.5300
HB	 0.6900	 0.4690
HC	 0.5190	 0.3900
I	 0.8360	 0.5530
IA	 0.8540	 0.5600



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Chain	Atom inclusion	Q-score
IB	 0.7810	 0.5240
IC	 0.6500	 0.5330
J	 0.7810	 0.5090
JA	 0.7400	 0.5010
JB	 0.7860	 0.5110
K	 0.8040	 0.5330
KA	 0.8150	 0.5380
KB	 0.7140	 0.4630
L	 0.8070	 0.5250
LA	 0.8370	 0.5480
LB	 0.8210	 0.5560
M	 0.8650	 0.5790
MA	 0.8300	 0.5630
MB	 0.4290	 0.2840
N	 0.8310	 0.5520
NA	 0.8400	 0.5690
NB	 0.8210	 0.5400
O	 0.8160	 0.5570
OA	 0.8190	 0.5650
OB	 0.7690	 0.5270
P	 0.8260	 0.5640
PA	 0.8300	 0.5460
PB	 0.6900	 0.4680
Q	 0.7920	 0.5230
QB	 0.7480	 0.4970
R	 0.8460	 0.5550
RA	 0.2220	 0.2720
RB	 0.7180	 0.4810
S	 0.8140	 0.5540
SA	 0.8290	 0.4830
SB	 0.7470	 0.4860
T	 0.7490	 0.4830
TA	 0.4550	 0.3210
TB	 0.7540	 0.4830
U	 0.7870	 0.5630
UA	 0.5900	 0.3390
UB	 0.6760	 0.4680
V	 0.7240	 0.4830
VA	 0.7310	 0.4440
VB	 0.7930	 0.5150
W	 0.7980	 0.5350
WA	 0.8880	 0.5200

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Chain	Atom inclusion	Q-score
WB	 0.8060	 0.5420
X	 0.8140	 0.5420
XA	 0.9520	 0.5520
XB	 0.8010	 0.5540
Y	 0.8270	 0.5360
YA	 0.8750	 0.5180
YB	 0.7590	 0.4980
Z	 0.8500	 0.5670
ZA	 0.8670	 0.5020
ZB	 0.6660	 0.4680
b	 0.3190	 0.2560
c	 0.1160	 0.3840