



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:33 PM EDT

PDB ID : 8SCB / pdb_00008scb
EMDB ID : EMD-40344
Title : Terminating ribosome with SRI-41315
Authors : Yip, M.C.J.; Coelho, J.P.L.; Oltion, K.; Tauton, J.; Shao, S.
Deposited on : 2023-04-05
Resolution : 2.50 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.dev133
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) : 2.50

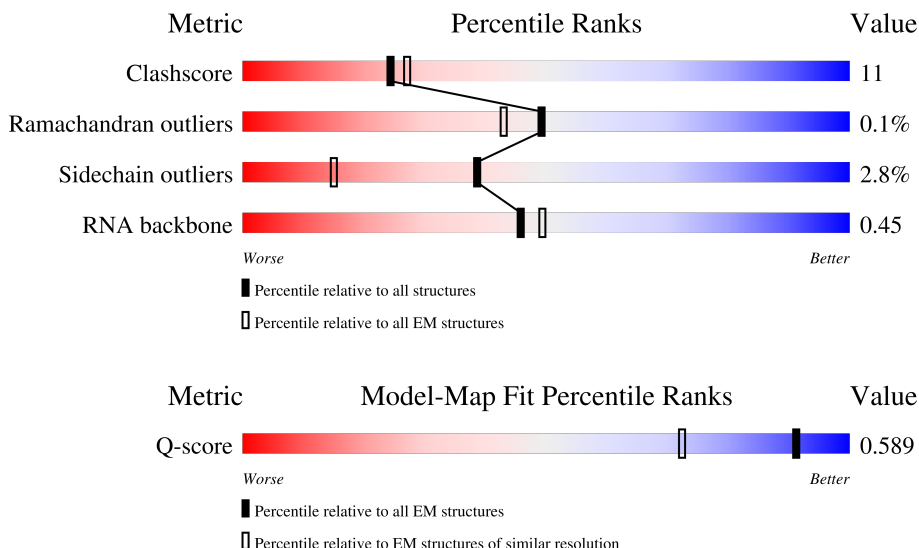
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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.



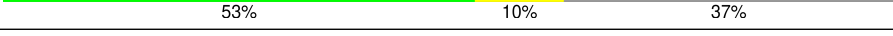
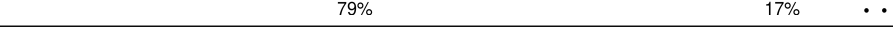
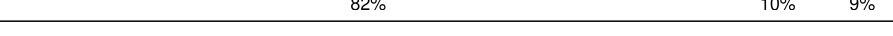
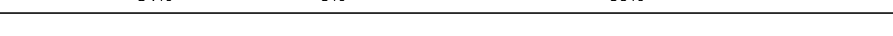
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	

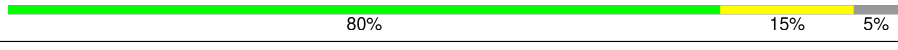
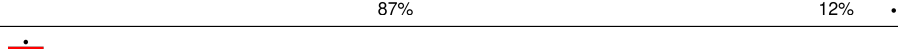
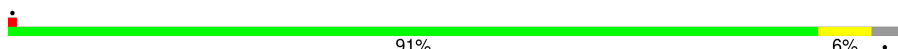
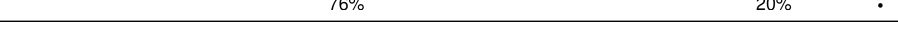
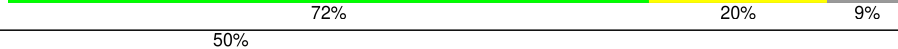
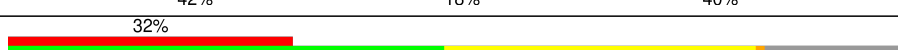
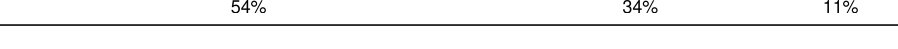
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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

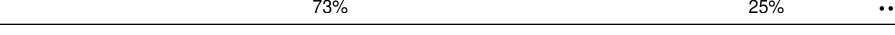
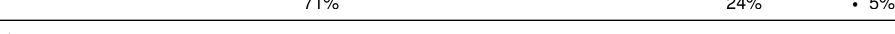
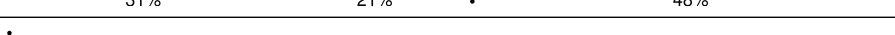
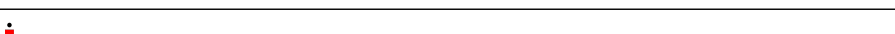
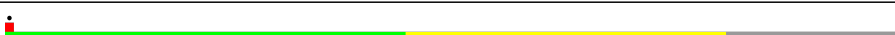
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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	93	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	130	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

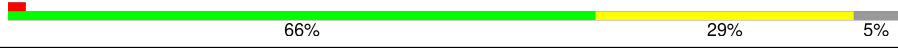
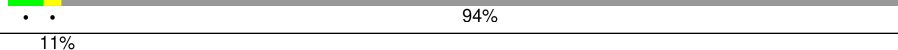
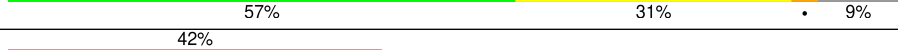
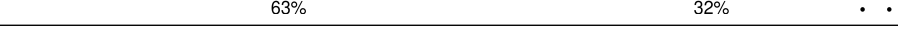
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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	197	
86	ii	459	
87	jj	599	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
90	ZVM	ii	501	X	-	-	-
91	SF4	jj	601	-	-	X	-

2 Entry composition

There are 92 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 Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

- Molecule 3 is a protein called 60S ribosomal protein L4.

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 Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	289	Total	C	N	O	S	0	0
			2361	1495	431	421	14		

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1726	1110	327	286	3		

- Molecule 6 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 7 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1768	1127	341	296	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called 60S ribosomal protein 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 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 10 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1336	846	249	235	6		

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called 60S ribosomal protein L14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	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	O	198	Total	C	N	O	S	0	0
			1621	1046	317	253	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 16 is a protein called Ribosomal protein L18.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	4	ASP	ASN	conflict	UNP G1TFE0
Q	14	ARG	TRP	conflict	UNP G1TFE0
Q	53	MET	LEU	conflict	UNP G1TFE0
Q	58	ARG	TRP	conflict	UNP G1TFE0
Q	75	ARG	GLN	conflict	UNP G1TFE0
Q	80	ALA	PRO	conflict	UNP G1TFE0
Q	86	VAL	ILE	conflict	UNP G1TFE0
Q	104	ARG	HIS	conflict	UNP G1TFE0
Q	110	ARG	CYS	conflict	UNP G1TFE0
Q	137	VAL	GLY	conflict	UNP G1TFE0
Q	157	GLY	ARG	conflict	UNP G1TFE0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 17 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	179	Total	C	N	O	S	0	0
			1502	930	327	236	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	CYS	conflict	UNP G1TJR3
R	64	ARG	GLN	conflict	UNP G1TJR3
R	94	THR	LYS	conflict	UNP G1TJR3

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	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	T	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	U	98	Total	C	N	O	S	0	0
			800	514	139	145	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	LEU	VAL	conflict	UNP G1TSG1
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	60	VAL	ALA	conflict	UNP G1TSG1
U	62	SER	THR	conflict	UNP G1TSG1
U	63	LEU	ILE	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1
U	106	THR	SER	conflict	UNP G1TSG1
U	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 21 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 22 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called eL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	116	Total	C	N	O	S	0	0
			949	606	178	164	1		

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called 60S ribosomal protein L27.

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

- Molecule 26 is a protein called 60S ribosomal protein L27a.

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

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	464	130	132	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	100	Total	C	N	O	S	0	0
			833	530	163	138	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called 60S ribosomal protein L34.

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

- Molecule 33 is a protein called eL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

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

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 36 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	49	Total	C	N	O	S	0	0
			438	280	95	62	1		

- Molecule 38 is a protein called Ubiquitin A-52 residue ribosomal protein fusion product 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	51	Total	C	N	O	S	0	0
			421	260	89	66	6		

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	190	Total	C	N	O	S	0	0
			1461	931	255	266	9		

- Molecule 44 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	141	Total	C	N	O	S	0	0
			1059	662	195	199	3		

- Molecule 45 is a protein called NC.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

- Molecule 46 is a RNA chain called P_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3530	Total	C	N	O	P	0	0
			75735	33780	13869	24556	3530		

- Molecule 49 is a RNA chain called 5S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

- Molecule 50 is a RNA chain called 5.8S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 51 is a RNA chain called 18S_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1692	Total	C	N	O	P	0	0
			36134	16163	6486	11794	1691		

- Molecule 52 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

- Molecule 53 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	216	Total	C	N	O	S	0	0
			1674	1085	286	294	9		

- Molecule 55 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	221	Total	C	N	O	S	0	0
			1723	1098	311	307	7		

- Molecule 56 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	259	Total	C	N	O	S	0	0
			2059	1316	383	352	8		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	181	Total	C	N	O	S	0	0
			1441	902	273	259	7		

- Molecule 58 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	GG	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	HH	177	Total	C	N	O	S	0	0
			1425	912	258	254	1		

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	II	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
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called S10_pectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	86	Total	C	N	O	S	0	0
			729	479	127	118	5		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	136	Total	C	N	O	S	0	0
			1123	717	210	190	6		

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	122	Total	C	N	O	S	0	0
			939	588	166	176	9		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 66 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	OO	127	Total	C	N	O	S	0	0
			957	585	189	177	6		

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	117	Total	C	N	O	S	0	0
			968	615	181	165	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	140	Total	C	N	O	S	0	0
			1117	710	211	193	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	118	Total	C	N	O	S	0	0
			962	604	179	176	3		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	140	Total	C	N	O	S	0	0
			1162	731	234	196	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	138	Total	C	N	O	S	0	0
			1075	674	206	192	3		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UU	102	Total	C	N	O	S	0	0
			807	507	153	143	4		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	123	Total	C	N	O	S	0	0
			1006	637	197	167	5		

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ZZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 78 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	aa	98	Total	C	N	O	S	0	0
			781	486	161	129	5		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 79 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	bb	79	Total	C	N	O	S	0	0
			628	395	117	110	6		

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	cc	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	47	Total	C	N	O	S	0	0
			380	231	86	62	1		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	63	Total	C	N	O	S	0	0
			527	336	99	86	6		

- Molecule 84 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	gg	304	Total	C	N	O	S	0	0
			2371	1496	414	449	12		

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	11	Total	C	N	O	P	0	0
			236	106	44	75	11		

- Molecule 86 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	expression tag	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495
ii	183	ALA	GLY	conflict	UNP P62495
ii	184	ALA	GLY	conflict	UNP P62495

- Molecule 87 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	578	Total	C	N	O	S	0	0
			4558	2914	780	835	29		

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A	2	Total	Mg	0
			2	2	
88	I	2	Total	Mg	0
			2	2	
88	N	1	Total	Mg	0
			1	1	
88	P	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	a	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
88	e	1	Total 1	Mg 1	0
88	f	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	o	1	Total 1	Mg 1	0
88	2	2	Total 2	Mg 2	0
88	5	221	Total 221	Mg 221	0
88	7	6	Total 6	Mg 6	0
88	8	2	Total 2	Mg 2	0
88	9	64	Total 64	Mg 64	0
88	EE	1	Total 1	Mg 1	0
88	LL	1	Total 1	Mg 1	0
88	OO	1	Total 1	Mg 1	0
88	XX	1	Total 1	Mg 1	0
88	hh	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

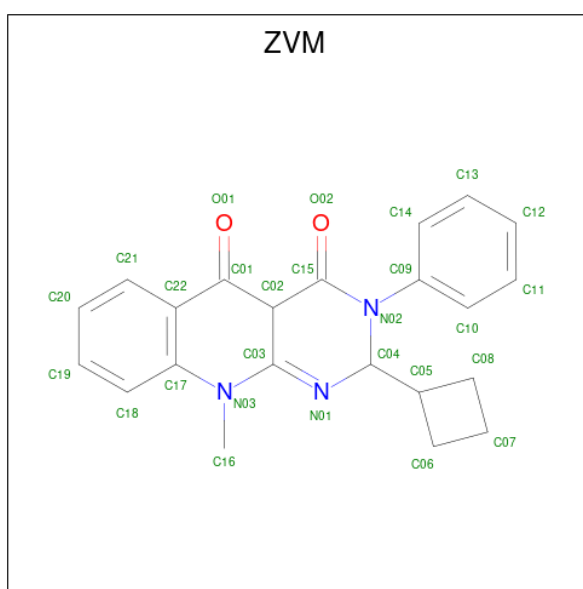
Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0

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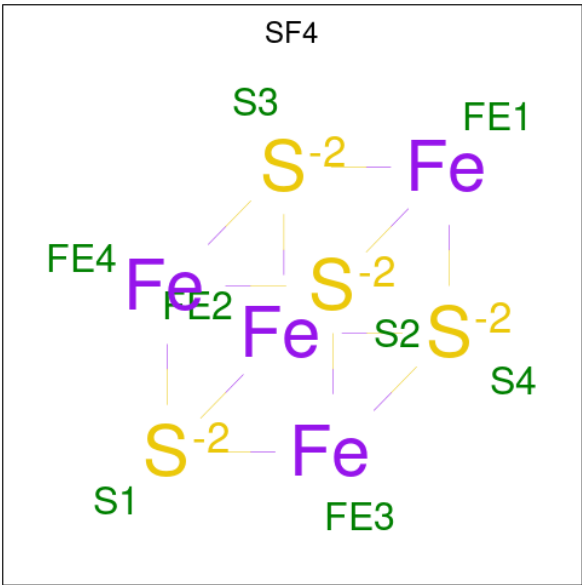
Mol	Chain	Residues	Atoms		AltConf
89	aa	1	Total	Zn	0
			1	1	
89	dd	1	Total	Zn	0
			1	1	
89	ff	1	Total	Zn	0
			1	1	

- Molecule 90 is (2S,4aS)-2-cyclobutyl-10-methyl-3-phenyl-2,10-dihydropyrimido[4,5-b]quinoline-4,5(3H,4aH)-dione (CCD ID: ZVM) (formula: C₂₂H₂₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
90	ii	1	Total	C	N	O	0
			27	22	3	2	

- Molecule 91 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
91	jj	1	Total	Fe	S	0
			8	4	4	
91	jj	1	Total	Fe	S	0
			8	4	4	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A	6	Total	O	0
			6	6	
92	B	2	Total	O	0
			2	2	
92	C	1	Total	O	0
			1	1	
92	F	1	Total	O	0
			1	1	
92	I	1	Total	O	0
			1	1	
92	L	1	Total	O	0
			1	1	
92	N	4	Total	O	0
			4	4	
92	Q	1	Total	O	0
			1	1	
92	R	1	Total	O	0
			1	1	
92	V	2	Total	O	0
			2	2	

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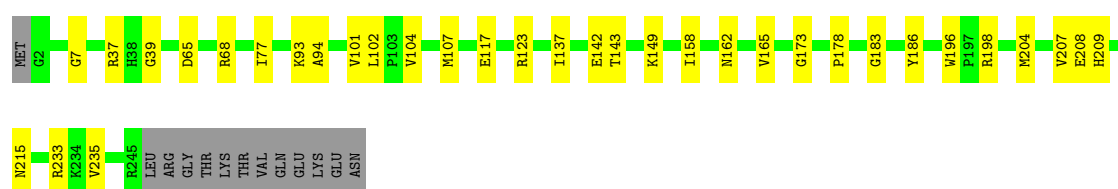
Mol	Chain	Residues	Atoms		AltConf
92	X	2	Total 2	O 2	0
92	a	5	Total 5	O 5	0
92	e	5	Total 5	O 5	0
92	j	1	Total 1	O 1	0
92	o	2	Total 2	O 2	0
92	5	723	Total 723	O 723	0
92	7	13	Total 13	O 13	0
92	8	8	Total 8	O 8	0
92	9	173	Total 173	O 173	0
92	II	1	Total 1	O 1	0
92	OO	1	Total 1	O 1	0
92	XX	1	Total 1	O 1	0
92	aa	1	Total 1	O 1	0
92	ii	2	Total 2	O 2	0

3 Residue-property plots

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

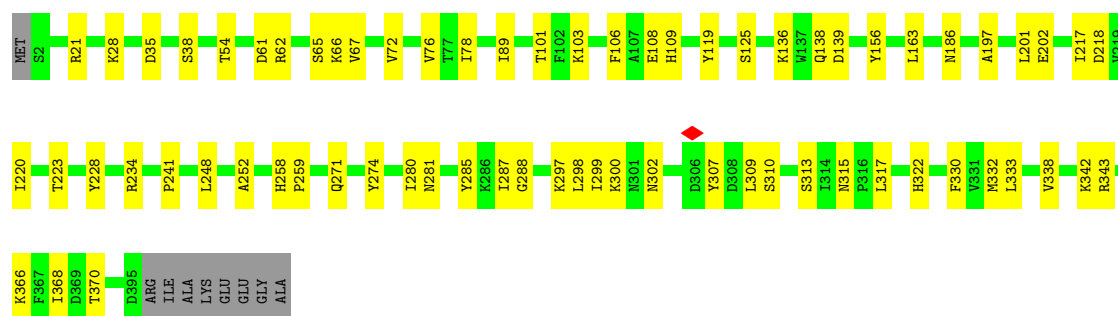
• Molecule 1: Ribosomal protein L8

Chain A: 



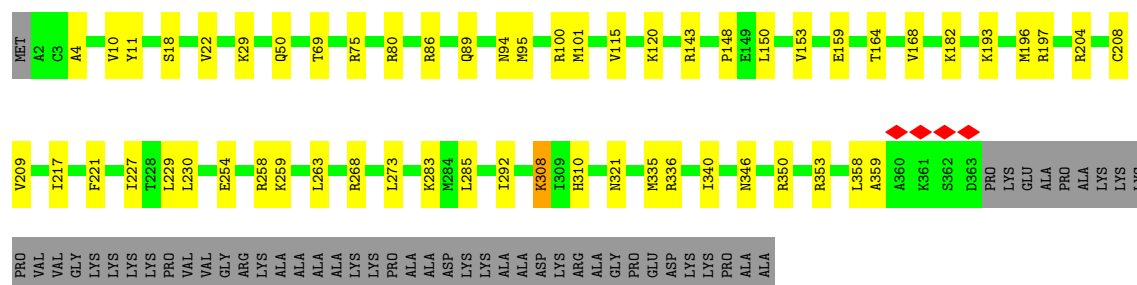
• Molecule 2: Ribosomal protein L3

Chain B: 

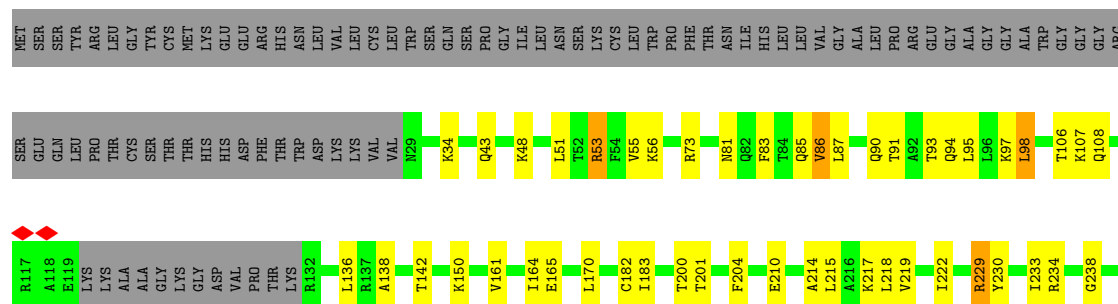
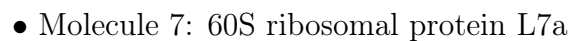
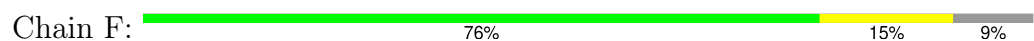
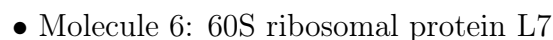
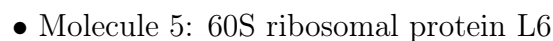


• Molecule 3: 60S ribosomal protein L4

Chain C: 



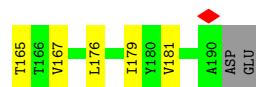
Chain D: 75% 21% ..





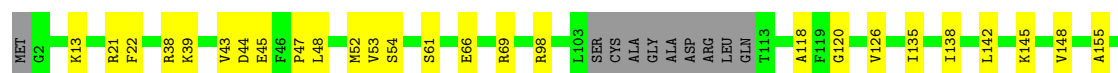
• Molecule 8: 60S ribosomal protein L9

Chain H: 80% 19%



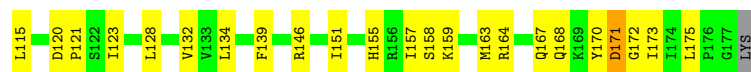
• Molecule 9: 60S ribosomal protein L10

Chain I: 79% 16% 5%



• Molecule 10: 60S ribosomal protein L11

Chain J: 67% 26% 6%



• Molecule 11: eL13

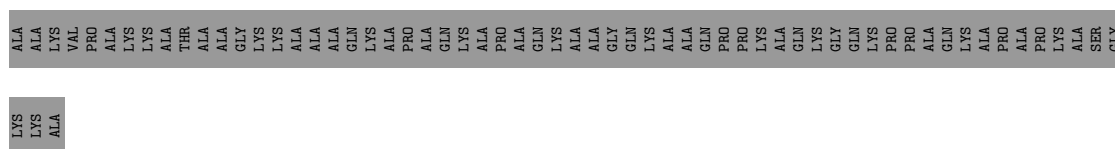
Chain L: 87% 12%



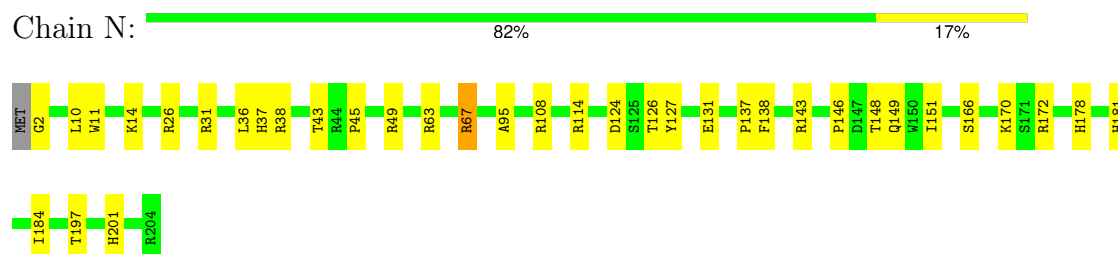
• Molecule 12: 60S ribosomal protein L14

Chain M: 53% 10% 37%

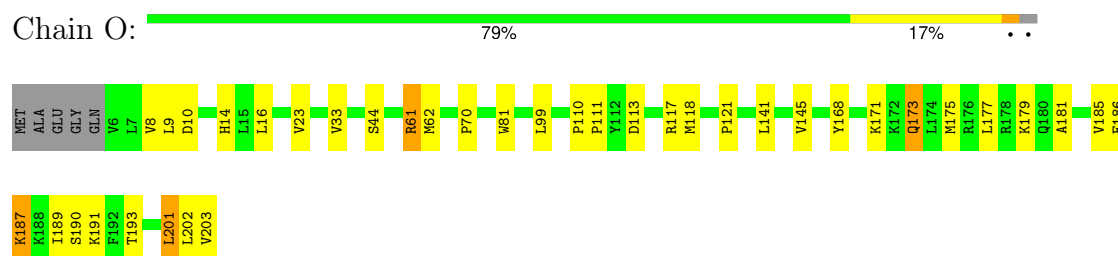




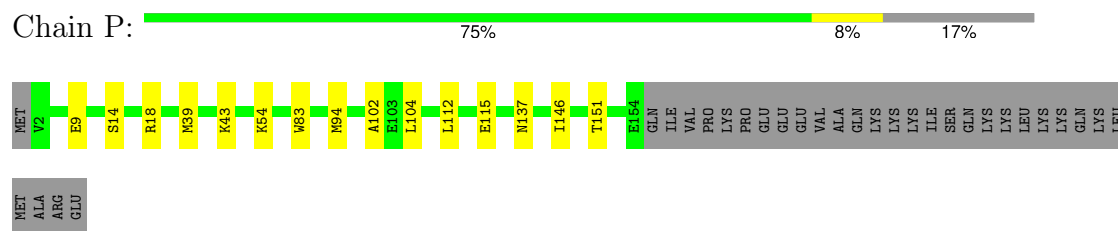
• Molecule 13: Ribosomal protein L15



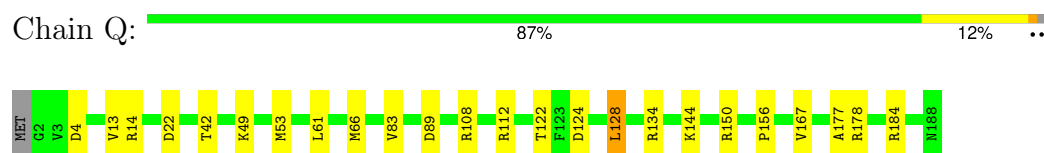
• Molecule 14: uL13



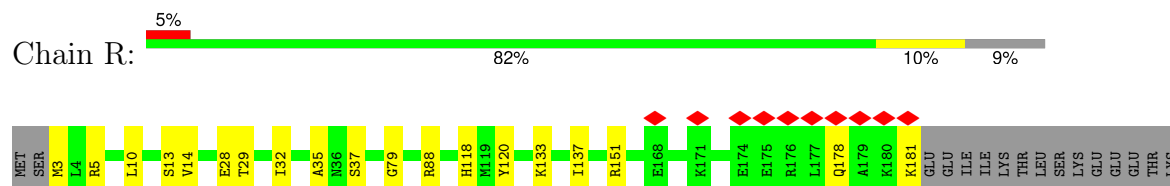
• Molecule 15: uL22



• Molecule 16: Ribosomal protein L18



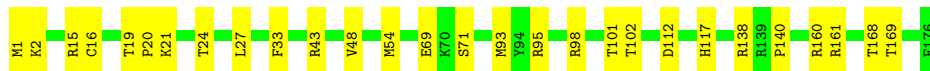
• Molecule 17: Ribosomal protein L19



LYS

- Molecule 18: eL20

Chain S: 84% 16%



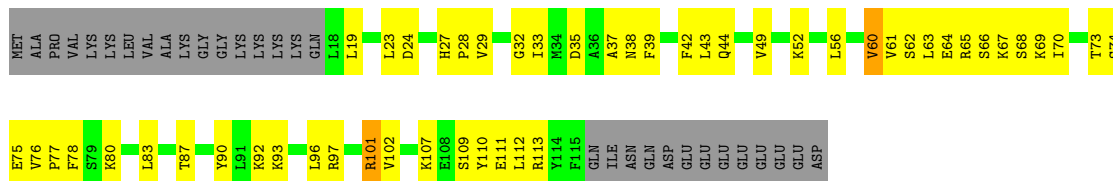
- Molecule 19: eL21

Chain T: 89% 10%



- Molecule 20: eL22

Chain U: 37% 38% 23%



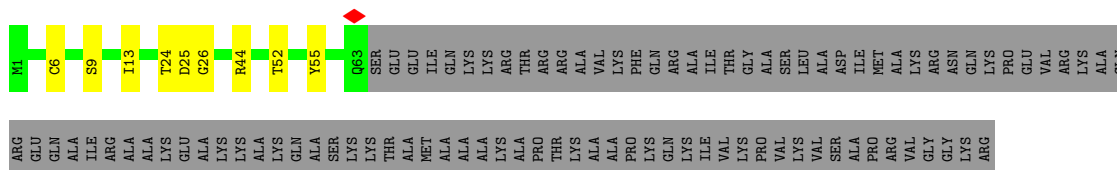
- Molecule 21: Ribosomal protein L23

Chain V: 86% 6% 7%



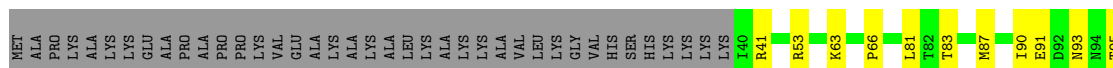
- Molecule 22: 60S ribosomal protein L24

Chain W: 34% 6% 60%



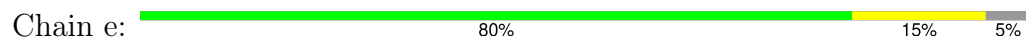
- Molecule 23: eL23

Chain X: 63% 12% 26%

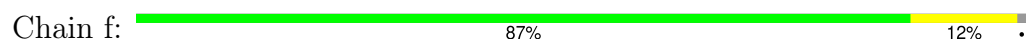




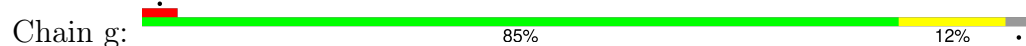
- Molecule 30: eL32



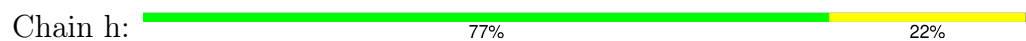
- Molecule 31: eL33



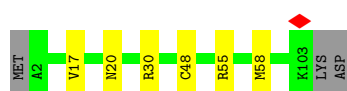
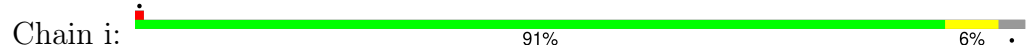
- Molecule 32: 60S ribosomal protein L34



- Molecule 33: eL35



- Molecule 34: 60S ribosomal protein L36



- Molecule 35: Ribosomal protein L37





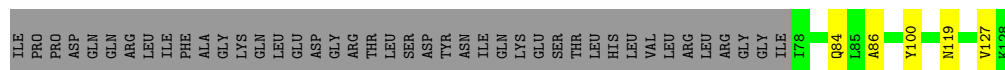
- Molecule 36: 60S ribosomal protein L38



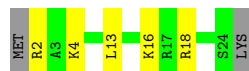
- Molecule 37: eL39



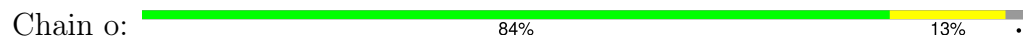
- Molecule 38: Ubiquitin A-52 residue ribosomal protein fusion product 1



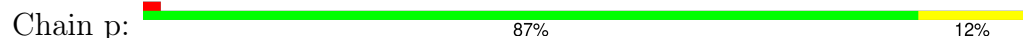
- Molecule 39: eL41



- Molecule 40: eL42

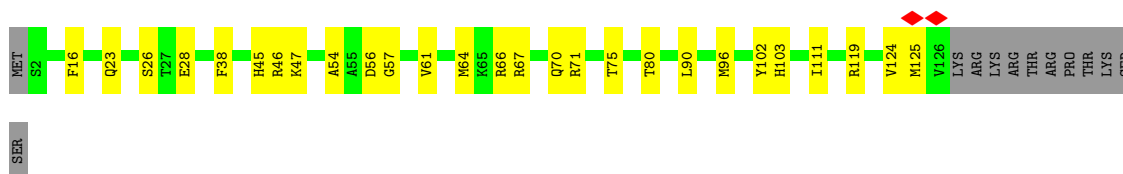


- Molecule 41: eL43

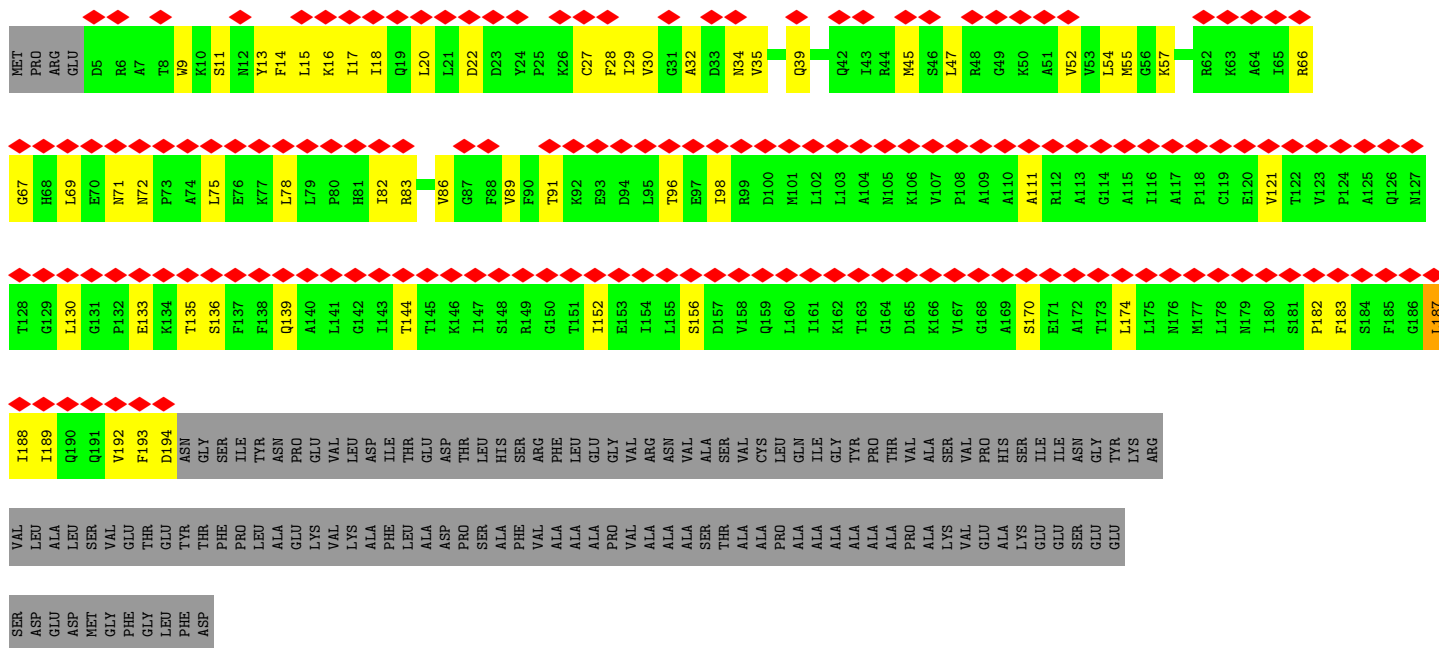


- Molecule 42: eL28

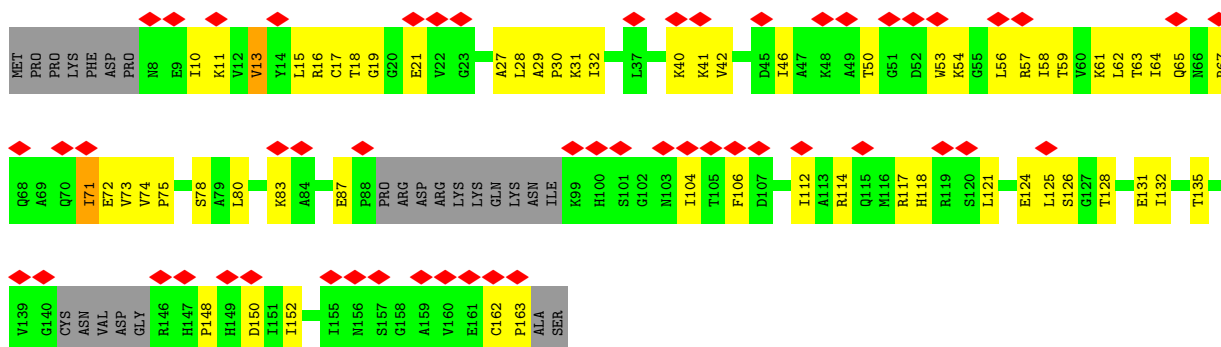




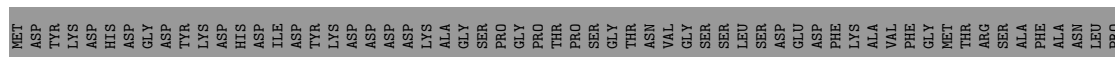
• Molecule 43: 60S acidic ribosomal protein P0

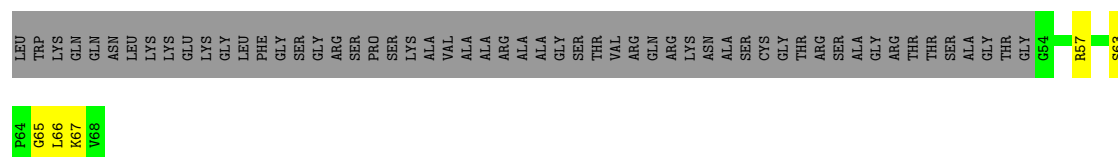


• Molecule 44: 60S ribosomal protein L12



• Molecule 45: NC





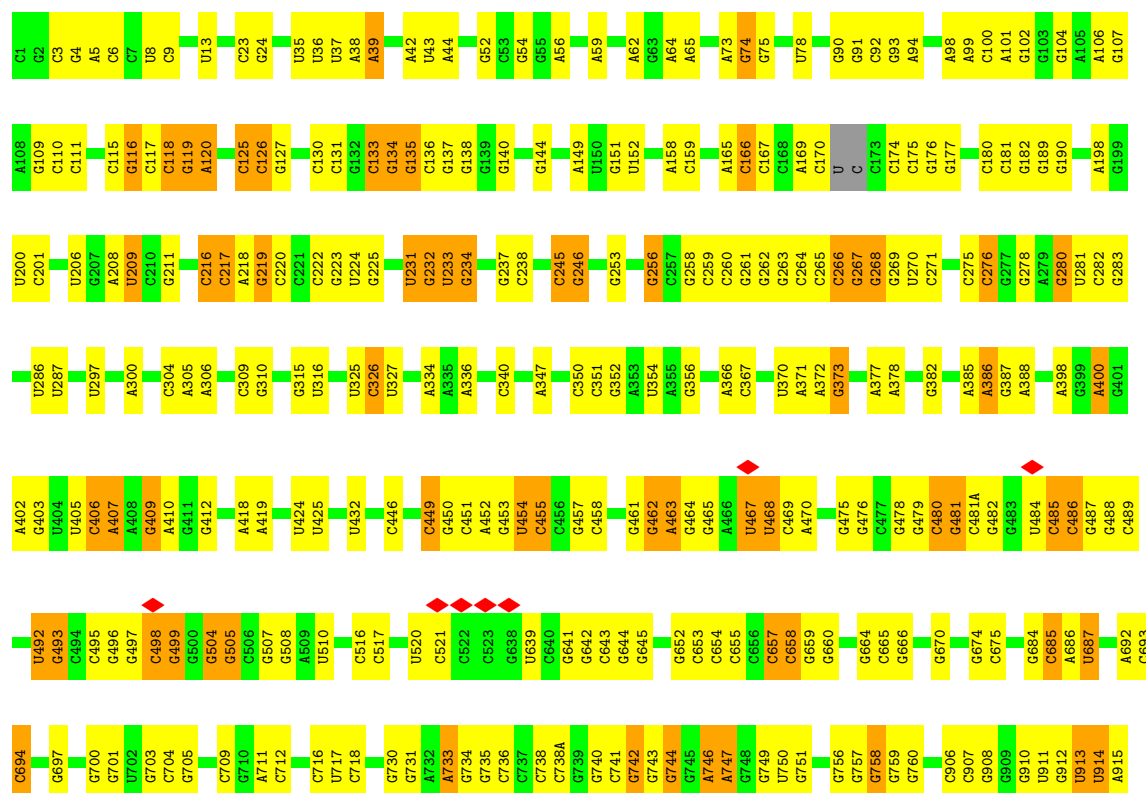
• Molecule 46: P_tRNA



• Molecule 47: E_tRNA

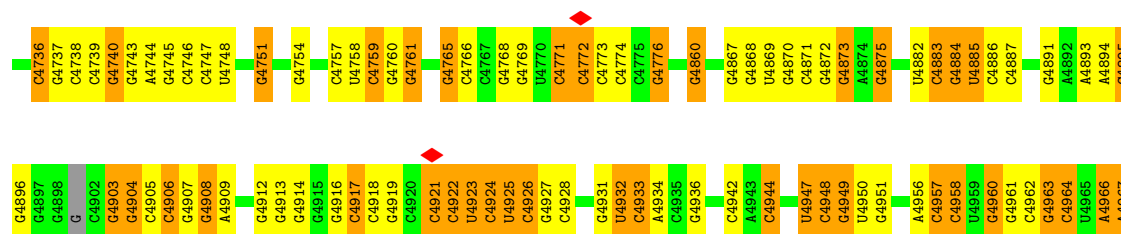


• Molecule 48: 28S_rRNA



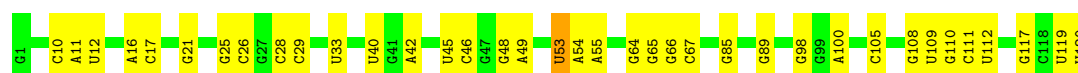
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C2447	G2328	U2084	G2000	U1930	G1836	G1760	A1635	G1523	A1433	U1339	U	G918
G2450	U2329	G2089	A2002	A1932	A1837	C1761	A1638	A1524	G1434	C1340	C	C922B
A2453	A2332	U2090	G2003	C1938	G1840	C1763	G1641	G1532	G1437	A1345	C	C924
G2457	G2333	C2091	U2004	A1939	C1841	G1764	U1641	A1533	U1440	C1346	C	G925
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C2466	U2352	C2099	G2016	G1952	A1858	U1771	A1666	A1547	U1449	G1361	G1277	G933
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G2518	G2429	A2069	C2067	A1990	G1919	U1820	A1742	G1612	C1411B	A1322	G1216	G1069
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					U3916	A3826	A3737	G3636	G2827	U2632	
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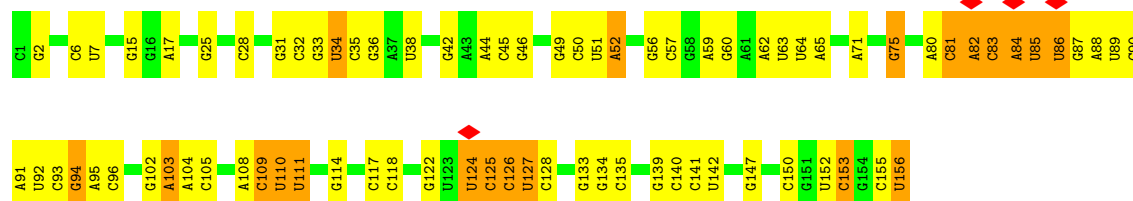
• Molecule 49: 5S_rRNA

Chain 7: 69% 30%



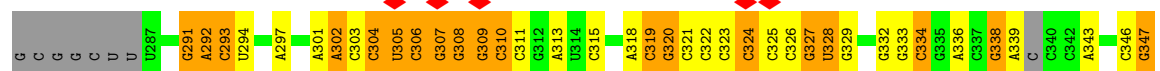
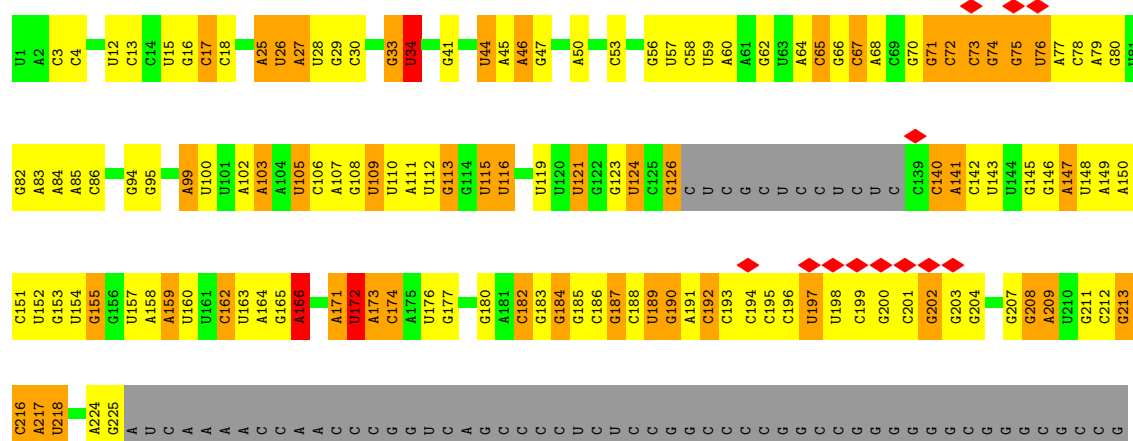
• Molecule 50: 5.8S_rRNA

Chain 8: 49% 38% 13%

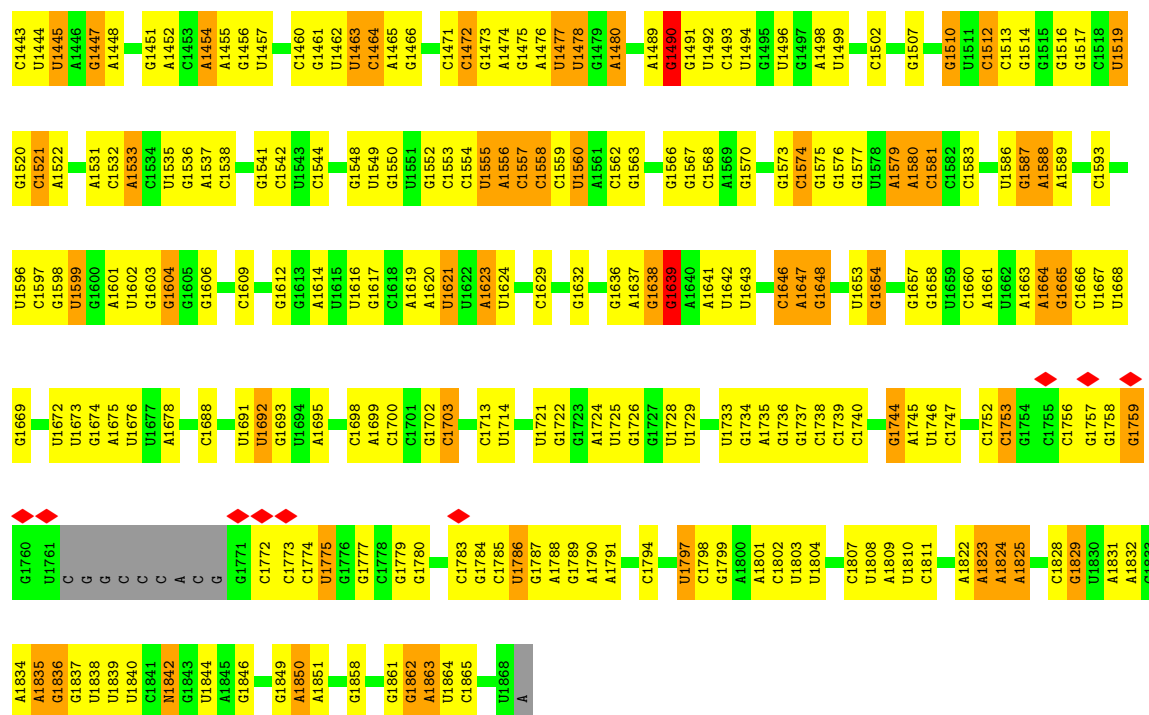


• Molecule 51: 18S_rRNA

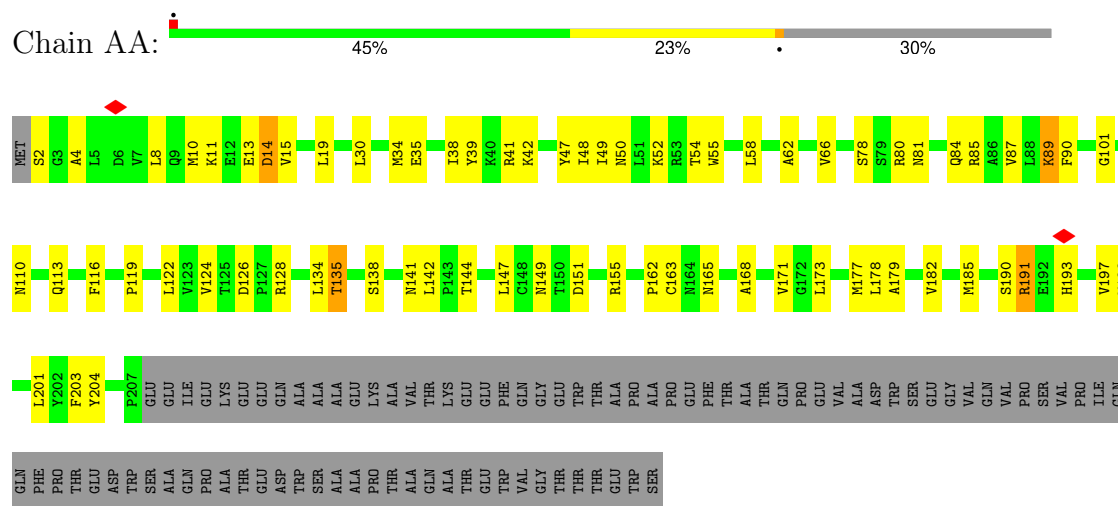
Chain 9: 39% 35% 16% 9%



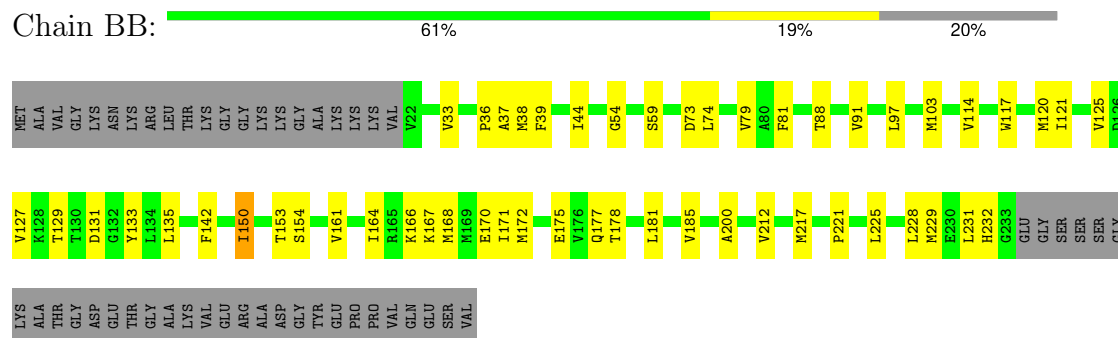




• Molecule 52: uS2 (SA)



• Molecule 53: eS1

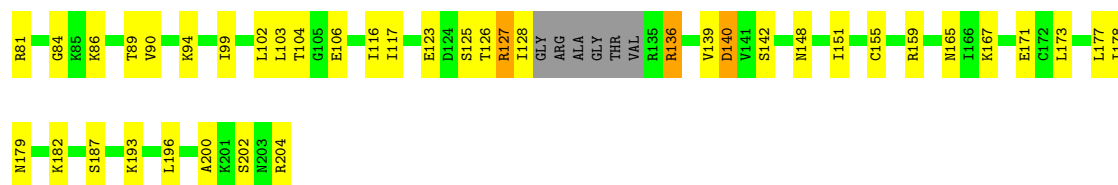


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V63	T64	V70	K71	D72	K73	K74	I75	K76	S77	L78	L83	I93	I94	L102	K108	I109	R121	K125	I130	G131	G135	V141	E146	V147	A148	R152	I162	V165	Y169	G175	K176	T184	V185	G186	I187	V191	R200	I204	P205						
MET	ALA	ASP	ALA	GLY	ALA	ALA	GLY	GLY	PRO	GLY	ASP	PRO	GLY	PRO	GLY	ILE	GLY	ARG	GLY	PHE	GLY	PHE	GLY	GLY	VAL	ARG	GLY	ARG	GLY	ARG	GLY	ARG	GLY	GLN	PRO	ALA	VAL	ALA	THR	LYS	ALA	GLU	ASP	LYS	E59

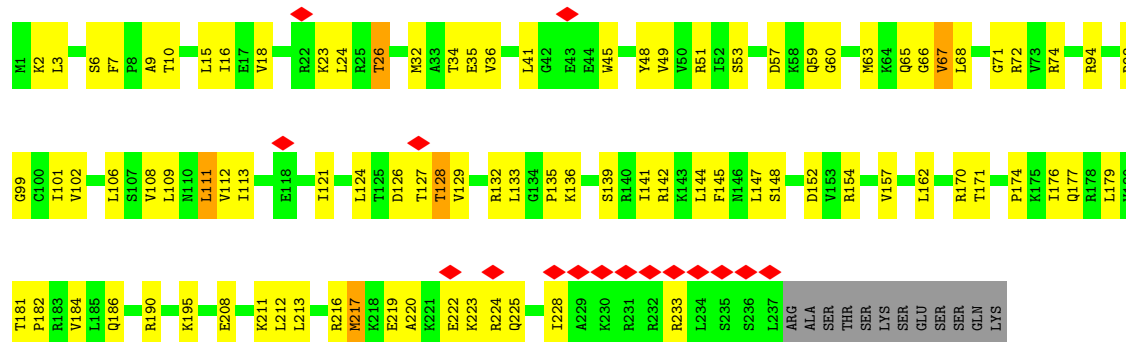
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A192	R84	VAL
D193	G95	Q4
P194	L96	I5
S195	I99	K8
G196	A100	V12
P203	Q101	I16
S209	A102	T26
I210	E103	R27
D215	S104	E28
E216	L113	D32
I217	R116	G33
L218	R117	S34
P219	A118	S35
T221	I122	G36
P222	T123	V37
I223	R124	E38
S224	F125	V41
E225	I126	THR
Q226	M127	PRO
G227	E128	THR
GLY	S129	R45
GLY	G133	I49
LYS	V138	L51
PRO	S139	I50
GLU	R143	A52
PRO	S149	T53
PRO	S149	R54
ALA	D154	E61
MET	G155	K62
PRO	L156	G63
GLN	M157	R64
PRO	I158	R65
VAL	H159	I66
PRO	S160	L69
THR	G161	T70
ALA	D162	A71
	P163	V72
	V164	V73
	Y167	Q74
	V172	F79
	R173	P90
	H174	E81
	V175	V84
	L176	E85
	L177	L86

MET	A2	K134	N232	K233	K138	H138	K134
	H8	L139		L140	L141		
M19	L20	L21	D21	K222	L23	T24	R20
L45	L46	F47	L48	L52	K53	Y54	D59
E60	V61	K62	K63	D73	Y92	T95	R100
Y103	D104	K105	K106	G107	R108	V111	H112
P116	E117	E118	K122	L123	G124	K125	F130
V131							

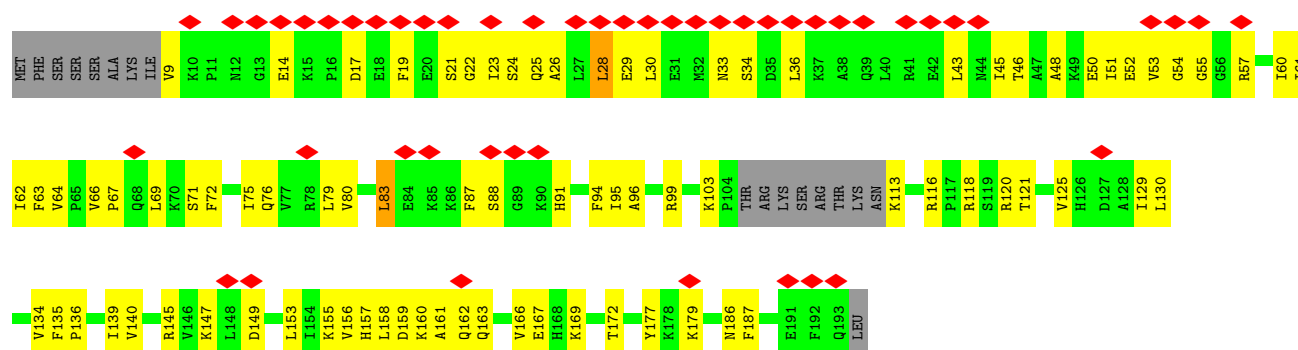
MET	THR	GLU	TRP	GLU	THR	ALA	ALA	PRO	PRO	VAL	ALA	GLU	THR	PRO	ASP	ILE	K18	L19	F20	T25	D26	D27	V28	Q29	I30	N31	I33	S34	L35	Q36	A40	V41	K42	E43	K44	Y45	A46	K47	Y48	H51	C56	P57	I68	V69	E70	R71	L72	T73	N74	S75	M78	H79	G80
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



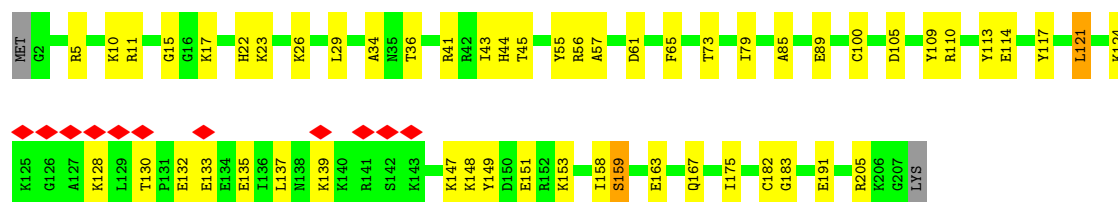
• Molecule 58: eS6



• Molecule 59: eS7

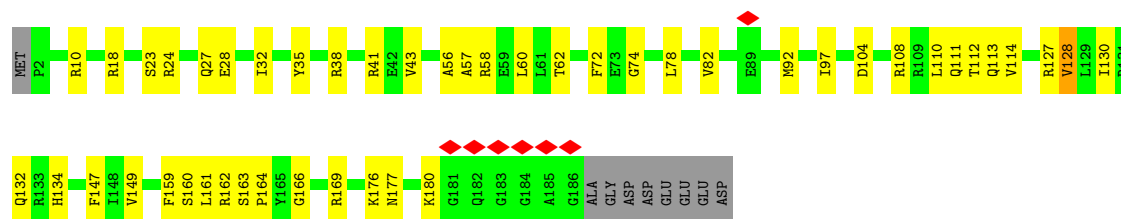


• Molecule 60: eS8

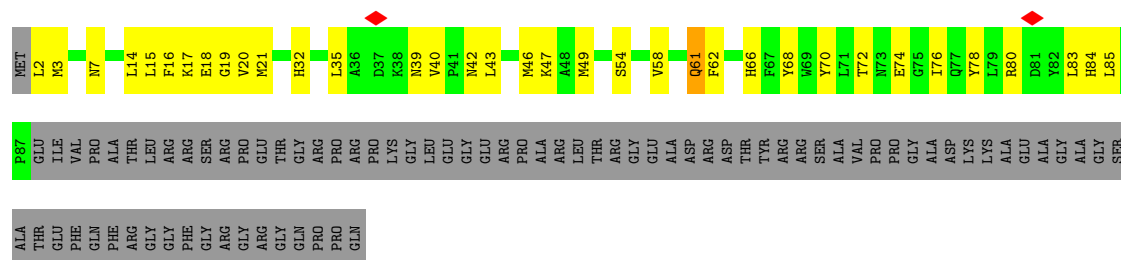
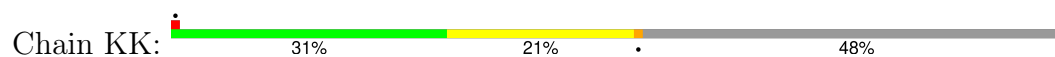


• Molecule 61: uS4





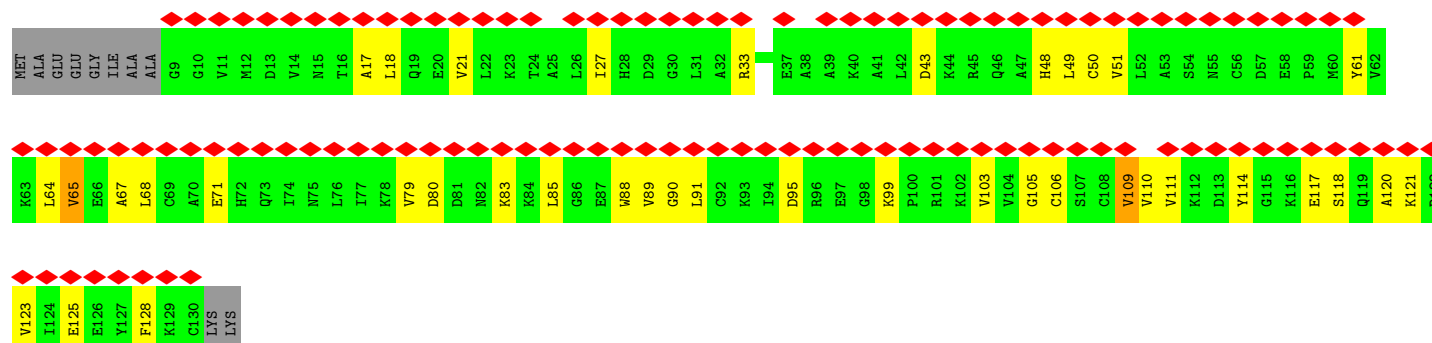
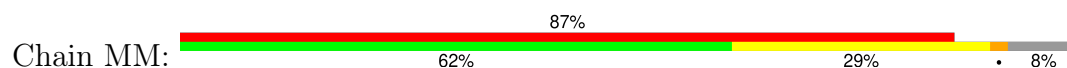
- Molecule 62: S10_pectin domain-containing protein



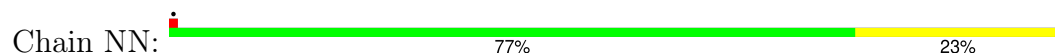
- Molecule 63: uS17

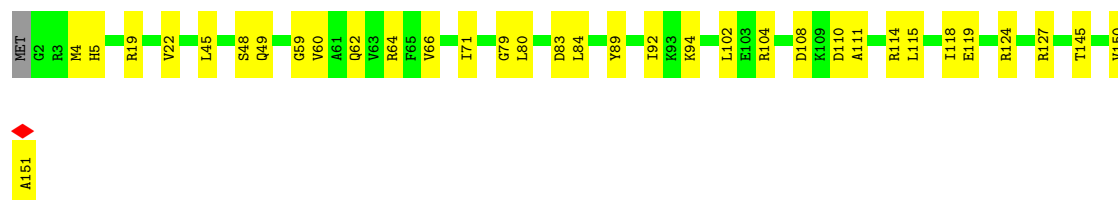


- Molecule 64: eS12



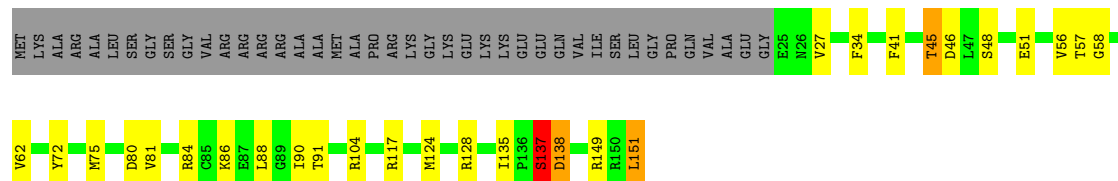
- Molecule 65: uS15





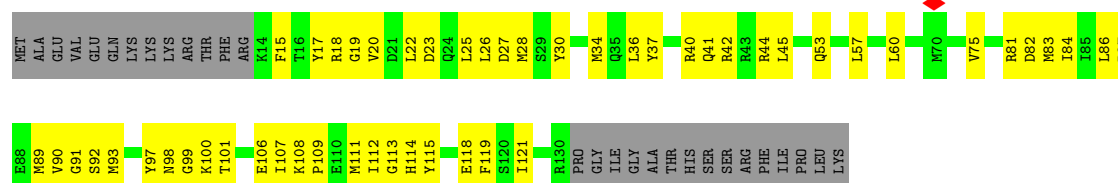
- Molecule 66: uS11

Chain OO: 58% 15% 24%



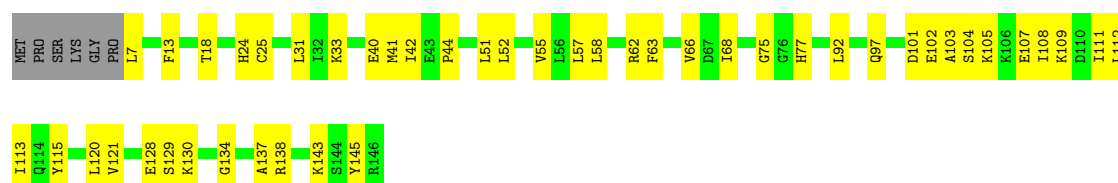
- Molecule 67: uS19

Chain PP: 45% 36% 19%



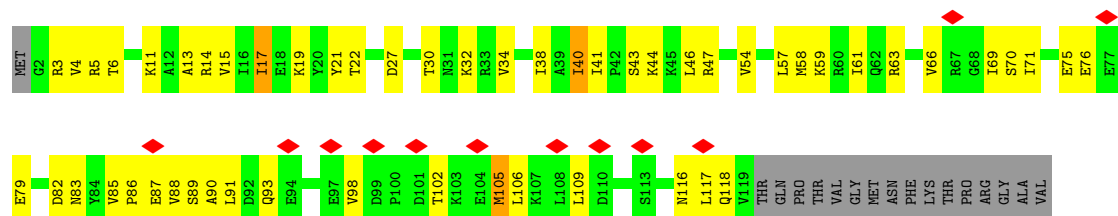
- Molecule 68: uS9

Chain QQ: 64% 32%



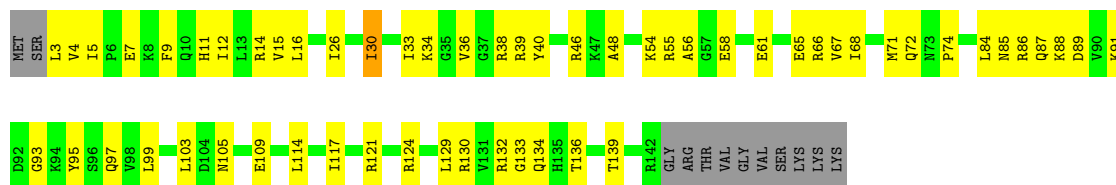
- Molecule 69: eS17

Chain RR: 10% 47% 38% 13%



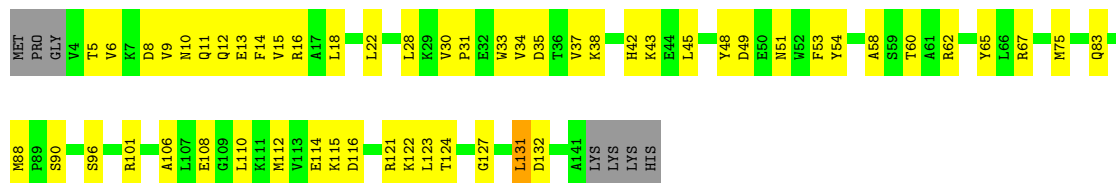
- Molecule 70: uS13

Chain SS:  55% 37% 8%



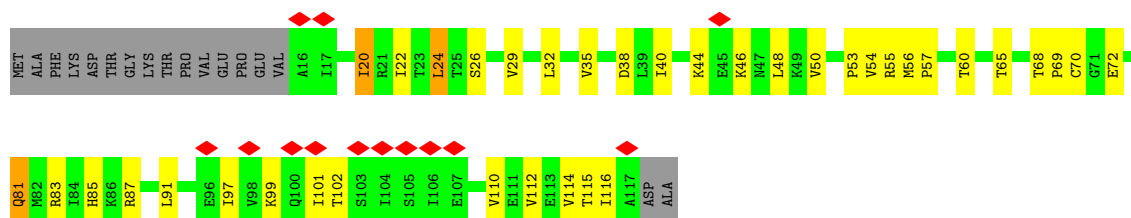
• Molecule 71: eS19

Chain TT:  58% 37% 5%



• Molecule 72: uS10

Chain UU:  11% 54% 29% 14%



• Molecule 73: eS21

Chain VV:  81% 17% 2%



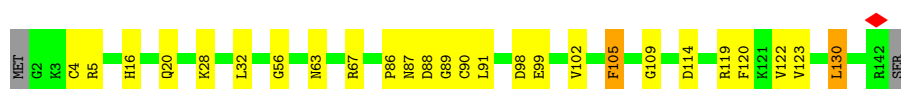
• Molecule 74: uS8

Chain WW:  82% 16% 2%



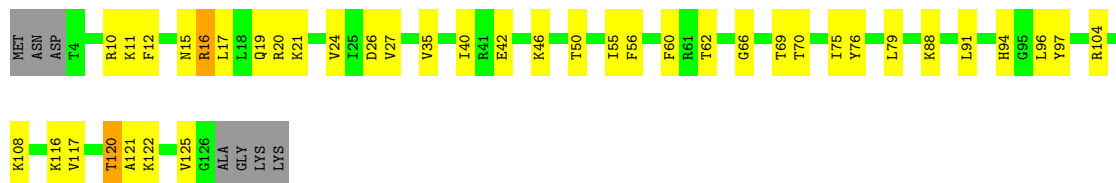
• Molecule 75: uS12

Chain XX:  80% 17% 3%

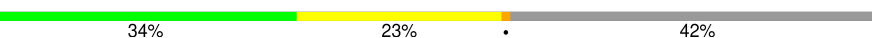


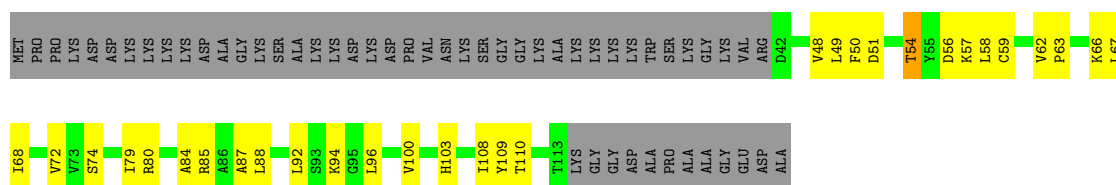
- Molecule 76: 40S ribosomal protein S24

Chain YY:  64% 29% 5%



- Molecule 77: eS25

Chain ZZ:  34% 23% 42%



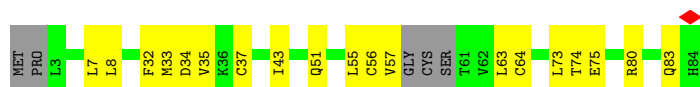
- Molecule 78: 40S ribosomal protein S26

Chain aa:  74% 10% 15%



- Molecule 79: eS27

Chain bb:  71% 23% 6%



- Molecule 80: eS28

Chain cc:  49% 35% 12%



- Molecule 81: uS14

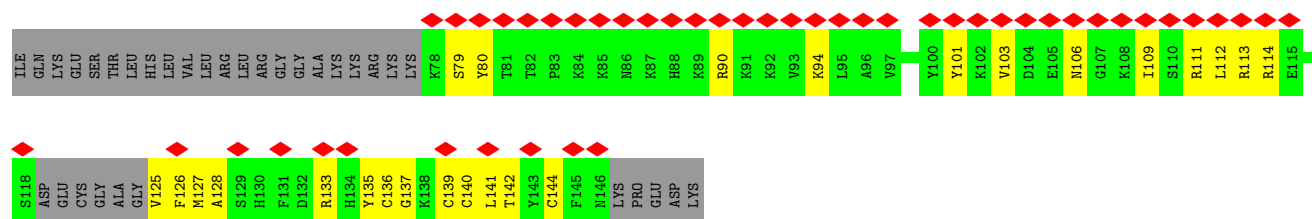
Chain dd:  66% 29% 5%



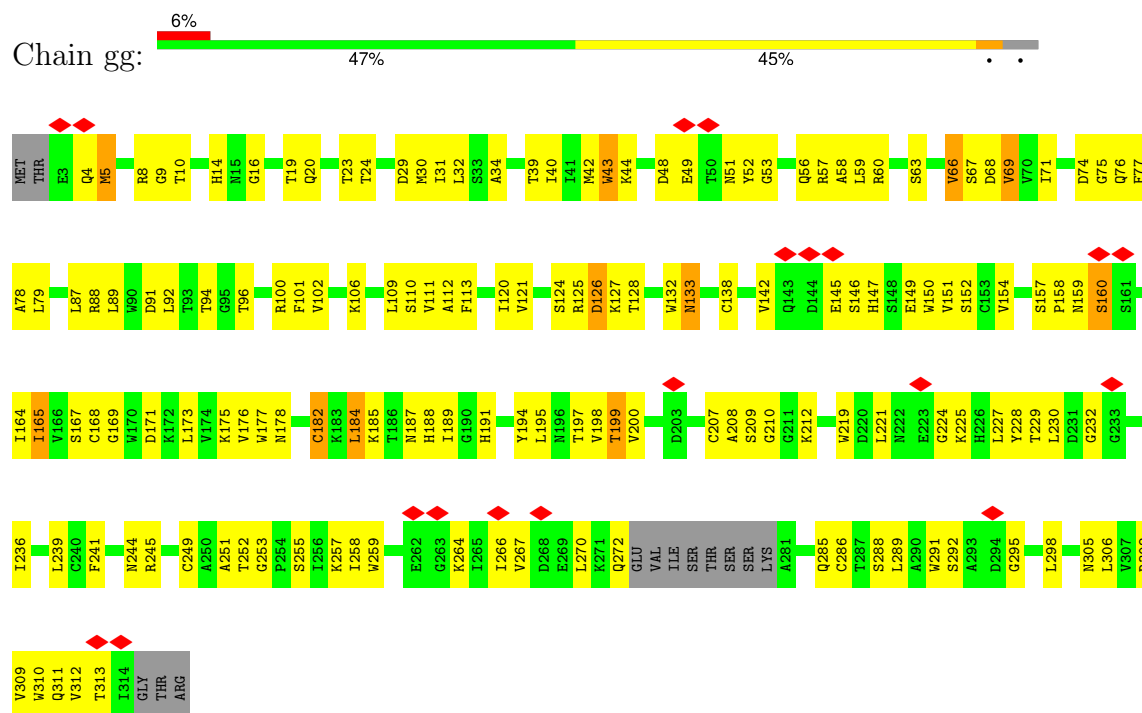
- Molecule 82: eS30



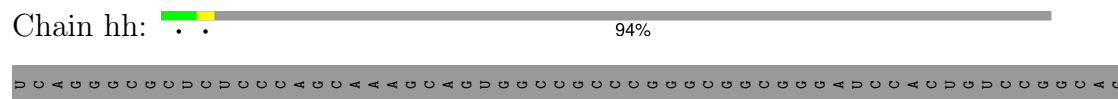
- Molecule 83: eS31

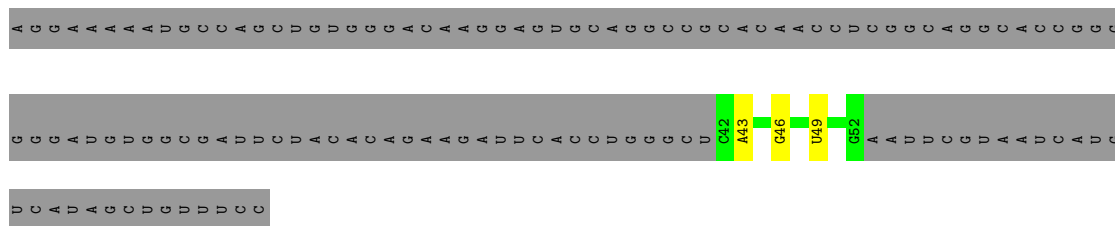


- Molecule 84: Receptor for Activated C Kinase 1 (RACK1)

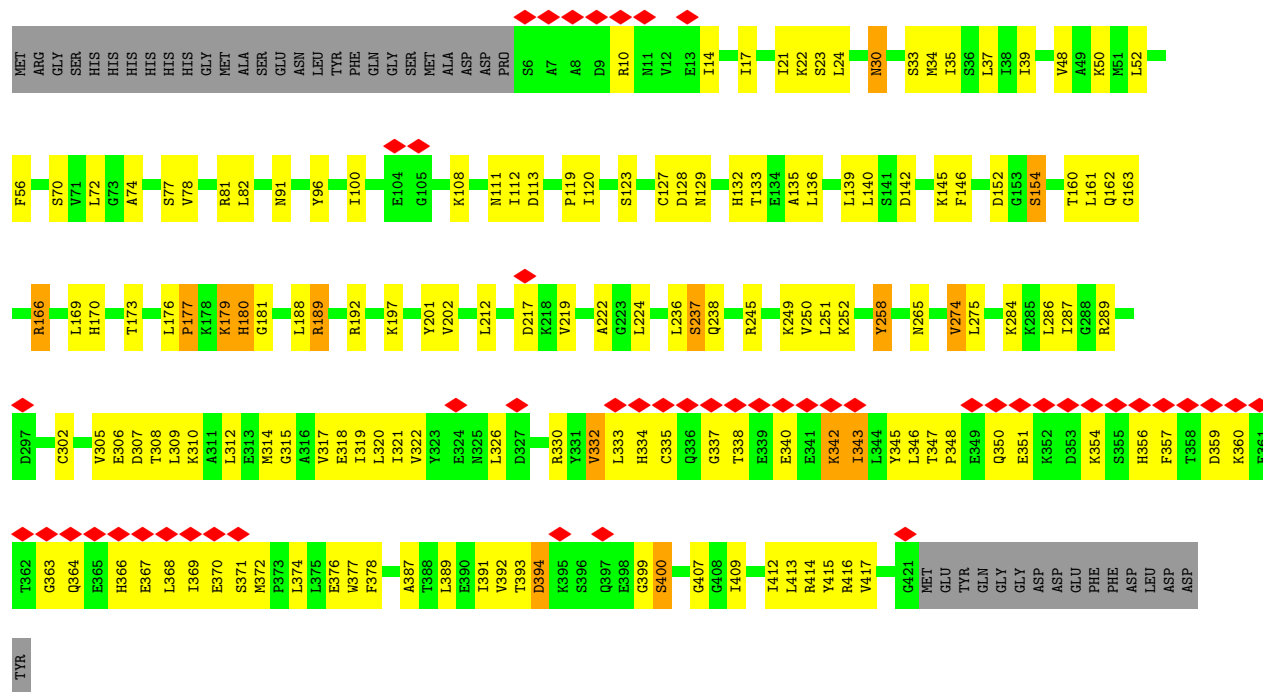


- Molecule 85: mRNA

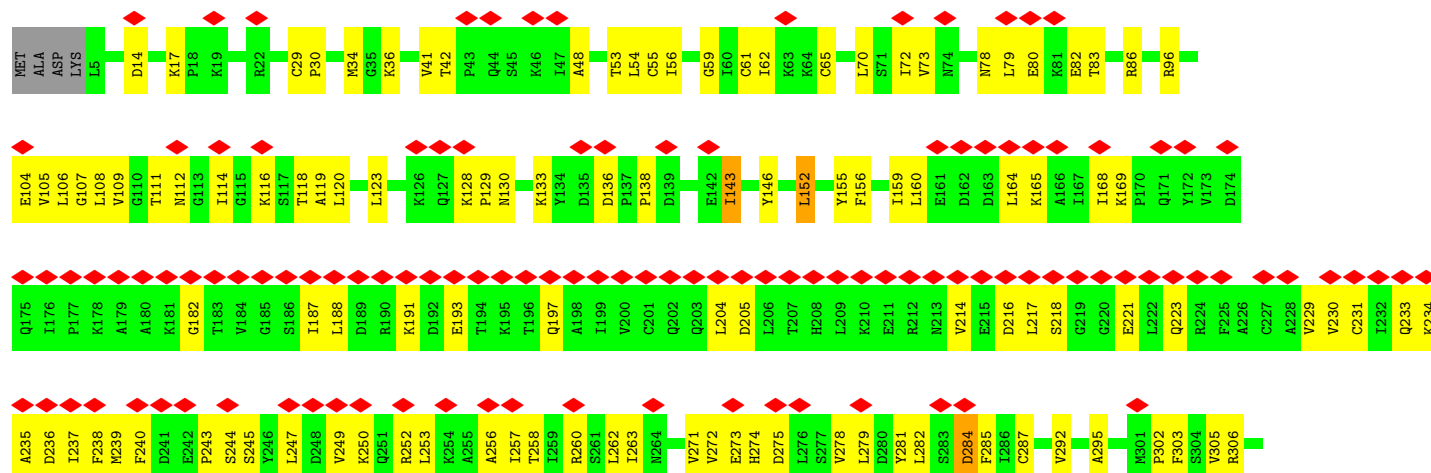
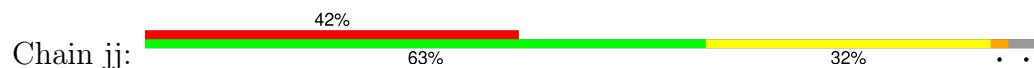


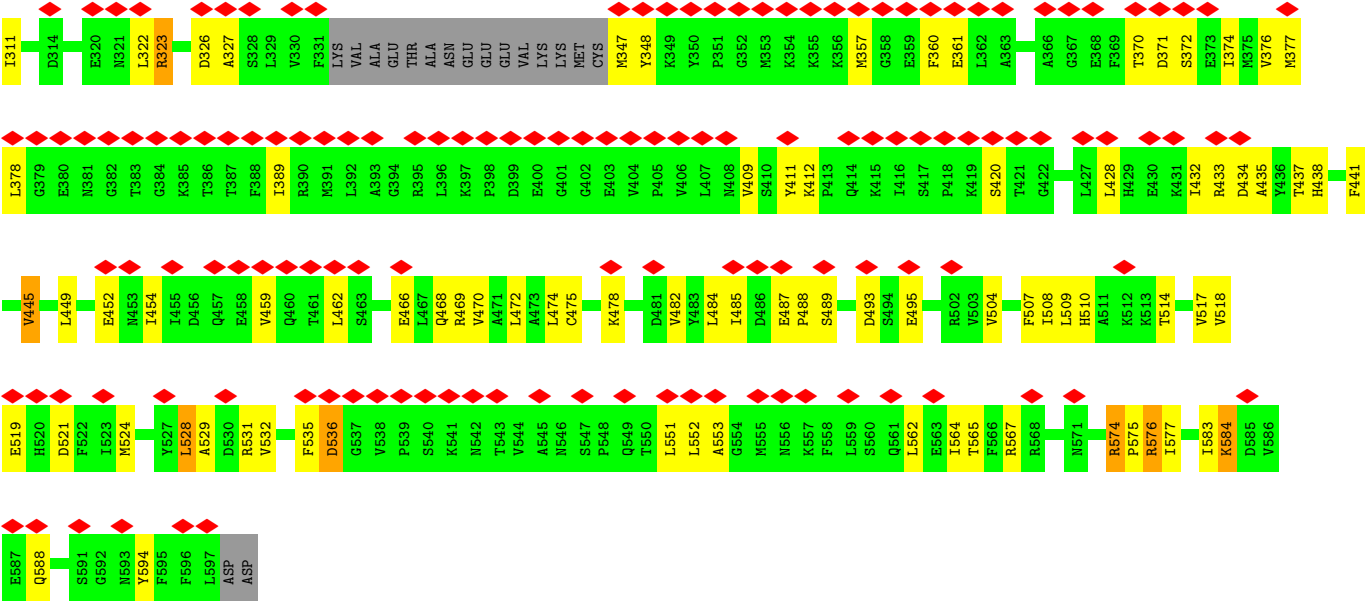


• Molecule 86: Eukaryotic peptide chain release factor subunit 1



• Molecule 87: ATP binding cassette subfamily E member 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90190	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 ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, UR3, B8N, 1MA, SF4, ZN, MG, OMC, 2MG, G7M, 5MC, PSU, UY1, MA6, ZVM, OMG, OMU, 4AC, B9B, A2M

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	0.33	0/1906	0.44	0/2556
2	B	0.32	0/3216	0.46	0/4311
3	C	0.33	0/2937	0.46	0/3946
4	D	0.30	0/2407	0.44	0/3224
5	E	0.28	0/1760	0.43	0/2362
6	F	0.32	0/1911	0.43	0/2549
7	G	0.30	0/1799	0.47	0/2424
8	H	0.29	0/1535	0.42	0/2063
9	I	0.29	0/1693	0.40	0/2260
10	J	0.27	0/1359	0.46	0/1817
11	L	0.30	0/1733	0.44	0/2316
12	M	0.28	0/1158	0.37	0/1547
13	N	0.35	0/1746	0.46	0/2338
14	O	0.31	0/1653	0.48	0/2210
15	P	0.33	0/1268	0.44	0/1700
16	Q	0.34	0/1539	0.45	0/2054
17	R	0.28	0/1518	0.41	0/2005
18	S	0.32	0/1501	0.43	0/2012
19	T	0.30	0/1326	0.41	0/1770
20	U	0.29	0/814	0.53	0/1092
21	V	0.30	0/987	0.43	0/1324
22	W	0.32	0/541	0.41	0/720
23	X	0.29	0/966	0.42	0/1301
24	Y	0.29	0/1132	0.42	0/1504
25	Z	0.39	0/1130	0.55	1/1507 (0.1%)
26	a	0.34	0/1191	0.44	0/1590
27	b	0.33	0/619	0.48	0/818
28	c	0.29	0/742	0.44	0/995
29	d	0.29	0/846	0.42	0/1136
30	e	0.34	0/1071	0.44	0/1429
31	f	0.35	0/895	0.47	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.29	0/916	0.39	0/1220
33	h	0.29	0/1021	0.43	0/1348
34	i	0.26	0/841	0.38	0/1112
35	j	0.36	0/720	0.51	0/952
36	k	0.41	0/565	0.62	0/750
37	l	0.32	0/450	0.47	0/597
38	m	0.30	0/427	0.39	0/564
39	n	0.34	0/223	0.46	0/284
40	o	0.30	0/855	0.41	0/1128
41	p	0.31	0/718	0.46	0/953
42	r	0.33	0/1017	0.43	0/1364
43	s	0.23	0/1483	0.41	0/2000
44	t	0.22	0/1071	0.48	0/1444
45	1	0.26	0/129	0.40	0/173
46	2	0.27	0/1805	0.43	0/2809
47	3	0.23	0/1777	0.45	0/2763
48	5	0.41	4/82331 (0.0%)	0.46	0/128398
49	7	0.37	0/2858	0.40	0/4455
50	8	0.40	0/3675	0.43	0/5725
51	9	0.35	6/38943 (0.0%)	0.46	0/60686
52	AA	0.29	0/1661	0.44	0/2259
53	BB	0.28	0/1749	0.45	1/2340 (0.0%)
54	CC	0.28	0/1710	0.43	0/2312
55	DD	0.26	0/1749	0.45	0/2350
56	EE	0.27	0/2101	0.48	0/2828
57	FF	0.26	0/1461	0.43	0/1961
58	GG	0.29	0/1946	0.49	0/2590
59	HH	0.25	0/1447	0.49	0/1939
60	II	0.27	0/1715	0.45	0/2287
61	JJ	0.26	0/1550	0.43	0/2069
62	KK	0.31	0/752	0.54	0/1014
63	LL	0.29	0/1143	0.43	0/1529
64	MM	0.23	0/949	0.44	0/1274
65	NN	0.26	0/1232	0.41	0/1656
66	OO	0.36	0/969	0.61	1/1298 (0.1%)
67	PP	0.25	0/986	0.47	0/1316
68	QQ	0.27	0/1134	0.45	0/1517
69	RR	0.26	0/973	0.45	0/1304
70	SS	0.25	0/1180	0.40	0/1581
71	TT	0.25	0/1093	0.42	0/1466
72	UU	0.25	0/817	0.44	0/1097
73	VV	0.27	0/623	0.42	0/833
74	WW	0.29	0/1051	0.45	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	XX	0.28	0/1116	0.42	0/1490
76	YY	0.25	0/1023	0.44	0/1359
77	ZZ	0.25	0/580	0.41	0/780
78	aa	0.28	0/794	0.46	0/1065
79	bb	0.26	0/640	0.45	0/856
80	cc	0.26	0/481	0.48	0/643
81	dd	0.27	0/455	0.48	0/603
82	ee	0.25	0/381	0.41	0/498
83	ff	0.22	0/538	0.43	0/713
84	gg	0.24	0/2427	0.48	0/3303
85	hh	0.33	0/264	0.47	0/409
86	ii	0.26	0/3333	0.47	0/4483
87	jj	0.22	0/4644	0.42	0/6272
All	All	0.35	10/233391 (0.0%)	0.45	3/341503 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
57	FF	0	1
63	LL	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3785	A2M	O3'-P	6.06	1.62	1.56
48	5	2787	A2M	O3'-P	5.54	1.61	1.56
51	9	1442	OMU	O3'-P	5.30	1.61	1.56
51	9	668	A2M	O3'-P	5.13	1.61	1.56
51	9	1031	A2M	O3'-P	5.12	1.61	1.56
51	9	27	A2M	O3'-P	5.08	1.61	1.56
51	9	484	A2M	O3'-P	5.07	1.61	1.56
51	9	1678	A2M	O3'-P	5.04	1.61	1.56
48	5	3825	A2M	O3'-P	5.04	1.61	1.56
48	5	3760	A2M	O3'-P	5.03	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	OO	137	SER	N-CA-C	-6.03	103.66	111.02
25	Z	26	VAL	N-CA-C	-5.90	107.06	112.96
53	BB	150	ILE	N-CA-C	-5.35	107.21	111.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
57	FF	136	ARG	Sidechain
63	LL	118	ARG	Sidechain

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	1868	0	1959	26	0
2	B	3148	0	3267	48	0
3	C	2883	0	3053	41	0
4	D	2361	0	2395	53	0
5	E	1726	0	1869	29	0
6	F	1875	0	1995	26	0
7	G	1768	0	1891	42	0
8	H	1516	0	1597	24	0
9	I	1655	0	1704	24	0
10	J	1336	0	1375	28	0
11	L	1702	0	1820	25	0
12	M	1137	0	1211	18	0
13	N	1701	0	1749	31	0
14	O	1621	0	1770	35	0
15	P	1242	0	1274	12	0
16	Q	1515	0	1634	23	0
17	R	1502	0	1659	13	0
18	S	1462	0	1508	19	0
19	T	1298	0	1366	17	0
20	U	800	0	825	37	0
21	V	973	0	1034	7	0
22	W	528	0	541	7	0
23	X	949	0	1016	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	1115	0	1205	14	0
25	Z	1107	0	1182	26	0
26	a	1162	0	1209	31	0
27	b	609	0	650	11	0
28	c	732	0	767	11	0
29	d	833	0	891	14	0
30	e	1053	0	1147	15	0
31	f	876	0	912	10	0
32	g	906	0	998	10	0
33	h	1013	0	1147	20	0
34	i	830	0	916	4	0
35	j	705	0	737	13	0
36	k	559	0	624	15	0
37	l	438	0	469	10	0
38	m	421	0	454	4	0
39	n	222	0	264	4	0
40	o	842	0	912	8	0
41	p	708	0	756	7	0
42	r	1001	0	1060	21	0
43	s	1461	0	1524	55	0
44	t	1059	0	1106	51	0
45	1	125	0	117	5	0
46	2	1616	0	823	30	0
47	3	1593	0	811	35	0
48	5	75735	0	38351	1073	0
49	7	2558	0	1296	19	0
50	8	3315	0	1685	66	0
51	9	36134	0	18306	822	0
52	AA	1624	0	1634	57	0
53	BB	1722	0	1794	40	0
54	CC	1674	0	1759	37	0
55	DD	1723	0	1815	81	0
56	EE	2059	0	2164	65	0
57	FF	1441	0	1493	60	0
58	GG	1923	0	2089	87	0
59	HH	1425	0	1504	74	0
60	II	1686	0	1772	47	0
61	JJ	1525	0	1640	35	0
62	KK	729	0	742	34	0
63	LL	1123	0	1186	20	0
64	MM	939	0	967	41	0
65	NN	1208	0	1294	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	OO	957	0	982	36	0
67	PP	968	0	1016	43	0
68	QQ	1117	0	1185	44	0
69	RR	962	0	1013	57	0
70	SS	1162	0	1221	51	0
71	TT	1075	0	1103	45	0
72	UU	807	0	874	32	0
73	VV	617	0	622	11	0
74	WW	1034	0	1080	19	0
75	XX	1098	0	1167	24	0
76	YY	1006	0	1078	34	0
77	ZZ	574	0	627	27	0
78	aa	781	0	828	10	0
79	bb	628	0	650	17	0
80	cc	479	0	507	25	0
81	dd	445	0	438	16	0
82	ee	380	0	417	14	0
83	ff	527	0	543	30	0
84	gg	2371	0	2324	137	0
85	hh	236	0	119	0	0
86	ii	3280	0	3326	118	0
87	jj	4558	0	4679	172	0
88	2	2	0	0	0	0
88	5	221	0	0	0	0
88	7	6	0	0	0	0
88	8	2	0	0	0	0
88	9	64	0	0	0	0
88	A	2	0	0	0	0
88	EE	1	0	0	0	0
88	I	2	0	0	0	0
88	LL	1	0	0	0	0
88	N	1	0	0	0	0
88	OO	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	XX	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	f	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
88	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	ii	27	0	0	0	0
91	jj	16	0	0	4	0
92	5	723	0	0	30	0
92	7	13	0	0	3	0
92	8	8	0	0	0	0
92	9	173	0	0	12	0
92	A	6	0	0	0	0
92	B	2	0	0	0	0
92	C	1	0	0	0	0
92	F	1	0	0	0	0
92	I	1	0	0	0	0
92	II	1	0	0	0	0
92	L	1	0	0	0	0
92	N	4	0	0	0	0
92	OO	1	0	0	0	0
92	Q	1	0	0	0	0
92	R	1	0	0	0	0
92	V	2	0	0	0	0
92	X	2	0	0	0	0
92	XX	1	0	0	0	0
92	a	5	0	0	0	0
92	aa	1	0	0	0	0
92	e	5	0	0	0	0
92	ii	2	0	0	1	0
92	j	1	0	0	0	0
92	o	2	0	0	0	0
All	All	222478	0	166483	4092	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 11.

All (4092) 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)
48:5:2638:G:N2	48:5:2697:A:N1	1.92	1.18
48:5:461:G:N2	48:5:694:C:O2	1.82	1.13
5:E:96:THR:HG22	5:E:109:VAL:HG22	1.33	1.07
48:5:973:G:N2	48:5:1282:G:N7	2.03	1.07
69:RR:105:MET:HE2	69:RR:109:LEU:HD11	1.36	1.05
51:9:197:U:O2	51:9:202:G:O6	1.74	1.04
43:s:20:LEU:HD22	43:s:52:VAL:HG11	1.39	1.03
51:9:1109:C:O2'	51:9:1110:G:O5'	1.75	1.02
69:RR:41:ILE:HG23	69:RR:46:LEU:HD23	1.41	1.02
48:5:1072:C:O2'	48:5:1073:G:O5'	1.77	1.01
48:5:1235:G:O2'	48:5:1236:C:OP2	1.78	1.00
51:9:1418:C:O2'	51:9:1421:A:OP2	1.80	0.99
48:5:1981:G:O2'	86:ii:314:MET:O	1.81	0.98
48:5:1999:A:O2'	48:5:2000:G:O4'	1.81	0.98
48:5:4903:G:N2	48:5:4918:C:O2	1.97	0.98
46:2:18:G:O2'	46:2:57:G:N2	1.97	0.97
48:5:4633:G:O2'	48:5:4635:A:OP2	1.81	0.97
51:9:1396:A:O2'	51:9:1398:G:N7	1.99	0.96
86:ii:330:ARG:O	86:ii:371:SER:OG	1.82	0.96
48:5:2797:C:OP1	92:5:5401:HOH:O	1.83	0.96
48:5:1992:U:O2'	48:5:2002:A:OP1	1.83	0.96
51:9:1085:C:OP2	92:9:2001:HOH:O	1.84	0.96
48:5:3692:A:H62	48:5:3823:G:H21	0.99	0.95
50:8:110:U:O2'	50:8:111:U:O4'	1.84	0.95
48:5:913:U:O2'	48:5:914:U:OP2	1.83	0.95
51:9:1480:A:O2'	81:dd:56:ASP:OD1	1.83	0.95
51:9:1109:C:O2'	51:9:1110:G:O4'	1.81	0.95
58:GG:102:VAL:HG21	58:GG:109:LEU:HD21	1.46	0.95
58:GG:157:VAL:HG11	58:GG:176:ILE:HD11	1.47	0.95
43:s:22:ASP:OD1	43:s:66:ARG:NH2	1.98	0.95
51:9:73:C:O2'	51:9:74:G:N3	2.01	0.94
50:8:109:C:O2'	50:8:110:U:OP2	1.86	0.94
51:9:417:C:O2'	51:9:418:A:OP1	1.83	0.94
51:9:1441:U:O2	51:9:1443:C:N4	1.99	0.94
65:NN:60:VAL:HG13	65:NN:66:VAL:HG21	1.47	0.94
48:5:922(B):C:O2'	48:5:923:C:OP1	1.86	0.93
68:QQ:42:ILE:HD11	68:QQ:51:LEU:HD11	1.48	0.93
4:D:253:TYR:OH	49:7:117:G:OP1	1.86	0.93
59:HH:17:ASP:OD2	59:HH:22:GLY:N	2.02	0.92
32:g:76:ARG:NH2	48:5:2583:C:OP2	2.02	0.92
51:9:1757:G:O6	51:9:1775:U:O2	1.89	0.91
86:ii:326:LEU:HD21	86:ii:409:ILE:HD11	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:208:G:O2'	51:9:209:A:O5'	1.87	0.91
48:5:1956:A:O2'	48:5:1957:U:OP1	1.88	0.90
51:9:607:U:O2'	51:9:608:C:OP1	1.89	0.90
51:9:1663:A:O2'	51:9:1664:A:OP2	1.89	0.90
51:9:1512:C:O2'	81:dd:7:TYR:O	1.87	0.90
55:DD:103:GLU:OE2	55:DD:173:ARG:NE	2.05	0.90
58:GG:18:VAL:HG11	58:GG:24:LEU:HD21	1.51	0.90
49:7:21:G:N7	92:7:301:HOH:O	2.05	0.90
48:5:2104:A:O2'	48:5:2105:A:O5'	1.88	0.90
51:9:1298:G:O2'	51:9:1299:A:O5'	1.89	0.89
51:9:1068:G:O6	92:9:2002:HOH:O	1.89	0.89
48:5:4136:G:N2	48:5:4148:C:O2	2.05	0.89
51:9:1395:C:O2'	51:9:1396:A:OP1	1.89	0.89
51:9:103:A:OP2	51:9:356:C:N4	2.06	0.88
59:HH:52:GLU:N	59:HH:52:GLU:OE1	2.07	0.88
31:f:58:VAL:O	48:5:4944:C:N4	2.07	0.88
48:5:1076:C:O2	48:5:1235:G:N2	2.07	0.88
48:5:1990:A:O2'	48:5:1991:A:OP1	1.92	0.87
76:YY:122:LYS:O	76:YY:125:VAL:HG22	1.73	0.87
48:5:1481:C:O2'	48:5:1482:G:O5'	1.91	0.87
86:ii:189:ARG:NH2	92:ii:601:HOH:O	2.06	0.87
48:5:3717:A:OP2	48:5:3735:G:N2	2.07	0.87
48:5:3751:G:H21	48:5:3775:A:H8	1.19	0.86
51:9:1456:G:OP1	69:RR:59:LYS:NZ	2.08	0.86
76:YY:26:ASP:OD1	76:YY:70:THR:OG1	1.92	0.86
86:ii:217:ASP:OD1	86:ii:245:ARG:NH1	2.08	0.86
4:D:286:SER:OG	48:5:1179:U:O2	1.93	0.86
48:5:245:C:O2'	48:5:246:G:OP2	1.92	0.86
70:SS:15:VAL:HG12	70:SS:68:ILE:HD11	1.57	0.86
48:5:480:C:O2'	48:5:481:G:OP1	1.92	0.86
48:5:1233:G:O2'	48:5:1234:G:OP2	1.92	0.86
56:EE:21:ASP:OD2	56:EE:24:THR:OG1	1.92	0.85
87:jj:62:ILE:HD11	87:jj:72:ILE:HG12	1.56	0.85
48:5:5047:C:O2'	48:5:5050:C:OP2	1.94	0.85
51:9:1061:U:OP1	92:9:2003:HOH:O	1.93	0.85
77:ZZ:56:ASP:OD1	77:ZZ:57:LYS:N	2.09	0.85
48:5:4927:G:OP2	48:5:4928:C:N4	2.09	0.85
47:3:54:U:O4	47:3:58:A:N7	2.09	0.85
68:QQ:101:ASP:OD1	68:QQ:103:ALA:N	2.09	0.85
51:9:71:G:O2'	51:9:72:C:OP1	1.94	0.85
37:l:21:ARG:NH1	50:8:52:A:OP1	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1890:G:N2	48:5:1939:A:H61	1.75	0.85
87:jj:432:ILE:O	87:jj:432:ILE:HD12	1.76	0.85
48:5:3759:A:OP2	92:5:5402:HOH:O	1.94	0.85
48:5:4415:A:N6	48:5:4427:G:O2'	2.09	0.85
51:9:1231:C:OP2	70:SS:139:THR:OG1	1.94	0.85
65:NN:19:ARG:NH2	79:bb:83:GLN:OE1	2.10	0.84
80:cc:44:ARG:NH2	80:cc:60:GLU:O	2.09	0.84
4:D:212:MET:HE1	4:D:233:PRO:HG2	1.59	0.84
51:9:1432:U:O2'	51:9:1433:C:OP1	1.94	0.84
24:Y:88:GLU:OE1	24:Y:88:GLU:N	2.09	0.84
51:9:1408:U:O2'	51:9:1409:A:O5'	1.95	0.84
48:5:3692:A:H62	48:5:3823:G:N2	1.74	0.84
50:8:122:G:H21	50:8:128:C:H41	1.19	0.84
1:A:142:GLU:O	1:A:143:THR:OG1	1.94	0.83
48:5:1998:A:N3	48:5:2019:C:O2'	2.10	0.83
55:DD:226:GLN:NE2	84:gg:224:GLY:O	2.12	0.83
51:9:100:U:OP2	92:9:2004:HOH:O	1.96	0.83
48:5:3672:G:O2'	48:5:3673:C:OP1	1.95	0.83
51:9:1616:U:O2'	51:9:1661:A:O2'	1.95	0.82
55:DD:167:TYR:OH	55:DD:193:ASP:OD1	1.97	0.82
60:II:114:GLU:OE2	60:II:128:LYS:NZ	2.12	0.82
77:ZZ:74:SER:OG	77:ZZ:79:ILE:O	1.97	0.82
48:5:1455:G:O2'	48:5:1456:C:OP1	1.96	0.82
25:Z:30:ASP:O	25:Z:39:SER:OG	1.96	0.82
48:5:1982:G:O2'	48:5:1983:A:OP1	1.96	0.82
54:CC:255:LEU:HD23	73:VV:1:MET:HE2	1.59	0.82
51:9:1303:C:OP2	83:ff:90:ARG:NH2	2.13	0.82
51:9:306:C:O4'	60:II:41:ARG:NH2	2.13	0.82
59:HH:139:ILE:HD12	59:HH:139:ILE:O	1.79	0.82
48:5:4487:A:N7	92:5:5415:HOH:O	2.13	0.81
48:5:1077:C:N4	48:5:1233:G:O6	2.11	0.81
51:9:537:C:N3	51:9:547:G:N2	2.27	0.81
55:DD:158:ILE:HD12	55:DD:164:VAL:HG12	1.61	0.81
51:9:1521:C:OP2	70:SS:136:THR:OG1	1.99	0.81
13:N:124:ASP:OD1	48:5:3937:C:O2'	1.97	0.81
48:5:1444:G:N2	48:5:2110:G:O6	2.13	0.81
53:BB:125:VAL:HG12	53:BB:172:MET:HE3	1.63	0.81
87:jj:389:ILE:HD13	87:jj:484:LEU:HD23	1.61	0.81
51:9:95:G:O6	92:9:2006:HOH:O	1.98	0.81
10:J:113:ILE:HD12	70:SS:14:ARG:HD3	1.63	0.80
48:5:3603:G:O2'	48:5:3604:A:OP1	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:70:G:HO2'	48:5:3740:G:HO2'	1.21	0.80
48:5:738(A):C:O2'	48:5:740:G:OP2	1.98	0.80
50:8:110:U:HO2'	50:8:111:U:C4'	1.92	0.80
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.63	0.80
51:9:1560:U:O2'	51:9:1583:C:O2'	1.88	0.80
56:EE:195:ILE:O	56:EE:196:THR:OG1	1.99	0.80
55:DD:28:GLU:OE1	55:DD:65:ARG:NH2	2.16	0.79
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.80	0.79
9:I:66:GLU:OE1	9:I:69:ARG:NH2	2.15	0.79
51:9:488:U:O2'	51:9:489:A:OP1	1.99	0.79
52:AA:50:ASN:HA	69:RR:105:MET:HE1	1.64	0.79
68:QQ:130:LYS:NZ	68:QQ:134:GLY:O	2.15	0.79
20:U:111:GLU:OE2	20:U:113:ARG:NE	2.15	0.79
48:5:1611:C:OP1	92:5:5404:HOH:O	2.01	0.79
48:5:2457:G:H21	48:5:3672:G:N2	1.81	0.79
43:s:9:TRP:NE1	48:5:1999:A:OP1	2.16	0.79
57:FF:74:ASN:OD1	57:FF:86:LYS:NZ	2.14	0.79
51:9:44:U:O4	51:9:485:A:N6	2.16	0.79
51:9:1249:C:O2'	68:QQ:143:LYS:NZ	2.15	0.79
9:I:162:ARG:NH2	48:5:2033:A:OP1	2.16	0.79
48:5:4572:U:O2'	48:5:4573:G:O4'	2.01	0.78
51:9:71:G:O6	58:GG:170:ARG:NH1	2.17	0.78
48:5:1991:A:O2'	48:5:1992:U:O4'	2.00	0.78
75:XX:98:ASP:OD1	75:XX:99:GLU:N	2.15	0.78
86:ii:24:LEU:HD21	86:ii:112:ILE:HD12	1.64	0.78
48:5:3860:A:H61	48:5:4560:C:H5	1.31	0.78
51:9:1291:A:HO2'	83:ff:135:TYR:HH	1.11	0.78
86:ii:24:LEU:HD21	86:ii:112:ILE:CD1	2.13	0.78
48:5:1629:G:OP1	92:5:5403:HOH:O	2.00	0.78
51:9:872:A:O2'	51:9:873:G:O5'	2.00	0.78
87:jj:165:LYS:NZ	87:jj:234:LYS:O	2.16	0.78
87:jj:168:ILE:HG22	87:jj:239:MET:HB2	1.65	0.78
13:N:2:GLY:N	48:5:116:G:OP2	2.17	0.78
52:AA:90:PHE:CD2	52:AA:179:ALA:HB2	2.19	0.78
4:D:43:LYS:O	4:D:46:THR:HG22	1.82	0.78
48:5:3637:U:OP2	92:5:5405:HOH:O	2.02	0.78
51:9:1192:U:OP2	75:XX:119:ARG:NH2	2.17	0.78
48:5:3897:G:OP2	92:5:5406:HOH:O	2.02	0.78
78:aa:3:LYS:NZ	78:aa:8:ASN:OD1	2.17	0.78
4:D:75:VAL:O	4:D:112:ARG:NH1	2.16	0.77
48:5:2092:G:O2'	48:5:2262:G:O6	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2638:G:H1	48:5:2697:A:H61	1.33	0.77
66:OO:86:LYS:HD2	66:OO:124:MET:HE3	1.66	0.77
55:DD:66:ILE:HD11	55:DD:86:LEU:O	1.85	0.77
57:FF:73:THR:O	57:FF:89:THR:HG21	1.84	0.77
87:jj:377:MET:HA	87:jj:377:MET:HE3	1.65	0.77
71:TT:22:LEU:HD22	71:TT:28:LEU:HD13	1.67	0.77
7:G:95:LEU:HD13	7:G:218:LEU:HD13	1.66	0.77
51:9:197:U:O2	51:9:202:G:C6	2.38	0.77
72:UU:24:LEU:CD1	72:UU:112:VAL:HG13	2.15	0.77
76:YY:27:VAL:HG11	76:YY:35:VAL:HG21	1.66	0.77
51:9:165:G:N2	51:9:165:G:OP2	2.16	0.76
48:5:467:U:N3	48:5:685:C:N3	2.34	0.76
69:RR:105:MET:HE2	69:RR:109:LEU:CD1	2.15	0.76
48:5:2553:A:H2	48:5:2765:A:H62	1.34	0.76
51:9:399:C:N3	63:LL:104:LYS:NZ	2.33	0.76
66:OO:124:MET:HE2	66:OO:124:MET:HA	1.65	0.76
67:PP:89:MET:O	67:PP:107:ILE:HD11	1.85	0.76
4:D:284:LYS:O	4:D:288:LEU:HD22	1.85	0.76
84:gg:288:SER:O	84:gg:289:LEU:HD23	1.84	0.76
51:9:1407:U:H2'	51:9:1408:U:C5	2.20	0.76
58:GG:7:PHE:CE1	58:GG:9:ALA:HB3	2.21	0.76
26:a:77:LYS:CE	48:5:1502:G:H22	1.99	0.76
48:5:2100:G:O2'	48:5:2101:A:OP2	2.03	0.76
51:9:1560:U:HO2'	51:9:1583:C:HO2'	0.98	0.76
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.67	0.76
80:cc:14:VAL:HG22	80:cc:30:VAL:HG21	1.67	0.76
25:Z:24:VAL:HG21	25:Z:87:VAL:HG22	1.68	0.76
44:t:114:ARG:NH2	44:t:126:SER:OG	2.19	0.76
87:jj:552:LEU:HD12	87:jj:553:ALA:H	1.50	0.76
31:f:106:TYR:O	31:f:108:SER:N	2.19	0.75
70:SS:58:GLU:OE2	77:ZZ:49:LEU:HD11	1.86	0.75
5:E:209:VAL:HG22	5:E:259:GLN:HB3	1.69	0.75
48:5:115:C:O2'	48:5:276:C:OP1	2.03	0.75
48:5:1449:C:O2	48:5:2105:A:O2'	2.03	0.75
51:9:1292:C:N4	51:9:1307:U:O2	2.19	0.75
51:9:1491:G:OP2	92:9:2007:HOH:O	2.05	0.75
51:9:33:G:H2'	51:9:34:PSU:H5''	1.67	0.75
51:9:217:A:O2'	51:9:218:PSU:H5''	1.87	0.75
87:jj:374:ILE:HG21	87:jj:528:LEU:HG	1.69	0.75
48:5:1322:1MA:OP1	92:5:5407:HOH:O	2.05	0.75
51:9:1407:U:O2	51:9:1407:U:O2'	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:ASN:ND2	5:E:274:LEU:O	2.20	0.75
87:jj:454:ILE:HD13	87:jj:466:GLU:HB3	1.67	0.75
48:5:2457:G:H21	48:5:3672:G:H21	1.35	0.74
48:5:2465:C:H1'	48:5:3672:G:H22	1.49	0.74
84:gg:5:MET:SD	84:gg:270:LEU:HD11	2.27	0.74
51:9:872:A:HO2'	51:9:873:G:C5'	1.99	0.74
86:ii:160:THR:HG23	86:ii:169:LEU:HD11	1.68	0.74
58:GG:126:ASP:OD1	58:GG:127:THR:HG23	1.87	0.74
7:G:73:ARG:NE	48:5:4076:G:OP1	2.21	0.74
48:5:3692:A:N6	48:5:3823:G:H21	1.81	0.74
24:Y:126:ARG:NH2	48:5:198:A:OP2	2.19	0.74
51:9:160:U:O2'	51:9:162:C:OP2	2.06	0.74
7:G:98:LEU:HD13	7:G:218:LEU:HD12	1.69	0.74
87:jj:237:ILE:HG22	87:jj:239:MET:HE2	1.69	0.74
59:HH:30:LEU:O	59:HH:36:LEU:HD23	1.88	0.74
64:MM:48:HIS:O	64:MM:49:LEU:HD12	1.88	0.74
5:E:58:ARG:NH1	5:E:58:ARG:O	2.19	0.74
51:9:291:G:N2	51:9:293:C:OP2	2.12	0.74
51:9:688:U:OP2	59:HH:116:ARG:NH2	2.19	0.74
87:jj:244:SER:O	87:jj:252:ARG:NH2	2.21	0.74
26:a:2:PRO:HG2	26:a:5:LEU:HD12	1.70	0.74
51:9:535:G:O6	51:9:547:G:N1	2.20	0.74
80:cc:13:ARG:HH22	80:cc:35:MET:HE3	1.50	0.74
33:h:7:ARG:NH1	50:8:86:U:O4'	2.21	0.73
87:jj:260:ARG:O	87:jj:263:ILE:HG22	1.88	0.73
48:5:1072:C:N4	48:5:1239:C:H42	1.86	0.73
52:AA:66:VAL:HG21	52:AA:185:MET:HB3	1.71	0.73
55:DD:138:VAL:HG12	55:DD:184:ILE:HD12	1.69	0.73
8:H:134:CYS:SG	8:H:144:LEU:HD13	2.27	0.73
42:r:26:SER:OG	42:r:28:GLU:OE1	2.05	0.73
48:5:2351:OMC:HM22	48:5:2352:U:H5'	1.70	0.73
25:Z:74:VAL:HG23	25:Z:101:PHE:CE2	2.23	0.73
48:5:4189:U:O4	92:5:5408:HOH:O	2.06	0.73
66:OO:84:ARG:CZ	66:OO:88:LEU:HD21	2.19	0.73
48:5:451:C:OP2	48:5:1294:A:N6	2.20	0.73
48:5:1072:C:H42	48:5:1239:C:H42	1.33	0.73
48:5:1369:C:OP2	48:5:1370:G:O2'	2.00	0.73
84:gg:272:GLN:OE1	84:gg:272:GLN:N	2.22	0.73
3:C:10:VAL:O	3:C:18:SER:OG	2.04	0.73
84:gg:176:VAL:O	84:gg:185:LYS:N	2.22	0.73
51:9:197:U:C2	51:9:202:G:O6	2.41	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1617:G:N1	51:9:1620:A:OP2	2.22	0.72
87:jj:495:GLU:OE1	87:jj:495:GLU:N	2.21	0.72
24:Y:74:TYR:OH	50:8:75:OMG:OP2	2.06	0.72
51:9:860:G:H21	74:WW:107:SER:HB3	1.53	0.72
53:BB:228:LEU:HD23	53:BB:229:MET:CE	2.20	0.72
84:gg:39:THR:HG22	84:gg:60:ARG:HD2	1.70	0.72
9:I:184:MET:HB2	9:I:190:LEU:HD12	1.72	0.72
51:9:654:A:N7	92:9:2010:HOH:O	2.21	0.72
48:5:2647:A:H62	48:5:2686:G:H8	1.36	0.72
9:I:13:LYS:NZ	48:5:1867:A:OP1	2.21	0.72
48:5:2819:U:OP2	92:5:5411:HOH:O	2.08	0.72
51:9:935:G:O2'	65:NN:108:ASP:OD1	2.07	0.72
51:9:1785:C:O2'	51:9:1786:U:O5'	2.07	0.72
58:GG:126:ASP:O	58:GG:127:THR:OG1	2.06	0.72
84:gg:79:LEU:HD21	84:gg:120:ILE:HG21	1.70	0.72
87:jj:284:ASP:N	87:jj:284:ASP:OD1	2.23	0.72
59:HH:134:VAL:HG23	59:HH:134:VAL:O	1.90	0.71
10:J:22:LEU:HD13	10:J:43:LEU:HD23	1.71	0.71
48:5:267:G:O2'	48:5:268:G:OP1	2.06	0.71
51:9:1612:G:OP1	67:PP:18:ARG:NH2	2.22	0.71
72:UU:48:LEU:HD22	72:UU:101:ILE:HD11	1.70	0.71
6:F:65:ARG:CZ	48:5:1210:C:H42	2.02	0.71
51:9:1348:G:H1	51:9:1381:G:H22	1.37	0.71
48:5:746:A:O2'	48:5:747:A:OP2	2.04	0.71
51:9:840:C:O2'	51:9:841:G:O5'	2.08	0.71
67:PP:37:TYR:O	67:PP:42:ARG:NH2	2.23	0.71
51:9:688:U:O2'	51:9:689:U:OP2	2.09	0.71
51:9:1316:C:O2'	51:9:1317:C:OP2	2.06	0.71
58:GG:181:THR:HG22	58:GG:182:PRO:HD2	1.73	0.71
1:A:93:LYS:NZ	48:5:4115:G:OP1	2.23	0.71
2:B:223:THR:HG22	2:B:338:VAL:HG23	1.72	0.71
43:s:34:ASN:ND2	48:5:1969:G:OP1	2.23	0.71
48:5:1481:C:O2'	48:5:1482:G:O4'	2.08	0.71
57:FF:43:GLU:OE1	57:FF:43:GLU:N	2.23	0.71
59:HH:25:GLN:O	59:HH:29:GLU:OE1	2.09	0.71
61:JJ:177:ASN:OD1	61:JJ:180:LYS:NZ	2.23	0.71
1:A:123:ARG:NH1	48:5:4083:U:OP1	2.24	0.71
48:5:4921:C:O2'	48:5:4922:C:OP2	2.09	0.71
51:9:1102:G:H22	51:9:1130:G:N2	1.89	0.71
87:jj:371:ASP:O	87:jj:372:SER:OG	2.07	0.71
87:jj:588:GLN:NE2	87:jj:594:TYR:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:GLN:OE1	7:G:229:ARG:NH1	2.24	0.71
48:5:1904:G:O6	92:5:5409:HOH:O	2.06	0.71
62:KK:16:PHE:CE1	62:KK:76:ILE:HG23	2.26	0.71
51:9:488:U:H3'	51:9:489:A:H5'	1.71	0.70
67:PP:19:GLY:N	70:SS:91:LYS:O	2.24	0.70
50:8:85:U:O2'	50:8:87:G:OP1	2.05	0.70
51:9:33:G:C2'	51:9:34:PSU:H5''	2.20	0.70
64:MM:64:LEU:HD22	83:ff:103:VAL:HG23	1.71	0.70
48:5:981:C:H42	48:5:1274:A:H61	1.38	0.70
51:9:213:G:O2'	51:9:214:U:OP1	2.08	0.70
25:Z:95:VAL:HG12	25:Z:110:ALA:HA	1.73	0.70
51:9:525:A:O2'	82:ee:31:ARG:NH2	2.23	0.70
64:MM:64:LEU:CD2	83:ff:103:VAL:HG23	2.21	0.70
71:TT:108:GLU:OE2	71:TT:115:LYS:NZ	2.24	0.70
84:gg:4:GLN:O	84:gg:313:THR:N	2.23	0.70
87:jj:347:MET:SD	87:jj:348:TYR:N	2.64	0.70
13:N:148:THR:O	13:N:151:ILE:HG22	1.91	0.70
67:PP:17:TYR:HB3	67:PP:25:LEU:HD11	1.74	0.70
87:jj:322:LEU:HD13	87:jj:323:ARG:N	2.07	0.70
51:9:1616:U:HO2'	51:9:1661:A:HO2'	1.37	0.70
4:D:107:ARG:NH1	4:D:169:GLY:O	2.24	0.70
72:UU:48:LEU:HD21	72:UU:97:ILE:CG2	2.22	0.70
76:YY:10:ARG:NH1	76:YY:26:ASP:OD2	2.24	0.70
49:7:65:G:N7	92:7:303:HOH:O	2.25	0.69
76:YY:55:ILE:HD12	76:YY:75:ILE:HD12	1.72	0.69
51:9:1570:G:O2'	51:9:1614:A:O2'	2.09	0.69
48:5:3786:U:OP1	48:5:4550:G:O2'	2.10	0.69
51:9:64:A:H2	51:9:83:A:H62	1.38	0.69
79:bb:35:VAL:HG11	79:bb:73:LEU:HD11	1.75	0.69
84:gg:9:GLY:O	84:gg:309:VAL:HG12	1.92	0.69
87:jj:409:VAL:HG22	87:jj:482:VAL:CG2	2.22	0.69
87:jj:519:GLU:OE2	87:jj:521:ASP:N	2.25	0.69
2:B:302:ASN:ND2	2:B:370:THR:OG1	2.26	0.69
32:g:29:ARG:NH2	48:5:2522:G:OP2	2.26	0.69
43:s:144:THR:OG1	43:s:156:SER:OG	2.11	0.69
48:5:4627:U:OP2	92:5:5412:HOH:O	2.11	0.69
51:9:583:A:OP1	61:JJ:162:ARG:NH2	2.26	0.69
51:9:835:C:O2'	51:9:838:G:OP2	2.07	0.69
51:9:1394:G:O2'	51:9:1395:C:OP1	2.11	0.69
48:5:52:G:N7	92:5:5437:HOH:O	2.24	0.69
51:9:1752:C:H2'	51:9:1753:C:O4'	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:19:LEU:HD11	69:RR:106:LEU:HD11	1.74	0.69
58:GG:74:ARG:NH2	58:GG:94:ARG:O	2.26	0.69
87:jj:218:SER:OG	87:jj:221:GLU:OE1	2.09	0.69
44:t:50:THR:HG21	44:t:72:GLU:HG2	1.75	0.69
51:9:1744:G:O2'	51:9:1745:A:OP2	2.10	0.69
53:BB:38:MET:HE2	53:BB:231:LEU:HD11	1.75	0.69
53:BB:97:LEU:HD12	53:BB:232:HIS:CD2	2.28	0.69
57:FF:171:GLU:OE2	77:ZZ:72:VAL:HG23	1.92	0.69
62:KK:15:LEU:O	62:KK:18:GLU:O	2.11	0.69
21:V:99:GLU:OE1	22:W:24:THR:HG22	1.92	0.68
40:o:2:VAL:N	40:o:90:HIS:O	2.26	0.68
74:WW:26:LEU:HB2	79:bb:7:LEU:HD23	1.76	0.68
75:XX:109:GLY:O	75:XX:119:ARG:NE	2.26	0.68
4:D:208:MET:CB	4:D:233:PRO:HG3	2.23	0.68
48:5:4635:A:H2	48:5:4663:G:H21	1.41	0.68
62:KK:15:LEU:O	62:KK:19:GLY:HA2	1.93	0.68
86:ii:407:GLY:HA2	87:jj:34:MET:HE2	1.74	0.68
51:9:292:A:OP2	63:LL:42:LEU:HD21	1.94	0.68
51:9:1598:G:O2'	51:9:1599:U:OP2	2.11	0.68
3:C:335:MET:HE1	48:5:943:A:N3	2.08	0.68
20:U:76:VAL:HG13	20:U:77:PRO:HD2	1.76	0.68
48:5:4743:G:O2'	48:5:4744:A:O4'	2.10	0.68
51:9:65:C:C2	58:GG:133:LEU:HD22	2.28	0.68
67:PP:81:ARG:NH1	67:PP:97:TYR:O	2.26	0.68
71:TT:30:VAL:HG12	71:TT:34:VAL:HG21	1.74	0.68
87:jj:466:GLU:OE1	87:jj:469:ARG:NH1	2.27	0.68
2:B:217:ILE:HD11	2:B:333:LEU:HD21	1.76	0.68
7:G:34:LYS:NZ	48:5:4129:G:O2'	2.22	0.68
67:PP:17:TYR:CB	67:PP:25:LEU:HD11	2.24	0.68
48:5:1413:C:O2'	48:5:1414:C:O5'	2.08	0.68
51:9:1507:G:HO2'	83:ff:80:TYR:HH	0.84	0.68
7:G:161:VAL:O	7:G:161:VAL:HG12	1.94	0.68
48:5:4244:A:O2'	48:5:4268:A:OP1	2.12	0.68
55:DD:177:LEU:HD12	55:DD:182:LEU:HD12	1.75	0.68
8:H:12:ILE:HG12	8:H:18:ILE:HD12	1.76	0.68
17:R:88:ARG:O	48:5:2725:A:N6	2.26	0.68
47:3:58:A:O2'	47:3:60:U:OP2	2.05	0.68
83:ff:103:VAL:HG13	83:ff:106:ASN:O	1.94	0.68
84:gg:270:LEU:HD22	84:gg:310:TRP:CZ3	2.28	0.68
56:EE:95:THR:HG22	76:YY:16:ARG:HG2	1.74	0.67
79:bb:63:LEU:O	79:bb:64:CYS:SG	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:235:ALA:HB3	87:jj:238:PHE:CE1	2.28	0.67
48:5:2562:G:N1	48:5:2565:A:OP2	2.27	0.67
52:AA:34:MET:HE2	52:AA:149:ASN:O	1.94	0.67
87:jj:152:LEU:HD22	87:jj:156:PHE:CE2	2.28	0.67
12:M:96:GLU:OE2	12:M:100:ARG:NH2	2.28	0.67
13:N:67:ARG:NH1	48:5:2458:C:OP1	2.27	0.67
44:t:41:LYS:HE3	86:ii:343:ILE:HD11	1.76	0.67
51:9:1490:OMG:HM22	51:9:1491:G:O4'	1.95	0.67
55:DD:93:THR:HG23	55:DD:93:THR:O	1.94	0.67
58:GG:157:VAL:CG1	58:GG:176:ILE:HD11	2.24	0.67
2:B:322:HIS:O	2:B:342:LYS:NZ	2.19	0.67
12:M:11:ARG:NH1	12:M:61:ILE:HD11	2.09	0.67
30:e:117:GLN:O	42:r:119:ARG:NH2	2.27	0.67
50:8:122:G:N2	50:8:128:C:H41	1.92	0.67
51:9:1566:G:N7	71:TT:101:ARG:NH2	2.42	0.67
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.77	0.67
84:gg:292:SER:O	84:gg:295:GLY:N	2.26	0.67
48:5:261:G:H2'	48:5:262:G:O4'	1.93	0.67
2:B:370:THR:O	2:B:370:THR:HG22	1.94	0.67
4:D:208:MET:HB2	4:D:233:PRO:HG3	1.76	0.67
48:5:2758:G:O2'	48:5:2765:A:N3	2.25	0.67
51:9:218:PSU:O2'	51:9:305:U:N3	2.28	0.67
51:9:846:G:C5	56:EE:19:MET:HE3	2.29	0.67
86:ii:287:ILE:HD11	86:ii:392:VAL:HB	1.77	0.67
51:9:551:U:N3	51:9:552:G:O6	2.25	0.67
63:LL:14:PRO:O	63:LL:15:THR:OG1	2.11	0.67
86:ii:287:ILE:HD13	86:ii:399:GLY:HA2	1.77	0.67
7:G:161:VAL:HG13	7:G:200:THR:HG22	1.77	0.67
48:5:2811:G:N1	48:5:2814:C:OP2	2.23	0.67
87:jj:114:ILE:HG22	87:jj:114:ILE:O	1.94	0.67
48:5:5068:G:N2	48:5:5069:U:O4	2.19	0.67
29:d:36:VAL:HG21	29:d:44:ARG:HG2	1.76	0.67
48:5:4903:G:N1	48:5:4918:C:N3	2.39	0.67
53:BB:225:LEU:HD23	53:BB:229:MET:HE3	1.76	0.67
71:TT:30:VAL:CG1	71:TT:34:VAL:HG21	2.24	0.67
48:5:4682:U:OP2	92:5:5413:HOH:O	2.12	0.66
7:G:182:CYS:HB3	7:G:222:ILE:HD12	1.78	0.66
17:R:151:ARG:NH1	63:LL:119:ASP:OD2	2.28	0.66
51:9:834:C:H2'	51:9:835:C:O4'	1.96	0.66
51:9:1160:U:OP2	75:XX:4:CYS:O	2.13	0.66
55:DD:51:LEU:HG	55:DD:91:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:135:LYS:N	11:L:138:ASP:OD2	2.29	0.66
43:s:139:GLN:OE1	87:jj:433:ARG:NH2	2.28	0.66
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	1.78	0.66
58:GG:6:SER:OG	58:GG:112:VAL:HG12	1.95	0.66
8:H:37:ASP:OD1	8:H:39:ASN:OD1	2.13	0.66
51:9:1403:C:N4	51:9:1436:C:OP2	2.29	0.66
47:3:54:U:H3	47:3:58:A:H62	1.44	0.66
55:DD:8:LYS:O	55:DD:12:VAL:HG23	1.94	0.66
46:2:18:G:OP2	46:2:60:A:O2'	2.13	0.66
84:gg:288:SER:C	84:gg:289:LEU:HD23	2.21	0.66
86:ii:326:LEU:HD21	86:ii:409:ILE:CD1	2.25	0.66
48:5:3865:A:OP2	92:5:5416:HOH:O	2.13	0.66
69:RR:106:LEU:HD23	69:RR:109:LEU:HD12	1.78	0.66
43:s:20:LEU:HD22	43:s:52:VAL:CG1	2.21	0.66
70:SS:30:ILE:CG2	70:SS:36:VAL:HG11	2.26	0.66
42:r:124:VAL:HG13	42:r:125:MET:H	1.61	0.65
51:9:217:A:H2	51:9:309:G:H22	1.43	0.65
72:UU:26:SER:HB3	72:UU:110:VAL:HG22	1.78	0.65
6:F:52:LYS:NZ	6:F:188:ASP:OD2	2.18	0.65
43:s:91:THR:HG21	43:s:98:ILE:HD11	1.78	0.65
59:HH:158:LEU:HD11	59:HH:187:PHE:HD2	1.61	0.65
60:II:36:THR:OG1	60:II:57:ALA:O	2.07	0.65
46:2:74:C:OP1	48:5:4548:A:O2'	2.13	0.65
48:5:4719:G:H4'	48:5:4720:C:OP1	1.95	0.65
56:EE:21:ASP:OD1	56:EE:23:LEU:N	2.30	0.65
56:EE:54:TYR:O	76:YY:15:ASN:ND2	2.30	0.65
56:EE:176:ASP:OD1	56:EE:177:THR:N	2.29	0.65
4:D:150:LEU:HD12	10:J:146:ARG:HG3	1.79	0.65
20:U:92:LYS:NZ	48:5:2627:C:OP1	2.30	0.65
24:Y:38:LEU:HD22	24:Y:42:TYR:HE2	1.61	0.65
48:5:1480:C:C2'	48:5:1483:C:H42	2.09	0.65
48:5:2047:A:C8	48:5:2047:A:OP2	2.50	0.65
48:5:2459:G:OP1	92:5:5414:HOH:O	2.13	0.65
48:5:4743:G:O2'	48:5:4744:A:O5'	2.14	0.65
51:9:208:G:HO2'	51:9:209:A:P	2.20	0.65
70:SS:15:VAL:CG1	70:SS:68:ILE:HD11	2.27	0.65
48:5:1976:G:N2	48:5:1991:A:N7	2.45	0.65
51:9:1419:C:O2	51:9:1429:G:N2	2.30	0.65
69:RR:117:LEU:HD23	69:RR:118:GLN:N	2.11	0.65
84:gg:253:GLY:O	84:gg:286:CYS:N	2.29	0.65
29:d:33:ILE:HG22	29:d:44:ARG:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DD:53:THR:HG22	55:DD:91:VAL:HB	1.78	0.65
59:HH:155:LYS:NZ	74:WW:51:GLU:OE2	2.23	0.65
24:Y:102:SER:OG	24:Y:103:LYS:NZ	2.30	0.65
29:d:20:VAL:HG12	29:d:20:VAL:O	1.97	0.65
76:YY:40:ILE:HD13	76:YY:60:PHE:CE2	2.32	0.65
87:jj:552:LEU:HD12	87:jj:553:ALA:N	2.11	0.65
48:5:1077:C:N3	48:5:1233:G:N1	2.40	0.65
84:gg:173:LEU:HD23	84:gg:189:ILE:HG12	1.78	0.65
84:gg:236:ILE:HG21	84:gg:239:LEU:HD21	1.79	0.65
86:ii:188:LEU:O	86:ii:192:ARG:HG3	1.96	0.65
86:ii:310:LYS:NZ	86:ii:314:MET:SD	2.70	0.65
5:E:64:MET:HE2	5:E:64:MET:HA	1.78	0.64
55:DD:210:ILE:HG21	69:RR:19:LYS:HZ3	1.62	0.64
80:cc:13:ARG:NH2	80:cc:35:MET:HE3	2.12	0.64
83:ff:112:LEU:HD12	83:ff:113:ARG:HH12	1.61	0.64
87:jj:378:LEU:HD11	87:jj:532:VAL:HG11	1.78	0.64
48:5:1991:A:O2'	48:5:1992:U:O5'	2.14	0.64
52:AA:178:LEU:O	52:AA:182:VAL:HG23	1.97	0.64
86:ii:146:PHE:CD1	86:ii:275:LEU:HD22	2.32	0.64
36:k:7:GLU:N	36:k:7:GLU:OE1	2.30	0.64
51:9:985:G:H4'	66:OO:138:ASP:CG	2.22	0.64
51:9:1542:C:OP1	71:TT:62:ARG:NH1	2.28	0.64
55:DD:32:ASP:O	55:DD:34:TYR:N	2.29	0.64
61:JJ:58:ARG:O	61:JJ:62:THR:HG23	1.97	0.64
48:5:3888:G:O2'	48:5:3889:G:OP1	2.15	0.64
62:KK:39:ASN:OD1	62:KK:39:ASN:O	2.15	0.64
51:9:691:G:N2	51:9:692:G:N7	2.45	0.64
51:9:190:G:O2'	51:9:209:A:N6	2.29	0.64
59:HH:153:LEU:HD21	59:HH:186:ASN:OD1	1.98	0.64
68:QQ:63:PHE:CE2	68:QQ:92:LEU:HD22	2.33	0.64
84:gg:145:GLU:O	84:gg:175:LYS:NZ	2.30	0.64
4:D:209:ARG:HA	4:D:212:MET:HE2	1.80	0.64
16:Q:122:THR:OG1	16:Q:124:ASP:OD1	2.14	0.64
35:j:49:TRP:O	48:5:1646:A:O2'	2.12	0.64
48:5:4378:A:O2'	48:5:4379:A:H2'	1.98	0.64
84:gg:48:ASP:N	84:gg:51:ASN:O	2.31	0.64
84:gg:270:LEU:HD13	84:gg:310:TRP:CD2	2.33	0.64
48:5:37:U:OP1	92:5:5417:HOH:O	2.14	0.64
51:9:1354:G:N2	51:9:1357:A:OP2	2.30	0.64
57:FF:20:PHE:CE2	57:FF:69:VAL:HG21	2.33	0.64
1:A:37:ARG:NH2	48:5:4088:C:OP1	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:173:GLN:OE1	14:O:177:LEU:HD12	1.98	0.64
51:9:1281:G:O2'	51:9:1282:A:OP1	2.10	0.64
11:L:158:ARG:NH2	48:5:1378:C:C5	2.66	0.64
72:UU:48:LEU:CD2	72:UU:101:ILE:HD11	2.28	0.64
48:5:2489:C:O2'	48:5:2491:C:N4	2.31	0.63
53:BB:225:LEU:CD2	53:BB:229:MET:HE3	2.28	0.63
48:5:749:G:O2'	48:5:750:U:OP2	2.16	0.63
51:9:1429:G:H2'	51:9:1430:C:O4'	1.97	0.63
51:9:1461:G:O2'	51:9:1464:C:N4	2.31	0.63
54:CC:94:ILE:HG21	54:CC:162:ILE:HD12	1.80	0.63
33:h:35:LYS:HA	33:h:44:LEU:HD11	1.80	0.63
48:5:3654:G:O2'	48:5:3693:U:OP1	2.15	0.63
48:5:4944:C:OP1	48:5:4944:C:H4'	1.97	0.63
51:9:75:G:O2'	51:9:76:U:H3'	1.97	0.63
51:9:1351:G:O2'	51:9:1378:A:N1	2.31	0.63
55:DD:93:THR:OG1	55:DD:96:LEU:HD12	1.98	0.63
66:OO:117:ARG:NH1	78:aa:48:ALA:O	2.30	0.63
87:jj:235:ALA:HB3	87:jj:238:PHE:HE1	1.64	0.63
48:5:978:G:N2	48:5:1277:G:H22	1.96	0.63
48:5:4098:A:H61	48:5:4110:C:H42	1.46	0.63
48:5:4635:A:H8	48:5:5048:A:H61	1.46	0.63
70:SS:55:ARG:HD2	77:ZZ:48:VAL:HG22	1.80	0.63
84:gg:249:CYS:SG	84:gg:291:TRP:NE1	2.71	0.63
19:T:70:HIS:NE2	48:5:4327:C:OP1	2.31	0.63
58:GG:157:VAL:HG11	58:GG:176:ILE:CD1	2.25	0.63
64:MM:85:LEU:HD22	64:MM:106:CYS:O	1.98	0.63
67:PP:93:MET:HE2	67:PP:106:GLU:HB2	1.80	0.63
3:C:95:MET:HG3	48:5:2351:OMC:HM23	1.78	0.63
10:J:105:PHE:HE1	10:J:134:LEU:HD11	1.63	0.63
48:5:406:C:O2'	48:5:407:A:OP1	2.14	0.63
59:HH:95:ILE:HD12	59:HH:129:ILE:HG23	1.81	0.63
63:LL:111:VAL:HG12	63:LL:140:PHE:HB2	1.80	0.63
84:gg:8:ARG:HA	84:gg:8:ARG:HE	1.64	0.63
84:gg:270:LEU:HD22	84:gg:310:TRP:CE3	2.34	0.63
46:2:54:U:H2'	46:2:55:U:O4'	1.99	0.63
51:9:176:U:H2'	51:9:177:G:O4'	1.98	0.63
80:cc:26:GLN:OE1	80:cc:26:GLN:N	2.31	0.63
32:g:45:ALA:HB3	32:g:82:MET:HE2	1.81	0.63
63:LL:65:ASN:O	63:LL:132:ARG:NH1	2.32	0.63
72:UU:26:SER:CB	72:UU:110:VAL:HG22	2.28	0.63
84:gg:198:VAL:HA	84:gg:209:SER:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:271:VAL:HG11	87:jj:282:LEU:HD21	1.81	0.63
44:t:21:GLU:HG2	44:t:56:LEU:HD12	1.81	0.62
51:9:495:U:H2'	51:9:496:C:O4'	1.99	0.62
67:PP:60:LEU:HD12	67:PP:92:SER:OG	1.99	0.62
86:ii:374:LEU:O	86:ii:374:LEU:HD23	1.99	0.62
4:D:166:ALA:HB1	4:D:171:LEU:HD12	1.81	0.62
7:G:86:VAL:HG13	7:G:183:ILE:HG22	1.81	0.62
20:U:23:LEU:HD21	20:U:87:THR:OG1	1.99	0.62
51:9:1406:G:N2	51:9:1442:OMU:O4	2.32	0.62
51:9:1490:OMG:N2	72:UU:72:GLU:OE1	2.32	0.62
52:AA:34:MET:HE2	52:AA:149:ASN:C	2.24	0.62
3:C:254:GLU:OE2	3:C:258:ARG:NH1	2.30	0.62
47:3:43:A:H2'	47:3:44:G:C8	2.33	0.62
52:AA:119:PRO:O	52:AA:142:LEU:HD13	1.99	0.62
72:UU:48:LEU:HD21	72:UU:97:ILE:HG22	1.82	0.62
74:WW:86:LEU:HD21	74:WW:104:LEU:HD11	1.80	0.62
48:5:3689:G:O2'	48:5:3818:UY1:OP2	2.17	0.62
51:9:1347:PSU:H2'	51:9:1348:G:C8	2.34	0.62
56:EE:248:ILE:HD12	61:JJ:72:PHE:CD2	2.33	0.62
84:gg:23:THR:HG22	84:gg:24:THR:H	1.65	0.62
18:S:169:THR:HG21	48:5:4875:G:C5	2.34	0.62
30:e:21:ILE:HD11	30:e:53:ILE:HD11	1.81	0.62
51:9:1740:C:OP1	60:II:44:HIS:ND1	2.30	0.62
62:KK:72:THR:O	62:KK:76:ILE:HG13	1.99	0.62
84:gg:199:THR:OG1	84:gg:200:VAL:N	2.32	0.62
48:5:1477:C:O2'	48:5:1478:C:OP1	2.18	0.62
51:9:1664:A:O2'	51:9:1666:C:N4	2.33	0.62
62:KK:16:PHE:HE1	62:KK:76:ILE:HG23	1.63	0.62
69:RR:90:ALA:O	69:RR:93:GLN:NE2	2.32	0.62
74:WW:50:PHE:HB3	74:WW:63:VAL:HG13	1.82	0.62
86:ii:308:THR:O	86:ii:312:LEU:HD12	1.99	0.62
48:5:914:U:O2'	48:5:915:A:O4'	2.18	0.62
48:5:3899:OMG:OP2	92:5:5418:HOH:O	2.16	0.62
48:5:4605:A:H2'	48:5:4606:G:O4'	2.00	0.62
51:9:846:G:C4	56:EE:19:MET:HE3	2.34	0.62
35:j:26:ALA:O	35:j:34:CYS:O	2.18	0.62
48:5:734:G:H1	48:5:929:A:H62	1.47	0.62
50:8:83:C:H4'	50:8:85:U:O2	2.00	0.62
58:GG:102:VAL:HG23	58:GG:106:LEU:CD1	2.29	0.62
87:jj:128:LYS:NZ	87:jj:138:PRO:O	2.32	0.62
69:RR:11:LYS:O	69:RR:15:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2409:U:H5	48:5:2783:A:N1	1.97	0.62
56:EE:19:MET:SD	56:EE:108:ARG:HD2	2.40	0.62
57:FF:99:ILE:HG22	57:FF:103:LEU:HD12	1.82	0.62
6:F:25:ALA:O	6:F:29:ILE:HD13	1.99	0.61
51:9:1589:A:N3	51:9:1653:U:O2'	2.29	0.61
67:PP:100:LYS:HG3	67:PP:101:THR:HG23	1.82	0.61
72:UU:40:ILE:HG23	72:UU:50:VAL:HG11	1.81	0.61
83:ff:127:MET:HE2	83:ff:136:CYS:N	2.16	0.61
84:gg:79:LEU:HD21	84:gg:120:ILE:CG2	2.30	0.61
12:M:119:ARG:NE	14:O:193:THR:OG1	2.32	0.61
49:7:98:G:O6	92:7:302:HOH:O	2.12	0.61
84:gg:191:HIS:CG	84:gg:195:LEU:HD21	2.34	0.61
3:C:193:LYS:HD2	3:C:196:MET:HE2	1.82	0.61
4:D:3:PHE:HD2	48:5:1753:G:H21	1.49	0.61
36:k:23:VAL:HG23	36:k:64:LEU:HG	1.81	0.61
51:9:3:C:O2	61:JJ:18:ARG:NH2	2.29	0.61
51:9:586:G:OP1	61:JJ:176:LYS:NZ	2.31	0.61
51:9:1350:U:O2'	52:AA:110:ASN:OD1	2.09	0.61
58:GG:102:VAL:HG21	58:GG:109:LEU:CD2	2.26	0.61
60:II:149:TYR:O	60:II:153:LYS:HG2	2.00	0.61
48:5:1979:A:H2'	48:5:1980:U:C1'	2.30	0.61
51:9:833:C:O2'	51:9:834:C:O5'	2.16	0.61
51:9:1348:G:H22	51:9:1381:G:N2	1.98	0.61
68:QQ:128:GLU:CD	68:QQ:137:ALA:HB1	2.25	0.61
61:JJ:108:ARG:O	61:JJ:149:VAL:HG22	2.00	0.61
70:SS:30:ILE:HD11	70:SS:67:VAL:HG11	1.82	0.61
81:dd:31:ILE:HB	81:dd:36:LEU:HD23	1.83	0.61
84:gg:207:CYS:HB2	84:gg:221:LEU:HD11	1.82	0.61
87:jj:428:LEU:HD23	87:jj:474:LEU:HD23	1.82	0.61
1:A:137:ILE:HD11	1:A:149:LYS:HB2	1.82	0.61
48:5:711:A:H2'	48:5:712:C:C6	2.36	0.61
51:9:488:U:O2	51:9:488:U:H2'	2.01	0.61
51:9:1588:A:H2'	51:9:1589:A:C8	2.36	0.61
53:BB:73:ASP:OD1	66:OO:128:ARG:NE	2.29	0.61
8:H:43:VAL:HG21	8:H:73:ILE:HD13	1.83	0.61
16:Q:150:ARG:NH1	48:5:1498:G:OP1	2.29	0.61
48:5:2502:A:O2'	48:5:2503:G:OP1	2.09	0.61
51:9:333:G:H2'	51:9:334:C:O4'	2.00	0.61
51:9:1745:A:H1'	58:GG:66:GLY:HA2	1.82	0.61
67:PP:107:ILE:HA	67:PP:111:MET:SD	2.40	0.61
87:jj:529:ALA:HB3	87:jj:551:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:125:VAL:HG22	33:h:123:ALA:HB3	1.82	0.61
42:r:80:THR:HG21	42:r:96:MET:HE1	1.83	0.61
51:9:1348:G:H22	51:9:1381:G:H22	1.47	0.61
53:BB:114:VAL:HG22	53:BB:120:MET:CE	2.31	0.61
76:YY:55:ILE:CD1	76:YY:75:ILE:HD12	2.30	0.61
13:N:45:PRO:O	13:N:49:ARG:HG3	2.01	0.61
54:CC:102:LEU:HD22	54:CC:130:ILE:HG12	1.83	0.61
48:5:758:G:H2'	48:5:759:G:O4'	2.01	0.60
48:5:2568:C:N4	48:5:2569:G:O6	2.32	0.60
55:DD:177:LEU:CD1	55:DD:182:LEU:HD12	2.30	0.60
63:LL:42:LEU:HD13	63:LL:72:ILE:HD11	1.83	0.60
86:ii:347:THR:OG1	86:ii:350:GLN:OE1	2.13	0.60
87:jj:240:PHE:HB2	87:jj:271:VAL:HG12	1.82	0.60
13:N:108:ARG:NH2	48:5:54:G:O2'	2.32	0.60
18:S:24:THR:O	18:S:24:THR:HG22	1.99	0.60
58:GG:7:PHE:HB2	58:GG:113:ILE:HD12	1.83	0.60
48:5:1234:G:O2'	48:5:1235:G:OP2	2.17	0.60
48:5:1377:G:H21	48:5:1380:G:H5'	1.65	0.60
56:EE:112:HIS:NE2	56:EE:237:SER:OG	2.34	0.60
58:GG:145:PHE:HB2	58:GG:147:LEU:HD11	1.83	0.60
87:jj:223:GLN:HE21	87:jj:247:LEU:HD21	1.66	0.60
7:G:83:PHE:HA	7:G:183:ILE:HD13	1.82	0.60
7:G:254:GLU:OE1	7:G:255:LYS:N	2.34	0.60
45:1:63:SER:O	45:1:66:LEU:HD13	2.01	0.60
49:7:111:C:H2'	49:7:112:U:O4'	2.01	0.60
51:9:1466:G:C5'	69:RR:4:VAL:HG22	2.30	0.60
86:ii:145:LYS:O	86:ii:222:ALA:N	2.32	0.60
22:W:44:ARG:NE	48:5:3615:G:N3	2.46	0.60
48:5:1235:G:HO2'	48:5:1236:C:P	2.21	0.60
76:YY:55:ILE:O	76:YY:94:HIS:NE2	2.31	0.60
48:5:4407:G:N7	92:5:5458:HOH:O	2.31	0.60
51:9:94:G:N7	92:9:2019:HOH:O	2.31	0.60
52:AA:62:ALA:O	52:AA:66:VAL:HG23	2.02	0.60
59:HH:169:LYS:O	59:HH:172:THR:OG1	2.16	0.60
48:5:263:G:H2'	48:5:264:C:O4'	2.02	0.60
48:5:1432:G:O2'	48:5:1451:G:N2	2.33	0.60
54:CC:146:GLU:OE1	55:DD:116:ARG:NH1	2.35	0.60
58:GG:66:GLY:O	58:GG:68:LEU:HD12	2.02	0.60
48:5:4739:C:N4	48:5:4740:G:O6	2.34	0.60
51:9:1535:U:O4	57:FF:159:ARG:NH1	2.33	0.60
53:BB:120:MET:HE2	53:BB:142:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:UU:44:LYS:HE2	72:UU:44:LYS:HA	1.82	0.60
84:gg:305:ASN:O	84:gg:306:LEU:HD12	2.02	0.60
47:3:6:G:H2'	47:3:7:A:C8	2.36	0.60
48:5:3641:U:H5	48:5:3646:A:N7	1.99	0.60
87:jj:59:GLY:HA2	87:jj:62:ILE:HD13	1.84	0.60
13:N:67:ARG:NH2	48:5:3673:C:OP2	2.34	0.60
48:5:470:A:N6	48:5:684:G:O2'	2.34	0.60
48:5:1238:A:O2'	48:5:1239:C:OP1	2.18	0.60
60:II:57:ALA:HB2	60:II:183:GLY:HA2	1.84	0.60
80:cc:20:ARG:CD	80:cc:28:THR:HG22	2.32	0.60
84:gg:40:ILE:HD11	84:gg:66:VAL:HG21	1.84	0.60
84:gg:198:VAL:O	84:gg:198:VAL:HG12	2.01	0.60
86:ii:372:MET:HE3	86:ii:376:GLU:OE2	2.02	0.60
87:jj:428:LEU:O	87:jj:432:ILE:O	2.20	0.60
51:9:695:C:N4	51:9:735:C:H42	2.00	0.59
51:9:862:A:O2'	51:9:863:PSU:H5''	2.02	0.59
56:EE:115:THR:OG1	56:EE:117:GLU:O	2.18	0.59
86:ii:34:MET:HE1	86:ii:100:ILE:HG22	1.82	0.59
87:jj:485:ILE:HB	87:jj:517:VAL:HG22	1.84	0.59
25:Z:136:PHE:OXT	48:5:4122:G:O2'	2.20	0.59
51:9:932:G:O2'	51:9:934:G:OP2	2.10	0.59
68:QQ:31:LEU:HD11	68:QQ:33:LYS:HD3	1.84	0.59
75:XX:89:GLY:HA2	82:ee:9:VAL:HG12	1.82	0.59
86:ii:77:SER:OG	86:ii:111:ASN:OD1	2.19	0.59
87:jj:169:LYS:HB2	87:jj:230:VAL:HG21	1.84	0.59
1:A:207:VAL:HG13	1:A:208:GLU:HG3	1.83	0.59
29:d:87:ARG:NH2	29:d:122:VAL:HG11	2.17	0.59
47:3:70:G:O2'	48:5:3740:G:O2'	1.98	0.59
51:9:1306:U:H3'	51:9:1307:U:H5''	1.84	0.59
53:BB:114:VAL:HG22	53:BB:120:MET:HE1	1.84	0.59
51:9:1466:G:OP2	69:RR:5:ARG:NH1	2.35	0.59
57:FF:71:ARG:NH2	57:FF:148:ASN:OD1	2.34	0.59
57:FF:142:SER:HB2	80:cc:50:VAL:HG12	1.84	0.59
42:r:66:ARG:NH1	42:r:75:THR:O	2.32	0.59
67:PP:26:LEU:HD12	67:PP:26:LEU:O	2.02	0.59
87:jj:371:ASP:HA	87:jj:514:THR:HG22	1.83	0.59
44:t:28:LEU:HD23	44:t:28:LEU:C	2.28	0.59
48:5:1547:A:O2'	48:5:2814:C:O2	2.18	0.59
51:9:546:G:H2'	51:9:547:G:O4'	2.02	0.59
51:9:1109:C:HO2'	51:9:1110:G:C1'	2.13	0.59
51:9:1298:G:O2'	51:9:1299:A:O4'	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1408:U:O2'	51:9:1409:A:C5'	2.51	0.59
61:JJ:163:SER:O	61:JJ:166:GLY:N	2.34	0.59
67:PP:87:PRO:HA	67:PP:112:ILE:HD11	1.83	0.59
86:ii:219:VAL:HG11	86:ii:249:LYS:HG3	1.83	0.59
51:9:1261:C:O2	81:dd:10:HIS:NE2	2.35	0.59
52:AA:190:SER:O	52:AA:191:ARG:HB3	2.02	0.59
9:I:38:ARG:NH1	9:I:45:GLU:OE2	2.34	0.59
35:j:36:LYS:NZ	48:5:372:A:OP1	2.33	0.59
36:k:15:ALA:O	36:k:64:LEU:HD22	2.03	0.59
43:s:13:TYR:CE1	43:s:54:LEU:HD21	2.38	0.59
51:9:1295:A:H2'	51:9:1296:U:O4'	2.02	0.59
26:a:39:HIS:O	26:a:40:HIS:ND1	2.35	0.59
48:5:2501:C:H2'	48:5:2502:A:O4'	2.02	0.59
48:5:2639:U:H2'	48:5:2694:G:H1	1.68	0.59
52:AA:42:LYS:HD2	52:AA:48:ILE:HD11	1.83	0.59
20:U:97:ARG:NH1	48:5:2626:U:O4	2.35	0.59
51:9:1139:C:H5	51:9:1149:A:H62	1.49	0.59
57:FF:32:ASP:O	57:FF:34:SER:N	2.36	0.59
44:t:18:THR:OG1	44:t:59:THR:O	2.18	0.58
47:3:75:C:O2'	47:3:76:A:H4'	2.03	0.58
48:5:165:A:H2'	48:5:166:C:O4'	2.02	0.58
54:CC:255:LEU:HD23	73:VV:1:MET:CE	2.29	0.58
58:GG:181:THR:CG2	58:GG:182:PRO:HD2	2.33	0.58
68:QQ:105:LYS:C	68:QQ:105:LYS:HD3	2.28	0.58
42:r:38:PHE:O	42:r:45:HIS:NE2	2.29	0.58
43:s:45:MET:HA	43:s:45:MET:HE3	1.86	0.58
51:9:323:C:H3'	51:9:324:C:H5''	1.85	0.58
51:9:563:G:O2'	51:9:564:A:O5'	2.19	0.58
55:DD:210:ILE:N	55:DD:210:ILE:HD12	2.19	0.58
59:HH:79:LEU:HD23	59:HH:83:LEU:HD13	1.84	0.58
69:RR:14:ARG:HG2	69:RR:69:ILE:HD11	1.84	0.58
86:ii:305:VAL:HG13	86:ii:306:GLU:N	2.19	0.58
48:5:1098:G:N3	48:5:1198:G:N2	2.52	0.58
57:FF:35:LEU:HD12	57:FF:117:ILE:HG12	1.85	0.58
58:GG:102:VAL:HG23	58:GG:106:LEU:HD11	1.85	0.58
69:RR:40:ILE:O	69:RR:40:ILE:HG13	2.04	0.58
27:b:44:ARG:NH2	48:5:1466:G:OP2	2.35	0.58
28:c:99:PRO:HG3	28:c:105:ILE:HD12	1.84	0.58
39:n:18:ARG:NH2	51:9:1183:A:OP2	2.37	0.58
43:s:29:ILE:HD11	43:s:78:LEU:HD13	1.85	0.58
52:AA:85:ARG:NH2	69:RR:82:ASP:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:146:GLU:OE1	55:DD:116:ARG:HD2	2.04	0.58
70:SS:36:VAL:HG22	70:SS:40:TYR:CD2	2.38	0.58
87:jj:78:ASN:OD1	87:jj:79:LEU:N	2.36	0.58
87:jj:79:LEU:O	87:jj:82:GLU:N	2.33	0.58
3:C:196:MET:HE3	48:5:352:G:C5	2.39	0.58
4:D:261:VAL:HG21	49:7:119:U:C2	2.38	0.58
51:9:465:A:OP1	87:jj:584:LYS:NZ	2.36	0.58
87:jj:221:GLU:OE1	87:jj:221:GLU:N	2.37	0.58
7:G:136:LEU:HD21	7:G:204:PHE:CD2	2.39	0.58
48:5:1198:G:H2'	48:5:1199:G:C1'	2.34	0.58
48:5:1475:G:O2'	48:5:1476:C:O4'	2.10	0.58
51:9:986:G:C8	66:OO:137:SER:O	2.56	0.58
60:II:100:CYS:SG	60:II:175:ILE:HD12	2.43	0.58
75:XX:123:VAL:C	75:XX:130:LEU:HD12	2.29	0.58
23:X:95:THR:HG22	23:X:139:ARG:HA	1.85	0.58
48:5:1320:U:O2'	48:5:1891:A:N1	2.34	0.58
67:PP:30:TYR:O	67:PP:34:MET:HG3	2.03	0.58
86:ii:34:MET:HE1	86:ii:100:ILE:CG2	2.33	0.58
4:D:278:ASP:OD2	48:5:1185:G:O2'	2.22	0.58
11:L:7:GLY:O	26:a:49:HIS:NE2	2.37	0.58
26:a:77:LYS:HE2	48:5:1502:G:H22	1.69	0.58
53:BB:225:LEU:O	53:BB:229:MET:HG2	2.04	0.58
84:gg:32:LEU:HB3	84:gg:71:ILE:HD11	1.85	0.58
86:ii:317:VAL:O	86:ii:317:VAL:HG13	2.02	0.58
3:C:4:ALA:O	3:C:29:LYS:NZ	2.32	0.58
48:5:1978:C:N4	48:5:1979:A:C2	2.72	0.58
48:5:2564:G:O2'	48:5:2565:A:O4'	2.17	0.58
48:5:2795:A:OP1	92:5:5423:HOH:O	2.17	0.58
48:5:3603:G:HO2'	48:5:3604:A:P	2.25	0.58
48:5:4348:A:O2'	48:5:4350:C:OP2	2.22	0.58
51:9:77:A:O2'	58:GG:174:PRO:O	2.15	0.58
67:PP:41:GLN:HG3	67:PP:84:ILE:HD12	1.85	0.58
25:Z:74:VAL:HG23	25:Z:101:PHE:HE2	1.69	0.57
48:5:4208:U:OP1	48:5:4334:U:O2'	2.21	0.57
51:9:25:A:O2'	51:9:26:U:O5'	2.22	0.57
51:9:420:G:O2'	51:9:660:C:N3	2.33	0.57
51:9:1240:A:H8	51:9:1267:C:HO2'	1.52	0.57
61:JJ:110:LEU:O	61:JJ:114:VAL:HG23	2.03	0.57
84:gg:178:ASN:O	84:gg:182:CYS:N	2.32	0.57
48:5:4444:C:OP1	92:5:5424:HOH:O	2.17	0.57
51:9:308:G:N3	60:II:45:THR:HG22	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:27:ASP:OD2	69:RR:30:THR:OG1	2.09	0.57
84:gg:210:GLY:HA3	84:gg:239:LEU:HD11	1.86	0.57
25:Z:97:ASN:OD1	25:Z:100:VAL:HG13	2.05	0.57
51:9:147:A:H2'	51:9:148:U:C6	2.39	0.57
53:BB:39:PHE:CE2	53:BB:74:LEU:HD13	2.39	0.57
55:DD:138:VAL:HG12	55:DD:184:ILE:CD1	2.33	0.57
58:GG:7:PHE:CZ	58:GG:9:ALA:HB3	2.38	0.57
84:gg:74:ASP:HB3	84:gg:76:GLN:HG2	1.86	0.57
7:G:106:THR:HG22	7:G:107:LYS:H	1.69	0.57
48:5:130:C:H2'	48:5:131:C:O4'	2.04	0.57
48:5:504:G:O2'	48:5:505:G:OP1	2.21	0.57
48:5:1098:G:N1	48:5:1196:G:O6	2.36	0.57
48:5:4393:G:O4'	48:5:4447:5MC:HM53	2.05	0.57
48:5:5016:A:H2	48:5:5033:G:H21	1.44	0.57
51:9:1391:OMC:HM23	81:dd:56:ASP:HB2	1.87	0.57
56:EE:117:GLU:OE2	56:EE:118:GLU:N	2.35	0.57
67:PP:22:LEU:O	67:PP:25:LEU:N	2.37	0.57
70:SS:5:ILE:N	77:ZZ:50:PHE:O	2.36	0.57
80:cc:52:GLU:OE1	80:cc:52:GLU:N	2.33	0.57
48:5:158:A:N1	48:5:276:C:O2'	2.32	0.57
48:5:4118:U:O2'	48:5:4119:C:OP2	2.21	0.57
51:9:562:U:H2'	51:9:563:G:C8	2.40	0.57
86:ii:100:ILE:HD11	86:ii:108:LYS:HD3	1.86	0.57
48:5:485:C:O2'	48:5:486:C:O5'	2.22	0.57
48:5:930:G:O2'	48:5:931:C:P	2.63	0.57
51:9:942:G:H2'	51:9:943:U:C6	2.40	0.57
51:9:1018:U:H5''	65:NN:71:ILE:HD12	1.87	0.57
67:PP:37:TYR:OH	67:PP:86:LEU:HD23	2.05	0.57
75:XX:91:LEU:HB3	82:ee:9:VAL:HG11	1.87	0.57
86:ii:169:LEU:HB2	86:ii:212:LEU:HD13	1.86	0.57
42:r:66:ARG:O	48:5:479:G:OP1	2.21	0.57
48:5:1380:G:H4'	48:5:1381:U:O2	2.05	0.57
48:5:4635:A:H3'	48:5:4636:U:H4'	1.85	0.57
52:AA:168:ALA:HB1	52:AA:204:TYR:HB3	1.85	0.57
11:L:36:ARG:NH1	48:5:1364:U:OP2	2.37	0.57
51:9:57:U:OP1	51:9:504:G:O2'	2.20	0.57
51:9:1394:G:HO2'	51:9:1395:C:P	2.27	0.57
52:AA:11:LYS:O	52:AA:15:VAL:HG13	2.05	0.57
71:TT:13:GLU:OE2	71:TT:16:ARG:NH1	2.38	0.57
25:Z:102:ARG:HG2	25:Z:102:ARG:HH11	1.70	0.57
51:9:561:A:H2'	51:9:562:U:O4'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1373:C:O2'	51:9:1465:A:O2'	2.07	0.57
60:II:61:ASP:OD1	60:II:61:ASP:N	2.38	0.57
61:JJ:113:GLN:OE1	61:JJ:113:GLN:HA	2.04	0.57
31:f:106:TYR:HB2	31:f:107:PRO:HD3	1.85	0.57
44:t:128:THR:O	44:t:132:ILE:HG13	2.05	0.57
48:5:4136:G:N1	48:5:4148:C:N3	2.44	0.57
51:9:686:PSU:O4	59:HH:118:ARG:NH2	2.38	0.57
51:9:1536:G:H2'	51:9:1537:A:C8	2.39	0.57
70:SS:84:LEU:HD12	70:SS:95:TYR:HB3	1.86	0.57
84:gg:52:TYR:CZ	84:gg:309:VAL:HG21	2.39	0.57
7:G:161:VAL:O	7:G:161:VAL:CG1	2.53	0.56
16:Q:49:LYS:HG2	16:Q:53:MET:HE3	1.87	0.56
48:5:1980:U:O2'	48:5:1982:G:H3'	2.05	0.56
51:9:147:A:O2'	51:9:148:U:O5'	2.22	0.56
51:9:691:G:C2	51:9:692:G:N7	2.72	0.56
53:BB:129:THR:OG1	53:BB:131:ASP:O	2.18	0.56
57:FF:20:PHE:HE1	57:FF:94:LYS:HZ1	1.53	0.56
77:ZZ:92:LEU:HD22	77:ZZ:109:TYR:HE1	1.70	0.56
84:gg:76:GLN:O	84:gg:77:PHE:C	2.48	0.56
5:E:209:VAL:HG23	5:E:263:LYS:HE3	1.87	0.56
14:O:110:PRO:HA	14:O:113:ASP:OD1	2.05	0.56
20:U:33:ILE:HG22	20:U:96:LEU:HD21	1.87	0.56
48:5:497:G:O2'	48:5:499:G:O4'	2.23	0.56
48:5:964:A:H2'	48:5:965:G:O4'	2.04	0.56
51:9:1452:A:OP2	69:RR:32:LYS:NZ	2.36	0.56
51:9:1797:U:H2'	51:9:1798:C:C6	2.40	0.56
87:jj:62:ILE:HD11	87:jj:72:ILE:CG1	2.32	0.56
4:D:265:ARG:NE	4:D:267:ASN:O	2.39	0.56
44:t:42:VAL:O	44:t:46:ILE:HD12	2.05	0.56
48:5:692:A:H2'	48:5:693:C:C6	2.41	0.56
51:9:308:G:C2	60:II:45:THR:HG22	2.41	0.56
51:9:466:G:O2'	58:GG:72:ARG:NH2	2.38	0.56
51:9:1427:C:N4	51:9:1428:G:O6	2.38	0.56
54:CC:70:VAL:HG21	54:CC:93:ILE:HG23	1.87	0.56
55:DD:113:LEU:HD23	55:DD:118:ALA:HB2	1.87	0.56
59:HH:69:LEU:HD12	59:HH:96:ALA:HB2	1.88	0.56
68:QQ:41:MET:SD	71:TT:10:ASN:N	2.79	0.56
70:SS:86:ARG:NE	70:SS:89:ASP:OD1	2.34	0.56
84:gg:14:HIS:O	84:gg:305:ASN:HB3	2.05	0.56
84:gg:24:THR:HB	84:gg:71:ILE:HG21	1.86	0.56
12:M:31:ILE:O	18:S:98:ARG:NE	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1866:U:H2'	48:5:1867:A:O4'	2.06	0.56
51:9:1447:G:OP1	72:UU:87:ARG:NH2	2.35	0.56
56:EE:47:PHE:CE2	56:EE:52:LEU:HD11	2.41	0.56
56:EE:95:THR:HG22	76:YY:16:ARG:CG	2.35	0.56
58:GG:152:ASP:OD2	58:GG:154:ARG:NH2	2.38	0.56
15:P:39:MET:HE2	15:P:43:LYS:HZ2	1.69	0.56
40:o:56:PHE:N	47:3:76:A:OP1	2.36	0.56
48:5:261:G:C2'	48:5:262:G:O4'	2.52	0.56
48:5:1072:C:HO2'	48:5:1073:G:P	2.24	0.56
48:5:1073:G:H1	48:5:1238:A:H2	1.49	0.56
48:5:1764:G:O2'	48:5:1767:A:N6	2.38	0.56
51:9:1430:C:O2	51:9:1431:G:N7	2.39	0.56
53:BB:117:TRP:O	53:BB:153:THR:O	2.24	0.56
53:BB:228:LEU:HD23	53:BB:229:MET:HE1	1.88	0.56
42:r:125:MET:HA	42:r:125:MET:HE3	1.87	0.56
43:s:28:PHE:CE2	43:s:98:ILE:HG21	2.41	0.56
48:5:1100:U:N3	48:5:1168:G:N7	2.54	0.56
48:5:2259:G:H3'	48:5:2260:C:H5'	1.88	0.56
48:5:4111:U:H2'	48:5:4112:C:C6	2.41	0.56
51:9:873:G:O2'	51:9:874:G:OP1	2.17	0.56
51:9:1308:U:O2'	83:ff:128:ALA:HB1	2.05	0.56
59:HH:43:LEU:HD21	59:HH:71:SER:OG	2.05	0.56
10:J:92:TYR:O	10:J:172:GLY:O	2.23	0.56
36:k:57:LYS:HA	36:k:60:LEU:HD12	1.88	0.56
48:5:4574:U:H3'	48:5:4575:G:H5''	1.88	0.56
51:9:940:U:H2'	51:9:941:C:C6	2.41	0.56
52:AA:10:MET:HE2	52:AA:55:TRP:HB2	1.86	0.56
55:DD:12:VAL:HG21	81:dd:34:TYR:HB3	1.87	0.56
84:gg:197:THR:O	84:gg:239:LEU:HD12	2.05	0.56
84:gg:232:GLY:O	84:gg:257:LYS:NZ	2.39	0.56
3:C:196:MET:HE3	48:5:352:G:C6	2.40	0.56
19:T:32:ARG:HG2	19:T:32:ARG:HH11	1.69	0.56
46:2:19:G:OP1	46:2:60:A:N6	2.33	0.56
48:5:4131:G:H2'	48:5:4132:C:C6	2.40	0.56
48:5:4751:G:H1	48:5:4948:C:H5	1.54	0.56
48:5:4771:C:HO2'	48:5:4772:C:H6	1.53	0.56
51:9:1596:U:H2'	51:9:1597:C:O4'	2.06	0.56
64:MM:83:LYS:HG2	64:MM:103:VAL:HG12	1.87	0.56
72:UU:60:THR:HG23	72:UU:60:THR:O	2.05	0.56
47:3:25:C:H2'	47:3:26:A:O4'	2.06	0.56
48:5:1477:C:HO2'	48:5:1478:C:P	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:176:LYS:O	54:CC:200:ARG:NH2	2.39	0.56
62:KK:43:LEU:C	62:KK:43:LEU:HD13	2.31	0.56
72:UU:48:LEU:HD21	72:UU:97:ILE:HG21	1.87	0.56
86:ii:251:LEU:HD11	86:ii:274:VAL:HG13	1.88	0.56
87:jj:411:TYR:CD1	87:jj:484:LEU:HD12	2.40	0.56
48:5:1802:A:O2'	48:5:1837:A:OP1	2.14	0.56
51:9:913:A:H1'	59:HH:66:VAL:HB	1.88	0.56
52:AA:10:MET:SD	52:AA:15:VAL:HG12	2.46	0.56
59:HH:14:GLU:OE1	59:HH:14:GLU:N	2.37	0.56
1:A:65:ASP:OD2	1:A:68:ARG:HG2	2.07	0.55
7:G:136:LEU:HD21	7:G:204:PHE:CE2	2.41	0.55
56:EE:153:LEU:HD11	58:GG:216:ARG:HH11	1.71	0.55
69:RR:17:ILE:HD11	69:RR:54:VAL:HG13	1.88	0.55
86:ii:96:TYR:OH	86:ii:132:HIS:O	2.22	0.55
45:1:65:GLY:O	48:5:3908:A:N6	2.38	0.55
60:II:113:TYR:CD2	60:II:121:LEU:HD22	2.42	0.55
61:JJ:113:GLN:HG3	61:JJ:149:VAL:HG21	1.87	0.55
76:YY:27:VAL:HG11	76:YY:35:VAL:CG2	2.36	0.55
87:jj:123:LEU:O	87:jj:155:TYR:OH	2.25	0.55
14:O:175:MET:HE1	14:O:179:LYS:CE	2.36	0.55
34:i:30:ARG:NH1	48:5:327:U:O2'	2.39	0.55
51:9:190:G:OP1	60:II:149:TYR:OH	2.24	0.55
51:9:319:C:N4	58:GG:186:GLN:OE1	2.39	0.55
51:9:1623:A:H5''	70:SS:133:GLY:HA3	1.87	0.55
56:EE:125:LYS:O	56:EE:142:HIS:N	2.40	0.55
57:FF:125:SER:HB2	57:FF:136:ARG:NH2	2.21	0.55
64:MM:21:VAL:HG23	64:MM:121:LYS:CD	2.37	0.55
84:gg:124:SER:OG	84:gg:125:ARG:N	2.39	0.55
35:j:82:THR:HB	50:8:94:G:H21	1.70	0.55
43:s:121:VAL:HG21	43:s:183:PHE:CE1	2.41	0.55
48:5:407:A:O2'	48:5:410:A:OP1	2.18	0.55
48:5:1755:C:O2'	48:5:1757:U:OP2	2.20	0.55
51:9:213:G:HO2'	51:9:214:U:P	2.30	0.55
51:9:1801:A:H2'	51:9:1802:C:C6	2.41	0.55
54:CC:252:THR:HG22	74:WW:99:PHE:CE1	2.42	0.55
84:gg:10:THR:HB	84:gg:306:LEU:HD23	1.88	0.55
87:jj:106:LEU:HD23	87:jj:106:LEU:C	2.30	0.55
2:B:35:ASP:HB3	2:B:186:ASN:CG	2.32	0.55
47:3:37:A:C5	47:3:38:A:C8	2.95	0.55
48:5:930:G:O2'	48:5:931:C:OP1	2.22	0.55
48:5:2759:G:O2'	48:5:2760:G:O4'	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:203:G:P	60:II:147:LYS:NZ	2.80	0.55
51:9:1084:A:OP1	51:9:1858:G:O2'	2.25	0.55
51:9:1126:G:OP1	52:AA:41:ARG:NH1	2.39	0.55
58:GG:98:ARG:NH1	58:GG:101:ILE:O	2.38	0.55
58:GG:145:PHE:HB3	58:GG:147:LEU:HD21	1.88	0.55
77:ZZ:56:ASP:OD1	77:ZZ:56:ASP:C	2.50	0.55
23:X:93:ASN:O	23:X:95:THR:HG23	2.07	0.55
24:Y:111:LEU:HD12	24:Y:116:LYS:HG3	1.89	0.55
48:5:3773:U:O2'	48:5:3775:A:C2	2.58	0.55
51:9:629:A:O2'	51:9:631:U:OP1	2.24	0.55
51:9:687:C:O3'	59:HH:121:THR:HG23	2.07	0.55
51:9:955:A:N1	51:9:968:U:O2'	2.37	0.55
51:9:1408:U:HO2'	51:9:1409:A:C5'	2.16	0.55
51:9:1563:G:OP1	71:TT:121:ARG:NE	2.37	0.55
56:EE:45:ILE:HA	56:EE:61:VAL:HG21	1.89	0.55
59:HH:50:GLU:HA	59:HH:60:ILE:HD13	1.87	0.55
60:II:34:ALA:HB2	60:II:56:ARG:HD3	1.88	0.55
75:XX:122:VAL:HG12	75:XX:130:LEU:HD11	1.87	0.55
10:J:105:PHE:CE1	10:J:134:LEU:HD11	2.41	0.55
23:X:63:LYS:HZ1	23:X:66:PRO:HA	1.72	0.55
25:Z:115:LYS:NZ	25:Z:119:GLU:OE2	2.40	0.55
35:j:59:THR:O	50:8:42:G:OP1	2.24	0.55
48:5:1199:G:O2'	48:5:1200:G:O5'	2.25	0.55
51:9:464:A:OP1	87:jj:576:ARG:NH1	2.38	0.55
51:9:1416:C:H2'	51:9:1417:C:C2	2.41	0.55
56:EE:103:TYR:CD1	56:EE:189:LEU:HD21	2.41	0.55
75:XX:63:ASN:ND2	75:XX:114:ASP:OD2	2.38	0.55
8:H:111:LEU:HD11	8:H:125:ARG:HG2	1.89	0.55
16:Q:83:VAL:O	16:Q:83:VAL:HG12	2.07	0.55
33:h:110:LYS:NZ	48:5:111:C:OP1	2.39	0.55
48:5:1978:C:HO2'	48:5:1979:A:P	2.30	0.55
48:5:2093:G:H4'	48:5:2094:C:H5'	1.89	0.55
48:5:4992:G:H2'	48:5:4993:G:C8	2.42	0.55
51:9:1757:G:C6	51:9:1775:U:O2	2.59	0.55
84:gg:120:ILE:HD12	84:gg:133:ASN:O	2.07	0.55
86:ii:389:LEU:HD21	86:ii:391:ILE:HD11	1.88	0.55
7:G:93:THR:HG22	7:G:97:LYS:HZ2	1.72	0.55
8:H:140:GLN:OE1	8:H:140:GLN:HA	2.07	0.55
56:EE:105:THR:HG21	56:EE:245:ARG:H	1.71	0.55
7:G:142:THR:HG23	48:5:151:G:O6	2.07	0.55
15:P:104:LEU:HD23	48:5:400:A2M:CM'	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:48:ARG:NH2	48:5:2279:A:O2'	2.39	0.55
48:5:1414:C:C4	48:5:1415:G:N7	2.75	0.55
51:9:1255:G:OP1	51:9:1256:G:O2'	2.17	0.55
53:BB:131:ASP:O	53:BB:133:TYR:N	2.39	0.55
60:II:22:HIS:ND1	60:II:23:LYS:O	2.38	0.55
65:NN:79:GLY:O	65:NN:80:LEU:HD23	2.06	0.55
84:gg:94:THR:HG23	84:gg:96:THR:HG22	1.89	0.55
87:jj:61:CYS:SG	87:jj:62:ILE:HD12	2.47	0.55
33:h:60:VAL:O	33:h:64:THR:HG22	2.07	0.54
48:5:1484:G:H2'	48:5:1484:G:N3	2.22	0.54
48:5:1996:C:H3'	48:5:1997:U:H5''	1.89	0.54
48:5:4382:G:O2'	48:5:4544:A:N1	2.37	0.54
51:9:71:G:O2'	51:9:71:G:N3	2.41	0.54
51:9:1636:G:H2'	51:9:1636:G:N3	2.22	0.54
51:9:1663:A:HO2'	51:9:1664:A:P	2.24	0.54
51:9:1757:G:O6	51:9:1775:U:C2	2.59	0.54
52:AA:42:LYS:CD	52:AA:48:ILE:HD11	2.37	0.54
55:DD:209:SER:O	69:RR:40:ILE:HG22	2.06	0.54
66:OO:117:ARG:HD3	80:cc:62:GLU:OE1	2.06	0.54
84:gg:16:GLY:N	84:gg:305:ASN:OD1	2.40	0.54
86:ii:251:LEU:HD23	86:ii:275:LEU:HD23	1.88	0.54
87:jj:428:LEU:HD23	87:jj:474:LEU:CD2	2.38	0.54
3:C:292:ILE:HG23	16:Q:128:LEU:CD1	2.38	0.54
5:E:94:THR:OG1	48:5:2258:C:O2	2.24	0.54
28:c:81:LEU:HD21	28:c:94:LEU:CD2	2.37	0.54
33:h:24:LEU:HD22	33:h:53:SER:OG	2.07	0.54
48:5:1982:G:HO2'	48:5:1983:A:P	2.29	0.54
48:5:2046:G:O2'	48:5:2047:A:OP2	2.14	0.54
48:5:5001:U:H2'	48:5:5002:U:O4'	2.06	0.54
51:9:65:C:OP1	58:GG:136:LYS:NZ	2.39	0.54
51:9:77:A:H1'	58:GG:176:ILE:HD13	1.88	0.54
51:9:654:A:N6	92:9:2021:HOH:O	2.32	0.54
51:9:877:C:C4	51:9:879:C:OP1	2.60	0.54
51:9:1834:A:N3	51:9:1834:A:O2'	2.35	0.54
68:QQ:112:LEU:HB2	68:QQ:120:LEU:HD11	1.88	0.54
30:e:17:THR:HG21	48:5:1301:C:O2	2.07	0.54
48:5:2024:G:O2'	48:5:2025:A:OP2	2.19	0.54
51:9:531:A:H3'	51:9:532:C:H5''	1.89	0.54
51:9:563:G:O2'	51:9:564:A:P	2.65	0.54
64:MM:21:VAL:HG23	64:MM:121:LYS:HD3	1.88	0.54
11:L:128:PRO:HD2	11:L:144:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:22:THR:HG23	29:d:122:VAL:HB	1.88	0.54
48:5:2259:G:H5'	48:5:2260:C:OP2	2.07	0.54
48:5:3807:A:N7	92:5:5462:HOH:O	2.33	0.54
51:9:203:G:H2'	51:9:204:G:O4'	2.07	0.54
69:RR:105:MET:CE	69:RR:109:LEU:HD11	2.24	0.54
6:F:28:LYS:HE2	6:F:32:LEU:HD11	1.90	0.54
10:J:170:TYR:O	10:J:171:ASP:OD2	2.26	0.54
15:P:54:LYS:HA	15:P:83:TRP:CD1	2.42	0.54
37:l:2:SER:N	48:5:2407:G:O6	2.40	0.54
48:5:1307:A:H2'	48:5:1308:C:C6	2.43	0.54
48:5:2394:G:O6	92:5:5422:HOH:O	2.17	0.54
48:5:2415:U:H2'	48:5:2416:G:O4'	2.07	0.54
48:5:3910:C:H2'	48:5:3911:C:C6	2.42	0.54
51:9:216:C:OP1	56:EE:134:LYS:HE3	2.08	0.54
51:9:376:A:H2'	51:9:377:G:O4'	2.07	0.54
51:9:1059:G:C6	51:9:1060:A:N1	2.75	0.54
51:9:1228:A:H2'	51:9:1229:G:C8	2.43	0.54
51:9:1439:A:H2'	51:9:1440:C:C6	2.42	0.54
51:9:1646:C:O2'	51:9:1647:A:OP2	2.22	0.54
56:EE:180:LEU:HD11	56:EE:192:ILE:HG22	1.90	0.54
70:SS:48:ALA:O	70:SS:66:ARG:NH2	2.41	0.54
84:gg:8:ARG:N	84:gg:309:VAL:O	2.38	0.54
87:jj:377:MET:HE2	87:jj:535:PHE:CZ	2.42	0.54
48:5:1890:G:N2	48:5:1938:C:N4	2.55	0.54
51:9:928:G:H1	51:9:1013:U:H3	1.56	0.54
56:EE:180:LEU:HD11	56:EE:192:ILE:CG2	2.38	0.54
58:GG:57:ASP:OD1	58:GG:59:GLN:N	2.32	0.54
69:RR:38:ILE:C	69:RR:38:ILE:HD12	2.33	0.54
84:gg:68:ASP:HB3	84:gg:111:VAL:HG22	1.90	0.54
87:jj:435:ALA:HB1	87:jj:441:PHE:CG	2.42	0.54
16:Q:61:LEU:HD23	16:Q:66:MET:HE2	1.90	0.54
16:Q:134:ARG:NH2	48:5:1449:C:OP1	2.40	0.54
48:5:261:G:O2'	48:5:262:G:O4'	2.26	0.54
48:5:1804:A:O4'	48:5:1806:G:C8	2.61	0.54
51:9:929:G:H2'	51:9:930:C:O4'	2.07	0.54
51:9:1223:A:OP1	57:FF:79:HIS:N	2.39	0.54
55:DD:52:ALA:O	55:DD:91:VAL:HG23	2.08	0.54
55:DD:158:ILE:HD12	55:DD:164:VAL:CG1	2.36	0.54
59:HH:140:VAL:HG11	59:HH:159:ASP:OD1	2.08	0.54
80:cc:25:GLY:N	80:cc:26:GLN:OE1	2.41	0.54
43:s:17:ILE:HG22	43:s:54:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4065:G:O3'	48:5:4066:U:O4'	2.26	0.54
52:AA:203:PHE:CE2	69:RR:91:LEU:HD13	2.42	0.54
54:CC:270:THR:O	54:CC:274:VAL:HG23	2.07	0.54
59:HH:139:ILE:HG22	59:HH:156:VAL:CG1	2.38	0.54
87:jj:459:VAL:HA	87:jj:462:LEU:HD13	1.89	0.54
4:D:76:CYS:SG	4:D:112:ARG:NH2	2.81	0.54
33:h:3:LYS:NZ	50:8:80:A:O2'	2.39	0.54
36:k:15:ALA:CB	36:k:61:PRO:HG2	2.38	0.54
48:5:966:A:H62	48:5:2096:G:H2'	1.73	0.54
48:5:1979:A:H2'	48:5:1980:U:O4'	2.07	0.54
48:5:4894:A:O2'	48:5:4895:C:OP1	2.24	0.54
51:9:1409:A:H4'	68:QQ:24:HIS:NE2	2.23	0.54
55:DD:38:GLU:O	55:DD:49:ILE:HD12	2.08	0.54
59:HH:51:ILE:HG23	59:HH:179:LYS:HD3	1.89	0.54
87:jj:86:ARG:O	87:jj:130:ASN:ND2	2.39	0.54
3:C:358:LEU:C	3:C:358:LEU:HD23	2.33	0.54
6:F:107:VAL:HG13	6:F:131:MET:HE2	1.90	0.54
7:G:93:THR:HG22	7:G:97:LYS:NZ	2.23	0.54
9:I:21:ARG:NH2	48:5:1789:C:OP1	2.40	0.54
9:I:39:LYS:NZ	48:5:1750:G:OP1	2.30	0.54
14:O:168:TYR:OH	48:5:4768:G:OP1	2.23	0.54
14:O:189:ILE:O	14:O:190:SER:OG	2.24	0.54
48:5:2639:U:O2'	48:5:2640:G:O5'	2.26	0.54
51:9:123:G:H3'	51:9:124:U:H5''	1.90	0.54
51:9:862:A:C2'	51:9:863:PSU:H5''	2.37	0.54
51:9:1541:G:N3	71:TT:12:GLN:NE2	2.56	0.54
60:II:148:LYS:O	60:II:151:GLU:HG3	2.08	0.54
83:ff:136:CYS:CB	83:ff:139:CYS:SG	2.95	0.54
87:jj:41:VAL:HG22	87:jj:48:ALA:HA	1.90	0.54
14:O:181:ALA:O	14:O:185:VAL:HG22	2.08	0.53
51:9:799:U:H2'	51:9:800:U:C6	2.43	0.53
56:EE:100:ARG:NH2	56:EE:118:GLU:O	2.41	0.53
87:jj:217:LEU:HD12	87:jj:221:GLU:HB3	1.90	0.53
5:E:48:ARG:O	5:E:67:ARG:NH2	2.40	0.53
5:E:184:LEU:O	48:5:4883:C:N4	2.41	0.53
6:F:40:MET:HE2	6:F:40:MET:N	2.24	0.53
9:I:179:ASP:OD1	9:I:180:GLU:N	2.40	0.53
13:N:126:THR:HG23	13:N:127:TYR:CD2	2.43	0.53
33:h:121:VAL:HG12	33:h:122:LYS:N	2.23	0.53
51:9:17:C:O2'	51:9:1194:A:N1	2.37	0.53
51:9:1629:C:OP1	70:SS:39:ARG:NE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:135:THR:O	52:AA:138:SER:OG	2.25	0.53
54:CC:206:SER:HB2	54:CC:224:THR:HG21	1.90	0.53
59:HH:25:GLN:O	59:HH:28:LEU:HB2	2.08	0.53
69:RR:17:ILE:HG21	69:RR:69:ILE:HD13	1.90	0.53
3:C:164:THR:O	3:C:168:VAL:HG23	2.08	0.53
4:D:208:MET:HB3	4:D:233:PRO:HG3	1.90	0.53
15:P:104:LEU:HD23	48:5:400:A2M:HM'3	1.90	0.53
43:s:83:ARG:O	43:s:86:VAL:HG23	2.08	0.53
48:5:1455:G:HO2'	48:5:1456:C:P	2.29	0.53
48:5:1755:C:H42	48:5:1775:A:H61	1.57	0.53
48:5:1890:G:N2	48:5:1939:A:N6	2.51	0.53
48:5:1990:A:HO2'	48:5:1991:A:P	2.25	0.53
48:5:4927:G:H2'	48:5:4928:C:O2	2.08	0.53
58:GG:41:LEU:O	58:GG:41:LEU:HD13	2.09	0.53
87:jj:129:PRO:O	87:jj:143:ILE:HD11	2.08	0.53
87:jj:326:ASP:OD1	87:jj:327:ALA:N	2.41	0.53
3:C:143:ARG:NH1	48:5:2300:A:N7	2.56	0.53
29:d:46:LEU:HD22	29:d:72:VAL:HG11	1.90	0.53
44:t:15:LEU:C	44:t:15:LEU:HD12	2.33	0.53
48:5:2544:G:C8	50:8:126:C:O4'	2.62	0.53
57:FF:20:PHE:HE2	57:FF:69:VAL:HG21	1.73	0.53
58:GG:171:THR:HG23	58:GG:171:THR:O	2.09	0.53
87:jj:111:THR:HG23	87:jj:495:GLU:OE2	2.08	0.53
87:jj:245:SER:O	87:jj:247:LEU:HD23	2.08	0.53
30:e:86:GLU:OE2	30:e:118:LEU:HD11	2.09	0.53
43:s:66:ARG:NH1	43:s:69:LEU:HD23	2.24	0.53
48:5:206:U:O2'	48:5:208:A:N7	2.32	0.53
51:9:1284:A:O2'	64:MM:105:GLY:O	2.25	0.53
57:FF:127:ARG:O	57:FF:128:ILE:HG23	2.08	0.53
59:HH:147:LYS:HD3	74:WW:49:GLU:OE2	2.09	0.53
84:gg:197:THR:HG21	84:gg:239:LEU:H	1.74	0.53
87:jj:120:LEU:HD22	87:jj:239:MET:HG2	1.90	0.53
87:jj:168:ILE:HG22	87:jj:239:MET:CB	2.35	0.53
2:B:139:ASP:OD1	2:B:139:ASP:N	2.41	0.53
4:D:15:ARG:HD2	48:5:1743:A:O4'	2.09	0.53
25:Z:24:VAL:HG21	25:Z:87:VAL:CG2	2.37	0.53
47:3:10:G:N2	47:3:26:A:H1'	2.23	0.53
48:5:4162:C:O2	48:5:4162:C:O5'	2.27	0.53
48:5:4904:G:C2	48:5:4918:C:C2	2.97	0.53
51:9:75:G:HO2'	51:9:76:U:H3'	1.72	0.53
51:9:141:A:H61	51:9:177:G:H21	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:196:C:H3'	51:9:197:U:C6	2.44	0.53
51:9:643:A:OP1	61:JJ:41:ARG:NH2	2.38	0.53
87:jj:165:LYS:HZ3	87:jj:235:ALA:HB2	1.73	0.53
26:a:132:ARG:HA	26:a:135:GLU:OE1	2.09	0.53
51:9:53:C:O2'	51:9:507:G:N7	2.24	0.53
51:9:108:G:C2'	51:9:109:PSU:H5''	2.39	0.53
51:9:1493:C:OP1	51:9:1494:U:O2'	2.26	0.53
58:GG:220:ALA:HB3	58:GG:224:ARG:HH21	1.74	0.53
70:SS:16:LEU:HD11	70:SS:72:GLN:HE21	1.73	0.53
84:gg:199:THR:HG21	84:gg:239:LEU:O	2.08	0.53
87:jj:65:CYS:HB2	87:jj:70:LEU:HD12	1.90	0.53
12:M:11:ARG:CZ	12:M:61:ILE:HD11	2.39	0.53
48:5:1662:C:H2'	48:5:1663:C:C6	2.44	0.53
48:5:4459:U:H2'	48:5:4460:U:C6	2.44	0.53
51:9:872:A:O2'	51:9:873:G:P	2.67	0.53
51:9:1102:G:H1	51:9:1130:G:H1	1.57	0.53
51:9:1118:C:O2'	79:bb:75:GLU:OE2	2.20	0.53
55:DD:113:LEU:CD2	55:DD:118:ALA:HB2	2.38	0.53
57:FF:32:ASP:C	57:FF:34:SER:H	2.17	0.53
64:MM:50:CYS:HB2	64:MM:110:VAL:HG22	1.91	0.53
80:cc:42:ILE:HD11	80:cc:64:GLU:HB2	1.91	0.53
87:jj:14:ASP:O	87:jj:17:LYS:NZ	2.35	0.53
13:N:43:THR:OG1	13:N:131:GLU:OE2	2.25	0.53
25:Z:58:GLY:O	25:Z:62:ILE:HG12	2.09	0.53
44:t:15:LEU:CA	44:t:62:LEU:HD12	2.39	0.53
48:5:4872:G:H4'	48:5:4873:G:H5'	1.90	0.53
51:9:962:A:N1	51:9:1055:A:O2'	2.41	0.53
55:DD:172:VAL:O	55:DD:173:ARG:NH1	2.42	0.53
61:JJ:128:VAL:HG13	61:JJ:132:GLN:OE1	2.08	0.53
87:jj:449:LEU:HD11	87:jj:472:LEU:HD12	1.90	0.53
8:H:106:GLN:HG2	8:H:111:LEU:HD12	1.91	0.53
12:M:85:LYS:O	12:M:89:THR:HG23	2.09	0.53
51:9:1315:U:OP1	62:KK:2:LEU:HD22	2.09	0.53
51:9:1429:G:H2'	51:9:1430:C:C1'	2.39	0.53
70:SS:46:ARG:HG2	71:TT:35:ASP:HB2	1.91	0.53
71:TT:6:VAL:HG23	71:TT:14:PHE:CZ	2.44	0.53
72:UU:24:LEU:HD12	72:UU:112:VAL:HG22	1.91	0.53
81:dd:38:MET:SD	81:dd:43:PHE:HA	2.49	0.53
86:ii:287:ILE:HD13	86:ii:399:GLY:CA	2.38	0.53
1:A:198:ARG:NH2	48:5:3687:A:OP2	2.42	0.52
48:5:1452:A:H2'	48:5:1453:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2567:G:H2'	48:5:2568:C:O4'	2.09	0.52
48:5:4635:A:H8	48:5:5048:A:N6	2.08	0.52
51:9:305:U:H6	60:II:182:CYS:O	1.91	0.52
51:9:1451:G:N7	69:RR:44:LYS:NZ	2.49	0.52
52:AA:14:ASP:OD1	52:AA:14:ASP:N	2.40	0.52
84:gg:127:LYS:HD2	84:gg:149:GLU:O	2.09	0.52
87:jj:377:MET:HB2	87:jj:518:VAL:HG22	1.90	0.52
6:F:49:ILE:HD11	6:F:184:ILE:HD12	1.90	0.52
6:F:59:GLU:HG2	6:F:63:MET:HE2	1.92	0.52
6:F:85:GLU:OE2	19:T:136:ARG:NH2	2.43	0.52
48:5:4584:A:H1'	48:5:4719:G:C2	2.45	0.52
48:5:4967:A:H2'	48:5:4968:A:C8	2.44	0.52
48:5:5016:A:C2	48:5:5033:G:N2	2.65	0.52
51:9:1007:C:O2'	65:NN:104:ARG:NH1	2.41	0.52
54:CC:263:LYS:HG2	54:CC:267:GLN:NE2	2.24	0.52
62:KK:21:MET:HE2	62:KK:32:HIS:CE1	2.44	0.52
72:UU:68:THR:HG23	72:UU:70:CYS:O	2.09	0.52
84:gg:42:MET:HE2	84:gg:57:ARG:HB2	1.92	0.52
16:Q:13:VAL:O	16:Q:13:VAL:HG12	2.08	0.52
18:S:15:ARG:HB3	18:S:27:LEU:HD23	1.91	0.52
43:s:135:THR:HG22	43:s:152:ILE:HD13	1.90	0.52
46:2:8:U:O2'	46:2:21:A:N1	2.41	0.52
46:2:15:G:N2	46:2:48:C:O2	2.33	0.52
48:5:1087:A:H2'	48:5:1088:C:C6	2.45	0.52
48:5:1214:C:H3'	48:5:1215:C:C5'	2.39	0.52
48:5:1990:A:H2'	48:5:1990:A:N3	2.23	0.52
48:5:4260:U:H2'	48:5:4261:C:C6	2.44	0.52
48:5:4963:G:H2'	48:5:4964:C:O5'	2.08	0.52
51:9:71:G:H1	51:9:74:G:H22	1.57	0.52
51:9:837:A:N1	51:9:840:C:C2	2.77	0.52
54:CC:262:THR:HG22	54:CC:263:LYS:N	2.24	0.52
56:EE:48:LEU:HA	56:EE:52:LEU:HD12	1.91	0.52
79:bb:35:VAL:HG11	79:bb:73:LEU:CD1	2.39	0.52
87:jj:281:TYR:CD1	87:jj:281:TYR:C	2.87	0.52
87:jj:564:ILE:HG23	87:jj:577:ILE:CD1	2.39	0.52
32:g:62:LYS:NZ	48:5:2516:G:O2'	2.42	0.52
33:h:116:LEU:HD13	33:h:117:ARG:O	2.09	0.52
44:t:148:PRO:O	44:t:150:ASP:N	2.42	0.52
48:5:1199:G:N3	48:5:1200:G:N7	2.57	0.52
48:5:1999:A:H2'	48:5:2000:G:C4	2.44	0.52
51:9:1598:G:N7	77:ZZ:85:ARG:NH2	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:QQ:57:LEU:HD23	68:QQ:112:LEU:HD23	1.91	0.52
84:gg:152:SER:OG	84:gg:195:LEU:O	2.22	0.52
87:jj:441:PHE:CE1	87:jj:445:VAL:HG21	2.43	0.52
46:2:75:C:H2'	46:2:76:A:O4'	2.10	0.52
51:9:488:U:H3'	51:9:489:A:C5'	2.39	0.52
52:AA:52:LYS:HB2	69:RR:109:LEU:HD22	1.92	0.52
54:CC:252:THR:OG1	54:CC:254:ASP:OD1	2.25	0.52
55:DD:139:SER:OG	55:DD:149:SER:OG	2.06	0.52
57:FF:79:HIS:O	57:FF:81:ARG:N	2.43	0.52
59:HH:145:ARG:NE	74:WW:51:GLU:HG3	2.25	0.52
70:SS:34:LYS:HG2	70:SS:103:LEU:HD23	1.91	0.52
2:B:67:VAL:HG21	2:B:72:VAL:CG1	2.40	0.52
44:t:13:VAL:HG23	44:t:64:ILE:HD12	1.91	0.52
48:5:2095:A:H2'	48:5:2096:G:C8	2.44	0.52
51:9:928:G:H2'	51:9:929:G:C8	2.45	0.52
53:BB:135:LEU:HD23	53:BB:217:MET:SD	2.49	0.52
58:GG:48:TYR:OH	58:GG:121:ILE:HG12	2.09	0.52
59:HH:53:VAL:HG12	59:HH:54:GLY:N	2.25	0.52
59:HH:76:GLN:HG2	59:HH:135:PHE:CD2	2.44	0.52
68:QQ:63:PHE:CZ	68:QQ:92:LEU:HD22	2.44	0.52
76:YY:117:VAL:HG21	76:YY:125:VAL:HG11	1.92	0.52
86:ii:319:ILE:HG22	86:ii:321:ILE:HD13	1.92	0.52
13:N:184:ILE:O	48:5:78:U:OP1	2.27	0.52
48:5:1976:G:C6	48:5:2002:A:O2'	2.62	0.52
48:5:2814:C:O2	48:5:2814:C:H2'	2.10	0.52
48:5:3783:A:O5'	48:5:3784:A:H5''	2.09	0.52
48:5:3786:U:O2	48:5:3814:U:H4'	2.09	0.52
48:5:4591:U:H2'	48:5:4592:C:C6	2.45	0.52
48:5:4884:G:O2'	48:5:4885:U:P	2.68	0.52
48:5:5057:C:H2'	48:5:5058:A:C8	2.44	0.52
51:9:491:C:O2'	51:9:493:A:N7	2.37	0.52
3:C:335:MET:HE2	6:F:57:HIS:CG	2.45	0.52
11:L:39:ARG:NH2	48:5:1362:G:OP1	2.38	0.52
21:V:48:ARG:HD2	48:5:4621:C:OP1	2.10	0.52
48:5:480:C:HO2'	48:5:481:G:P	2.25	0.52
48:5:3867:A2M:HM'3	48:5:3880:G:N2	2.24	0.52
51:9:303:C:H2'	51:9:304:C:O4'	2.09	0.52
51:9:1658:G:OP2	51:9:1660:C:N4	2.36	0.52
55:DD:193:ASP:CB	55:DD:194:PRO:HD3	2.40	0.52
59:HH:43:LEU:HD12	59:HH:75:ILE:HD11	1.92	0.52
66:OO:58:GLY:O	66:OO:62:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:PP:111:MET:HE2	67:PP:119:PHE:CD1	2.45	0.52
84:gg:32:LEU:CB	84:gg:71:ILE:HD11	2.40	0.52
87:jj:56:ILE:N	91:jj:601:SF4:S3	2.74	0.52
48:5:643:C:H2'	48:5:644:G:C8	2.45	0.52
51:9:546:G:C2'	51:9:547:G:O4'	2.58	0.52
56:EE:107:GLY:HA3	56:EE:189:LEU:HD22	1.92	0.52
59:HH:17:ASP:OD1	59:HH:19:PHE:N	2.42	0.52
63:LL:20:LYS:O	63:LL:21:LYS:CB	2.57	0.52
2:B:78:ILE:N	2:B:78:ILE:HD12	2.24	0.52
3:C:89:GLN:O	48:5:2353:U:OP1	2.28	0.52
30:e:57:ASN:OD1	48:5:1899:G:O2'	2.24	0.52
48:5:1358:G:O2'	48:5:1360:G:O6	2.20	0.52
48:5:1755:C:H42	48:5:1775:A:N6	2.06	0.52
48:5:2055:G:H4'	48:5:2056:G:OP2	2.10	0.52
51:9:1227:G:C2	51:9:1228:A:C8	2.98	0.52
51:9:1344:A:H4'	51:9:1345:G:OP1	2.10	0.52
76:YY:56:PHE:CZ	76:YY:91:LEU:HD23	2.45	0.52
87:jj:377:MET:HG3	87:jj:518:VAL:HG22	1.91	0.52
7:G:56:LYS:HA	48:5:4085:A:C8	2.45	0.51
7:G:108:GLN:OE1	7:G:108:GLN:N	2.38	0.51
42:r:64:MET:HE3	42:r:102:TYR:CD2	2.45	0.51
48:5:23:C:H2'	48:5:24:G:O4'	2.10	0.51
48:5:99:A:H2'	48:5:100:C:O2	2.10	0.51
48:5:496:G:H2'	48:5:497:G:O4'	2.10	0.51
48:5:1996:C:H42	48:5:2000:G:H22	1.58	0.51
48:5:2706:G:O2'	48:5:2709:C:N4	2.43	0.51
48:5:3701:OMC:N4	48:5:3745:U:H2'	2.26	0.51
50:8:81:C:H5'	50:8:82:A:O5'	2.10	0.51
51:9:507:G:O2'	51:9:508:A:OP1	2.24	0.51
51:9:1444:U:O2'	51:9:1445:PSU:H5''	2.09	0.51
51:9:1477:U:O2'	51:9:1478:U:P	2.67	0.51
57:FF:32:ASP:C	57:FF:34:SER:N	2.67	0.51
83:ff:114:ARG:O	83:ff:127:MET:HG3	2.11	0.51
84:gg:244:ASN:OD1	84:gg:245:ARG:N	2.43	0.51
86:ii:188:LEU:HD21	86:ii:192:ARG:NH2	2.25	0.51
87:jj:164:LEU:HD22	87:jj:236:ASP:CB	2.40	0.51
87:jj:472:LEU:HD13	87:jj:472:LEU:C	2.34	0.51
2:B:252:ALA:HB1	48:5:4524:G:N3	2.24	0.51
3:C:80:ARG:NH2	48:5:1645:C:OP1	2.42	0.51
37:l:44:TRP:CE3	48:5:2409:U:O2	2.63	0.51
48:5:1957:U:O2'	48:5:1958:A:O5'	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3625:G:O2'	48:5:3626:G:P	2.68	0.51
54:CC:102:LEU:HD23	54:CC:131:GLY:C	2.35	0.51
59:HH:33:ASN:OD1	59:HH:34:SER:N	2.43	0.51
65:NN:45:LEU:HD23	65:NN:49:GLN:HB3	1.92	0.51
86:ii:332:VAL:O	86:ii:332:VAL:HG13	2.09	0.51
87:jj:133:LYS:HD2	87:jj:136:ASP:O	2.10	0.51
8:H:106:GLN:CG	8:H:111:LEU:HD12	2.41	0.51
24:Y:92:GLY:O	24:Y:93:THR:OG1	2.28	0.51
48:5:2490:U:H2'	48:5:2491:C:C2	2.46	0.51
51:9:688:U:OP1	59:HH:103:LYS:HD2	2.10	0.51
51:9:1411:G:H8	51:9:1411:G:O5'	1.94	0.51
84:gg:178:ASN:O	84:gg:178:ASN:OD1	2.29	0.51
87:jj:470:VAL:O	87:jj:474:LEU:HG	2.10	0.51
26:a:2:PRO:CG	26:a:5:LEU:HD12	2.39	0.51
26:a:100:ILE:N	26:a:100:ILE:HD12	2.26	0.51
35:j:39:TYR:C	35:j:39:TYR:CD1	2.87	0.51
44:t:28:LEU:HD23	44:t:29:ALA:N	2.26	0.51
44:t:50:THR:HG21	44:t:72:GLU:CG	2.41	0.51
48:5:266:C:OP1	48:5:266:C:O4'	2.28	0.51
48:5:4152:G:H2'	48:5:4153:C:O4'	2.10	0.51
51:9:306:C:O2	51:9:307:G:N2	2.39	0.51
51:9:1310:U:OP1	83:ff:126:PHE:N	2.43	0.51
51:9:1404:U:O2	51:9:1580:A:H5'	2.11	0.51
51:9:1550:G:O2'	51:9:1558:C:O2	2.27	0.51
51:9:1809:A:H2'	51:9:1810:U:C6	2.46	0.51
71:TT:11:GLN:O	71:TT:15:VAL:HG23	2.10	0.51
2:B:223:THR:HA	2:B:338:VAL:HG22	1.92	0.51
10:J:167:GLN:HA	10:J:172:GLY:CA	2.41	0.51
11:L:128:PRO:CD	11:L:144:LEU:HD11	2.40	0.51
42:r:70:GLN:O	42:r:71:ARG:HG2	2.09	0.51
48:5:2504:C:O2	48:5:2505:C:C4	2.63	0.51
48:5:3706:C:H2'	48:5:3707:U:O4'	2.10	0.51
48:5:4397:A:OP1	92:5:5425:HOH:O	2.19	0.51
48:5:5006:U:H4'	48:5:5007:A:H5'	1.92	0.51
51:9:857:U:H2'	51:9:858:A:C8	2.45	0.51
51:9:1406:G:O3'	51:9:1407:U:H4'	2.11	0.51
57:FF:102:LEU:HD21	77:ZZ:100:VAL:HG21	1.91	0.51
64:MM:18:LEU:HD23	64:MM:18:LEU:C	2.35	0.51
68:QQ:109:LYS:HG2	68:QQ:120:LEU:HD13	1.93	0.51
73:VV:39:VAL:HG12	73:VV:45:ARG:O	2.09	0.51
87:jj:263:ILE:HG23	87:jj:263:ILE:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:118:ALA:O	48:5:1865:G:H5'	2.10	0.51
15:P:39:MET:HE2	15:P:43:LYS:NZ	2.26	0.51
25:Z:53:VAL:HB	25:Z:62:ILE:HD12	1.92	0.51
48:5:106:A:H2'	48:5:107:G:O4'	2.11	0.51
48:5:1905:U:OP1	92:5:5426:HOH:O	2.19	0.51
48:5:1931:C:O2'	48:5:1932:A:O5'	2.26	0.51
48:5:2002:A:N3	48:5:2002:A:H2'	2.26	0.51
48:5:2040:A:H4'	48:5:2041:A:O5'	2.10	0.51
48:5:2100:G:OP2	48:5:2100:G:H4'	2.11	0.51
51:9:13:C:H4'	51:9:1355:C:O2	2.10	0.51
51:9:327:G:H1'	51:9:328:U:OP2	2.10	0.51
51:9:526:A:OP1	82:ee:35:ARG:NH1	2.43	0.51
51:9:833:C:O2'	51:9:834:C:O4'	2.28	0.51
55:DD:127:MET:HE1	55:DD:133:GLY:HA2	1.91	0.51
59:HH:136:PRO:HB2	59:HH:166:VAL:HG23	1.92	0.51
62:KK:76:ILE:O	62:KK:80:ARG:HG2	2.11	0.51
87:jj:377:MET:CB	87:jj:518:VAL:HG22	2.41	0.51
8:H:165:THR:HG21	8:H:179:ILE:HG13	1.93	0.51
14:O:23:VAL:HG13	14:O:33:VAL:HG11	1.93	0.51
28:c:48:LEU:HD21	28:c:60:ILE:HG21	1.91	0.51
48:5:2065:G:H2'	48:5:2066:C:O4'	2.10	0.51
48:5:4395:U:OP2	92:5:5428:HOH:O	2.20	0.51
51:9:1039:C:H2'	51:9:1040:G:H5''	1.93	0.51
53:BB:154:SER:O	53:BB:154:SER:OG	2.27	0.51
59:HH:158:LEU:HD11	59:HH:187:PHE:CD2	2.44	0.51
62:KK:78:TYR:CD1	62:KK:78:TYR:C	2.88	0.51
68:QQ:25:CYS:SG	68:QQ:66:VAL:HG11	2.50	0.51
86:ii:135:ALA:O	86:ii:139:LEU:HD13	2.10	0.51
87:jj:281:TYR:HB2	87:jj:577:ILE:HG21	1.92	0.51
4:D:56:THR:HG22	4:D:57:ASN:H	1.75	0.51
12:M:136:LEU:HD13	12:M:136:LEU:C	2.36	0.51
48:5:1072:C:O2'	48:5:1073:G:P	2.67	0.51
48:5:1197:C:H2'	48:5:1198:G:C8	2.45	0.51
48:5:4508:C:N3	48:5:4512:U:H5	2.09	0.51
51:9:71:G:O2'	51:9:72:C:P	2.69	0.51
51:9:140:C:O2'	51:9:141:A:OP1	2.27	0.51
51:9:690:G:H3'	51:9:691:G:H8	1.74	0.51
58:GG:102:VAL:HG13	58:GG:102:VAL:O	2.10	0.51
1:A:215:ASN:ND2	48:5:4546:A:N7	2.57	0.51
32:g:56:VAL:HG13	32:g:72:LYS:HA	1.92	0.51
37:l:2:SER:O	37:l:3:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:100:TYR:O	48:5:4472:G:O2'	2.26	0.51
48:5:1980:U:H2'	48:5:1982:G:H5'	1.92	0.51
48:5:4906:C:H2'	48:5:4906:C:O2	2.11	0.51
51:9:985:G:H5'	66:OO:138:ASP:OD2	2.11	0.51
51:9:1418:C:H4'	51:9:1419:C:OP1	2.11	0.51
51:9:1746:U:H2'	51:9:1747:C:O4'	2.10	0.51
58:GG:142:ARG:HA	58:GG:147:LEU:HD12	1.92	0.51
20:U:23:LEU:HD21	20:U:87:THR:HG1	1.76	0.51
20:U:38:ASN:OD1	20:U:38:ASN:N	2.41	0.51
20:U:93:LYS:HE3	20:U:93:LYS:HA	1.92	0.51
44:t:62:LEU:HB2	44:t:75:PRO:CD	2.41	0.51
51:9:465:A:H4'	51:9:466:G:O5'	2.11	0.51
51:9:1102:G:N2	51:9:1130:G:N2	2.56	0.51
51:9:1531:A:H2'	51:9:1532:C:C6	2.45	0.51
53:BB:178:THR:O	53:BB:178:THR:CG2	2.59	0.51
55:DD:50:ILE:H	55:DD:50:ILE:HD12	1.75	0.51
58:GG:176:ILE:HG22	58:GG:179:LEU:HD23	1.93	0.51
59:HH:139:ILE:HG22	59:HH:156:VAL:HG11	1.93	0.51
71:TT:28:LEU:HA	71:TT:110:LEU:HD11	1.92	0.51
87:jj:188:LEU:HD23	87:jj:197:GLN:OE1	2.11	0.51
18:S:93:MET:HG2	48:5:1952:G:H4'	1.92	0.50
27:b:69:ALA:O	27:b:73:LYS:HG3	2.11	0.50
35:j:9:GLY:HA3	48:5:2800:G:H1'	1.93	0.50
48:5:922(B):C:C2'	48:5:923:C:OP1	2.59	0.50
48:5:1957:U:HO2'	48:5:1958:A:P	2.32	0.50
48:5:2503:G:H2'	48:5:2504:C:C1'	2.41	0.50
48:5:2528:G:H2'	48:5:2529:A:O4'	2.10	0.50
50:8:122:G:H21	50:8:128:C:N4	1.97	0.50
51:9:1019:C:H2'	51:9:1020:A:O4'	2.11	0.50
51:9:1130:G:H2'	51:9:1131:G:H5''	1.92	0.50
51:9:1744:G:HO2'	51:9:1745:A:P	2.33	0.50
57:FF:116:ILE:HD11	57:FF:151:ILE:HD11	1.93	0.50
58:GG:224:ARG:O	58:GG:228:ILE:HD12	2.11	0.50
68:QQ:42:ILE:CD1	68:QQ:51:LEU:HD11	2.31	0.50
72:UU:24:LEU:HD11	72:UU:112:VAL:HG13	1.89	0.50
74:WW:94:LEU:HD11	74:WW:102:ILE:HG23	1.93	0.50
76:YY:117:VAL:HG21	76:YY:125:VAL:CG1	2.41	0.50
87:jj:292:VAL:HG23	87:jj:292:VAL:O	2.10	0.50
25:Z:57:MET:HB2	25:Z:62:ILE:HD11	1.93	0.50
35:j:44:LYS:NZ	48:5:23:C:OP1	2.43	0.50
43:s:30:VAL:HG12	43:s:189:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:67:GLY:N	43:s:75:LEU:HD12	2.27	0.50
48:5:258:G:O2'	48:5:259:C:H5'	2.11	0.50
54:CC:78:LEU:HD23	54:CC:78:LEU:H	1.75	0.50
57:FF:40:ALA:HB1	57:FF:45:TYR:CG	2.46	0.50
59:HH:118:ARG:C	59:HH:121:THR:HG1	2.19	0.50
63:LL:76:VAL:HG22	63:LL:125:ILE:HD13	1.92	0.50
64:MM:21:VAL:CG2	64:MM:121:LYS:HD3	2.41	0.50
86:ii:332:VAL:O	86:ii:332:VAL:CG1	2.60	0.50
87:jj:564:ILE:HG23	87:jj:577:ILE:HD11	1.92	0.50
2:B:223:THR:HA	2:B:338:VAL:CG2	2.42	0.50
25:Z:91:LEU:HD22	25:Z:96:VAL:HG21	1.93	0.50
40:o:99:ARG:NH1	40:o:102:GLN:OE1	2.44	0.50
43:s:121:VAL:HG22	43:s:182:PRO:HB2	1.93	0.50
48:5:267:G:O2'	48:5:268:G:P	2.69	0.50
48:5:1316:OMG:HM22	48:5:1317:U:H5'	1.93	0.50
48:5:3736:A:H2'	48:5:3737:A:C8	2.46	0.50
48:5:4963:G:C2'	48:5:4964:C:O5'	2.59	0.50
51:9:532:C:C2'	51:9:533:A:O5'	2.60	0.50
51:9:640:A:H2'	51:9:641:A:C8	2.46	0.50
51:9:1287:A:H2'	51:9:1288:U:H5''	1.91	0.50
51:9:1441:U:H1'	51:9:1442:OMU:H5	1.92	0.50
54:CC:186:GLY:HA2	54:CC:242:ASP:OD2	2.11	0.50
55:DD:113:LEU:HD21	55:DD:117:ARG:HG2	1.92	0.50
64:MM:71:GLU:HG2	83:ff:109:ILE:HD12	1.93	0.50
76:YY:35:VAL:HG23	76:YY:40:ILE:HD11	1.93	0.50
78:aa:32:LYS:O	78:aa:37:LYS:NZ	2.40	0.50
84:gg:51:ASN:C	84:gg:51:ASN:OD1	2.55	0.50
84:gg:133:ASN:OD1	84:gg:133:ASN:N	2.44	0.50
14:O:190:SER:HA	14:O:193:THR:HB	1.93	0.50
16:Q:14:ARG:NH2	48:5:2083:C:OP1	2.44	0.50
30:e:98:GLU:OE1	30:e:123:THR:OG1	2.29	0.50
48:5:4990:C:OP2	48:5:4990:C:H4'	2.12	0.50
51:9:1088:U:H4'	51:9:1089:G:OP2	2.10	0.50
51:9:1395:C:HO2'	51:9:1396:A:P	2.26	0.50
51:9:1660:C:O5'	51:9:1660:C:O2	2.29	0.50
56:EE:73:ASP:OD2	56:EE:122:LYS:NZ	2.35	0.50
56:EE:195:ILE:C	56:EE:196:THR:HG1	2.10	0.50
71:TT:123:LEU:HD22	71:TT:127:GLY:HA3	1.94	0.50
72:UU:81:GLN:OE1	72:UU:83:ARG:NE	2.41	0.50
87:jj:484:LEU:HD13	87:jj:484:LEU:C	2.36	0.50
18:S:19:THR:HB	18:S:20:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1218:G:H2'	48:5:1219:G:O4'	2.12	0.50
48:5:1445:U:H2'	48:5:1446:C:C6	2.45	0.50
51:9:1037:G:OP2	92:9:2008:HOH:O	2.20	0.50
51:9:1324:G:H21	51:9:1510:G:C5'	2.24	0.50
75:XX:122:VAL:HG12	75:XX:130:LEU:CD1	2.41	0.50
86:ii:81:ARG:NE	86:ii:113:ASP:OD1	2.45	0.50
87:jj:258:THR:O	87:jj:262:LEU:HG	2.11	0.50
8:H:56:ARG:NE	8:H:58:ASP:OD2	2.45	0.50
10:J:164:ARG:HG3	10:J:168:GLN:OE1	2.12	0.50
27:b:53:GLY:O	27:b:57:MET:HG3	2.12	0.50
29:d:63:ARG:HD3	29:d:103:TYR:CD1	2.47	0.50
33:h:7:ARG:NH1	50:8:86:U:C2	2.80	0.50
48:5:269:G:H2'	48:5:270:U:C6	2.47	0.50
48:5:366:A:H2'	48:5:367:C:O4'	2.12	0.50
48:5:492:U:O2'	48:5:493:G:OP1	2.21	0.50
48:5:1982:G:O2'	48:5:1983:A:P	2.69	0.50
48:5:2092:G:N3	48:5:2093:G:N2	2.59	0.50
48:5:2465:C:H1'	48:5:3672:G:N2	2.23	0.50
51:9:196:C:H3'	51:9:197:U:H6	1.77	0.50
51:9:1823:A:N6	51:9:1824:A:C6	2.80	0.50
58:GG:113:ILE:HD11	58:GG:124:LEU:HD23	1.94	0.50
67:PP:87:PRO:HA	67:PP:90:VAL:HG23	1.94	0.50
70:SS:114:LEU:HD13	70:SS:121:ARG:HG2	1.93	0.50
2:B:285:TYR:HB2	2:B:332:MET:HG2	1.94	0.50
3:C:336:ARG:O	3:C:340:ILE:HD12	2.12	0.50
18:S:1:MET:HE1	18:S:33:PHE:O	2.12	0.50
38:m:127:VAL:HG13	38:m:127:VAL:O	2.12	0.50
48:5:978:G:H22	48:5:1277:G:H1	1.58	0.50
48:5:1397:A:N1	48:5:1498:G:O2'	2.42	0.50
51:9:108:G:H2'	51:9:109:PSU:H5''	1.93	0.50
51:9:838:G:H4'	51:9:839:C:H3'	1.93	0.50
51:9:1700:C:C2	51:9:1834:A:N6	2.79	0.50
86:ii:152:ASP:OD1	86:ii:154:SER:N	2.36	0.50
2:B:21:ARG:NH2	48:5:4981:G:O6	2.44	0.50
13:N:172:ARG:NH1	48:5:62:A:OP1	2.44	0.50
28:c:37:MET:SD	28:c:97:ILE:HD11	2.52	0.50
39:n:2:ARG:NE	51:9:1842:4AC:OP2	2.39	0.50
48:5:2412:A:H2'	48:5:2413:U:C6	2.47	0.50
57:FF:25:THR:O	57:FF:28:VAL:HG12	2.12	0.50
62:KK:83:LEU:HB3	62:KK:85:LEU:HD23	1.93	0.50
67:PP:111:MET:HE2	67:PP:119:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:21:TYR:CE1	69:RR:61:ILE:HG21	2.47	0.50
86:ii:289:ARG:HD3	86:ii:412:ILE:HD13	1.92	0.50
1:A:142:GLU:C	1:A:143:THR:HG1	2.08	0.50
2:B:228:TYR:O	48:5:2835:A:O2'	2.28	0.50
7:G:90:GLN:NE2	7:G:94:GLN:OE1	2.45	0.50
10:J:57:VAL:HG11	10:J:60:PHE:CD2	2.46	0.50
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.93	0.50
14:O:201:LEU:HD22	14:O:201:LEU:N	2.27	0.50
48:5:2588:C:OP1	48:5:2768:C:O2'	2.26	0.50
48:5:5003:U:H2'	48:5:5004:C:C6	2.47	0.50
51:9:157:U:H5''	87:jj:583:ILE:HD11	1.94	0.50
56:EE:111:VAL:HG23	56:EE:111:VAL:O	2.12	0.50
60:II:11:ARG:CZ	60:II:17:LYS:HE3	2.42	0.50
62:KK:74:GLU:OE1	62:KK:74:GLU:N	2.40	0.50
87:jj:111:THR:HG22	87:jj:112:ASN:H	1.76	0.50
44:t:112:ILE:H	44:t:112:ILE:HD12	1.76	0.49
51:9:1288:U:O2'	51:9:1289:U:OP2	2.28	0.49
51:9:1466:G:H5'	69:RR:4:VAL:HG22	1.93	0.49
64:MM:89:VAL:HG22	64:MM:109:VAL:HG21	1.92	0.49
68:QQ:107:GLU:O	68:QQ:111:ILE:HD13	2.11	0.49
69:RR:98:VAL:O	69:RR:118:GLN:HA	2.12	0.49
84:gg:112:ALA:HB3	84:gg:121:VAL:HG23	1.92	0.49
86:ii:318:GLU:C	86:ii:319:ILE:HD13	2.36	0.49
12:M:46:ARG:NH1	48:5:937:U:OP1	2.45	0.49
43:s:187:LEU:HD23	43:s:187:LEU:H	1.76	0.49
47:3:76:A:C8	48:5:4341:C:N4	2.73	0.49
54:CC:63:VAL:O	54:CC:64:THR:HB	2.11	0.49
58:GG:18:VAL:CG1	58:GG:24:LEU:HD21	2.35	0.49
69:RR:17:ILE:HG21	69:RR:61:ILE:HD11	1.93	0.49
81:dd:19:ARG:O	81:dd:27:ARG:NH1	2.45	0.49
84:gg:91:ASP:HB3	84:gg:94:THR:HG22	1.94	0.49
84:gg:109:LEU:HD13	84:gg:152:SER:HA	1.94	0.49
87:jj:434:ASP:OD1	87:jj:435:ALA:N	2.45	0.49
87:jj:531:ARG:HG2	87:jj:531:ARG:HH11	1.76	0.49
4:D:56:THR:HG21	49:7:26:C:OP1	2.12	0.49
9:I:203:ARG:NH1	49:7:105:C:OP2	2.46	0.49
11:L:59:VAL:HB	48:5:74:G:H5'	1.94	0.49
14:O:61:ARG:NH1	48:5:4587:G:OP1	2.40	0.49
14:O:81:TRP:CZ2	14:O:99:LEU:HD21	2.47	0.49
33:h:103:LYS:O	33:h:108:GLN:NE2	2.45	0.49
36:k:16:ARG:CD	36:k:61:PRO:HG3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:29:ILE:CD1	43:s:78:LEU:HD13	2.42	0.49
47:3:21:A:N6	47:3:46:G:O2'	2.46	0.49
48:5:2750:G:H2'	48:5:2751:G:O4'	2.13	0.49
48:5:3773:U:C2'	48:5:3775:A:C2	2.96	0.49
48:5:3773:U:C2'	48:5:3775:A:H2	2.26	0.49
48:5:3792:OMG:H2'	48:5:3793:U:C6	2.47	0.49
48:5:3810:C:O2'	48:5:3811:G:P	2.70	0.49
51:9:899:U:H2'	51:9:900:C:O4'	2.12	0.49
51:9:1432:U:O2'	51:9:1433:C:P	2.70	0.49
51:9:1661:A:C8	81:dd:14:PHE:CD1	3.00	0.49
51:9:1693:G:N2	51:9:1834:A:C8	2.81	0.49
59:HH:17:ASP:OD2	59:HH:21:SER:OG	2.20	0.49
84:gg:177:TRP:HA	84:gg:184:LEU:HA	1.94	0.49
87:jj:377:MET:CG	87:jj:518:VAL:HG22	2.42	0.49
20:U:113:ARG:NH1	48:5:2703:G:OP1	2.46	0.49
29:d:114:PHE:HA	29:d:117:LEU:HD12	1.94	0.49
31:f:52:LYS:NZ	48:5:4751:G:N7	2.57	0.49
48:5:3603:G:H2'	48:5:3604:A:C8	2.47	0.49
48:5:4119:C:C4'	48:5:4120:U:OP1	2.60	0.49
48:5:4331:G:O2'	48:5:4332:C:OP1	2.26	0.49
51:9:1421:A:H3'	51:9:1422:G:C8	2.47	0.49
51:9:1779:G:H2'	51:9:1780:G:C8	2.48	0.49
58:GG:147:LEU:O	58:GG:148:SER:C	2.56	0.49
59:HH:55:GLY:HA3	59:HH:57:ARG:HH11	1.78	0.49
62:KK:21:MET:HE1	62:KK:35:LEU:CD1	2.42	0.49
64:MM:18:LEU:HD22	64:MM:88:TRP:CZ3	2.48	0.49
72:UU:24:LEU:HB3	72:UU:32:LEU:HD11	1.95	0.49
76:YY:15:ASN:O	76:YY:19:GLN:N	2.45	0.49
84:gg:19:THR:OG1	84:gg:66:VAL:O	2.21	0.49
84:gg:24:THR:HG22	84:gg:30:MET:CE	2.43	0.49
10:J:128:LEU:N	10:J:128:LEU:HD23	2.28	0.49
14:O:9:LEU:HD23	14:O:118:MET:HB2	1.93	0.49
36:k:10:ASP:O	36:k:14:THR:OG1	2.30	0.49
48:5:467:U:O4'	48:5:467:U:OP2	2.30	0.49
48:5:4440:G:OP2	86:ii:189:ARG:HD2	2.12	0.49
48:5:4966:A:H2'	48:5:4967:A:O4'	2.11	0.49
51:9:799:U:O2'	51:9:800:U:O5'	2.23	0.49
51:9:925:G:N2	65:NN:48:SER:OG	2.45	0.49
51:9:1562:C:C2	51:9:1563:G:C8	3.00	0.49
51:9:1617:G:C2	51:9:1620:A:C2	3.01	0.49
55:DD:93:THR:O	55:DD:93:THR:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.75	0.49
59:HH:46:THR:HG22	59:HH:63:PHE:C	2.37	0.49
65:NN:94:LYS:HG2	65:NN:118:ILE:HD13	1.94	0.49
68:QQ:113:ILE:HG12	68:QQ:120:LEU:HD12	1.93	0.49
69:RR:82:ASP:OD1	69:RR:83:ASN:N	2.45	0.49
75:XX:56:GLY:N	82:ee:6:LEU:HD21	2.28	0.49
2:B:223:THR:HG22	2:B:338:VAL:CG2	2.39	0.49
47:3:73:G:O2'	47:3:74:C:H5'	2.12	0.49
48:5:5:A:H2'	48:5:6:C:O4'	2.12	0.49
48:5:914:U:H1'	48:5:915:A:C5	2.47	0.49
48:5:2627:C:O4'	48:5:2627:C:O2	2.30	0.49
48:5:4583:C:O2	48:5:4719:G:O6	2.31	0.49
51:9:115:U:H2'	51:9:116:OMU:C6	2.43	0.49
51:9:1124:C:H5''	53:BB:150:ILE:HG12	1.95	0.49
51:9:1407:U:O2'	51:9:1408:U:H5'	2.12	0.49
51:9:1606:G:N2	51:9:1632:G:H1'	2.28	0.49
53:BB:167:LYS:HE2	53:BB:200:ALA:HB1	1.94	0.49
64:MM:99:LYS:HG3	64:MM:99:LYS:O	2.13	0.49
68:QQ:40:GLU:OE1	68:QQ:40:GLU:HA	2.13	0.49
69:RR:98:VAL:HG13	69:RR:102:THR:HB	1.94	0.49
83:ff:136:CYS:SG	83:ff:137:GLY:N	2.85	0.49
5:E:97:LYS:HD3	48:5:687:U:O2'	2.12	0.49
14:O:186:GLU:O	14:O:187:LYS:HB2	2.11	0.49
21:V:129:TRP:CB	21:V:132:ILE:HD12	2.43	0.49
48:5:1440:U:H2'	48:5:1441:C:O5'	2.13	0.49
48:5:2104:A:O2'	48:5:2105:A:O4'	2.27	0.49
48:5:4395:U:H6	48:5:4395:U:H5'	1.77	0.49
50:8:124:U:O5'	50:8:124:U:H6	1.96	0.49
51:9:147:A:HO2'	51:9:148:U:C5'	2.25	0.49
51:9:1533:A:H2	51:9:1536:G:N3	2.11	0.49
55:DD:27:ARG:O	62:KK:61:GLN:NE2	2.46	0.49
63:LL:55:TYR:OH	63:LL:116:CYS:HB3	2.13	0.49
86:ii:170:HIS:HB2	86:ii:212:LEU:HD11	1.95	0.49
11:L:170:THR:HG22	11:L:171:GLU:N	2.28	0.49
26:a:132:ARG:NH2	48:5:1468:C:OP1	2.43	0.49
48:5:978:G:H22	48:5:1277:G:H22	1.61	0.49
48:5:1077:C:H4'	48:5:1215:C:H5	1.76	0.49
48:5:1755:C:C2	48:5:1757:U:C5	3.00	0.49
48:5:2089:G:H1'	48:5:2090:U:OP2	2.12	0.49
50:8:110:U:HO2'	50:8:111:U:C1'	2.13	0.49
50:8:141:C:H2'	50:8:142:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:151:C:OP1	76:YY:120:THR:OG1	2.28	0.49
51:9:184:G:C4	51:9:185:G:C8	3.01	0.49
51:9:216:C:O2	51:9:216:C:O4'	2.31	0.49
51:9:687:C:H4'	59:HH:121:THR:HG21	1.94	0.49
51:9:1313:A:OP1	64:MM:33:ARG:NH1	2.42	0.49
51:9:1538:C:O2	71:TT:48:TYR:OH	2.25	0.49
52:AA:30:LEU:HD22	52:AA:47:TYR:HE2	1.78	0.49
59:HH:118:ARG:O	59:HH:121:THR:OG1	2.30	0.49
64:MM:49:LEU:O	64:MM:111:VAL:HG12	2.12	0.49
76:YY:56:PHE:HZ	76:YY:91:LEU:HD23	1.78	0.49
86:ii:166:ARG:NH1	86:ii:265:ASN:OD1	2.41	0.49
3:C:321:ASN:OD1	48:5:1280:C:O2'	2.30	0.49
4:D:204:VAL:O	4:D:208:MET:HG3	2.13	0.49
7:G:215:LEU:O	7:G:219:VAL:HG13	2.11	0.49
27:b:52:LYS:O	48:5:1813:U:C5'	2.61	0.49
36:k:60:LEU:HD23	36:k:61:PRO:HD2	1.94	0.49
43:s:29:ILE:CD1	43:s:78:LEU:HD22	2.43	0.49
48:5:1771:U:H2'	48:5:1772:C:C1'	2.43	0.49
51:9:301:A:H2'	51:9:302:A:O4'	2.13	0.49
51:9:736:C:H2'	51:9:737:G:C8	2.48	0.49
51:9:1790:A:H2'	51:9:1791:A:O4'	2.13	0.49
70:SS:26:ILE:HD13	70:SS:56:ALA:HA	1.93	0.49
73:VV:67:ASP:O	73:VV:71:ARG:HG3	2.13	0.49
4:D:232:THR:O	4:D:233:PRO:C	2.56	0.49
43:s:32:ALA:HB1	43:s:35:VAL:HG11	1.95	0.49
43:s:170:SER:O	43:s:174:LEU:HG	2.12	0.49
44:t:15:LEU:HA	44:t:62:LEU:HD12	1.95	0.49
46:2:18:G:HO2'	46:2:57:G:H22	1.52	0.49
46:2:74:C:C5'	48:5:4548:A:H2'	2.43	0.49
48:5:169:A:C6	48:5:267:G:C6	3.01	0.49
48:5:449:C:H4'	48:5:449:C:OP1	2.12	0.49
48:5:978:G:N2	48:5:1277:G:H1	2.11	0.49
48:5:1586:G:O2'	48:5:1587:G:H5'	2.13	0.49
48:5:1693:U:H2'	48:5:1694:C:O4'	2.13	0.49
48:5:3598:C:H2'	48:5:3599:A:C8	2.47	0.49
48:5:4072:C:H2'	48:5:4073:A:O4'	2.13	0.49
48:5:4448:G:H4'	48:5:4449:A:OP2	2.12	0.49
48:5:4932:U:H2'	48:5:4933:C:O5'	2.13	0.49
51:9:50:A:N1	51:9:488:U:C5	2.81	0.49
51:9:1617:G:H4'	81:dd:14:PHE:CE2	2.48	0.49
51:9:1786:U:H2'	51:9:1787:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:197:VAL:HG12	52:AA:198:MET:H	1.78	0.49
53:BB:164:ILE:O	53:BB:168:MET:HG3	2.13	0.49
57:FF:28:VAL:O	57:FF:42:LYS:NZ	2.35	0.49
63:LL:88:ILE:HG21	63:LL:126:VAL:HG21	1.94	0.49
70:SS:7:GLU:OE1	70:SS:7:GLU:N	2.46	0.49
84:gg:121:VAL:HG11	84:gg:165:ILE:HD13	1.94	0.49
84:gg:184:LEU:HD12	84:gg:184:LEU:O	2.12	0.49
2:B:61:ASP:O	2:B:61:ASP:OD2	2.31	0.48
8:H:92:MET:HE3	8:H:181:VAL:HG23	1.94	0.48
43:s:30:VAL:O	43:s:86:VAL:HA	2.13	0.48
43:s:189:ILE:HG23	43:s:189:ILE:O	2.12	0.48
44:t:28:LEU:HD22	44:t:40:LYS:HD3	1.95	0.48
46:2:28:U:OP2	86:ii:50:LYS:NZ	2.46	0.48
48:5:658:C:OP1	48:5:658:C:H4'	2.13	0.48
51:9:914:U:O2	51:9:914:U:O4'	2.31	0.48
51:9:1394:G:O2'	51:9:1395:C:P	2.71	0.48
51:9:1435:C:O3'	51:9:1436:C:O4'	2.31	0.48
51:9:1665:G:C8	71:TT:88:MET:HE3	2.48	0.48
52:AA:30:LEU:HD21	52:AA:35:GLU:HG3	1.94	0.48
55:DD:72:VAL:HG13	62:KK:20:VAL:HG21	1.94	0.48
59:HH:30:LEU:C	59:HH:36:LEU:HD23	2.36	0.48
83:ff:111:ARG:NE	83:ff:113:ARG:O	2.46	0.48
86:ii:179:LYS:O	86:ii:180:HIS:CG	2.66	0.48
87:jj:116:LYS:HD2	87:jj:116:LYS:C	2.38	0.48
7:G:55:VAL:HG21	23:X:41:ARG:CD	2.43	0.48
7:G:138:ALA:O	7:G:201:THR:O	2.31	0.48
14:O:141:LEU:O	14:O:145:VAL:HG22	2.13	0.48
16:Q:108:ARG:NH2	48:5:1355:G:OP1	2.45	0.48
36:k:15:ALA:HB3	36:k:61:PRO:HG2	1.94	0.48
48:5:507:G:O2'	48:5:508:G:H5'	2.13	0.48
48:5:1238:A:HO2'	48:5:1239:C:P	2.35	0.48
48:5:1381:U:O2	48:5:1381:U:O4'	2.31	0.48
48:5:2695:A:H1'	48:5:2696:A:OP2	2.13	0.48
48:5:4128:A:H2'	48:5:4129:G:O4'	2.12	0.48
48:5:4302:U:H3'	48:5:4303:C:O2	2.12	0.48
48:5:4525:C:OP1	92:5:5427:HOH:O	2.19	0.48
51:9:310:C:H2'	51:9:311:C:C6	2.48	0.48
51:9:852:G:H3'	51:9:853:C:O2	2.14	0.48
51:9:996:A:H2'	51:9:997:A:C8	2.48	0.48
51:9:1406:G:C4	51:9:1407:U:H1'	2.48	0.48
56:EE:123:LEU:HD12	56:EE:236:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:ZZ:66:LYS:O	77:ZZ:110:THR:OG1	2.26	0.48
80:cc:46:VAL:HG11	80:cc:50:VAL:HG11	1.94	0.48
84:gg:10:THR:HG22	84:gg:308:ARG:CG	2.43	0.48
84:gg:229:THR:OG1	84:gg:230:LEU:N	2.46	0.48
84:gg:245:ARG:NH2	84:gg:312:VAL:HG11	2.28	0.48
86:ii:52:LEU:HD12	86:ii:82:LEU:HD12	1.95	0.48
2:B:297:LYS:HG3	2:B:299:ILE:HG23	1.95	0.48
3:C:193:LYS:CD	3:C:196:MET:HE2	2.43	0.48
48:5:743:G:H2'	48:5:744:G:O4'	2.13	0.48
48:5:3603:G:O2'	48:5:3604:A:P	2.70	0.48
48:5:4274:A:H2'	48:5:4275:G:C8	2.48	0.48
51:9:112:U:OP1	51:9:292:A:N1	2.46	0.48
51:9:927:C:H1'	79:bb:51:GLN:OE1	2.13	0.48
51:9:1401:A:H2'	51:9:1402:A:C8	2.49	0.48
51:9:1646:C:OP1	68:QQ:138:ARG:NH1	2.42	0.48
84:gg:74:ASP:HB3	84:gg:76:GLN:CG	2.42	0.48
1:A:117:GLU:HB2	1:A:162:ASN:HB2	1.95	0.48
36:k:16:ARG:HD3	36:k:61:PRO:HG3	1.94	0.48
48:5:749:G:HO2'	48:5:750:U:P	2.36	0.48
48:5:1214:C:O2	48:5:1214:C:O4'	2.32	0.48
51:9:661:U:OP2	51:9:662:G:O2'	2.31	0.48
51:9:1310:U:H4'	83:ff:137:GLY:HA3	1.95	0.48
70:SS:55:ARG:CD	77:ZZ:48:VAL:HG22	2.42	0.48
74:WW:51:GLU:OE1	79:bb:8:LEU:CD1	2.61	0.48
86:ii:356:HIS:CG	86:ii:356:HIS:O	2.66	0.48
4:D:234:ASP:O	4:D:235:MET:CB	2.61	0.48
15:P:9:GLU:CD	15:P:9:GLU:N	2.71	0.48
20:U:60:VAL:O	20:U:74:SER:HA	2.14	0.48
32:g:37:LYS:NZ	48:5:2516:G:OP2	2.40	0.48
35:j:9:GLY:HA2	48:5:2792:C:O2	2.13	0.48
38:m:119:ASN:C	38:m:119:ASN:OD1	2.56	0.48
48:5:405:U:O2'	48:5:407:A:N7	2.41	0.48
48:5:504:G:HO2'	48:5:505:G:P	2.35	0.48
48:5:1198:G:H2'	48:5:1199:G:N9	2.28	0.48
48:5:1345:A:H2'	48:5:1346:C:C6	2.48	0.48
48:5:1599:G:H21	48:5:1601:A:C4'	2.26	0.48
48:5:2504:C:O2'	48:5:2505:C:O2	2.22	0.48
51:9:368:U:C2'	51:9:369:C:OP2	2.62	0.48
51:9:544:G:H2'	51:9:545:A:C8	2.48	0.48
51:9:1120:U:H2'	51:9:1121:G:C8	2.48	0.48
51:9:1199:A:H2'	51:9:1200:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1415:C:H2'	51:9:1416:C:C6	2.49	0.48
51:9:1434:C:O3'	51:9:1435:C:O4'	2.31	0.48
56:EE:8:HIS:O	56:EE:30:ARG:NH1	2.47	0.48
70:SS:36:VAL:HG22	70:SS:40:TYR:CE2	2.48	0.48
84:gg:87:LEU:HB2	84:gg:101:PHE:HB2	1.95	0.48
19:T:87:LYS:NZ	48:5:4305:G:H22	2.12	0.48
19:T:144:ASN:ND2	19:T:144:ASN:O	2.46	0.48
27:b:18:ARG:NH1	48:5:1669:A:OP1	2.36	0.48
43:s:14:PHE:HA	43:s:17:ILE:HG12	1.95	0.48
43:s:29:ILE:HD12	43:s:78:LEU:HD22	1.95	0.48
47:3:37:A:H2'	47:3:38:A:H5'	1.96	0.48
48:5:911:U:H2'	48:5:912:G:O4'	2.13	0.48
48:5:2045:G:O6	48:5:3870:C:O2'	2.32	0.48
48:5:2862:G:N3	48:5:3624:A:H2'	2.28	0.48
48:5:3718:A2M:H8	48:5:3718:A2M:O5'	2.13	0.48
51:9:115:U:O2'	51:9:381:C:O2	2.21	0.48
51:9:1265:A:C2'	51:9:1265:A:N3	2.76	0.48
54:CC:272:HIS:ND1	54:CC:272:HIS:O	2.47	0.48
84:gg:16:GLY:CA	84:gg:305:ASN:OD1	2.61	0.48
8:H:103:VAL:HG11	8:H:144:LEU:HD21	1.95	0.48
26:a:94:LYS:O	26:a:95:THR:HG23	2.13	0.48
42:r:90:LEU:HG	42:r:111:ILE:HG23	1.96	0.48
44:t:19:GLY:HA2	44:t:58:ILE:HA	1.96	0.48
48:5:709:C:H1'	48:5:4942:C:H5	1.79	0.48
48:5:1767:A:H3'	48:5:1769:G:N7	2.29	0.48
48:5:1810:G:H2'	48:5:1811:G:O4'	2.13	0.48
48:5:1981:G:H5''	48:5:1982:G:H4'	1.94	0.48
48:5:2673:G:H5''	48:5:2675:G:O4'	2.14	0.48
48:5:3923:A:H2'	48:5:3924:C:C6	2.48	0.48
48:5:4548:A:N1	86:ii:181:GLY:O	2.47	0.48
48:5:4583:C:O2'	48:5:4718:G:N2	2.40	0.48
51:9:66:G:H2'	51:9:67:C:H4'	1.94	0.48
51:9:484:A2M:H8	51:9:484:A2M:O5'	2.13	0.48
51:9:880:G:C8	51:9:907:G:N1	2.82	0.48
51:9:1130:G:O5'	51:9:1130:G:H8	1.95	0.48
52:AA:30:LEU:HD11	52:AA:35:GLU:HA	1.95	0.48
56:EE:123:LEU:HD11	56:EE:235:TRP:HB2	1.96	0.48
57:FF:75:SER:O	57:FF:78:MET:HE3	2.13	0.48
63:LL:48:LYS:NZ	63:LL:52:GLU:OE1	2.47	0.48
70:SS:3:LEU:HD23	70:SS:4:VAL:N	2.29	0.48
87:jj:529:ALA:O	87:jj:551:LEU:HD21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:151:ARG:HH21	63:LL:118:ARG:NH1	2.10	0.48
26:a:103:VAL:CG1	26:a:108:TYR:HB2	2.44	0.48
48:5:1096:C:O2'	48:5:1097:C:O5'	2.28	0.48
48:5:1098:G:C2	48:5:1198:G:N1	2.82	0.48
48:5:1378:C:H4'	48:5:1379:C:H5'	1.96	0.48
48:5:1444:G:H2'	48:5:1445:U:H6	1.79	0.48
48:5:1959:U:OP1	48:5:1960:A:O2'	2.28	0.48
48:5:2640:G:H2'	48:5:2641:A:C8	2.49	0.48
48:5:4559:A:O3'	48:5:4560:C:O2	2.32	0.48
51:9:84:A:N3	51:9:150:A:O2'	2.42	0.48
51:9:171:A:H5''	58:GG:177:GLN:OE1	2.13	0.48
51:9:546:G:O2'	51:9:547:G:O4'	2.30	0.48
51:9:697:G:N3	51:9:697:G:H2'	2.28	0.48
51:9:886:A:H3'	51:9:887:U:H5''	1.95	0.48
51:9:1025:U:H2'	51:9:1026:C:O4'	2.14	0.48
51:9:1190:A:H2'	51:9:1191:C:O4'	2.12	0.48
51:9:1348:G:N2	51:9:1381:G:H22	2.10	0.48
51:9:1744:G:H8	51:9:1744:G:OP2	1.97	0.48
51:9:1788:A:H2'	51:9:1789:G:O4'	2.13	0.48
53:BB:59:SER:HA	53:BB:91:VAL:HG21	1.95	0.48
55:DD:35:SER:O	55:DD:99:ILE:HD11	2.14	0.48
66:OO:84:ARG:O	66:OO:88:LEU:HD23	2.13	0.48
71:TT:116:ASP:OD1	71:TT:116:ASP:C	2.57	0.48
87:jj:357:MET:HE2	87:jj:357:MET:HA	1.96	0.48
2:B:54:THR:HG22	2:B:78:ILE:HD11	1.95	0.48
9:I:22:PHE:CZ	48:5:1788:A:H2'	2.48	0.48
14:O:175:MET:HE1	14:O:179:LYS:NZ	2.29	0.48
14:O:185:VAL:O	14:O:187:LYS:O	2.31	0.48
27:b:38:LYS:NZ	48:5:1816:C:O3'	2.47	0.48
48:5:504:G:O2'	48:5:505:G:P	2.71	0.48
48:5:2276:A:H2'	48:5:2277:C:O4'	2.13	0.48
48:5:2726:G:H2'	48:5:2727:C:C6	2.49	0.48
50:8:102:G:OP2	50:8:104:A:O2'	2.29	0.48
51:9:642:U:OP2	82:ee:34:ARG:NH2	2.42	0.48
51:9:1520:G:H5''	51:9:1521:C:OP2	2.14	0.48
51:9:1667:U:H2'	51:9:1668:U:C6	2.49	0.48
67:PP:17:TYR:HB2	67:PP:25:LEU:HD11	1.96	0.48
68:QQ:44:PRO:HD3	68:QQ:77:HIS:HB3	1.95	0.48
18:S:1:MET:HG2	18:S:2:LYS:N	2.29	0.48
42:r:124:VAL:HG13	42:r:125:MET:N	2.28	0.48
43:s:78:LEU:HD11	43:s:193:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2:74:C:H5'	48:5:4548:A:H2'	1.95	0.48
47:3:52:G:H2'	47:3:53:G:O4'	2.13	0.48
48:5:1308:C:H2'	48:5:1309:C:C6	2.49	0.48
48:5:1444:G:C2	48:5:1445:U:C5	3.02	0.48
48:5:2550:G:O2'	48:5:2587:A:N1	2.43	0.48
48:5:2639:U:O2'	48:5:2640:G:P	2.72	0.48
48:5:4625:C:O2'	48:5:4626:A:H5'	2.14	0.48
48:5:4932:U:C2'	48:5:4933:C:O5'	2.62	0.48
50:8:126:C:H1'	50:8:127:U:C6	2.49	0.48
51:9:16:G:H2'	51:9:17:C:C6	2.49	0.48
51:9:29:G:H2'	51:9:30:C:C6	2.49	0.48
51:9:684:G:OP1	92:9:2009:HOH:O	2.20	0.48
51:9:1409:A:C8	51:9:1410:C:O4'	2.67	0.48
51:9:1533:A:C8	51:9:1604:G:H1'	2.49	0.48
55:DD:12:VAL:HG21	81:dd:34:TYR:CB	2.43	0.48
58:GG:135:PRO:HB2	58:GG:141:ILE:HD12	1.96	0.48
87:jj:111:THR:HG22	87:jj:112:ASN:N	2.29	0.48
2:B:101:THR:HG21	48:5:4724:A:H1'	1.96	0.47
7:G:81:ASN:CG	7:G:238:GLY:HA3	2.39	0.47
48:5:1455:G:O2'	48:5:1456:C:P	2.72	0.47
48:5:1870:C:H2'	48:5:1871:A2M:H8	1.96	0.47
48:5:1920:C:H3'	48:5:1921:C:H5''	1.96	0.47
48:5:4305:G:H2'	48:5:4305:G:N3	2.29	0.47
51:9:1507:G:C2	83:ff:80:TYR:CG	3.02	0.47
51:9:1673:U:O2'	57:FF:84:GLY:O	2.27	0.47
54:CC:217:ALA:HB3	54:CC:219:ILE:HD12	1.94	0.47
55:DD:52:ALA:C	55:DD:91:VAL:HG23	2.39	0.47
55:DD:122:VAL:HG22	55:DD:126:ILE:HD12	1.95	0.47
58:GG:41:LEU:HD12	58:GG:45:TRP:CE3	2.48	0.47
61:JJ:28:GLU:OE1	61:JJ:43:VAL:HG11	2.14	0.47
67:PP:22:LEU:O	67:PP:23:ASP:C	2.57	0.47
84:gg:187:ASN:O	84:gg:188:HIS:ND1	2.46	0.47
86:ii:128:ASP:OD1	86:ii:129:ASN:N	2.42	0.47
86:ii:202:VAL:HG13	86:ii:236:LEU:HD12	1.96	0.47
1:A:142:GLU:OE1	1:A:142:GLU:N	2.47	0.47
16:Q:89:ASP:O	16:Q:112:ARG:NH2	2.47	0.47
33:h:53:SER:O	33:h:57:VAL:HG23	2.14	0.47
48:5:1981:G:C5'	48:5:1982:G:H4'	2.44	0.47
48:5:2487:G:H8	48:5:2487:G:O5'	1.97	0.47
48:5:2501:C:C2'	48:5:2502:A:O4'	2.62	0.47
50:8:91:A:H2'	50:8:92:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:28:U:H2'	51:9:29:G:H8	1.79	0.47
51:9:183:G:C2	51:9:184:G:C8	3.02	0.47
51:9:213:G:O2'	51:9:214:U:P	2.72	0.47
51:9:547:G:O2'	51:9:548:C:H5''	2.14	0.47
51:9:1055:A:N1	51:9:1063:C:N4	2.59	0.47
51:9:1302:G:O6	51:9:1307:U:C2	2.67	0.47
51:9:1474:A:H5''	68:QQ:121:VAL:HG13	1.97	0.47
57:FF:33:ILE:O	57:FF:33:ILE:CG2	2.62	0.47
58:GG:71:GLY:O	58:GG:98:ARG:HD2	2.15	0.47
59:HH:76:GLN:O	59:HH:80:VAL:HG12	2.14	0.47
63:LL:20:LYS:O	63:LL:21:LYS:HB3	2.15	0.47
74:WW:28:ARG:HB3	74:WW:29:PRO:CD	2.44	0.47
84:gg:236:ILE:CG2	84:gg:239:LEU:HD21	2.43	0.47
86:ii:142:ASP:C	86:ii:142:ASP:OD1	2.57	0.47
1:A:158:ILE:HB	1:A:162:ASN:HD21	1.80	0.47
2:B:258:HIS:HA	2:B:259:PRO:C	2.39	0.47
5:E:164:ARG:O	5:E:185:ASN:OD1	2.31	0.47
26:a:29:PRO:O	48:5:39:A:N7	2.47	0.47
40:o:37:GLY:HA3	48:5:4342:C:O3'	2.14	0.47
46:2:18:G:H4'	46:2:60:A:C2	2.48	0.47
48:5:978:G:H1	48:5:1277:G:H1	1.62	0.47
48:5:1214:C:H3'	48:5:1215:C:H5''	1.96	0.47
48:5:1920:C:O2'	48:5:1922:G:O5'	2.31	0.47
48:5:2843:U:O2'	48:5:4632:U:OP1	2.25	0.47
48:5:3866:C:H2'	48:5:3867:A2M:O4'	2.14	0.47
48:5:4121:G:H4'	48:5:4122:G:OP2	2.14	0.47
48:5:4962:C:C4	48:5:4963:G:N7	2.82	0.47
51:9:12:U:H2'	51:9:13:C:C6	2.49	0.47
51:9:301:A:N3	60:II:73:THR:HG21	2.30	0.47
51:9:876:C:H2'	51:9:878:G:H1'	1.96	0.47
51:9:1533:A:C2	51:9:1536:G:N3	2.82	0.47
53:BB:33:VAL:HG12	53:BB:44:ILE:HD12	1.96	0.47
56:EE:181:CYS:SG	56:EE:225:ILE:HD12	2.55	0.47
57:FF:33:ILE:O	57:FF:33:ILE:HG22	2.14	0.47
57:FF:72:LEU:HD12	57:FF:155:CYS:SG	2.54	0.47
58:GG:127:THR:O	58:GG:128:THR:O	2.31	0.47
65:NN:84:LEU:HD21	65:NN:89:TYR:HD1	1.79	0.47
86:ii:22:LYS:HG3	86:ii:23:SER:N	2.28	0.47
87:jj:191:LYS:HD2	87:jj:229:VAL:HG13	1.96	0.47
2:B:103:LYS:NZ	48:5:4725:C:OP1	2.33	0.47
4:D:67:ALA:HA	4:D:72:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:39:PHE:CZ	20:U:43:LEU:HD11	2.49	0.47
26:a:117:LEU:HD23	26:a:140:VAL:HG21	1.95	0.47
43:s:35:VAL:HG23	43:s:39:GLN:OE1	2.14	0.47
44:t:16:ARG:HH21	44:t:18:THR:HG22	1.80	0.47
48:5:1066:G:H2'	48:5:1067:G:O4'	2.14	0.47
50:8:6:C:H2'	50:8:7:U:C6	2.49	0.47
50:8:155:C:H2'	50:8:156:U:O4'	2.14	0.47
51:9:551:U:H2'	51:9:552:G:C8	2.49	0.47
51:9:581:U:H4'	76:YY:66:GLY:HA2	1.96	0.47
51:9:1117:C:O2	51:9:1117:C:O4'	2.32	0.47
51:9:1344:A:N1	51:9:1385:G:O2'	2.41	0.47
53:BB:178:THR:O	53:BB:178:THR:HG22	2.15	0.47
64:MM:43:ASP:OD1	83:ff:101:TYR:OH	2.27	0.47
65:NN:92:ILE:HG22	65:NN:150:VAL:HG11	1.97	0.47
68:QQ:143:LYS:HD3	68:QQ:145:TYR:CZ	2.50	0.47
84:gg:219:TRP:C	84:gg:227:LEU:HD12	2.39	0.47
86:ii:312:LEU:HD21	86:ii:320:LEU:HD22	1.96	0.47
87:jj:531:ARG:HG2	87:jj:531:ARG:NH1	2.30	0.47
12:M:29:ASP:OD1	12:M:30:VAL:N	2.47	0.47
26:a:35:ALA:HB2	48:5:38:A:H5''	1.96	0.47
36:k:32:VAL:HG21	36:k:53:ALA:CB	2.44	0.47
44:t:73:VAL:HG12	44:t:74:VAL:N	2.30	0.47
48:5:750:U:H2'	48:5:751:G:O4'	2.14	0.47
48:5:1195:G:C6	48:5:1196:G:N7	2.82	0.47
48:5:1296:G:HO2'	48:5:1297:U:H6	1.57	0.47
48:5:1339:U:H2'	48:5:1340:OMC:C6	2.49	0.47
48:5:1846:G:H2'	48:5:1847:C:C6	2.49	0.47
48:5:2504:C:H2'	48:5:2505:C:C2	2.49	0.47
48:5:4263:C:H2'	48:5:4264:G:O4'	2.14	0.47
51:9:217:A:C2'	51:9:218:PSU:H5''	2.45	0.47
51:9:319:C:C2'	51:9:320:G:OP1	2.62	0.47
51:9:1675:A:O2'	57:FF:74:ASN:HB3	2.15	0.47
64:MM:125:GLU:HA	64:MM:128:PHE:CD2	2.50	0.47
71:TT:114:GLU:HG3	71:TT:122:LYS:HG3	1.95	0.47
77:ZZ:68:ILE:HD12	77:ZZ:110:THR:HA	1.96	0.47
86:ii:251:LEU:HD12	86:ii:251:LEU:O	2.14	0.47
87:jj:155:TYR:CE2	87:jj:159:ILE:HD11	2.50	0.47
87:jj:305:VAL:HG13	87:jj:306:ARG:N	2.30	0.47
6:F:240:ASN:O	6:F:244:ARG:HG2	2.14	0.47
45:1:67:LYS:HD3	48:5:4452:U:H1'	1.97	0.47
48:5:485:C:O2'	48:5:486:C:P	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1076:C:O2'	48:5:1077:C:H5'	2.14	0.47
48:5:1535:C:H2'	48:5:1536:U:O4'	2.15	0.47
48:5:1992:U:H4'	48:5:1993:C:O4'	2.15	0.47
51:9:70:G:N1	58:GG:170:ARG:NH1	2.63	0.47
51:9:146:G:HO2'	51:9:147:A:C5'	2.28	0.47
51:9:688:U:H1'	51:9:689:U:C5	2.48	0.47
51:9:984:C:O2'	66:OO:138:ASP:OD2	2.29	0.47
51:9:1281:G:C6	51:9:1282:A:H1'	2.49	0.47
52:AA:2:SER:N	52:AA:8:LEU:HD12	2.30	0.47
55:DD:210:ILE:HG21	69:RR:19:LYS:NZ	2.28	0.47
58:GG:144:LEU:HD22	58:GG:145:PHE:CE1	2.49	0.47
59:HH:147:LYS:HA	74:WW:49:GLU:OE2	2.13	0.47
84:gg:48:ASP:O	84:gg:49:GLU:C	2.58	0.47
84:gg:75:GLY:O	84:gg:76:GLN:NE2	2.47	0.47
87:jj:273:GLU:OE2	87:jj:275:ASP:HB3	2.14	0.47
13:N:114:ARG:HD3	13:N:151:ILE:O	2.15	0.47
21:V:41:SER:CB	48:5:4507:A:O2'	2.63	0.47
25:Z:57:MET:CB	25:Z:62:ILE:HD11	2.45	0.47
47:3:33:U:C3'	47:3:34:U:H2'	2.45	0.47
48:5:233:U:H2'	48:5:234:G:C8	2.50	0.47
48:5:377:A:H2'	48:5:378:A:O4'	2.15	0.47
48:5:1371:A:N1	50:8:28:C:O2'	2.44	0.47
48:5:1633:G:H5'	48:5:1634:A:OP1	2.15	0.47
48:5:1956:A:O2'	48:5:1957:U:P	2.72	0.47
48:5:2090:U:H4'	48:5:2091:C:OP2	2.14	0.47
48:5:2494:U:O3'	48:5:2495:U:O4'	2.33	0.47
48:5:3707:U:H2'	48:5:3708:C:C6	2.50	0.47
48:5:4119:C:O2	48:5:4120:U:N3	2.48	0.47
48:5:4758:U:O2	48:5:4758:U:O4'	2.33	0.47
51:9:15:U:H2'	51:9:16:G:O4'	2.14	0.47
51:9:201:C:H2'	51:9:202:G:H5'	1.97	0.47
51:9:867:G:C2	51:9:868:G:C6	3.03	0.47
51:9:1553:C:H2'	51:9:1554:C:O4'	2.14	0.47
51:9:1653:U:H2'	51:9:1654:G:C8	2.49	0.47
51:9:1842:4AC:O7	51:9:1842:4AC:H5	2.14	0.47
52:AA:89:LYS:HD3	52:AA:201:LEU:HG	1.97	0.47
52:AA:197:VAL:HG12	52:AA:198:MET:N	2.30	0.47
57:FF:51:HIS:HB2	57:FF:90:VAL:HG21	1.95	0.47
57:FF:139:VAL:HG12	57:FF:140:ASP:O	2.15	0.47
61:JJ:24:ARG:O	61:JJ:28:GLU:HG2	2.14	0.47
64:MM:89:VAL:CG2	64:MM:109:VAL:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:MM:114:TYR:HA	64:MM:121:LYS:HZ2	1.79	0.47
69:RR:41:ILE:HG21	69:RR:47:ARG:HB3	1.97	0.47
70:SS:54:LYS:NZ	70:SS:58:GLU:OE1	2.47	0.47
70:SS:84:LEU:N	70:SS:84:LEU:HD23	2.30	0.47
70:SS:89:ASP:O	70:SS:93:GLY:N	2.45	0.47
71:TT:18:LEU:HD23	71:TT:58:ALA:HA	1.95	0.47
78:aa:45:VAL:O	78:aa:45:VAL:CG1	2.62	0.47
86:ii:326:LEU:HD11	86:ii:409:ILE:CG1	2.45	0.47
86:ii:347:THR:HB	86:ii:348:PRO:CD	2.45	0.47
87:jj:164:LEU:HD22	87:jj:236:ASP:HB3	1.96	0.47
4:D:7:VAL:HG13	4:D:8:LYS:N	2.29	0.47
11:L:21:ARG:O	13:N:197:THR:HG23	2.15	0.47
26:a:39:HIS:O	26:a:40:HIS:CG	2.68	0.47
27:b:49:HIS:NE2	48:5:1815:G:O6	2.34	0.47
40:o:75:PRO:O	40:o:76:ASN:HB2	2.15	0.47
46:2:20(A):U:O2'	46:2:21:A:H5''	2.14	0.47
48:5:1591:U:OP2	48:5:2856:C:O2'	2.28	0.47
48:5:4537:C:H2'	48:5:4538:G:C8	2.50	0.47
51:9:82:G:O2'	51:9:83:A:O5'	2.33	0.47
51:9:319:C:H2'	51:9:320:G:OP1	2.15	0.47
51:9:463:C:OP2	87:jj:306:ARG:NH2	2.48	0.47
51:9:551:U:H2'	51:9:552:G:N7	2.29	0.47
51:9:587:A:HO2'	51:9:588:G:N2	2.13	0.47
51:9:1094:C:OP1	74:WW:28:ARG:NH2	2.48	0.47
51:9:1265:A:H4'	51:9:1327:G:OP1	2.14	0.47
51:9:1348:G:H1	51:9:1381:G:N2	2.11	0.47
52:AA:80:ARG:HH22	52:AA:126:ASP:CB	2.28	0.47
56:EE:107:GLY:CA	56:EE:189:LEU:HD22	2.45	0.47
68:QQ:57:LEU:HD21	68:QQ:115:TYR:CB	2.45	0.47
69:RR:66:VAL:HG11	69:RR:69:ILE:HD12	1.97	0.47
78:aa:36:ILE:HD12	78:aa:36:ILE:N	2.29	0.47
86:ii:394:ASP:HB3	86:ii:400:SER:HA	1.95	0.47
86:ii:416:ARG:O	86:ii:417:VAL:HG23	2.15	0.47
87:jj:106:LEU:CD2	87:jj:108:LEU:HD23	2.44	0.47
9:I:48:LEU:HD11	9:I:145:LYS:HG3	1.95	0.47
9:I:52:MET:HE1	9:I:155:ALA:HB3	1.96	0.47
20:U:76:VAL:CG1	20:U:77:PRO:HD2	2.44	0.47
22:W:44:ARG:HD3	48:5:3615:G:H21	1.80	0.47
48:5:35:U:H2'	48:5:36:U:H5'	1.96	0.47
48:5:1548:G:O2'	48:5:2812:A:N3	2.46	0.47
48:5:2486:G:C6	48:5:2493:G:O6	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:833:C:O2'	51:9:834:C:C6	2.68	0.47
51:9:1374:C:H2'	51:9:1375:G:O4'	2.15	0.47
51:9:1406:G:N3	51:9:1407:U:H1'	2.30	0.47
51:9:1834:A:H2	51:9:1837:G:H22	1.63	0.47
55:DD:161:GLY:O	55:DD:164:VAL:HG22	2.15	0.47
59:HH:161:ALA:O	59:HH:162:GLN:HB2	2.15	0.47
79:bb:55:LEU:HD22	79:bb:55:LEU:N	2.30	0.47
7:G:170:LEU:CD2	7:G:201:THR:HG21	2.45	0.47
8:H:115:ARG:HE	8:H:123:ILE:HD13	1.80	0.47
48:5:516:C:O2'	48:5:517:C:H5'	2.15	0.47
48:5:1776:A:H3'	48:5:1777:C:H6	1.79	0.47
48:5:1998:A:O2'	48:5:1999:A:O5'	2.33	0.47
48:5:3604:A:H2'	48:5:3605:C:C6	2.50	0.47
48:5:3880:G:H2'	48:5:3881:G:C8	2.50	0.47
48:5:4420:PSU:O2	48:5:4475:G:N2	2.48	0.47
51:9:153:G:C2'	51:9:154:U:O5'	2.63	0.47
51:9:598:G:O2'	51:9:605:A:N1	2.37	0.47
51:9:886:A:C5	51:9:901:G:C2	3.03	0.47
51:9:926:A:H61	51:9:1015:U:H3	1.63	0.47
51:9:1401:A:O3'	51:9:1402:A:O4'	2.33	0.47
51:9:1698:C:H4'	51:9:1699:A:OP2	2.14	0.47
51:9:1835:A:O2'	51:9:1836:G:P	2.73	0.47
55:DD:102:ALA:HB1	55:DD:173:ARG:HG3	1.96	0.47
57:FF:103:LEU:HD11	77:ZZ:67:LEU:HD22	1.97	0.47
60:II:132:GLU:O	60:II:133:GLU:C	2.56	0.47
65:NN:102:LEU:HD11	65:NN:111:ALA:C	2.40	0.47
66:OO:41:PHE:HA	66:OO:57:THR:HG22	1.97	0.47
83:ff:133:ARG:HD2	83:ff:142:THR:CG2	2.44	0.47
84:gg:158:PRO:O	84:gg:160:SER:N	2.47	0.47
84:gg:191:HIS:CD2	84:gg:195:LEU:HD11	2.50	0.47
86:ii:35:ILE:HD12	86:ii:74:ALA:CB	2.45	0.47
3:C:94:ASN:HA	3:C:100:ARG:O	2.15	0.46
10:J:83:LEU:HD12	10:J:83:LEU:O	2.14	0.46
25:Z:10:VAL:HG11	25:Z:129:TRP:HZ3	1.80	0.46
36:k:12:LEU:HD11	36:k:59:SER:O	2.15	0.46
48:5:652:G:H2'	48:5:653:C:C6	2.50	0.46
48:5:978:G:H22	48:5:1277:G:N2	2.13	0.46
48:5:5015:G:O2'	48:5:5034:A:N6	2.46	0.46
51:9:1016:U:O2	51:9:1016:U:H2'	2.14	0.46
51:9:1304:U:OP1	83:ff:90:ARG:N	2.48	0.46
51:9:1420:G:H2'	51:9:1421:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1435:C:H2'	51:9:1436:C:C2	2.50	0.46
52:AA:58:LEU:HD22	52:AA:178:LEU:HD13	1.97	0.46
58:GG:67:VAL:HG11	58:GG:99:GLY:HA2	1.97	0.46
87:jj:55:CYS:HA	91:jj:601:SF4:S3	2.55	0.46
87:jj:274:HIS:CG	87:jj:493:ASP:HA	2.49	0.46
9:I:138:ILE:HG21	9:I:148:VAL:HG12	1.97	0.46
20:U:78:PHE:CE2	20:U:83:LEU:HD21	2.50	0.46
23:X:90:ILE:HD11	23:X:155:ILE:HD11	1.97	0.46
44:t:74:VAL:O	44:t:74:VAL:HG12	2.15	0.46
48:5:174:C:H2'	48:5:175:C:O4'	2.15	0.46
48:5:1986:U:H3'	48:5:1987:C:H5'	1.96	0.46
48:5:2708:U:O2'	48:5:2709:C:O4'	2.33	0.46
48:5:4273:A:H2'	48:5:4274:A:C8	2.50	0.46
48:5:4947:U:O2'	48:5:4948:C:OP1	2.32	0.46
51:9:26:U:H2'	51:9:27:A2M:H8	1.98	0.46
51:9:1118:C:O2	51:9:1118:C:O4'	2.33	0.46
51:9:1646:C:C2'	51:9:1647:A:OP2	2.63	0.46
52:AA:122:LEU:HB3	52:AA:144:THR:HG22	1.97	0.46
58:GG:225:GLN:HA	58:GG:228:ILE:CD1	2.45	0.46
59:HH:9:VAL:HG23	59:HH:9:VAL:O	2.16	0.46
62:KK:62:PHE:O	62:KK:66:HIS:O	2.34	0.46
69:RR:75:GLU:O	69:RR:79:GLU:HG2	2.14	0.46
72:UU:20:ILE:HG22	72:UU:91:LEU:HB2	1.97	0.46
84:gg:34:ALA:HB2	84:gg:40:ILE:HG12	1.96	0.46
4:D:163:LEU:HD13	4:D:173:ILE:HG21	1.97	0.46
8:H:1:MET:HE3	18:S:140:PRO:HB2	1.97	0.46
15:P:115:GLU:OE1	15:P:151:THR:OG1	2.33	0.46
47:3:35:U:H2'	47:3:36:U:C5'	2.45	0.46
48:5:1991:A:O2'	48:5:1992:U:C6	2.69	0.46
48:5:2505:C:O2	48:5:2505:C:O4'	2.33	0.46
48:5:4719:G:C4'	48:5:4720:C:OP1	2.64	0.46
48:5:4922:C:H3'	48:5:4923:U:C6	2.50	0.46
48:5:4925:U:C4'	48:5:4926:C:OP2	2.63	0.46
50:8:92:U:H2'	50:8:93:C:O4'	2.15	0.46
51:9:191:A:C2'	51:9:192:C:OP1	2.62	0.46
51:9:846:G:C6	56:EE:19:MET:HE3	2.51	0.46
51:9:1398:G:H1'	84:gg:63:SER:OG	2.15	0.46
51:9:1417:C:H2'	51:9:1419:C:H5''	1.97	0.46
54:CC:75:ILE:HD11	54:CC:265:PRO:CB	2.46	0.46
59:HH:69:LEU:CD1	59:HH:96:ALA:HB2	2.46	0.46
61:JJ:57:ALA:HB2	61:JJ:97:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JJ:82:VAL:HG11	61:JJ:92:MET:HG3	1.96	0.46
72:UU:20:ILE:HD12	72:UU:116:ILE:HA	1.96	0.46
86:ii:56:PHE:HE1	86:ii:72:LEU:O	1.97	0.46
86:ii:414:ARG:HG3	86:ii:415:TYR:CD1	2.50	0.46
87:jj:435:ALA:O	87:jj:441:PHE:CD2	2.68	0.46
2:B:218:ASP:OD1	2:B:280:ILE:HA	2.15	0.46
6:F:114:ARG:NH1	16:Q:4:ASP:O	2.42	0.46
18:S:95:ARG:NH2	18:S:112:ASP:OD2	2.48	0.46
22:W:6:CYS:HA	22:W:13:ILE:HD11	1.97	0.46
42:r:66:ARG:O	42:r:67:ARG:HB3	2.15	0.46
43:s:69:LEU:HG	43:s:71:ASN:HB2	1.97	0.46
48:5:1604:G:H2'	48:5:1605:G:C8	2.50	0.46
48:5:1978:C:O2'	48:5:1979:A:OP1	2.33	0.46
48:5:2258:C:C2'	48:5:2259:G:OP1	2.63	0.46
48:5:2570:U:H2'	48:5:2571:C:C6	2.50	0.46
48:5:4305:G:N3	48:5:4305:G:C2'	2.79	0.46
48:5:4699:U:H1'	48:5:4700:A:H5''	1.98	0.46
51:9:107:A:H2'	51:9:108:G:C8	2.50	0.46
51:9:146:G:O2'	51:9:147:A:O5'	2.30	0.46
51:9:147:A:O2'	51:9:148:U:C5'	2.64	0.46
51:9:455:A:H2'	51:9:456:C:C6	2.51	0.46
51:9:524:U:OP2	82:ee:31:ARG:NH1	2.48	0.46
51:9:925:G:H1	51:9:1017:U:H3	1.63	0.46
51:9:1408:U:H1'	51:9:1409:A:C8	2.51	0.46
51:9:1646:C:O2'	51:9:1647:A:P	2.74	0.46
51:9:1798:C:H2'	51:9:1799:G:O4'	2.16	0.46
53:BB:166:LYS:O	53:BB:170:GLU:HG2	2.15	0.46
56:EE:195:ILE:O	56:EE:209:HIS:O	2.33	0.46
65:NN:59:GLY:HA2	79:bb:32:PHE:CE1	2.51	0.46
71:TT:28:LEU:O	71:TT:106:ALA:HB1	2.15	0.46
86:ii:346:LEU:HD23	86:ii:351:GLU:HA	1.96	0.46
2:B:300:LYS:HE3	2:B:300:LYS:O	2.14	0.46
15:P:18:ARG:C	15:P:94:MET:HE2	2.40	0.46
24:Y:65:GLN:HA	24:Y:65:GLN:OE1	2.16	0.46
35:j:31:LYS:NZ	48:5:1532:G:OP2	2.37	0.46
47:3:59:G:H2'	47:3:59:G:N3	2.30	0.46
48:5:100:C:H2'	48:5:101:A:O4'	2.14	0.46
48:5:717:U:H2'	48:5:718:C:C6	2.51	0.46
51:9:305:U:C6	60:II:55:TYR:CD2	3.03	0.46
51:9:618:C:H41	75:XX:67:ARG:NH2	2.14	0.46
51:9:853:C:O2	51:9:853:C:O4'	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1609:C:OP2	70:SS:134:GLN:NE2	2.46	0.46
55:DD:218:LEU:O	55:DD:218:LEU:HD23	2.15	0.46
68:QQ:52:LEU:O	68:QQ:55:VAL:HG22	2.16	0.46
71:TT:28:LEU:HD22	71:TT:54:TYR:HD1	1.81	0.46
79:bb:80:ARG:CZ	79:bb:80:ARG:HA	2.46	0.46
84:gg:20:GLN:HB3	84:gg:69:VAL:HG12	1.97	0.46
86:ii:389:LEU:HD21	86:ii:391:ILE:CD1	2.44	0.46
87:jj:83:THR:HG23	87:jj:83:THR:O	2.16	0.46
87:jj:564:ILE:HG22	87:jj:565:THR:N	2.31	0.46
5:E:209:VAL:HG21	5:E:260:ILE:HD13	1.98	0.46
17:R:151:ARG:NH2	63:LL:118:ARG:NH1	2.64	0.46
19:T:105:PHE:CD1	48:5:1802:A:H4'	2.51	0.46
31:f:47:CYS:SG	31:f:74:VAL:HG23	2.56	0.46
48:5:1477:C:O2'	48:5:1478:C:P	2.74	0.46
48:5:1695:U:H2'	48:5:1696:C:O4'	2.15	0.46
48:5:4948:C:O2	48:5:4949:G:H2'	2.16	0.46
50:8:83:C:H4'	50:8:85:U:C2	2.50	0.46
51:9:140:C:HO2'	51:9:141:A:P	2.38	0.46
51:9:981:A:H2'	51:9:982:G:C8	2.50	0.46
51:9:1746:U:H4'	58:GG:65:GLN:NE2	2.31	0.46
64:MM:114:TYR:HA	64:MM:121:LYS:NZ	2.31	0.46
65:NN:60:VAL:HG13	65:NN:66:VAL:CG2	2.32	0.46
66:OO:149:ARG:CZ	66:OO:151:LEU:HD13	2.45	0.46
67:PP:28:MET:CE	67:PP:36:LEU:HD11	2.46	0.46
68:QQ:105:LYS:C	68:QQ:105:LYS:CD	2.88	0.46
77:ZZ:58:LEU:HD11	77:ZZ:87:ALA:HB1	1.96	0.46
86:ii:286:LEU:HD11	86:ii:321:ILE:HD12	1.97	0.46
4:D:208:MET:HE2	4:D:233:PRO:HD3	1.97	0.46
6:F:92:ILE:HG21	6:F:246:MET:HE1	1.96	0.46
18:S:93:MET:HE1	18:S:117:HIS:CE1	2.51	0.46
20:U:24:ASP:OD1	20:U:69:LYS:HD3	2.16	0.46
48:5:700:G:O2'	48:5:701:G:H5'	2.16	0.46
48:5:1976:G:N2	48:5:1991:A:C8	2.84	0.46
48:5:1993:C:H5	48:5:2002:A:OP1	1.98	0.46
48:5:4739:C:C2	48:5:4961:G:N2	2.84	0.46
49:7:16:A:H2'	49:7:17:C:C6	2.50	0.46
50:8:152:U:H2'	50:8:153:C:O4'	2.16	0.46
51:9:154:U:O3'	58:GG:15:LEU:HD22	2.14	0.46
51:9:429:C:O2'	51:9:811:A:N1	2.44	0.46
51:9:526:A:H2'	51:9:527:C:O4'	2.15	0.46
51:9:535:G:O6	51:9:547:G:C2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:589:G:O6	51:9:591:U:H2'	2.16	0.46
51:9:816:A:H2'	51:9:817:G:H5'	1.98	0.46
51:9:952:G:H2'	51:9:953:C:C6	2.51	0.46
51:9:1345:G:OP1	51:9:1688:C:O2'	2.33	0.46
52:AA:197:VAL:HG13	52:AA:201:LEU:HD22	1.98	0.46
55:DD:176:LEU:HD13	55:DD:177:LEU:N	2.31	0.46
59:HH:61:ILE:HG13	59:HH:63:PHE:CE1	2.51	0.46
84:gg:168:CYS:SG	84:gg:198:VAL:HG23	2.56	0.46
84:gg:251:ALA:HB2	84:gg:289:LEU:HD21	1.98	0.46
86:ii:91:ASN:HA	86:ii:119:PRO:HA	1.97	0.46
8:H:71:ARG:HD3	48:5:4691:A:H4'	1.97	0.46
9:I:47:PRO:HG2	9:I:142:LEU:CD1	2.46	0.46
9:I:180:GLU:O	9:I:184:MET:HG3	2.16	0.46
9:I:184:MET:CB	9:I:190:LEU:HD12	2.44	0.46
19:T:39:ILE:N	19:T:39:ILE:HD13	2.31	0.46
19:T:105:PHE:O	19:T:109:VAL:HG23	2.15	0.46
20:U:44:GLN:HG3	20:U:56:LEU:HD21	1.97	0.46
20:U:61:VAL:HG22	20:U:74:SER:OG	2.15	0.46
20:U:62:SER:OG	20:U:73:THR:CG2	2.64	0.46
23:X:150:ALA:HB1	23:X:155:ILE:HG13	1.97	0.46
24:Y:37:GLU:OE2	24:Y:37:GLU:HA	2.16	0.46
28:c:98:ASP:C	28:c:98:ASP:OD1	2.59	0.46
33:h:35:LYS:NZ	50:8:49:G:O3'	2.49	0.46
41:p:58:GLY:O	48:5:2652:G:N1	2.38	0.46
42:r:47:LYS:O	42:r:103:HIS:CD2	2.69	0.46
43:s:57:LYS:HA	48:5:2020:U:O3'	2.15	0.46
44:t:27:ALA:O	44:t:31:LYS:HG3	2.16	0.46
48:5:8:U:H2'	48:5:9:C:O4'	2.16	0.46
48:5:746:A:O2'	48:5:747:A:H8	1.99	0.46
48:5:2461:G:H2'	48:5:2462:C:C6	2.51	0.46
48:5:2545:U:H3'	48:5:2546:G:C5'	2.46	0.46
48:5:3625:G:O2'	48:5:3626:G:OP1	2.34	0.46
48:5:4390:A:H2'	48:5:4391:G:O4'	2.16	0.46
48:5:5052:C:H2'	48:5:5053:U:O4'	2.15	0.46
51:9:292:A:OP2	63:LL:42:LEU:HD11	2.16	0.46
51:9:1220:A:H2'	51:9:1221:G:O4'	2.15	0.46
51:9:1307:U:N3	51:9:1308:U:O2	2.49	0.46
51:9:1425:G:H3'	51:9:1426:U:C5	2.51	0.46
51:9:1647:A:H1'	51:9:1648:G:OP2	2.16	0.46
53:BB:103:MET:HE1	53:BB:212:VAL:O	2.16	0.46
53:BB:121:ILE:HG23	53:BB:161:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:QQ:97:GLN:HG3	68:QQ:105:LYS:HG3	1.98	0.46
68:QQ:104:SER:HA	68:QQ:107:GLU:HG3	1.96	0.46
70:SS:36:VAL:HG23	70:SS:99:LEU:HD22	1.96	0.46
1:A:101:VAL:HG22	1:A:165:VAL:HG22	1.97	0.46
2:B:302:ASN:OD1	2:B:368:ILE:HG21	2.15	0.46
3:C:346:ASN:O	3:C:350:ARG:HG3	2.16	0.46
10:J:155:HIS:HB2	49:7:55:A:H4'	1.97	0.46
43:s:15:LEU:HA	43:s:18:ILE:HG22	1.98	0.46
44:t:41:LYS:CE	86:ii:343:ILE:HD11	2.45	0.46
48:5:176:G:C6	48:5:261:G:C2	3.03	0.46
48:5:1298:C:H2'	48:5:1299:G:C8	2.51	0.46
48:5:1588:U:H2'	48:5:1589:C:C6	2.50	0.46
48:5:1736:A:H2'	48:5:1737:A:O4'	2.16	0.46
48:5:1817:U:C4	48:5:1818:G:C6	3.04	0.46
48:5:4266:G:N3	48:5:4266:G:H2'	2.31	0.46
51:9:17:C:H2'	51:9:18:C:C6	2.51	0.46
51:9:113:G:N2	51:9:293:C:O5'	2.49	0.46
51:9:346:C:H2'	51:9:347:G:O4'	2.16	0.46
51:9:1243:U:H2'	51:9:1244:PSU:O4'	2.16	0.46
51:9:1277:C:O4'	62:KK:54:SER:OG	2.33	0.46
51:9:1407:U:O2	51:9:1407:U:C2'	2.62	0.46
51:9:1745:A:C2	51:9:1789:G:N2	2.80	0.46
56:EE:239:PRO:O	56:EE:240:ARG:C	2.59	0.46
59:HH:51:ILE:HD12	59:HH:61:ILE:HD13	1.98	0.46
65:NN:4:MET:O	65:NN:5:HIS:HB2	2.14	0.46
1:A:94:ALA:O	1:A:102:LEU:HD21	2.16	0.46
5:E:108:ARG:NH1	48:5:469:C:N3	2.58	0.46
7:G:51:LEU:HD11	48:5:4086:G:C4	2.51	0.46
11:L:165:LYS:O	26:a:100:ILE:HD13	2.16	0.46
17:R:120:TYR:CD1	17:R:120:TYR:C	2.93	0.46
30:e:76:LYS:NZ	30:e:98:GLU:OE2	2.48	0.46
44:t:46:ILE:O	44:t:50:THR:HG23	2.16	0.46
48:5:106:A:H1'	48:5:336:A:N3	2.31	0.46
48:5:211:G:H1'	48:5:233:U:O4	2.16	0.46
48:5:388:A:O2'	48:5:402:A:N1	2.39	0.46
48:5:914:U:HO2'	48:5:915:A:C1'	2.27	0.46
48:5:1672:U:H2'	48:5:1673:U:C6	2.51	0.46
48:5:4459:U:H2'	48:5:4460:U:O4'	2.16	0.46
51:9:617:G:OP1	82:ee:9:VAL:HG13	2.16	0.46
51:9:919:A:O2'	51:9:1020:A:N6	2.48	0.46
51:9:919:A:OP2	65:NN:64:ARG:NH1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1366:G:H2'	51:9:1367:PSU:O4'	2.16	0.46
51:9:1675:A:N3	51:9:1675:A:O4'	2.47	0.46
71:TT:5:THR:OG1	71:TT:6:VAL:N	2.48	0.46
79:bb:74:THR:HG22	79:bb:75:GLU:N	2.31	0.46
87:jj:468:GLN:NE2	87:jj:487:GLU:O	2.41	0.46
3:C:263:LEU:HG	3:C:273:LEU:HD12	1.98	0.45
4:D:43:LYS:HB3	4:D:46:THR:CG2	2.45	0.45
17:R:178:GLN:O	17:R:181:LYS:HD2	2.16	0.45
44:t:50:THR:HA	44:t:53:TRP:CE2	2.50	0.45
48:5:125:C:O2'	48:5:126:C:O5'	2.25	0.45
48:5:1734:G:N2	48:5:1735:U:O4	2.40	0.45
48:5:4893:A:H2'	48:5:4894:A:O4'	2.16	0.45
48:5:4962:C:H2'	48:5:4963:G:O4'	2.15	0.45
51:9:1559:C:H2'	51:9:1560:U:O4'	2.15	0.45
51:9:1620:A:N3	51:9:1620:A:H2'	2.30	0.45
51:9:1621:U:O4	67:PP:82:ASP:HB3	2.17	0.45
57:FF:204:ARG:HD3	80:cc:60:GLU:HG3	1.98	0.45
59:HH:160:LYS:HA	59:HH:163:GLN:HB2	1.98	0.45
64:MM:85:LEU:HD23	64:MM:85:LEU:C	2.40	0.45
66:OO:128:ARG:HG2	66:OO:128:ARG:HH11	1.80	0.45
84:gg:154:VAL:HG12	84:gg:167:SER:CB	2.45	0.45
87:jj:79:LEU:O	87:jj:80:GLU:C	2.58	0.45
18:S:1:MET:HE3	18:S:43:ARG:HG3	1.97	0.45
30:e:4:LEU:O	30:e:121:ARG:NH1	2.46	0.45
44:t:135:THR:HB	48:5:1993:C:O2	2.16	0.45
48:5:3:C:H2'	48:5:4:G:O4'	2.15	0.45
48:5:37:U:H2'	48:5:38:A:O4'	2.16	0.45
48:5:1328:G:O2'	48:5:2349:A:OP1	2.33	0.45
48:5:1433:A:H2'	48:5:1434:G:O4'	2.16	0.45
48:5:1759:G:C6	48:5:1760:G:N7	2.85	0.45
48:5:1979:A:H2'	48:5:1980:U:H1'	1.99	0.45
48:5:2627:C:O2	48:5:2627:C:O5'	2.34	0.45
51:9:309:G:OP2	51:9:309:G:O3'	2.34	0.45
51:9:1822:A:H2'	51:9:1823:A:O4'	2.17	0.45
56:EE:255:ARG:O	56:EE:259:LYS:HG2	2.17	0.45
59:HH:19:PHE:O	59:HH:48:ALA:HB3	2.16	0.45
62:KK:84:HIS:C	62:KK:85:LEU:HD22	2.41	0.45
67:PP:44:ARG:NH1	67:PP:82:ASP:O	2.42	0.45
83:ff:136:CYS:HB3	83:ff:141:LEU:N	2.31	0.45
84:gg:173:LEU:HD23	84:gg:189:ILE:CG1	2.45	0.45
6:F:198:LYS:HE3	6:F:198:LYS:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:55:VAL:HG21	23:X:41:ARG:HD3	1.98	0.45
16:Q:156:PRO:O	26:a:50:PRO:HD3	2.17	0.45
25:Z:61:LYS:O	25:Z:65:ARG:HG2	2.17	0.45
26:a:75:LEU:HD11	26:a:133:ALA:HA	1.98	0.45
43:s:91:THR:HG21	43:s:98:ILE:CD1	2.46	0.45
44:t:135:THR:OG1	48:5:1973:G:N2	2.49	0.45
48:5:419:A:N6	50:8:15:G:H1'	2.31	0.45
48:5:2899:C:C2	48:5:2900:U:C5	3.04	0.45
48:5:5061:A:H3'	48:5:5062:G:H5'	1.98	0.45
51:9:85:A:N3	51:9:149:A:H2	2.15	0.45
51:9:203:G:O2'	51:9:204:G:H5'	2.17	0.45
51:9:301:A:N3	60:II:73:THR:CG2	2.80	0.45
51:9:555:A:H5''	51:9:556:U:OP2	2.17	0.45
51:9:887:U:O2	51:9:887:U:O4'	2.33	0.45
51:9:1059:G:H2'	51:9:1060:A:H5'	1.97	0.45
51:9:1664:A:HO2'	51:9:1666:C:H41	1.64	0.45
53:BB:39:PHE:CD2	53:BB:74:LEU:HD13	2.51	0.45
60:II:41:ARG:HD3	60:II:43:ILE:HD12	1.99	0.45
70:SS:38:ARG:CG	71:TT:45:LEU:HD21	2.47	0.45
72:UU:46:LYS:HB3	72:UU:48:LEU:HD13	1.98	0.45
75:XX:28:LYS:CE	75:XX:32:LEU:HD13	2.46	0.45
83:ff:136:CYS:HB3	83:ff:141:LEU:H	1.82	0.45
3:C:86:ARG:HG3	3:C:86:ARG:O	2.16	0.45
5:E:185:ASN:HD21	5:E:274:LEU:C	2.24	0.45
10:J:94:LEU:O	10:J:175:LEU:N	2.41	0.45
25:Z:46:ILE:HG23	25:Z:68:ILE:HG23	1.97	0.45
47:3:76:A:N6	48:5:4371:G:N7	2.64	0.45
48:5:233:U:H5	48:5:2304:U:O2'	1.99	0.45
48:5:1413:C:H2'	48:5:1414:C:C6	2.51	0.45
48:5:1817:U:O2'	48:5:1818:G:H5'	2.16	0.45
48:5:2543:A:H4'	50:8:127:U:O2	2.17	0.45
51:9:964:A:H1'	51:9:1054:G:O2'	2.17	0.45
51:9:1303:C:O2	51:9:1303:C:O4'	2.34	0.45
51:9:1314:U:H5'	51:9:1315:U:OP2	2.16	0.45
51:9:1733:U:H2'	51:9:1734:G:O4'	2.16	0.45
55:DD:37:VAL:O	55:DD:37:VAL:HG13	2.15	0.45
59:HH:130:LEU:HD11	59:HH:156:VAL:HG21	1.98	0.45
65:NN:4:MET:HE2	65:NN:124:ARG:NH2	2.31	0.45
68:QQ:57:LEU:HD23	68:QQ:112:LEU:CD2	2.46	0.45
68:QQ:58:LEU:HD22	68:QQ:108:ILE:HG22	1.98	0.45
77:ZZ:58:LEU:HD23	77:ZZ:59:CYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:ii:52:LEU:CD1	86:ii:78:VAL:HG12	2.46	0.45
1:A:204:MET:HE2	48:5:1631:A:N1	2.31	0.45
5:E:199:ALA:HB3	31:f:110:ILE:OXT	2.15	0.45
6:F:112:ARG:HD2	48:5:1840:G:H5''	1.99	0.45
8:H:44:GLU:OE2	12:M:2:VAL:N	2.50	0.45
44:t:11:LYS:HA	44:t:65:GLN:O	2.17	0.45
48:5:137:G:O2'	48:5:138:G:H5'	2.16	0.45
48:5:488:G:H2'	48:5:489:C:C6	2.52	0.45
48:5:1178:G:H2'	48:5:1179:U:H5'	1.99	0.45
48:5:2028:C:H2'	48:5:2029:A:O4'	2.17	0.45
48:5:2379:A:H2'	48:5:2380:G:O4'	2.17	0.45
48:5:2601:A:N6	48:5:2744:A:OP2	2.44	0.45
48:5:4653:C:H2'	48:5:4654:C:C6	2.52	0.45
51:9:333:G:OP2	58:GG:190:ARG:NH2	2.32	0.45
51:9:1287:A:C2	51:9:1313:A:C4	3.05	0.45
51:9:1401:A:O2'	72:UU:53:PRO:O	2.28	0.45
53:BB:168:MET:O	53:BB:172:MET:HG3	2.15	0.45
53:BB:171:ILE:O	53:BB:175:GLU:HG2	2.16	0.45
63:LL:91:ASP:OD1	63:LL:104:LYS:NZ	2.42	0.45
67:PP:98:ASN:OD1	67:PP:121:ILE:O	2.34	0.45
76:YY:24:VAL:HG13	76:YY:70:THR:HG23	1.98	0.45
79:bb:37:CYS:HB2	79:bb:63:LEU:HD11	1.98	0.45
87:jj:106:LEU:HG	87:jj:285:PHE:CE2	2.51	0.45
87:jj:187:ILE:O	87:jj:191:LYS:HG2	2.17	0.45
1:A:7:GLY:O	48:5:3667:C:H4'	2.17	0.45
2:B:370:THR:O	2:B:370:THR:CG2	2.64	0.45
4:D:186:GLU:O	4:D:187:SER:HB3	2.16	0.45
9:I:184:MET:HE2	9:I:190:LEU:HG	1.99	0.45
14:O:110:PRO:O	14:O:113:ASP:OD1	2.34	0.45
43:s:9:TRP:HE1	48:5:1999:A:P	2.40	0.45
48:5:2538:U:H2'	48:5:2539:C:C6	2.51	0.45
48:5:4419:U:OP1	48:5:4421:C:N4	2.47	0.45
48:5:4765:G:O6	48:5:4869:U:H5	1.98	0.45
48:5:4924:C:H2'	48:5:4925:U:O4'	2.17	0.45
51:9:643:A:OP2	61:JJ:38:ARG:NH2	2.44	0.45
51:9:1133:A:H4'	78:aa:13:LYS:HD3	1.98	0.45
51:9:1810:U:O2'	51:9:1811:C:H5'	2.16	0.45
52:AA:30:LEU:HD22	52:AA:47:TYR:CE2	2.52	0.45
60:II:158:ILE:HB	60:II:163:GLU:OE2	2.17	0.45
66:OO:56:VAL:HG21	66:OO:80:ASP:CG	2.41	0.45
66:OO:56:VAL:HG12	66:OO:57:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:QQ:40:GLU:OE1	68:QQ:40:GLU:CA	2.64	0.45
84:gg:146:SER:O	84:gg:147:HIS:CD2	2.70	0.45
84:gg:197:THR:HG21	84:gg:239:LEU:N	2.31	0.45
86:ii:24:LEU:HD21	86:ii:112:ILE:HD13	1.96	0.45
1:A:209:HIS:CE1	1:A:235:VAL:HG21	2.52	0.45
5:E:286:PRO:HB2	31:f:41:PHE:CZ	2.52	0.45
7:G:165:GLU:OE1	13:N:26:ARG:NH2	2.46	0.45
17:R:10:LEU:O	17:R:14:VAL:HG23	2.17	0.45
20:U:66:SER:OG	20:U:67:LYS:N	2.46	0.45
28:c:18:LEU:O	28:c:22:MET:HG2	2.16	0.45
40:o:38:LYS:HA	47:3:75:C:N4	2.31	0.45
48:5:418:A:C2	50:8:17:A:H1'	2.51	0.45
48:5:462:G:H2'	48:5:463:A:N9	2.32	0.45
48:5:978:G:N2	48:5:1278:C:C2	2.85	0.45
48:5:1420:A:H4'	48:5:1421:G:C5'	2.47	0.45
48:5:5004:C:H2'	48:5:5005:G:O4'	2.17	0.45
51:9:224:A:H2'	51:9:225:G:C8	2.52	0.45
51:9:379:C:O2	60:II:5:ARG:NE	2.44	0.45
51:9:1491:G:H2'	51:9:1492:U:C6	2.52	0.45
51:9:1536:G:H2'	51:9:1537:A:H8	1.82	0.45
51:9:1587:G:N3	51:9:1587:G:H2'	2.32	0.45
51:9:1839:U:H2'	51:9:1840:U:C6	2.52	0.45
61:JJ:104:ASP:OD1	61:JJ:104:ASP:N	2.49	0.45
76:YY:20:ARG:HB3	76:YY:76:TYR:CD1	2.52	0.45
87:jj:504:VAL:CG2	87:jj:528:LEU:HD13	2.47	0.45
1:A:173:GLY:O	41:p:69:TRP:NE1	2.49	0.45
2:B:156:TYR:OH	48:5:4909:A:OP2	2.28	0.45
25:Z:123:LYS:O	25:Z:124:THR:OG1	2.27	0.45
27:b:69:ALA:O	27:b:72:ILE:HG22	2.16	0.45
33:h:75:GLY:HA2	48:5:133:C:O2	2.17	0.45
44:t:73:VAL:HG12	44:t:74:VAL:H	1.82	0.45
48:5:125:C:O2'	48:5:126:C:P	2.74	0.45
48:5:325:U:H2'	48:5:326:C:C6	2.52	0.45
48:5:2552:G:O2'	48:5:2766:A:N6	2.44	0.45
48:5:2733:C:H2'	48:5:2734:U:O4'	2.16	0.45
50:8:126:C:O2	50:8:127:U:C4	2.69	0.45
51:9:113:G:C2	51:9:292:A:H1'	2.52	0.45
51:9:126:G:O5'	58:GG:195:LYS:HD2	2.16	0.45
51:9:203:G:P	60:II:147:LYS:HZ1	2.39	0.45
51:9:734:C:C4	51:9:735:C:C5	3.05	0.45
51:9:835:C:O2	51:9:837:A:H4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:876:C:H5'	51:9:877:C:P	2.57	0.45
51:9:1386:A:OP2	55:DD:160:SER:OG	2.34	0.45
54:CC:83:LEU:HD11	73:VV:15:ARG:HG3	1.99	0.45
55:DD:51:LEU:HD11	55:DD:91:VAL:HA	1.99	0.45
58:GG:10:THR:O	58:GG:129:VAL:HB	2.17	0.45
64:MM:51:VAL:HB	64:MM:109:VAL:HG12	1.98	0.45
66:OO:27:VAL:HG12	66:OO:90:ILE:HD13	1.99	0.45
86:ii:326:LEU:HD11	86:ii:409:ILE:HG13	1.98	0.45
3:C:268:ARG:NH1	48:5:655:C:OP2	2.49	0.45
4:D:41:LYS:HB2	19:T:68:THR:O	2.17	0.45
25:Z:100:VAL:HG12	25:Z:106:LEU:HB3	1.99	0.45
48:5:93:G:H2'	48:5:94:A:C8	2.51	0.45
48:5:733:A:H2'	48:5:734:G:O4'	2.16	0.45
48:5:1238:A:O2'	48:5:1239:C:P	2.75	0.45
48:5:2273:G:H2'	48:5:2274:C:C6	2.52	0.45
48:5:2555:G:H2'	48:5:2556:G:O4'	2.17	0.45
48:5:4349:C:H3'	48:5:4350:C:H5'	1.98	0.45
48:5:4394:A:H4'	48:5:4395:U:OP2	2.17	0.45
48:5:4922:C:OP2	48:5:4922:C:C6	2.70	0.45
51:9:158:A:H2'	51:9:159:A2M:O4'	2.17	0.45
51:9:338:G:H2'	51:9:339:A:N7	2.32	0.45
51:9:599:A:H2'	51:9:606:G:N2	2.31	0.45
51:9:953:C:H2'	51:9:954:U:O4'	2.16	0.45
51:9:1139:C:O2	51:9:1139:C:O4'	2.32	0.45
51:9:1298:G:O2'	51:9:1299:A:H8	1.99	0.45
51:9:1372:U:O2'	69:RR:6:THR:HG22	2.17	0.45
51:9:1380:C:H2'	51:9:1381:G:O4'	2.17	0.45
51:9:1516:G:H2'	51:9:1517:G:O4'	2.16	0.45
52:AA:84:GLN:O	52:AA:87:VAL:HG22	2.17	0.45
57:FF:18:LYS:HD2	57:FF:48:TYR:CZ	2.52	0.45
69:RR:82:ASP:OD1	69:RR:82:ASP:C	2.59	0.45
70:SS:124:ARG:NE	70:SS:130:ARG:O	2.48	0.45
84:gg:154:VAL:HG12	84:gg:167:SER:HB2	1.99	0.45
84:gg:252:THR:O	84:gg:255:SER:O	2.34	0.45
86:ii:177:PRO:HG2	86:ii:197:LYS:HG3	1.99	0.45
5:E:195:LYS:O	31:f:106:TYR:O	2.34	0.45
48:5:495:C:H2'	48:5:496:G:C8	2.52	0.45
48:5:2699:C:O2'	48:5:2700:G:H5'	2.16	0.45
51:9:320:G:OP1	51:9:320:G:C4'	2.65	0.45
51:9:1013:U:OP1	51:9:1129:G:O2'	2.35	0.45
51:9:1407:U:H2'	51:9:1408:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1577:G:O2'	51:9:1579:A:N3	2.42	0.45
53:BB:37:ALA:O	53:BB:38:MET:C	2.60	0.45
58:GG:16:ILE:HG22	58:GG:18:VAL:HG23	1.99	0.45
59:HH:51:ILE:CD1	59:HH:61:ILE:HD13	2.47	0.45
67:PP:119:PHE:CE1	70:SS:117:ILE:HG22	2.51	0.45
68:QQ:128:GLU:HG2	68:QQ:129:SER:N	2.32	0.45
76:YY:12:PHE:CZ	76:YY:21:LYS:HB3	2.51	0.45
86:ii:161:LEU:HG	86:ii:162:GLN:O	2.17	0.45
87:jj:41:VAL:O	87:jj:42:THR:HG23	2.17	0.45
4:D:234:ASP:O	4:D:235:MET:HB3	2.17	0.44
5:E:94:THR:HG22	5:E:111:LYS:HA	1.99	0.44
9:I:43:VAL:HG13	9:I:44:ASP:N	2.32	0.44
48:5:118:C:H3'	48:5:119:G:C5'	2.46	0.44
48:5:222:C:H2'	48:5:223:G:O4'	2.17	0.44
48:5:2390:G:H22	48:5:2825:A:H2	1.64	0.44
48:5:2480:G:C2	48:5:2481:G:C8	3.05	0.44
50:8:56:G:H2'	50:8:57:C:O4'	2.17	0.44
51:9:186:C:H2'	51:9:187:G:C8	2.52	0.44
51:9:371:A:OP2	60:II:10:LYS:HB2	2.16	0.44
51:9:532:C:H2'	51:9:533:A:O5'	2.18	0.44
51:9:674:C:H2'	51:9:675:U:C6	2.52	0.44
51:9:841:G:N7	76:YY:12:PHE:N	2.65	0.44
52:AA:128:ARG:NH2	52:AA:151:ASP:O	2.50	0.44
52:AA:141:ASN:ND2	73:VV:31:SER:O	2.40	0.44
58:GG:132:ARG:O	58:GG:133:LEU:HD23	2.18	0.44
58:GG:219:GLU:O	58:GG:223:LYS:HE2	2.17	0.44
59:HH:14:GLU:O	59:HH:14:GLU:CD	2.60	0.44
61:JJ:32:ILE:O	61:JJ:35:TYR:O	2.35	0.44
80:cc:28:THR:O	80:cc:30:VAL:HG13	2.16	0.44
84:gg:30:MET:HA	84:gg:43:TRP:O	2.17	0.44
84:gg:195:LEU:HD13	84:gg:195:LEU:HA	1.86	0.44
84:gg:241:PHE:N	84:gg:241:PHE:CD1	2.85	0.44
86:ii:33:SER:HB3	86:ii:70:SER:HB3	1.99	0.44
86:ii:389:LEU:HD23	86:ii:389:LEU:O	2.17	0.44
87:jj:372:SER:HA	87:jj:508:ILE:HG22	1.98	0.44
2:B:297:LYS:C	2:B:298:LEU:HD23	2.42	0.44
29:d:68:LEU:CD2	29:d:106:VAL:HG12	2.47	0.44
43:s:27:CYS:HA	43:s:89:VAL:O	2.17	0.44
48:5:475:G:H2'	48:5:476:G:O4'	2.16	0.44
48:5:692:A:H2'	48:5:693:C:H6	1.82	0.44
48:5:1480:C:H2'	48:5:1483:C:H42	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1685:G:H2'	48:5:1686:C:C6	2.52	0.44
48:5:3861:A:H2'	48:5:3862:A:C8	2.51	0.44
48:5:4418:G:H2'	48:5:4475:G:N2	2.32	0.44
48:5:4476:C:O2'	48:5:4478:G:OP2	2.31	0.44
48:5:4886:C:H2'	48:5:4887:C:C6	2.52	0.44
51:9:305:U:C2	60:II:55:TYR:CE2	3.05	0.44
51:9:816:A:C2'	51:9:817:G:H5'	2.47	0.44
51:9:876:C:H2'	51:9:878:G:C1'	2.47	0.44
51:9:926:A:H2'	51:9:927:C:O4'	2.17	0.44
51:9:1109:C:O2'	51:9:1110:G:P	2.75	0.44
51:9:1144:A:H2'	51:9:1145:A:C8	2.53	0.44
51:9:1364:U:O2	51:9:1364:U:O4'	2.35	0.44
59:HH:64:VAL:HG22	59:HH:95:ILE:O	2.16	0.44
60:II:133:GLU:O	60:II:137:LEU:HG	2.17	0.44
84:gg:23:THR:HG23	84:gg:31:ILE:HD13	2.00	0.44
84:gg:198:VAL:HG13	84:gg:209:SER:HB2	1.99	0.44
86:ii:337:GLY:C	86:ii:338:THR:HG23	2.42	0.44
87:jj:437:THR:O	87:jj:438:HIS:C	2.59	0.44
2:B:248:LEU:HD12	2:B:248:LEU:C	2.42	0.44
5:E:157:THR:HG23	5:E:158:GLY:N	2.31	0.44
8:H:62:GLY:HA2	8:H:66:GLU:OE1	2.17	0.44
10:J:24:ILE:HD12	10:J:40:LEU:HG	2.00	0.44
14:O:10:ASP:O	14:O:14:HIS:CE1	2.70	0.44
26:a:25:HIS:ND1	48:5:1338:G:N7	2.64	0.44
30:e:78:LEU:HD11	30:e:100:ALA:HA	1.98	0.44
44:t:114:ARG:CZ	44:t:118:HIS:NE2	2.80	0.44
48:5:102:G:HO2'	48:5:1381:U:HO2'	1.61	0.44
48:5:286:U:H2'	48:5:287:U:C6	2.52	0.44
48:5:462:G:N2	48:5:694:C:H1'	2.33	0.44
48:5:1217:G:O2'	48:5:1218:G:H5'	2.18	0.44
48:5:1967:A:C2	48:5:2021:G:C5	3.05	0.44
48:5:1972:G:C6	48:5:1995:G:C6	3.05	0.44
48:5:1993:C:N3	48:5:2002:A:C6	2.85	0.44
48:5:2104:A:O2'	48:5:2105:A:P	2.76	0.44
48:5:3673:C:O5'	48:5:3673:C:O2	2.35	0.44
48:5:4738:C:H2'	48:5:4739:C:C6	2.53	0.44
51:9:185:G:H2'	51:9:186:C:C6	2.53	0.44
51:9:559:G:O2'	51:9:560:A:O4'	2.36	0.44
51:9:730:C:N3	51:9:731:G:C8	2.85	0.44
51:9:821:G:C6	61:JJ:147:PHE:CZ	3.05	0.44
51:9:943:U:O2'	66:OO:135:ILE:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1109:C:H2'	51:9:1110:G:C8	2.53	0.44
51:9:1240:A:C8	51:9:1267:C:O2'	2.68	0.44
51:9:1259:A:N6	51:9:1519:U:H5''	2.32	0.44
51:9:1298:G:HO2'	51:9:1299:A:H8	1.64	0.44
51:9:1593:C:OP1	77:ZZ:103:HIS:NE2	2.40	0.44
51:9:1598:G:HO2'	51:9:1599:U:P	2.40	0.44
51:9:1803:U:H2'	51:9:1804:U:O4'	2.17	0.44
55:DD:28:GLU:HA	62:KK:61:GLN:NE2	2.33	0.44
56:EE:59:ASP:OD1	56:EE:62:LYS:NZ	2.32	0.44
63:LL:109:MET:HE1	63:LL:140:PHE:CE1	2.53	0.44
64:MM:17:ALA:O	64:MM:21:VAL:HG12	2.17	0.44
64:MM:49:LEU:HD21	64:MM:128:PHE:CE2	2.52	0.44
68:QQ:13:PHE:CD1	68:QQ:13:PHE:C	2.95	0.44
70:SS:105:ASN:O	70:SS:109:GLU:HG3	2.17	0.44
75:XX:98:ASP:OD1	75:XX:98:ASP:C	2.59	0.44
86:ii:161:LEU:HD23	86:ii:275:LEU:CD1	2.48	0.44
86:ii:335:CYS:HB2	86:ii:366:HIS:CE1	2.52	0.44
87:jj:80:GLU:O	87:jj:83:THR:HG22	2.18	0.44
1:A:198:ARG:NH1	48:5:3688:U:OP2	2.50	0.44
3:C:209:VAL:HB	3:C:229:LEU:HD13	1.99	0.44
12:M:74:ARG:NH2	48:5:736:C:OP1	2.43	0.44
15:P:83:TRP:O	48:5:3856:A:H5''	2.16	0.44
16:Q:49:LYS:CG	16:Q:53:MET:HE3	2.47	0.44
19:T:126:VAL:HG12	19:T:127:GLN:N	2.33	0.44
20:U:67:LYS:HD2	20:U:68:SER:N	2.32	0.44
26:a:100:ILE:HG13	26:a:123:ILE:HB	1.98	0.44
32:g:66:ARG:NH2	48:5:2517:A:O2'	2.50	0.44
43:s:121:VAL:HG22	43:s:182:PRO:CB	2.48	0.44
48:5:693:C:H2'	48:5:694:C:C6	2.52	0.44
48:5:1234:G:O2'	48:5:1235:G:P	2.74	0.44
48:5:1786:A:H2'	48:5:1789:C:C5	2.53	0.44
48:5:2292:C:H2'	48:5:2293:U:C6	2.52	0.44
48:5:2494:U:H2'	48:5:2495:U:N1	2.32	0.44
48:5:4173:G:H2'	48:5:4174:U:C6	2.52	0.44
48:5:4322:G:O2'	48:5:4324:A:N7	2.42	0.44
48:5:4344:U:H2'	48:5:4345:C:C6	2.52	0.44
48:5:4916:G:H2'	48:5:4917:C:C5'	2.47	0.44
51:9:906:U:N3	51:9:907:G:N7	2.66	0.44
51:9:1440:C:H2'	51:9:1441:U:C6	2.51	0.44
59:HH:43:LEU:HD11	59:HH:72:PHE:HA	2.00	0.44
66:OO:151:LEU:HD23	66:OO:151:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SS:30:ILE:HG23	70:SS:36:VAL:HG11	2.00	0.44
86:ii:305:VAL:CG1	86:ii:306:GLU:N	2.81	0.44
87:jj:191:LYS:CD	87:jj:229:VAL:HG13	2.47	0.44
87:jj:594:TYR:N	87:jj:594:TYR:CD1	2.84	0.44
2:B:307:TYR:CD2	2:B:366:LYS:HA	2.53	0.44
7:G:34:LYS:O	48:5:4128:A:N3	2.51	0.44
12:M:34:ASN:ND2	48:5:1925:G:OP1	2.46	0.44
29:d:30:HIS:NE2	48:5:4637:OMG:OP1	2.42	0.44
32:g:75:SER:OG	48:5:2584:G:O6	2.34	0.44
35:j:79:ARG:HE	50:8:94:G:H5'	1.81	0.44
39:n:13:LEU:HD12	39:n:16:LYS:HE2	2.00	0.44
44:t:162:CYS:HB2	44:t:163:PRO:HD3	1.99	0.44
46:2:70:A:N6	46:2:71:A:N6	2.66	0.44
48:5:216:C:O2'	48:5:217:C:O2'	2.31	0.44
48:5:373:OMG:HM21	48:5:1645:C:H4'	1.99	0.44
48:5:741:C:H2'	48:5:742:G:O4'	2.17	0.44
48:5:1078:A:C2	48:5:1233:G:C6	3.06	0.44
48:5:1201:U:H2'	48:5:1202:C:O4'	2.18	0.44
48:5:1979:A:C2	48:5:1988:G:O6	2.71	0.44
48:5:2027:U:O2'	48:5:2028:C:H5'	2.18	0.44
48:5:2370:A:N1	48:5:2390:G:O2'	2.45	0.44
48:5:3871:A:H2'	48:5:3872:A:C8	2.52	0.44
48:5:4194:U:H5	48:5:4198:G:OP2	2.00	0.44
48:5:4572:U:HO2'	48:5:4573:G:H8	1.60	0.44
51:9:64:A:OP1	58:GG:177:GLN:NE2	2.44	0.44
51:9:126:G:C5'	58:GG:195:LYS:HD2	2.48	0.44
51:9:297:A:H5'	56:EE:131:VAL:O	2.18	0.44
51:9:897:U:N3	51:9:898:U:C6	2.86	0.44
51:9:1406:G:C3'	51:9:1407:U:H4'	2.47	0.44
51:9:1456:G:H2'	51:9:1457:U:C6	2.52	0.44
51:9:1724:A:H2'	51:9:1725:U:C6	2.52	0.44
56:EE:179:ASN:OD1	56:EE:230:LYS:HA	2.18	0.44
58:GG:225:GLN:HA	58:GG:228:ILE:HD12	2.00	0.44
60:II:79:ILE:HD11	60:II:105:ASP:CA	2.47	0.44
60:II:113:TYR:CD1	60:II:117:TYR:HD2	2.35	0.44
73:VV:1:MET:O	73:VV:9:VAL:HG22	2.17	0.44
84:gg:251:ALA:HB1	84:gg:286:CYS:SG	2.57	0.44
86:ii:334:HIS:CG	86:ii:369:ILE:HD13	2.53	0.44
87:jj:168:ILE:HG22	87:jj:239:MET:SD	2.57	0.44
5:E:245:ILE:HG22	5:E:246:THR:N	2.32	0.44
14:O:191:LYS:HE2	14:O:191:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:160:ARG:O	18:S:161:ARG:HB2	2.17	0.44
19:T:87:LYS:CD	48:5:4305:G:H22	2.31	0.44
23:X:106:LYS:NZ	48:5:2438:A:OP1	2.43	0.44
44:t:50:THR:HA	44:t:53:TRP:CZ2	2.52	0.44
44:t:54:LYS:O	44:t:54:LYS:NZ	2.41	0.44
44:t:87:GLU:HG3	44:t:104:ILE:HD12	1.99	0.44
47:3:54:U:H2'	47:3:55:U:O4'	2.17	0.44
48:5:644:G:H8	48:5:644:G:O5'	2.01	0.44
48:5:2005:G:C2	48:5:2015:U:H1'	2.53	0.44
48:5:2611:A:OP1	48:5:2688:G:O2'	2.32	0.44
48:5:4188:U:H2'	48:5:4189:U:C6	2.52	0.44
49:7:53:U:H4'	49:7:54:A:OP1	2.17	0.44
51:9:458:A:H2'	51:9:459:C:O4'	2.17	0.44
51:9:839:C:O2	51:9:839:C:H2'	2.17	0.44
51:9:1354:G:H2'	51:9:1356:G:N7	2.33	0.44
51:9:1406:G:H2'	51:9:1407:U:C4'	2.48	0.44
51:9:1620:A:H1'	51:9:1624:U:OP2	2.18	0.44
52:AA:10:MET:HE2	52:AA:55:TRP:CB	2.48	0.44
55:DD:94:ARG:O	55:DD:101:GLN:NE2	2.50	0.44
57:FF:20:PHE:CZ	57:FF:69:VAL:HG21	2.53	0.44
64:MM:95:ASP:N	64:MM:95:ASP:OD1	2.51	0.44
65:NN:62:GLN:O	65:NN:66:VAL:HG23	2.18	0.44
67:PP:92:SER:HB3	67:PP:107:ILE:HG12	2.00	0.44
70:SS:40:TYR:CD1	70:SS:97:GLN:OE1	2.70	0.44
77:ZZ:68:ILE:HB	77:ZZ:109:TYR:HB2	2.00	0.44
86:ii:407:GLY:HA2	87:jj:34:MET:CE	2.44	0.44
13:N:31:ARG:NH1	48:5:4078:C:OP1	2.44	0.44
19:T:35:LYS:NZ	48:5:1824:G:OP1	2.51	0.44
20:U:75:GLU:OE1	20:U:75:GLU:N	2.44	0.44
36:k:49:ASP:HB2	36:k:52:LYS:HD3	1.99	0.44
43:s:55:MET:C	43:s:55:MET:SD	3.00	0.44
48:5:468:U:O2'	48:5:469:C:C5	2.69	0.44
48:5:966:A:H2'	48:5:966:A:N3	2.32	0.44
48:5:1411:C:H2'	48:5:1411(A):G:C8	2.53	0.44
48:5:1967:A:C2	48:5:2021:G:C4	3.06	0.44
49:7:45:U:H2'	49:7:46:C:O4'	2.17	0.44
51:9:73:C:O3'	51:9:74:G:O4'	2.36	0.44
51:9:189:U:H3'	51:9:190:G:C8	2.53	0.44
51:9:689:U:C5	51:9:690:G:N2	2.86	0.44
51:9:1466:G:H5''	69:RR:4:VAL:HG22	2.00	0.44
54:CC:169:TYR:OH	54:CC:175:GLY:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:25:THR:HG21	57:FF:46:ALA:HB1	1.99	0.44
57:FF:51:HIS:ND1	57:FF:51:HIS:C	2.76	0.44
60:II:132:GLU:O	60:II:135:GLU:N	2.51	0.44
66:OO:56:VAL:HG21	66:OO:80:ASP:OD2	2.18	0.44
69:RR:17:ILE:HG13	69:RR:58:MET:HE2	2.00	0.44
84:gg:58:ALA:C	84:gg:59:LEU:HD12	2.42	0.44
84:gg:149:GLU:O	84:gg:150:TRP:CD1	2.70	0.44
84:gg:258:ILE:O	84:gg:267:VAL:HB	2.18	0.44
86:ii:21:ILE:HG23	86:ii:133:THR:HB	2.00	0.44
87:jj:285:PHE:CE1	87:jj:302:PRO:HB3	2.52	0.44
1:A:183:GLY:HA2	48:5:1613:A:H5''	2.00	0.44
2:B:76:VAL:HG21	2:B:332:MET:HE2	2.00	0.44
3:C:100:ARG:HG2	3:C:101:MET:O	2.17	0.44
3:C:208:CYS:SG	3:C:230:LEU:HD12	2.57	0.44
3:C:350:ARG:HG2	3:C:353:ARG:NH2	2.33	0.44
7:G:254:GLU:OE1	7:G:254:GLU:C	2.61	0.44
30:e:86:GLU:OE2	30:e:86:GLU:HA	2.18	0.44
40:o:73:VAL:O	40:o:78:ARG:NH2	2.51	0.44
48:5:180:C:H2'	48:5:181:C:C6	2.53	0.44
48:5:1411(C):C:O5'	48:5:1411(C):C:H6	2.01	0.44
48:5:1767:A:H2'	48:5:1769:G:C8	2.52	0.44
48:5:1977:C:C4	48:5:1978:C:N4	2.85	0.44
51:9:197:U:O2'	51:9:198:U:H5'	2.18	0.44
51:9:309:G:O2'	51:9:310:C:H5'	2.18	0.44
51:9:872:A:H2'	51:9:872:A:N3	2.33	0.44
51:9:1221:G:O2'	51:9:1676:U:O2	2.35	0.44
51:9:1305:C:H2'	51:9:1306:U:C6	2.53	0.44
51:9:1408:U:H3'	51:9:1408:U:OP2	2.18	0.44
55:DD:95:GLY:HA3	55:DD:129:SER:OG	2.17	0.44
60:II:26:LYS:O	60:II:29:LEU:HD23	2.17	0.44
60:II:113:TYR:CE1	60:II:117:TYR:CD2	3.06	0.44
69:RR:87:GLU:O	69:RR:88:VAL:HG23	2.18	0.44
70:SS:33:ILE:HD13	70:SS:71:MET:CE	2.48	0.44
87:jj:106:LEU:HD21	87:jj:287:CYS:SG	2.58	0.44
87:jj:108:LEU:HB2	87:jj:272:VAL:HG22	2.00	0.44
3:C:358:LEU:HD23	3:C:359:ALA:N	2.32	0.44
4:D:187:SER:OG	4:D:188:LYS:N	2.51	0.44
7:G:210:GLU:OE1	7:G:210:GLU:N	2.48	0.44
14:O:110:PRO:C	14:O:113:ASP:OD1	2.61	0.44
16:Q:156:PRO:O	26:a:47:LYS:O	2.36	0.44
48:5:219:G:OP2	48:5:219:G:O4'	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1194:G:N3	48:5:1195:G:H1'	2.33	0.44
48:5:1477:C:H2'	48:5:1478:C:H6	1.82	0.44
48:5:1921:C:H4'	48:5:1922:G:OP2	2.18	0.44
48:5:2519:U:H1'	48:5:2520:C:C6	2.53	0.44
48:5:4960:G:H2'	48:5:4961:G:C8	2.53	0.44
51:9:441:C:H4'	51:9:1737:G:O2'	2.17	0.44
51:9:808:A:H5''	56:EE:219:ALA:O	2.16	0.44
51:9:833:C:O2'	51:9:834:C:P	2.76	0.44
51:9:889:U:O5'	51:9:889:U:H6	2.01	0.44
51:9:1274:G:H5'	51:9:1274:G:N3	2.32	0.44
51:9:1402:A:H1'	72:UU:54:VAL:HG22	1.99	0.44
51:9:1828:C:H2'	51:9:1829:G:O4'	2.18	0.44
52:AA:203:PHE:HE2	69:RR:91:LEU:HD13	1.83	0.44
61:JJ:56:ALA:O	61:JJ:60:LEU:HG	2.18	0.44
64:MM:110:VAL:HG12	64:MM:111:VAL:N	2.33	0.44
70:SS:61:GLU:O	70:SS:65:GLU:HG2	2.18	0.44
5:E:205:ASP:C	5:E:205:ASP:OD1	2.60	0.43
7:G:214:ALA:HA	7:G:217:LYS:NZ	2.33	0.43
13:N:114:ARG:HD3	13:N:151:ILE:HG13	2.00	0.43
23:X:117:TYR:O	23:X:119:ILE:HG23	2.17	0.43
25:Z:116:VAL:O	25:Z:120:GLU:HG2	2.17	0.43
26:a:76:ASP:OD1	26:a:76:ASP:C	2.61	0.43
35:j:65:ARG:O	35:j:69:ILE:HD12	2.18	0.43
41:p:26:VAL:O	41:p:30:GLU:HG2	2.17	0.43
42:r:16:PHE:CG	42:r:28:GLU:HB3	2.52	0.43
48:5:309:C:H5''	48:5:310:G:O4'	2.18	0.43
48:5:734:G:C2	48:5:735:G:C8	3.06	0.43
48:5:1291:G:O2'	48:5:1292:C:O5'	2.30	0.43
48:5:2637:U:O2'	48:5:2718:U:O2'	2.24	0.43
48:5:3732:A:H2'	48:5:3733:A:C8	2.53	0.43
48:5:3810:C:C2	86:ii:258:TYR:HE1	2.36	0.43
48:5:3911:C:H2'	48:5:3912:U:C6	2.53	0.43
48:5:4094:G:C2	48:5:4115:G:N2	2.86	0.43
48:5:4476:C:O2	48:5:4476:C:O4'	2.34	0.43
48:5:4584:A:H2'	48:5:4585:U:O4'	2.18	0.43
49:7:12:U:OP2	49:7:67:C:O2'	2.33	0.43
51:9:201:C:C4	51:9:202:G:H1'	2.53	0.43
51:9:1395:C:O2'	51:9:1396:A:P	2.75	0.43
51:9:1597:C:H4'	51:9:1603:G:C6	2.53	0.43
51:9:1713:C:H2'	51:9:1714:U:C6	2.53	0.43
52:AA:39:TYR:CE2	69:RR:105:MET:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:78:SER:O	52:AA:101:GLY:N	2.40	0.43
57:FF:123:GLU:HG2	57:FF:200:ALA:HB1	2.00	0.43
58:GG:222:GLU:O	58:GG:225:GLN:HG2	2.18	0.43
60:II:113:TYR:CE1	60:II:158:ILE:HD11	2.53	0.43
66:OO:27:VAL:CG1	66:OO:90:ILE:HD13	2.48	0.43
84:gg:29:ASP:N	84:gg:29:ASP:OD1	2.51	0.43
84:gg:51:ASN:OD1	84:gg:53:GLY:N	2.51	0.43
86:ii:35:ILE:HD12	86:ii:74:ALA:HB3	2.00	0.43
86:ii:343:ILE:H	86:ii:343:ILE:HD12	1.83	0.43
87:jj:484:LEU:HD13	87:jj:485:ILE:N	2.33	0.43
2:B:119:TYR:HE1	48:5:4967:A:H5'	1.83	0.43
2:B:252:ALA:HB1	48:5:4524:G:C2	2.53	0.43
4:D:188:LYS:O	4:D:189:GLU:CB	2.66	0.43
10:J:120:ASP:HB3	10:J:123:ILE:HB	1.99	0.43
10:J:159:LYS:O	10:J:163:MET:HG3	2.17	0.43
13:N:138:PHE:HA	13:N:143:ARG:HD2	2.00	0.43
14:O:8:VAL:HG12	14:O:117:ARG:HG3	2.00	0.43
30:e:127:ALA:O	48:5:2327:G:OP1	2.37	0.43
43:s:17:ILE:HG13	43:s:18:ILE:N	2.32	0.43
44:t:104:ILE:O	44:t:106:PHE:CE1	2.71	0.43
46:2:18:G:H21	46:2:58:A:H5'	1.82	0.43
48:5:657:C:H5'	48:5:658:C:OP2	2.19	0.43
48:5:700:G:H2'	48:5:701:G:O5'	2.18	0.43
48:5:906:C:H2'	48:5:907:C:O4'	2.18	0.43
48:5:930:G:HO2'	48:5:931:C:P	2.36	0.43
48:5:1363:C:H2'	48:5:1364:U:O4'	2.19	0.43
48:5:1404:G:N2	48:5:1414:C:C2	2.86	0.43
48:5:3902:A:OP1	48:5:4450:U:H4'	2.17	0.43
51:9:172:OMU:OP1	51:9:315:C:O2'	2.31	0.43
51:9:318:A:H2	51:9:332:G:H22	1.66	0.43
51:9:588:G:H1'	51:9:589:G:H5''	1.99	0.43
51:9:898:U:H2'	51:9:898:U:O2	2.17	0.43
51:9:1535:U:O4	57:FF:159:ARG:HG3	2.17	0.43
51:9:1641:A:H2'	51:9:1642:U:O4'	2.18	0.43
52:AA:124:VAL:HG21	52:AA:134:LEU:HD11	1.99	0.43
56:EE:92:ILE:CG2	76:YY:17:LEU:HD21	2.48	0.43
56:EE:177:THR:HG23	56:EE:196:THR:HA	2.01	0.43
57:FF:25:THR:HG21	57:FF:46:ALA:CB	2.48	0.43
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD13	2.01	0.43
57:FF:99:ILE:HG13	77:ZZ:108:ILE:HD11	1.98	0.43
61:JJ:110:LEU:HD12	61:JJ:114:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:OO:46:ASP:OD1	66:OO:46:ASP:N	2.50	0.43
69:RR:34:VAL:O	69:RR:38:ILE:HG13	2.17	0.43
84:gg:16:GLY:O	84:gg:305:ASN:HA	2.18	0.43
87:jj:249:VAL:O	87:jj:252:ARG:HG2	2.18	0.43
87:jj:432:ILE:HD12	87:jj:432:ILE:C	2.39	0.43
6:F:150:ASN:HD21	48:5:943:A:H62	1.65	0.43
16:Q:177:ALA:O	16:Q:178:ARG:C	2.61	0.43
28:c:35:LEU:O	28:c:39:ARG:HG3	2.19	0.43
30:e:81:ASN:HA	30:e:111:ILE:HD11	2.00	0.43
42:r:54:ALA:HA	42:r:61:VAL:HG23	2.00	0.43
43:s:16:LYS:O	43:s:20:LEU:HG	2.19	0.43
44:t:117:ARG:O	44:t:121:LEU:HD12	2.18	0.43
46:2:19:G:H3'	46:2:20:U:C5'	2.48	0.43
48:5:457:G:C6	48:5:458:C:C4	3.07	0.43
48:5:924:C:O2'	48:5:925:C:OP1	2.34	0.43
48:5:970:G:H2'	48:5:971:U:O4'	2.18	0.43
48:5:1380:G:N2	48:5:1381:U:O4	2.43	0.43
48:5:1890:G:N2	48:5:1938:C:H42	2.16	0.43
48:5:3662:A:H5'	48:5:3664:G:O4'	2.19	0.43
48:5:4596:C:C4	48:5:4597:U:C4	3.06	0.43
51:9:293:C:OP1	63:LL:39:ASN:O	2.35	0.43
51:9:309:G:C2	51:9:310:C:C5	3.05	0.43
51:9:546:G:C6	51:9:547:G:C2	3.05	0.43
51:9:1170:A:H4'	51:9:1171:G:OP1	2.18	0.43
51:9:1435:C:H2'	51:9:1436:C:N1	2.33	0.43
51:9:1862:G:H4'	51:9:1863:A:OP1	2.17	0.43
54:CC:251:LEU:HA	73:VV:23:ILE:HD11	2.00	0.43
58:GG:108:VAL:HG12	58:GG:109:LEU:N	2.32	0.43
64:MM:117:GLU:O	64:MM:118:SER:OG	2.20	0.43
67:PP:15:PHE:CD2	67:PP:109:PRO:HB2	2.53	0.43
71:TT:114:GLU:HG2	71:TT:124:THR:HG23	1.99	0.43
86:ii:306:GLU:HG2	86:ii:307:ASP:N	2.34	0.43
4:D:35:ARG:HG2	48:5:4326:G:O2'	2.18	0.43
4:D:71:GLY:O	4:D:73:MET:HE3	2.18	0.43
6:F:156:ARG:HG3	6:F:247:ASN:OD1	2.18	0.43
8:H:45:LEU:HD22	8:H:57:VAL:HG22	1.99	0.43
11:L:125:VAL:CG2	33:h:123:ALA:HB3	2.48	0.43
11:L:201:GLU:OE1	11:L:202:ALA:N	2.51	0.43
14:O:186:GLU:O	14:O:187:LYS:CB	2.65	0.43
16:Q:178:ARG:HA	16:Q:184:ARG:O	2.18	0.43
23:X:154:GLY:O	33:h:37:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:84:ALA:HA	65:NN:151:ALA:O	2.18	0.43
44:t:64:ILE:HG23	44:t:71:ILE:HB	2.00	0.43
46:2:66:C:H2'	46:2:67:G:C8	2.52	0.43
47:3:32:C:H5'	57:FF:136:ARG:NH1	2.32	0.43
48:5:189:G:C2	48:5:190:G:C8	3.07	0.43
48:5:1297:U:H2'	48:5:1298:C:H6	1.84	0.43
48:5:1770:A:N1	48:5:1771:U:C4	2.87	0.43
48:5:2565:A:C2'	48:5:2566:G:OP1	2.66	0.43
48:5:2669:C:H2'	48:5:2670:C:O4'	2.17	0.43
48:5:2844:A:O2'	48:5:4631:G:H4'	2.18	0.43
48:5:4090:G:H2'	48:5:4091:G:O4'	2.18	0.43
51:9:553:U:H2'	51:9:554:A:O4'	2.17	0.43
51:9:587:A:O2'	51:9:588:G:N2	2.51	0.43
51:9:1239:U:O2'	51:9:1241:A:N7	2.29	0.43
51:9:1431:G:O5'	51:9:1432:U:O5'	2.37	0.43
51:9:1477:U:H1'	51:9:1478:U:OP1	2.18	0.43
51:9:1675:A:O3'	57:FF:74:ASN:HB3	2.19	0.43
57:FF:173:LEU:O	57:FF:177:LEU:HG	2.19	0.43
59:HH:125:VAL:O	59:HH:129:ILE:HG13	2.18	0.43
72:UU:22:ILE:HD13	72:UU:114:VAL:HG22	1.99	0.43
75:XX:28:LYS:HE2	75:XX:32:LEU:HD22	2.00	0.43
86:ii:251:LEU:CD2	86:ii:275:LEU:HD23	2.48	0.43
87:jj:204:LEU:O	87:jj:205:ASP:OD1	2.36	0.43
2:B:343:ARG:NH2	48:5:4976:U:O2'	2.51	0.43
4:D:185:SER:O	4:D:187:SER:O	2.36	0.43
11:L:108:GLU:H	11:L:108:GLU:CD	2.25	0.43
14:O:175:MET:HE3	14:O:175:MET:O	2.18	0.43
26:a:8:THR:OG1	48:5:1339:U:OP1	2.30	0.43
30:e:35:TRP:CE2	30:e:56:PRO:HD2	2.54	0.43
33:h:29:SER:O	33:h:33:VAL:HG23	2.19	0.43
36:k:11:PHE:CD1	36:k:11:PHE:C	2.97	0.43
43:s:82:ILE:O	43:s:83:ARG:HD3	2.18	0.43
47:3:8:U:O2	47:3:8:U:H3'	2.18	0.43
47:3:33:U:O5'	47:3:34:U:OP2	2.37	0.43
48:5:134:G:H1'	48:5:135:G:OP2	2.18	0.43
48:5:233:U:H5'	48:5:234:G:OP2	2.17	0.43
48:5:2503:G:O4'	48:5:4084:G:N2	2.51	0.43
48:5:2890:C:H4'	48:5:5034:A:O4'	2.19	0.43
48:5:3657:U:H5''	48:5:3657:U:H6	1.83	0.43
48:5:4187:G:H2'	48:5:4188:U:O4'	2.19	0.43
48:5:4412:C:H2'	48:5:4413:C:O2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4746:C:H2'	48:5:4747:C:O4'	2.18	0.43
50:8:71:A:C2	50:8:88:A:H1'	2.53	0.43
50:8:89:U:H2'	50:8:90:C:C6	2.53	0.43
51:9:71:G:C2'	51:9:72:C:H5''	2.49	0.43
51:9:547:G:C2	51:9:549:C:N4	2.87	0.43
51:9:606:G:O4'	82:ee:56:ASN:HB3	2.18	0.43
51:9:664:A:N1	51:9:1163:C:O2	2.51	0.43
51:9:917:U:O4'	59:HH:118:ARG:HG3	2.19	0.43
51:9:942:G:H21	66:OO:137:SER:HB2	1.82	0.43
51:9:1261:C:O2	81:dd:10:HIS:CE1	2.71	0.43
51:9:1672:U:OP1	68:QQ:18:THR:OG1	2.33	0.43
52:AA:54:THR:HG23	52:AA:162:PRO:O	2.19	0.43
55:DD:138:VAL:O	55:DD:138:VAL:HG23	2.18	0.43
55:DD:156:LEU:O	55:DD:157:MET:HE2	2.19	0.43
64:MM:79:VAL:HG13	64:MM:80:ASP:HB2	2.00	0.43
65:NN:127:ARG:HH11	65:NN:127:ARG:HG2	1.82	0.43
68:QQ:41:MET:SD	71:TT:9:VAL:C	3.01	0.43
86:ii:176:LEU:HD11	86:ii:201:TYR:CD2	2.54	0.43
87:jj:36:LYS:HB3	87:jj:54:LEU:HD21	2.00	0.43
10:J:120:ASP:OD1	10:J:121:PRO:HD2	2.18	0.43
26:a:78:LEU:HD21	26:a:124:VAL:HG22	2.00	0.43
27:b:10:HIS:NE2	48:5:1877:G:O6	2.52	0.43
45:1:57:ARG:HG3	48:5:3904:G:O3'	2.19	0.43
48:5:90:G:OP2	48:5:92:C:N4	2.40	0.43
48:5:487:G:H2'	48:5:488:G:O4'	2.19	0.43
48:5:498:C:H3'	48:5:499:G:H4'	2.00	0.43
48:5:1927:U:OP1	48:5:1949:U:O2'	2.33	0.43
48:5:1962:A:N3	48:5:1962:A:H2'	2.33	0.43
48:5:2062:C:O2'	48:5:2063:G:H5'	2.18	0.43
48:5:2589:C:H2'	48:5:2590:G:O4'	2.18	0.43
48:5:2898:G:H2'	48:5:2899:C:C6	2.53	0.43
48:5:3909:C:O2	48:5:4396:A:N1	2.51	0.43
48:5:4154:G:H2'	48:5:4155:C:C6	2.54	0.43
48:5:4413:C:H5	48:5:4429:C:H42	1.66	0.43
48:5:4413:C:H5	48:5:4429:C:N4	2.16	0.43
48:5:4522:G:O2'	48:5:4525:C:OP2	2.37	0.43
48:5:4771:C:O2'	48:5:4772:C:H5'	2.19	0.43
50:8:117:C:H2'	50:8:118:C:O4'	2.18	0.43
50:8:139:G:H2'	50:8:140:C:O4'	2.19	0.43
50:8:140:C:H2'	50:8:141:C:C6	2.53	0.43
51:9:594:A:C2	51:9:642:U:O2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1329:U:O2'	51:9:1332:A:OP2	2.19	0.43
51:9:1728:U:H2'	51:9:1729:U:O4'	2.18	0.43
51:9:1786:U:O2'	51:9:1787:G:H5'	2.18	0.43
52:AA:173:LEU:HD22	69:RR:91:LEU:HD21	2.00	0.43
54:CC:206:SER:CB	54:CC:224:THR:HG21	2.48	0.43
55:DD:61:GLU:C	55:DD:63:GLY:H	2.26	0.43
56:EE:139:LEU:HD23	56:EE:139:LEU:O	2.19	0.43
59:HH:134:VAL:O	59:HH:134:VAL:CG2	2.60	0.43
61:JJ:111:GLN:NE2	61:JJ:127:ARG:HB2	2.33	0.43
67:PP:89:MET:C	67:PP:107:ILE:HD11	2.44	0.43
69:RR:57:LEU:HD13	69:RR:69:ILE:HD11	2.01	0.43
70:SS:87:GLN:O	70:SS:88:LYS:C	2.62	0.43
75:XX:105:PHE:HB2	75:XX:119:ARG:C	2.43	0.43
84:gg:150:TRP:O	84:gg:169:GLY:HA3	2.18	0.43
86:ii:238:GLN:O	86:ii:238:GLN:CG	2.65	0.43
4:D:188:LYS:O	4:D:189:GLU:HB2	2.19	0.43
13:N:181:HIS:CD2	48:5:99:A:H4'	2.53	0.43
18:S:16:CYS:SG	18:S:54:MET:HG3	2.58	0.43
26:a:117:LEU:HD23	26:a:140:VAL:CG2	2.48	0.43
48:5:1411(B):C:H2'	48:5:1411(C):C:C6	2.52	0.43
48:5:2638:G:H22	48:5:2697:A:N6	2.17	0.43
48:5:4114:C:H2'	48:5:4115:G:O4'	2.18	0.43
48:5:4491:G:O2'	48:5:4511:A:N1	2.49	0.43
48:5:4504:C:H2'	48:5:4505:C:C6	2.53	0.43
48:5:4957:C:H3'	48:5:4958:C:H5''	2.01	0.43
50:8:31:G:H2'	50:8:32:C:O4'	2.17	0.43
51:9:67:C:C2	58:GG:162:LEU:HD11	2.54	0.43
51:9:529:A:H61	51:9:555:A:H61	1.65	0.43
51:9:953:C:H2'	51:9:954:U:C6	2.53	0.43
51:9:1240:A:H8	51:9:1267:C:O2'	2.01	0.43
51:9:1328:OMG:HM23	51:9:1328:OMG:H1'	1.80	0.43
51:9:1499:U:H4'	55:DD:176:LEU:HD23	2.00	0.43
51:9:1513:C:OP1	81:dd:10:HIS:HB3	2.19	0.43
51:9:1598:G:OP1	77:ZZ:80:ARG:NH1	2.52	0.43
51:9:1692:PSU:H2'	51:9:1693:G:C8	2.53	0.43
51:9:1702:G:H2'	51:9:1703:OMC:O4'	2.18	0.43
52:AA:191:ARG:HG3	52:AA:191:ARG:O	2.19	0.43
54:CC:187:ARG:NH1	54:CC:191:VAL:O	2.52	0.43
56:EE:122:LYS:HD3	56:EE:164:LEU:HD21	2.00	0.43
58:GG:181:THR:O	58:GG:182:PRO:C	2.62	0.43
59:HH:57:ARG:H	59:HH:57:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:159:SER:O	60:II:163:GLU:HG2	2.18	0.43
64:MM:114:TYR:HD1	64:MM:121:LYS:HD2	1.84	0.43
66:OO:117:ARG:NH2	78:aa:48:ALA:O	2.51	0.43
67:PP:89:MET:HB3	67:PP:107:ILE:HD11	2.00	0.43
80:cc:30:VAL:HG23	80:cc:32:VAL:HG13	2.00	0.43
83:ff:133:ARG:HD2	83:ff:142:THR:HG23	2.00	0.43
84:gg:171:ASP:OD1	84:gg:173:LEU:HB2	2.18	0.43
86:ii:162:GLN:O	86:ii:163:GLY:C	2.62	0.43
2:B:108:GLU:OE1	2:B:109:HIS:NE2	2.52	0.43
4:D:3:PHE:CD1	4:D:3:PHE:N	2.85	0.43
5:E:150:GLY:HA3	5:E:204:ILE:O	2.18	0.43
5:E:186:ARG:HD3	48:5:4936:G:C5	2.53	0.43
8:H:176:LEU:HB3	38:m:86:ALA:HB1	2.01	0.43
44:t:124:GLU:HG2	44:t:125:LEU:HG	2.01	0.43
48:5:119:G:H3'	48:5:120:A:H5''	2.01	0.43
48:5:406:C:HO2'	48:5:407:A:P	2.39	0.43
48:5:1761:G:C6	48:5:1762:C:C2	3.06	0.43
48:5:3944:G:O3'	53:BB:54:GLY:HA2	2.18	0.43
50:8:36:G:O2'	50:8:103:A:N1	2.37	0.43
51:9:488:U:O2	51:9:488:U:C2'	2.66	0.43
51:9:734:C:N4	51:9:735:C:C5	2.87	0.43
51:9:1164:G:O2'	51:9:1165:G:H5'	2.19	0.43
51:9:1240:A:H62	67:PP:99:GLY:HA3	1.84	0.43
51:9:1555:U:H6	51:9:1557:C:H41	1.66	0.43
51:9:1672:U:H5''	68:QQ:75:GLY:HA2	1.99	0.43
55:DD:225:GLU:O	55:DD:226:GLN:C	2.62	0.43
58:GG:3:LEU:HD22	58:GG:111:LEU:HD11	2.01	0.43
58:GG:108:VAL:CG1	58:GG:109:LEU:N	2.81	0.43
59:HH:95:ILE:CG1	59:HH:96:ALA:N	2.80	0.43
60:II:113:TYR:CE2	60:II:121:LEU:HB2	2.54	0.43
64:MM:120:ALA:O	64:MM:123:VAL:HG22	2.18	0.43
66:OO:91:THR:HA	66:OO:124:MET:HE1	2.00	0.43
74:WW:55:ASP:O	74:WW:56:HIS:HB2	2.18	0.43
84:gg:128:THR:H	84:gg:151:VAL:HG21	1.83	0.43
86:ii:48:VAL:HG12	86:ii:82:LEU:HD11	2.01	0.43
86:ii:136:LEU:O	86:ii:140:LEU:HG	2.18	0.43
87:jj:574:ARG:HG3	87:jj:575:PRO:N	2.34	0.43
3:C:22:VAL:HG22	3:C:258:ARG:CZ	2.49	0.43
4:D:237:GLU:CG	4:D:241:LYS:HZ2	2.31	0.43
6:F:60:TYR:HA	6:F:63:MET:HE3	2.01	0.43
7:G:93:THR:O	7:G:97:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:98:ARG:NE	48:5:4872:G:O6	2.49	0.43
20:U:23:LEU:HD11	20:U:83:LEU:HB3	2.00	0.43
20:U:35:ASP:O	20:U:38:ASN:OD1	2.37	0.43
30:e:76:LYS:O	42:r:23:GLN:NE2	2.50	0.43
41:p:29:ILE:HG23	41:p:69:TRP:HB3	2.01	0.43
44:t:10:ILE:HD11	44:t:67:ARG:HD2	2.01	0.43
48:5:356:G:O2'	50:8:25:G:N3	2.52	0.43
48:5:462:G:O3'	48:5:463:A:O4'	2.36	0.43
48:5:1472:C:H2'	48:5:1473:U:H6	1.83	0.43
48:5:2457:G:H4'	48:5:2470:C:N4	2.34	0.43
48:5:3605:C:H2'	48:5:3606:U:O4'	2.19	0.43
48:5:4747:C:H2'	48:5:4748:U:O4'	2.19	0.43
50:8:33:G:H5''	50:8:34:U:OP1	2.19	0.43
50:8:51:U:H2'	50:8:51:U:O2	2.18	0.43
51:9:116:OMU:O5'	51:9:116:OMU:H6	2.18	0.43
51:9:121:OMU:O5'	51:9:121:OMU:H6	2.19	0.43
51:9:155:G:C6	51:9:164:A:C6	3.07	0.43
51:9:464:A:H3'	51:9:465:A:H5'	2.00	0.43
51:9:870:A:H5''	51:9:872:A:O4'	2.19	0.43
51:9:877:C:H2'	51:9:879:C:OP2	2.19	0.43
51:9:1276:A:C2	51:9:1277:C:H1'	2.54	0.43
51:9:1646:C:HO2'	51:9:1647:A:P	2.41	0.43
51:9:1673:U:H2'	51:9:1674:G:O4'	2.19	0.43
51:9:1758:G:H2'	51:9:1759:G:O4'	2.18	0.43
55:DD:70:THR:HG22	55:DD:86:LEU:HB2	2.01	0.43
57:FF:140:ASP:OD2	80:cc:44:ARG:NH1	2.52	0.43
61:JJ:24:ARG:O	61:JJ:27:GLN:HG3	2.19	0.43
72:UU:115:THR:HG22	72:UU:116:ILE:N	2.34	0.43
75:XX:88:ASP:OD1	82:ee:10:GLY:HA2	2.19	0.43
77:ZZ:94:LYS:HD3	77:ZZ:96:LEU:HD13	2.00	0.43
83:ff:101:TYR:HB3	83:ff:109:ILE:CG2	2.49	0.43
86:ii:37:LEU:HD21	86:ii:39:ILE:HD11	2.01	0.43
86:ii:309:LEU:HD21	86:ii:345:TYR:CZ	2.54	0.43
87:jj:30:PRO:HD2	91:jj:601:SF4:S2	2.59	0.43
87:jj:56:ILE:O	87:jj:56:ILE:CG2	2.67	0.43
47:3:7:A:O2'	47:3:49:C:O4'	2.37	0.43
47:3:31:A:H2'	47:3:32:C:C6	2.54	0.43
48:5:1590:C:H5''	48:5:1591:U:O5'	2.19	0.43
48:5:1760:G:C4	48:5:1761:G:C8	3.06	0.43
48:5:2876:OMG:HM22	48:5:2877:G:O5'	2.19	0.43
48:5:4524:G:OP2	48:5:4524:G:H4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:8:84:A:N3	50:8:84:A:O5'	2.51	0.43
51:9:217:A:H2	51:9:309:G:N2	2.15	0.43
51:9:913:A:O3'	59:HH:67:PRO:HG3	2.19	0.43
51:9:1280:G:C2	51:9:1281:G:C4	3.07	0.43
51:9:1298:G:O2'	51:9:1299:A:P	2.76	0.43
51:9:1834:A:H2	51:9:1837:G:H1	1.66	0.43
53:BB:36:PRO:HB3	53:BB:231:LEU:HD23	2.00	0.43
55:DD:65:ARG:O	55:DD:69:LEU:HG	2.19	0.43
55:DD:210:ILE:HD12	55:DD:210:ILE:H	1.81	0.43
56:EE:48:LEU:CD1	56:EE:61:VAL:HG23	2.49	0.43
56:EE:149:TYR:N	56:EE:150:PRO:CD	2.82	0.43
56:EE:189:LEU:HD23	56:EE:190:GLY:N	2.34	0.43
61:JJ:163:SER:O	61:JJ:164:PRO:C	2.61	0.43
67:PP:20:VAL:HG21	67:PP:28:MET:HE2	2.00	0.43
67:PP:53:GLN:HB3	67:PP:83:MET:SD	2.58	0.43
71:TT:33:TRP:CE3	71:TT:37:VAL:HG11	2.54	0.43
75:XX:28:LYS:HE3	75:XX:32:LEU:HD13	2.00	0.43
84:gg:289:LEU:HD13	84:gg:298:LEU:HD21	2.01	0.43
87:jj:146:TYR:CD1	87:jj:146:TYR:C	2.97	0.43
87:jj:257:ILE:HG12	87:jj:281:TYR:OH	2.19	0.43
87:jj:322:LEU:HD13	87:jj:322:LEU:C	2.44	0.43
2:B:288:GLY:HA3	2:B:330:PHE:CZ	2.54	0.42
3:C:221:PHE:HB2	3:C:229:LEU:HD21	2.00	0.42
5:E:245:ILE:HG22	5:E:246:THR:H	1.84	0.42
12:M:90:ARG:NE	48:5:4868:G:H5''	2.34	0.42
20:U:43:LEU:CB	20:U:63:LEU:HD21	2.48	0.42
24:Y:43:ASN:OD1	24:Y:126:ARG:HD3	2.19	0.42
41:p:9:GLY:C	48:5:1554:A:H5'	2.44	0.42
43:s:72:ASN:OD1	43:s:193:PHE:HE2	2.01	0.42
48:5:914:U:H1'	48:5:915:A:C4	2.54	0.42
48:5:1440:U:C2'	48:5:1441:C:O5'	2.67	0.42
48:5:1811:G:H2'	48:5:1812:C:C6	2.53	0.42
48:5:1915:C:H5	92:5:6026:HOH:O	2.01	0.42
48:5:2521:G:H5'	48:5:2640:G:H1'	2.01	0.42
51:9:318:A:C2	51:9:333:G:C2	3.07	0.42
51:9:440:G:OP1	51:9:1798:C:O2'	2.34	0.42
51:9:441:C:H2'	51:9:442:C:C6	2.54	0.42
51:9:1101:U:H2'	51:9:1102:G:C8	2.54	0.42
52:AA:55:TRP:HZ3	52:AA:177:MET:SD	2.42	0.42
52:AA:147:LEU:HB3	52:AA:163:CYS:SG	2.59	0.42
54:CC:108:LYS:HD3	54:CC:109:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:2:LYS:O	58:GG:108:VAL:HG13	2.19	0.42
60:II:139:LYS:HG3	60:II:139:LYS:O	2.19	0.42
61:JJ:82:VAL:HG11	61:JJ:92:MET:CG	2.49	0.42
64:MM:110:VAL:CG1	64:MM:111:VAL:N	2.82	0.42
66:OO:117:ARG:NH1	78:aa:49:ALA:HB2	2.34	0.42
72:UU:29:VAL:HG22	72:UU:85:HIS:CE1	2.53	0.42
72:UU:69:PRO:HB3	81:dd:41:GLN:HG2	2.01	0.42
77:ZZ:84:ALA:O	77:ZZ:88:LEU:HG	2.18	0.42
83:ff:136:CYS:HB3	83:ff:140:CYS:N	2.34	0.42
84:gg:5:MET:HA	84:gg:311:GLN:O	2.18	0.42
86:ii:202:VAL:HG13	86:ii:236:LEU:CD1	2.49	0.42
87:jj:168:ILE:HG13	87:jj:168:ILE:O	2.18	0.42
2:B:62:ARG:HG3	2:B:65:SER:HB3	2.02	0.42
2:B:89:ILE:HG12	2:B:197:ALA:HB1	2.01	0.42
3:C:50:GLN:OE1	48:5:347:A:O2'	2.29	0.42
5:E:153:LEU:HD13	5:E:197:VAL:HG21	2.00	0.42
15:P:102:ALA:CB	15:P:112:LEU:HD11	2.49	0.42
17:R:32:ILE:O	17:R:35:ALA:HB3	2.17	0.42
25:Z:68:ILE:HD13	25:Z:119:GLU:HG2	2.01	0.42
40:o:70:LEU:HD11	40:o:83:LEU:HD23	2.02	0.42
44:t:58:ILE:O	44:t:80:LEU:HD22	2.19	0.42
45:1:57:ARG:CZ	48:5:3904:G:H4'	2.49	0.42
48:5:125:C:H2'	48:5:126:C:H6	1.84	0.42
48:5:700:G:C2'	48:5:701:G:O5'	2.67	0.42
48:5:1201:U:C2'	48:5:1202:C:H5'	2.49	0.42
48:5:1503:A:H4'	48:5:1504:G:H5'	2.01	0.42
48:5:1759:G:C3'	48:5:1760:G:H5''	2.49	0.42
48:5:2110:G:H2'	48:5:2111:U:H5'	2.00	0.42
48:5:2336:G:H2'	48:5:2337:C:C6	2.54	0.42
48:5:2557:G:H1	48:5:2570:U:H3	1.67	0.42
48:5:4918:C:N4	48:5:4919:G:O6	2.52	0.42
51:9:172:OMU:H6	51:9:315:C:O2'	2.19	0.42
51:9:1068:G:N7	92:9:2026:HOH:O	2.36	0.42
51:9:1279:C:H2'	51:9:1280:G:C1'	2.49	0.42
51:9:1507:G:C5	83:ff:80:TYR:CE2	3.06	0.42
51:9:1556:A:C2	51:9:1557:C:C5	3.07	0.42
52:AA:90:PHE:CD1	52:AA:90:PHE:C	2.97	0.42
53:BB:133:TYR:CE1	53:BB:221:PRO:HD2	2.54	0.42
54:CC:74:LYS:HB3	54:CC:269:PHE:CD2	2.53	0.42
55:DD:85:GLU:O	55:DD:86:LEU:HD12	2.19	0.42
65:NN:92:ILE:HG22	65:NN:150:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:UU:55:ARG:HG3	72:UU:55:ARG:NH1	2.34	0.42
75:XX:4:CYS:O	75:XX:5:ARG:HB3	2.18	0.42
76:YY:62:THR:HB	76:YY:69:THR:HB	2.01	0.42
86:ii:286:LEU:HD11	86:ii:321:ILE:CD1	2.50	0.42
87:jj:182:GLY:O	87:jj:214:VAL:HG13	2.19	0.42
87:jj:412:LYS:HA	87:jj:475:CYS:SG	2.59	0.42
87:jj:567:ARG:NH2	87:jj:577:ILE:O	2.51	0.42
1:A:39:GLY:HA2	1:A:93:LYS:HG3	2.00	0.42
2:B:201:LEU:O	2:B:202:GLU:HB2	2.20	0.42
8:H:5:LEU:HB2	8:H:60:TRP:CZ3	2.54	0.42
13:N:14:LYS:HE2	48:5:280:G:H5''	2.01	0.42
19:T:87:LYS:CE	48:5:4305:G:H1	2.32	0.42
46:2:50:U:H2'	46:2:51:C:C6	2.54	0.42
48:5:1332:C:H2'	48:5:1333:A:H8	1.85	0.42
48:5:1786:A:O2'	48:5:1788:A:OP2	2.22	0.42
48:5:4760:G:H2'	48:5:4761:G:O4'	2.19	0.42
51:9:46:A:H4'	51:9:47:G:C5'	2.49	0.42
51:9:50:A:N1	51:9:488:U:H5	2.17	0.42
51:9:302:A:H2'	51:9:303:C:O4'	2.19	0.42
51:9:305:U:C6	60:II:182:CYS:O	2.71	0.42
51:9:933:G:N7	51:9:992:A:N1	2.67	0.42
51:9:1336:C:H2'	51:9:1337:4AC:O4'	2.19	0.42
51:9:1422:G:N1	51:9:1425:G:OP2	2.53	0.42
51:9:1745:A:H2'	51:9:1746:U:O4'	2.20	0.42
51:9:1810:U:H2'	51:9:1811:C:O4'	2.18	0.42
52:AA:113:GLN:O	52:AA:116:PHE:N	2.52	0.42
57:FF:126:THR:HB	57:FF:139:VAL:HG21	2.01	0.42
59:HH:45:ILE:HD11	59:HH:62:ILE:HG23	2.01	0.42
62:KK:14:LEU:HA	62:KK:17:LYS:HZ2	1.85	0.42
64:MM:64:LEU:O	64:MM:67:ALA:HB3	2.18	0.42
73:VV:24:ILE:O	73:VV:24:ILE:HG22	2.18	0.42
86:ii:237:SER:OG	86:ii:238:GLN:N	2.51	0.42
4:D:60:ILE:HB	4:D:80:ALA:HB2	2.01	0.42
6:F:127:ALA:O	6:F:131:MET:HG3	2.18	0.42
10:J:85:LYS:O	10:J:89:VAL:HG23	2.19	0.42
10:J:89:VAL:HG21	10:J:115:LEU:HD23	2.01	0.42
17:R:118:HIS:ND1	48:5:2663:G:OP1	2.52	0.42
46:2:13:U:O4	46:2:22:U:O4	2.38	0.42
48:5:282:C:H2'	48:5:283:G:O4'	2.19	0.42
48:5:370:U:H2'	48:5:371:A:O4'	2.19	0.42
48:5:1450:C:O2'	48:5:2104:A:H1'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1578:U:H2'	48:5:1579:C:C6	2.54	0.42
48:5:2030:A:H2'	48:5:2031:C:O4'	2.19	0.42
48:5:2871:A:H2'	48:5:2872:C:O4'	2.20	0.42
48:5:4254:G:H22	48:5:4257:A:H8	1.67	0.42
48:5:4489:G:C6	48:5:4708:A:C5	3.07	0.42
51:9:407:G:H5''	51:9:408:A:H5'	2.01	0.42
51:9:1047:C:H2'	51:9:1048:G:O4'	2.20	0.42
51:9:1280:G:C6	51:9:1281:G:C6	3.07	0.42
51:9:1288:U:O4	51:9:1311:C:N3	2.52	0.42
51:9:1399:C:H4'	84:gg:100:ARG:NH2	2.33	0.42
54:CC:270:THR:HG23	54:CC:271:ASP:N	2.34	0.42
55:DD:16:ILE:HG21	81:dd:22:ARG:NH1	2.34	0.42
59:HH:91:HIS:CB	59:HH:172:THR:HG21	2.49	0.42
67:PP:115:TYR:HB2	67:PP:118:GLU:HG3	2.01	0.42
69:RR:85:VAL:HG22	69:RR:86:PRO:HD2	2.01	0.42
71:TT:28:LEU:HB3	71:TT:54:TYR:HE1	1.84	0.42
83:ff:127:MET:CE	83:ff:136:CYS:HB2	2.49	0.42
86:ii:302:CYS:SG	86:ii:413:LEU:HD21	2.60	0.42
86:ii:354:LYS:HD2	86:ii:357:PHE:CE2	2.55	0.42
4:D:215:ASP:OD1	4:D:215:ASP:N	2.50	0.42
10:J:54:ARG:NH2	10:J:55:TYR:OH	2.53	0.42
10:J:103:GLY:HA3	10:J:157:ILE:HG22	2.01	0.42
14:O:61:ARG:HA	14:O:70:PRO:HD2	2.01	0.42
16:Q:177:ALA:O	26:a:51:GLY:HA2	2.19	0.42
20:U:49:VAL:O	20:U:52:LYS:HG2	2.19	0.42
44:t:57:ARG:NE	44:t:83:LYS:HE3	2.34	0.42
47:3:71:G:H4'	48:5:3739:C:O2	2.19	0.42
48:5:1543:G:O2'	48:5:2513:A:N3	2.51	0.42
48:5:1757:U:C2	48:5:1758:G:C8	3.07	0.42
48:5:1857:C:H2'	48:5:1858:A:C8	2.54	0.42
48:5:1981:G:C4	48:5:1982:G:O4'	2.73	0.42
48:5:2046:G:C2'	48:5:2047:A:OP2	2.66	0.42
48:5:4736:C:H2'	48:5:4737:G:H8	1.85	0.42
50:8:81:C:OP1	50:8:82:A:OP2	2.37	0.42
51:9:145:G:H2'	51:9:146:G:C8	2.54	0.42
51:9:157:U:H1'	58:GG:60:GLY:HA3	2.00	0.42
51:9:328:U:H2'	51:9:329:G:O4'	2.19	0.42
51:9:546:G:HO2'	51:9:547:G:C4'	2.33	0.42
51:9:682:U:H5'	51:9:1160:U:OP1	2.20	0.42
51:9:688:U:O2	51:9:688:U:P	2.78	0.42
51:9:1279:C:H2'	51:9:1280:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1444:U:H2'	51:9:1445:PSU:O4'	2.20	0.42
55:DD:74:GLN:HA	55:DD:79:PHE:HB2	2.01	0.42
55:DD:95:GLY:O	55:DD:126:ILE:HG12	2.19	0.42
56:EE:157:ASN:OD1	56:EE:222:LEU:HD21	2.20	0.42
60:II:85:ALA:O	63:LL:8:ARG:HD2	2.20	0.42
68:QQ:108:ILE:O	68:QQ:112:LEU:HG	2.19	0.42
69:RR:40:ILE:O	69:RR:40:ILE:CG1	2.67	0.42
70:SS:38:ARG:HB3	71:TT:45:LEU:HD21	2.00	0.42
84:gg:252:THR:HG23	84:gg:255:SER:O	2.18	0.42
86:ii:333:LEU:HB2	86:ii:342:LYS:HB3	2.00	0.42
86:ii:363:GLY:O	86:ii:364:GLN:C	2.62	0.42
87:jj:119:ALA:O	87:jj:123:LEU:HG	2.19	0.42
87:jj:376:VAL:HG21	87:jj:529:ALA:HB2	2.02	0.42
7:G:230:TYR:HA	7:G:233:ILE:HD12	2.01	0.42
12:M:50:MET:HG3	12:M:54:CYS:SG	2.59	0.42
14:O:121:PRO:HD3	18:S:168:THR:HG22	2.01	0.42
20:U:27:HIS:N	20:U:28:PRO:HD2	2.34	0.42
31:f:49:TYR:HD2	31:f:70:ILE:HD12	1.84	0.42
34:i:55:ARG:HA	34:i:58:MET:HE3	2.02	0.42
37:l:27:ILE:HG13	50:8:52:A:N6	2.35	0.42
46:2:49:C:O2'	46:2:50:U:H5'	2.19	0.42
48:5:644:G:H2'	48:5:645:G:C8	2.54	0.42
48:5:1824:G:H2'	48:5:1825:A:O4'	2.19	0.42
48:5:2364:OMG:OP2	92:5:5429:HOH:O	2.22	0.42
48:5:2886:U:H2'	48:5:2887:U:C6	2.54	0.42
48:5:3783:A:OP2	48:5:3808:OMC:N4	2.37	0.42
48:5:4761:G:N2	48:5:4766:C:O3'	2.52	0.42
51:9:44:U:O2	51:9:482:G:H1'	2.20	0.42
51:9:501:C:O2	51:9:501:C:H2'	2.19	0.42
51:9:827:A:OP1	61:JJ:10:ARG:HD2	2.19	0.42
51:9:1232:PSU:H2'	51:9:1233:G:C8	2.54	0.42
51:9:1520:G:N3	51:9:1520:G:H2'	2.35	0.42
54:CC:148:ALA:O	54:CC:152:ARG:HG2	2.19	0.42
55:DD:193:ASP:OD1	55:DD:203:PRO:HA	2.20	0.42
55:DD:195:SER:OG	55:DD:196:GLY:N	2.53	0.42
56:EE:159:THR:HG23	56:EE:173:ILE:HB	2.00	0.42
56:EE:183:VAL:HG21	56:EE:220:THR:HG21	2.02	0.42
60:II:11:ARG:NH1	60:II:15:GLY:O	2.50	0.42
61:JJ:78:LEU:HD23	61:JJ:97:ILE:HD11	2.00	0.42
66:OO:72:TYR:HD1	66:OO:75:MET:HE3	1.83	0.42
76:YY:96:LEU:N	76:YY:96:LEU:HD23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:ZZ:51:ASP:OD2	77:ZZ:54:THR:OG1	2.37	0.42
79:bb:35:VAL:O	79:bb:43:ILE:HD12	2.19	0.42
87:jj:420:SER:O	87:jj:459:VAL:HG11	2.20	0.42
4:D:123:VAL:HG22	4:D:248:ARG:NH1	2.34	0.42
10:J:96:LYS:HG2	10:J:163:MET:SD	2.60	0.42
14:O:110:PRO:N	14:O:111:PRO:CD	2.83	0.42
14:O:175:MET:HE1	14:O:179:LYS:HE2	2.00	0.42
14:O:202:LEU:HD23	14:O:202:LEU:HA	1.90	0.42
19:T:83:LYS:NZ	48:5:4305:G:O5'	2.53	0.42
22:W:25:ASP:OD1	22:W:26:GLY:N	2.53	0.42
28:c:65:MET:HE2	28:c:65:MET:HB3	1.97	0.42
37:l:46:ARG:HH12	48:5:2796:G:P	2.42	0.42
43:s:57:LYS:HD3	48:5:2020:U:H5''	2.01	0.42
43:s:78:LEU:HD11	43:s:193:PHE:CB	2.49	0.42
46:2:19:G:C5	46:2:57:G:N2	2.88	0.42
48:5:115:C:O2	48:5:115:C:O4'	2.37	0.42
48:5:120:A:H2'	48:5:149:A:N6	2.34	0.42
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	2.19	0.42
48:5:1406(C):G:C2	48:5:1411(A):G:C2	3.08	0.42
48:5:1763:C:N3	48:5:1770:A:N1	2.66	0.42
48:5:1857:C:H2'	48:5:1858:A:H8	1.85	0.42
50:8:64:U:C2	50:8:65:A:C8	3.07	0.42
51:9:103:A:C2	51:9:105:PSU:O2	2.72	0.42
51:9:369:C:O2	51:9:369:C:O4'	2.36	0.42
51:9:662:G:H4'	51:9:663:C:OP1	2.20	0.42
51:9:963:A:H2'	51:9:964:A:C8	2.54	0.42
51:9:1229:G:H2'	51:9:1230:C:O4'	2.20	0.42
51:9:1280:G:N1	51:9:1281:G:C5	2.88	0.42
52:AA:38:ILE:HD12	52:AA:38:ILE:C	2.45	0.42
62:KK:17:LYS:NZ	62:KK:18:GLU:OE1	2.51	0.42
71:TT:28:LEU:HD23	71:TT:53:PHE:HD2	1.84	0.42
73:VV:39:VAL:HA	73:VV:45:ARG:O	2.19	0.42
80:cc:12:ALA:HB3	80:cc:58:LEU:HD21	2.01	0.42
84:gg:78:ALA:HB3	84:gg:92:LEU:HD11	2.02	0.42
86:ii:372:MET:CE	86:ii:377:TRP:HB2	2.50	0.42
86:ii:378:PHE:HB3	86:ii:389:LEU:CD1	2.50	0.42
87:jj:478:LYS:HE3	87:jj:478:LYS:HB3	1.95	0.42
2:B:223:THR:O	2:B:274:TYR:HA	2.19	0.42
2:B:241:PRO:HD3	48:5:4456:OMC:HM21	2.02	0.42
3:C:115:VAL:O	3:C:120:LYS:HE2	2.19	0.42
6:F:91:VAL:O	6:F:119:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:102:ARG:HA	48:5:75:G:C5	2.54	0.42
13:N:37:HIS:CE1	13:N:63:ARG:NH1	2.87	0.42
22:W:55:TYR:CD1	22:W:55:TYR:C	2.97	0.42
44:t:15:LEU:HD12	44:t:16:ARG:N	2.35	0.42
44:t:27:ALA:C	44:t:30:PRO:HD2	2.45	0.42
46:2:21:A:H2'	46:2:46:G:O6	2.20	0.42
47:3:35:U:C5	47:3:36:U:C5	3.08	0.42
48:5:684:G:H5''	48:5:685:C:OP2	2.20	0.42
48:5:924:C:HO2'	48:5:925:C:P	2.41	0.42
48:5:1211:G:C2'	48:5:1212:G:O5'	2.67	0.42
48:5:1882:U:C4	48:5:2279:A:C2	3.08	0.42
48:5:1929:A:H5'	48:5:1930:U:OP1	2.19	0.42
48:5:1964:A:C2	48:5:1965:G:H1'	2.55	0.42
48:5:1980:U:H2'	48:5:1982:G:C5'	2.50	0.42
48:5:2001:G:O6	48:5:2003:G:N2	2.53	0.42
48:5:3816:A:OP1	48:5:3818:UY1:N1	2.53	0.42
48:5:3911:C:H4'	48:5:4196:OMG:HM22	2.01	0.42
48:5:4512:U:H4'	48:5:4513:A:OP1	2.19	0.42
51:9:64:A:C2	51:9:83:A:N7	2.88	0.42
51:9:881:G:OP2	51:9:881:G:H8	2.02	0.42
51:9:883:U:C4	51:9:884:C:C5	3.07	0.42
51:9:959:G:OP1	66:OO:104:ARG:NH2	2.52	0.42
51:9:1228:A:H2'	51:9:1229:G:H8	1.81	0.42
51:9:1231:C:H2'	51:9:1232:PSU:O4'	2.20	0.42
51:9:1426:U:H2'	51:9:1427:C:O4'	2.19	0.42
51:9:1834:A:N3	51:9:1834:A:C2'	2.83	0.42
55:DD:159:HIS:O	55:DD:164:VAL:HG11	2.20	0.42
56:EE:180:LEU:CD1	56:EE:192:ILE:HG22	2.50	0.42
57:FF:165:ASN:OD1	57:FF:167:LYS:N	2.47	0.42
62:KK:58:VAL:HA	62:KK:70:TYR:O	2.19	0.42
72:UU:35:VAL:HA	72:UU:38:ASP:OD2	2.20	0.42
84:gg:106:LYS:HG3	84:gg:126:ASP:HB3	2.02	0.42
3:C:182:LYS:NZ	48:5:2299:G:OP1	2.44	0.42
4:D:160:PHE:CE2	4:D:179:ARG:HB3	2.55	0.42
5:E:277:VAL:HG11	31:f:2:SER:HB2	2.02	0.42
7:G:53:ARG:NH1	48:5:4163:U:OP2	2.44	0.42
7:G:90:GLN:HG3	7:G:91:THR:N	2.34	0.42
9:I:53:VAL:HG11	19:T:158:PHE:CZ	2.55	0.42
9:I:184:MET:O	9:I:187:GLU:O	2.37	0.42
11:L:39:ARG:HD2	48:5:1363:C:OP1	2.19	0.42
20:U:37:ALA:HA	20:U:65:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:81:LEU:HG	23:X:83:THR:HG23	2.02	0.42
28:c:83:THR:O	65:NN:151:ALA:O	2.37	0.42
42:r:80:THR:CG2	42:r:96:MET:HE1	2.49	0.42
46:2:11:U:H2'	46:2:12:G:C8	2.55	0.42
48:5:968:C:O2'	48:5:969:C:O5'	2.35	0.42
48:5:1978:C:N4	48:5:1979:A:N1	2.67	0.42
48:5:2416:G:N2	48:5:2427:G:N7	2.63	0.42
48:5:2639:U:H2'	48:5:2694:G:N1	2.32	0.42
48:5:4303:C:O2	48:5:4303:C:O5'	2.38	0.42
48:5:4916:G:H2'	48:5:4917:C:O5'	2.20	0.42
51:9:71:G:C2	51:9:72:C:C6	3.08	0.42
51:9:152:U:H3	51:9:166:A2M:H62	1.67	0.42
51:9:464:A:H4'	51:9:465:A:OP2	2.20	0.42
51:9:878:G:C2	51:9:909:G:C2	3.07	0.42
51:9:1109:C:O2'	51:9:1110:G:H8	2.02	0.42
51:9:1823:A:H2'	51:9:1824:A:H5'	2.02	0.42
51:9:1825:A:N6	86:ii:127:CYS:O	2.52	0.42
51:9:1834:A:H2	51:9:1837:G:N2	2.17	0.42
52:AA:2:SER:O	52:AA:4:ALA:N	2.52	0.42
53:BB:97:LEU:HD12	53:BB:232:HIS:CG	2.55	0.42
55:DD:66:ILE:O	55:DD:70:THR:HG23	2.19	0.42
55:DD:223:ILE:HG22	55:DD:224:SER:N	2.35	0.42
56:EE:111:VAL:O	56:EE:111:VAL:CG2	2.68	0.42
59:HH:157:HIS:CD2	59:HH:157:HIS:N	2.88	0.42
66:OO:80:ASP:OD1	66:OO:80:ASP:C	2.63	0.42
70:SS:132:ARG:HB2	70:SS:134:GLN:OE1	2.20	0.42
71:TT:14:PHE:CE2	71:TT:131:LEU:HD13	2.55	0.42
75:XX:86:PRO:O	75:XX:87:ASN:CB	2.67	0.42
80:cc:67:ARG:CG	80:cc:67:ARG:HH11	2.33	0.42
83:ff:79:SER:O	83:ff:80:TYR:CD1	2.73	0.42
84:gg:8:ARG:HB2	84:gg:309:VAL:HG13	2.01	0.42
84:gg:44:LYS:HD3	84:gg:56:GLN:CG	2.49	0.42
84:gg:48:ASP:O	84:gg:51:ASN:N	2.52	0.42
84:gg:87:LEU:HB2	84:gg:101:PHE:CD1	2.54	0.42
87:jj:507:PHE:CD2	87:jj:507:PHE:C	2.98	0.42
1:A:233:ARG:HB2	48:5:4184:G:H5'	2.02	0.42
4:D:205:ALA:O	4:D:209:ARG:HG3	2.20	0.42
7:G:214:ALA:HA	7:G:217:LYS:HE3	2.02	0.42
7:G:230:TYR:CE2	7:G:234:ARG:HD3	2.55	0.42
9:I:54:SER:HB2	9:I:135:ILE:HD11	2.00	0.42
14:O:62:MET:HA	48:5:2045:G:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:29:VAL:C	20:U:32:GLY:H	2.28	0.42
20:U:64:GLU:O	20:U:70:ILE:HA	2.20	0.42
26:a:117:LEU:HB3	26:a:140:VAL:HG11	2.01	0.42
43:s:35:VAL:O	43:s:35:VAL:HG13	2.19	0.42
44:t:17:CYS:SG	48:5:1975:G:C6	3.11	0.42
44:t:27:ALA:O	44:t:31:LYS:HE2	2.20	0.42
46:2:19:G:H3'	46:2:20:U:H5'	2.02	0.42
47:3:32:C:O2'	47:3:33:U:H5'	2.20	0.42
48:5:223:G:H4'	48:5:225:G:N7	2.35	0.42
48:5:1208:G:O2'	48:5:1209:U:O5'	2.38	0.42
48:5:1468:C:H2'	48:5:1469:C:C6	2.55	0.42
48:5:1804:A:H4'	48:5:1805:A:O5'	2.20	0.42
48:5:2006:U:H2'	48:5:2007:G:H5'	2.02	0.42
48:5:2602:G:H2'	48:5:2603:C:C6	2.55	0.42
48:5:2882:A:OP1	48:5:3625:G:N1	2.43	0.42
48:5:4119:C:H4'	48:5:4120:U:OP1	2.19	0.42
51:9:182:C:O4'	51:9:183:G:C2	2.73	0.42
51:9:191:A:H62	51:9:208:G:H21	1.68	0.42
51:9:407:G:H5''	51:9:408:A:C5'	2.50	0.42
51:9:1138:C:OP1	52:AA:155:ARG:CZ	2.68	0.42
51:9:1386:A:H2'	51:9:1387:G:O4'	2.18	0.42
51:9:1568:C:OP1	71:TT:96:SER:OG	2.36	0.42
56:EE:192:ILE:HB	56:EE:242:LYS:O	2.20	0.42
64:MM:33:ARG:O	64:MM:33:ARG:HD2	2.20	0.42
67:PP:111:MET:O	67:PP:112:ILE:C	2.63	0.42
71:TT:42:HIS:HB2	71:TT:83:GLN:HA	2.02	0.42
71:TT:51:ASN:ND2	71:TT:54:TYR:CD2	2.88	0.42
76:YY:79:LEU:HD12	76:YY:79:LEU:O	2.19	0.42
86:ii:335:CYS:HB3	86:ii:340:GLU:HB3	2.01	0.42
4:D:261:VAL:O	4:D:262:LYS:C	2.62	0.41
6:F:28:LYS:NZ	48:5:965:G:N7	2.55	0.41
6:F:154:TYR:CE1	6:F:186:MET:HG2	2.55	0.41
8:H:118:LEU:CD1	8:H:167:VAL:HG22	2.50	0.41
9:I:61:SER:HA	9:I:126:VAL:HG12	2.01	0.41
11:L:59:VAL:HB	48:5:74:G:C5'	2.50	0.41
18:S:69:GLU:HG2	18:S:101:THR:HG22	2.01	0.41
24:Y:89:LYS:HD2	24:Y:95:VAL:HG11	2.01	0.41
33:h:85:PRO:O	50:8:38:U:H5	2.03	0.41
42:r:46:ARG:NH2	42:r:67:ARG:HG2	2.35	0.41
43:s:55:MET:CE	48:5:1998:A:O4'	2.68	0.41
43:s:57:LYS:O	43:s:57:LYS:CD	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:119:G:H3'	48:5:120:A:C5'	2.49	0.41
48:5:982:U:H3	48:5:1273:G:H1	1.68	0.41
48:5:1169:G:O2'	48:5:1170:G:H5'	2.20	0.41
48:5:1199:G:C4	48:5:1200:G:N7	2.88	0.41
48:5:1201:U:O2'	48:5:1202:C:H5'	2.20	0.41
48:5:1481:C:C2'	48:5:1482:G:O5'	2.68	0.41
48:5:1567:U:H2'	48:5:1568:C:C6	2.55	0.41
48:5:2046:G:H1'	48:5:2047:A:OP2	2.20	0.41
48:5:2424:OMG:H2'	48:5:2426:U:C5	2.54	0.41
48:5:4114:C:C2'	48:5:4115:G:O4'	2.68	0.41
48:5:4776:G:C2	48:5:4860:G:C5	3.08	0.41
48:5:4884:G:O2'	48:5:4885:U:O5'	2.37	0.41
51:9:25:A:O2'	51:9:26:U:O4'	2.38	0.41
51:9:191:A:H3'	51:9:192:C:H5''	2.01	0.41
51:9:197:U:C6	51:9:197:U:OP2	2.73	0.41
51:9:199:C:C2	51:9:200:G:C8	3.08	0.41
51:9:1265:A:H2	51:9:1517:G:H22	1.66	0.41
51:9:1306:U:H2'	51:9:1307:U:O5'	2.20	0.41
51:9:1398:G:O2'	84:gg:88:ARG:NH2	2.53	0.41
51:9:1419:C:O2'	71:TT:132:ASP:OD2	2.37	0.41
51:9:1850:MA6:H8	51:9:1850:MA6:O5'	2.19	0.41
56:EE:130:PHE:HB3	56:EE:138:HIS:HB2	2.02	0.41
57:FF:99:ILE:CG1	77:ZZ:108:ILE:HD11	2.50	0.41
57:FF:204:ARG:HD2	66:OO:72:TYR:OH	2.20	0.41
58:GG:7:PHE:HD1	58:GG:10:THR:HG1	1.66	0.41
66:OO:46:ASP:CG	66:OO:51:GLU:HB2	2.45	0.41
68:QQ:58:LEU:HD21	68:QQ:112:LEU:HD21	2.02	0.41
75:XX:56:GLY:CA	82:ee:6:LEU:HD21	2.50	0.41
80:cc:42:ILE:CD1	80:cc:64:GLU:HB2	2.50	0.41
80:cc:66:ARG:O	80:cc:67:ARG:HG3	2.20	0.41
84:gg:78:ALA:O	84:gg:89:LEU:HD23	2.20	0.41
84:gg:270:LEU:HD13	84:gg:310:TRP:CG	2.55	0.41
87:jj:109:VAL:HB	87:jj:279:LEU:HD21	2.01	0.41
87:jj:292:VAL:O	87:jj:292:VAL:CG2	2.67	0.41
9:I:98:ARG:HD2	9:I:120:GLY:O	2.20	0.41
10:J:15:LEU:CD2	10:J:157:ILE:HD13	2.50	0.41
44:t:15:LEU:CB	44:t:62:LEU:HD12	2.50	0.41
46:2:51:C:H2'	46:2:52:G:O4'	2.20	0.41
48:5:245:C:O2'	48:5:246:G:P	2.76	0.41
48:5:449:C:OP1	48:5:449:C:C4'	2.67	0.41
48:5:1208:G:C2'	48:5:1209:U:O5'	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1479:G:O2'	48:5:1480:C:H5'	2.19	0.41
48:5:1510:G:H2'	48:5:1511:U:C6	2.55	0.41
48:5:1808:C:H2'	48:5:1809:C:H6	1.84	0.41
48:5:1940:G:O4'	48:5:1940:G:OP2	2.38	0.41
48:5:1942:A:N3	48:5:4432:C:O2'	2.45	0.41
48:5:2008:U:O2	48:5:2008:U:O4'	2.37	0.41
48:5:2489:C:OP1	48:5:2490:U:C5	2.74	0.41
48:5:2539:C:H2'	48:5:2540:C:C6	2.54	0.41
48:5:3684:G:H2'	48:5:3685:C:C6	2.55	0.41
48:5:4891:G:H1	48:5:4928:C:H5	1.67	0.41
48:5:4908:G:N3	48:5:4913:G:O4'	2.53	0.41
50:8:83:C:C5'	50:8:85:U:O2	2.68	0.41
50:8:103:A:H3'	50:8:104:A:H5''	2.03	0.41
51:9:70:G:C2	51:9:80:G:C6	3.09	0.41
51:9:305:U:O2'	51:9:309:G:H1'	2.20	0.41
51:9:407:G:C8	51:9:407:G:O5'	2.73	0.41
51:9:1115:U:O2'	51:9:1116:C:N3	2.53	0.41
51:9:1411:G:O3'	51:9:1412:C:H4'	2.19	0.41
51:9:1454:A:O4'	69:RR:3:ARG:HD3	2.20	0.41
51:9:1691:U:H2'	51:9:1692:PSU:O4'	2.20	0.41
51:9:1693:G:N2	51:9:1834:A:H8	2.18	0.41
55:DD:26:THR:HA	55:DD:34:TYR:CD2	2.55	0.41
56:EE:153:LEU:HD11	58:GG:216:ARG:NH1	2.34	0.41
66:OO:84:ARG:NE	66:OO:88:LEU:HD21	2.35	0.41
69:RR:63:ARG:O	69:RR:63:ARG:HG2	2.18	0.41
78:aa:51:ARG:O	78:aa:55:GLU:HG3	2.20	0.41
80:cc:34:PHE:C	80:cc:36:ASP:H	2.28	0.41
80:cc:50:VAL:O	80:cc:50:VAL:HG23	2.20	0.41
84:gg:142:VAL:O	84:gg:142:VAL:HG23	2.19	0.41
84:gg:228:TYR:CE2	84:gg:264:LYS:HG2	2.55	0.41
86:ii:10:ARG:HD2	86:ii:14:ILE:HD11	2.01	0.41
86:ii:120:ILE:HG22	86:ii:139:LEU:HD23	2.02	0.41
87:jj:56:ILE:O	87:jj:56:ILE:HG22	2.19	0.41
87:jj:193:GLU:OE1	87:jj:233:GLN:HA	2.21	0.41
1:A:178:PRO:HG3	41:p:25:MET:HE3	2.01	0.41
13:N:114:ARG:HH11	13:N:114:ARG:HG3	1.85	0.41
13:N:178:HIS:HA	13:N:181:HIS:NE2	2.35	0.41
25:Z:6:LYS:O	25:Z:25:ILE:HB	2.19	0.41
41:p:8:VAL:O	41:p:11:VAL:HG22	2.19	0.41
43:s:192:VAL:CG1	43:s:194:ASP:OD1	2.68	0.41
48:5:181:C:N3	48:5:256:G:C2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:258:G:H2'	48:5:259:C:O4'	2.20	0.41
48:5:1332:C:H2'	48:5:1333:A:C8	2.55	0.41
48:5:1546:C:H42	48:5:1612:G:H22	1.68	0.41
48:5:2465:C:H2'	48:5:2466:G:O4'	2.20	0.41
48:5:2488:C:H2'	48:5:2489:C:OP1	2.21	0.41
48:5:3810:C:HO2'	48:5:3811:G:P	2.43	0.41
48:5:3864:C:OP1	92:5:5430:HOH:O	2.22	0.41
48:5:4181:U:H2'	48:5:4182:G:O4'	2.21	0.41
48:5:4918:C:C4	48:5:4919:G:N7	2.88	0.41
51:9:25:A:H2'	51:9:26:U:C6	2.55	0.41
51:9:165:G:H21	51:9:165:G:P	2.36	0.41
51:9:587:A:C2	51:9:592:C:C2	3.09	0.41
51:9:637:U:H2'	51:9:638:C:O4'	2.21	0.41
51:9:656:G:H5'	51:9:662:G:N2	2.35	0.41
51:9:1109:C:O2'	51:9:1110:G:C8	2.73	0.41
51:9:1114:U:O2'	51:9:1115:U:P	2.79	0.41
51:9:1290:G:C2	51:9:1291:A:C8	3.09	0.41
51:9:1298:G:O2'	51:9:1299:A:C5'	2.67	0.41
51:9:1463:U:H4'	51:9:1464:C:O5'	2.21	0.41
51:9:1738:C:H2'	51:9:1739:C:C6	2.55	0.41
53:BB:79:VAL:HG21	53:BB:81:PHE:CZ	2.55	0.41
56:EE:175:PHE:HA	56:EE:227:VAL:HG21	2.02	0.41
58:GG:208:GLU:OE1	58:GG:211:LYS:HG2	2.20	0.41
60:II:110:ARG:O	60:II:114:GLU:HG3	2.20	0.41
65:NN:84:LEU:HD21	65:NN:89:TYR:CD1	2.55	0.41
65:NN:115:LEU:O	65:NN:119:GLU:HG3	2.20	0.41
67:PP:34:MET:HE2	67:PP:45:LEU:HB3	2.02	0.41
68:QQ:58:LEU:O	68:QQ:62:ARG:HD3	2.20	0.41
69:RR:41:ILE:HG22	69:RR:43:SER:H	1.85	0.41
70:SS:36:VAL:HG22	70:SS:40:TYR:HD2	1.82	0.41
79:bb:55:LEU:HD22	79:bb:55:LEU:H	1.85	0.41
87:jj:107:GLY:HA2	87:jj:271:VAL:HG23	2.02	0.41
87:jj:488:PRO:O	87:jj:524:MET:HE1	2.20	0.41
87:jj:536:ASP:OD1	87:jj:536:ASP:N	2.52	0.41
2:B:281:ASN:ND2	48:5:4676:G:OP1	2.53	0.41
2:B:315:ASN:O	2:B:370:THR:HG23	2.19	0.41
4:D:48:LYS:HE2	48:5:4325:A:O2'	2.21	0.41
11:L:108:GLU:CD	11:L:108:GLU:N	2.78	0.41
14:O:118:MET:HE1	18:S:169:THR:HG23	2.02	0.41
16:Q:144:LYS:NZ	48:5:1461:C:OP1	2.37	0.41
20:U:101:ARG:O	20:U:112:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:114:ASP:O	24:Y:117:LYS:HG2	2.21	0.41
37:l:31:THR:OG1	50:8:75:OMG:OP2	2.37	0.41
43:s:13:TYR:O	43:s:17:ILE:HG23	2.19	0.41
48:5:304:C:H2'	48:5:305:A:O4'	2.20	0.41
48:5:1398:A:N6	48:5:1419:G:O2'	2.53	0.41
48:5:1432:G:H1'	48:5:1452:A:H61	1.85	0.41
48:5:1996:C:C4	48:5:1997:U:C6	3.08	0.41
48:5:2460:A:H2'	48:5:2461:G:O4'	2.20	0.41
48:5:3720:G:H22	48:5:3733:A:H2	1.67	0.41
48:5:4112:C:O2'	48:5:4113:U:H5'	2.21	0.41
48:5:4589:A:N1	48:5:4621:C:O2'	2.50	0.41
50:8:60:G:O6	50:8:96:C:O2'	2.31	0.41
51:9:71:G:C6	58:GG:170:ARG:NH1	2.88	0.41
51:9:193:C:H2'	51:9:194:C:O4'	2.20	0.41
51:9:417:C:O2'	51:9:418:A:P	2.77	0.41
51:9:688:U:OP2	51:9:688:U:O2	2.39	0.41
51:9:863:PSU:C2	51:9:864:A:N7	2.88	0.41
51:9:913:A:OP2	59:HH:99:ARG:NH1	2.48	0.41
51:9:1152:U:O3'	74:WW:19:LYS:NZ	2.54	0.41
51:9:1208:A:O2'	51:9:1209:A:H5'	2.20	0.41
51:9:1549:U:OP2	55:DD:8:LYS:NZ	2.54	0.41
51:9:1587:G:O6	71:TT:67:ARG:HD3	2.20	0.41
52:AA:203:PHE:CZ	69:RR:91:LEU:HD13	2.55	0.41
54:CC:204:ILE:HD11	54:CC:219:ILE:O	2.18	0.41
56:EE:248:ILE:HD12	61:JJ:72:PHE:CE2	2.56	0.41
61:JJ:111:GLN:HA	61:JJ:130:ILE:CD1	2.51	0.41
64:MM:68:LEU:HD23	83:ff:109:ILE:CD1	2.51	0.41
66:OO:149:ARG:NH2	66:OO:151:LEU:HD13	2.35	0.41
72:UU:99:LYS:HA	72:UU:102:THR:HG22	2.02	0.41
84:gg:208:ALA:HB2	84:gg:241:PHE:CZ	2.55	0.41
87:jj:165:LYS:O	87:jj:235:ALA:HB1	2.20	0.41
87:jj:409:VAL:HG22	87:jj:482:VAL:HG22	2.01	0.41
6:F:34:LYS:N	6:F:34:LYS:HD3	2.36	0.41
7:G:48:LYS:NZ	48:5:4086:G:O6	2.39	0.41
8:H:106:GLN:HB2	8:H:111:LEU:HB3	2.02	0.41
16:Q:14:ARG:HH22	48:5:2083:C:P	2.43	0.41
18:S:48:VAL:HG12	19:T:151:LEU:HD12	2.02	0.41
37:l:18:LYS:NZ	50:8:46:G:OP1	2.41	0.41
42:r:47:LYS:O	42:r:103:HIS:NE2	2.53	0.41
43:s:57:LYS:O	43:s:57:LYS:HD2	2.20	0.41
43:s:111:ALA:HB1	43:s:183:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:130:LEU:HD13	43:s:133:GLU:HG2	2.03	0.41
46:2:18:G:H4'	46:2:60:A:C6	2.56	0.41
47:3:15:G:N2	47:3:59:G:C8	2.89	0.41
48:5:206:U:H1'	48:5:209:U:C4	2.56	0.41
48:5:1295:U:O2	48:5:1295:U:O4'	2.38	0.41
48:5:1472:C:H2'	48:5:1473:U:C6	2.55	0.41
48:5:1666:C:O2'	48:5:1688:G:OP1	2.34	0.41
48:5:1879:C:O2'	48:5:1891:A:N3	2.48	0.41
48:5:1977:C:O2	48:5:1990:A:N6	2.54	0.41
48:5:4152:G:H8	48:5:4152:G:O5'	2.03	0.41
48:5:5034:A:H2'	48:5:5035:U:O4'	2.20	0.41
50:8:103:A:C8	50:8:104:A:C8	3.09	0.41
51:9:103:A:H2	51:9:105:PSU:O2	2.04	0.41
51:9:688:U:O2'	51:9:689:U:P	2.78	0.41
51:9:1018:U:C5'	65:NN:71:ILE:HD12	2.48	0.41
51:9:1050:A:H4'	51:9:1846:G:O2'	2.20	0.41
51:9:1282:A:H3'	51:9:1283:C:H5'	2.02	0.41
51:9:1675:A:O2'	57:FF:74:ASN:O	2.38	0.41
51:9:1807:C:H2'	51:9:1808:U:O4'	2.20	0.41
55:DD:91:VAL:HG12	55:DD:92:ALA:O	2.20	0.41
56:EE:180:LEU:HB2	56:EE:232:ASN:HA	2.01	0.41
57:FF:116:ILE:HD11	57:FF:151:ILE:CD1	2.50	0.41
58:GG:35:GLU:HA	58:GG:51:ARG:HA	2.02	0.41
62:KK:7:ASN:HA	62:KK:40:VAL:HG22	2.02	0.41
66:OO:45:THR:HB	66:OO:51:GLU:O	2.20	0.41
68:QQ:102:GLU:HB2	84:gg:56:GLN:O	2.19	0.41
69:RR:21:TYR:CD2	69:RR:71:ILE:HG23	2.56	0.41
75:XX:16:HIS:O	75:XX:20:GLN:HG2	2.21	0.41
76:YY:104:ARG:NH2	76:YY:108:LYS:HE3	2.35	0.41
84:gg:31:ILE:HD13	84:gg:31:ILE:HA	1.96	0.41
84:gg:194:TYR:CZ	84:gg:212:LYS:HB2	2.55	0.41
86:ii:224:LEU:HD23	86:ii:250:VAL:HG12	2.03	0.41
87:jj:252:ARG:HD3	87:jj:278:VAL:HG21	2.01	0.41
2:B:309:LEU:O	2:B:310:SER:C	2.64	0.41
4:D:128:ASP:O	4:D:164:LYS:NZ	2.47	0.41
7:G:218:LEU:O	7:G:222:ILE:HG12	2.20	0.41
10:J:62:ILE:CG2	10:J:68:ILE:HD12	2.51	0.41
15:P:137:ASN:HB3	48:5:3860:A:O2'	2.21	0.41
24:Y:88:GLU:HA	24:Y:93:THR:O	2.21	0.41
24:Y:89:LYS:NZ	48:5:386:A:OP2	2.29	0.41
25:Z:92:ASP:HB3	25:Z:113:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:39:LYS:NZ	48:5:2369:U:O2	2.53	0.41
29:d:70:LYS:HE2	48:5:2389:A:H4'	2.02	0.41
39:n:4:LYS:NZ	51:9:1844:U:O4	2.49	0.41
44:t:64:ILE:CG2	44:t:71:ILE:HB	2.51	0.41
48:5:1565:A:C5	48:5:1566:C:H1'	2.55	0.41
48:5:1984:A:OP2	48:5:1986:U:OP1	2.39	0.41
48:5:2016:C:H2'	48:5:2017:A:H8	1.86	0.41
48:5:2616:C:O2'	48:5:2617:G:H5'	2.20	0.41
48:5:2898:G:H2'	48:5:2899:C:H6	1.85	0.41
48:5:3771:C:H2'	48:5:3772:U:O4'	2.20	0.41
48:5:4244:A:H2'	48:5:4245:G:O4'	2.20	0.41
48:5:4254:G:N3	48:5:4254:G:H2'	2.35	0.41
48:5:4439:U:OP1	86:ii:192:ARG:HD2	2.20	0.41
48:5:4543:G:H2'	48:5:4544:A:C8	2.56	0.41
50:8:81:C:H3'	50:8:82:A:H4'	2.02	0.41
51:9:106:C:H2'	51:9:107:A:C8	2.55	0.41
51:9:164:A:H2'	51:9:165:G:N3	2.36	0.41
51:9:194:C:C2	51:9:195:C:C5	3.08	0.41
51:9:691:G:N2	51:9:692:G:C8	2.88	0.41
51:9:1265:A:N3	51:9:1265:A:H2'	2.36	0.41
51:9:1420:G:OP2	71:TT:132:ASP:HB2	2.21	0.41
51:9:1471:C:H2'	51:9:1472:C:O4'	2.20	0.41
51:9:1863:A:OP2	78:aa:4:LYS:NZ	2.48	0.41
53:BB:181:LEU:O	53:BB:185:VAL:HG23	2.20	0.41
54:CC:63:VAL:HG22	54:CC:64:THR:N	2.35	0.41
58:GG:213:LEU:HD11	58:GG:217:MET:HE1	2.02	0.41
59:HH:79:LEU:HD22	59:HH:94:PHE:CE2	2.55	0.41
62:KK:84:HIS:HB3	64:MM:27:ILE:HG23	2.03	0.41
70:SS:11:HIS:O	70:SS:12:ILE:HD13	2.19	0.41
70:SS:40:TYR:OH	70:SS:74:PRO:HG3	2.21	0.41
71:TT:65:TYR:OH	71:TT:132:ASP:OD1	2.37	0.41
72:UU:56:MET:O	72:UU:57:PRO:C	2.63	0.41
73:VV:4:ASP:OD1	73:VV:5:ALA:N	2.53	0.41
86:ii:407:GLY:N	87:jj:34:MET:HE3	2.35	0.41
87:jj:231:CYS:SG	87:jj:258:THR:HG22	2.60	0.41
87:jj:250:LYS:HD2	87:jj:562:LEU:HD22	2.02	0.41
2:B:106:PHE:CZ	2:B:163:LEU:HD13	2.56	0.41
3:C:197:ARG:NH1	48:5:351:C:OP2	2.50	0.41
5:E:214:HIS:NE2	5:E:252:ASP:OD2	2.46	0.41
6:F:221:LYS:HE2	49:7:85:G:OP1	2.20	0.41
11:L:55:ILE:HA	11:L:154:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:108:GLU:N	11:L:108:GLU:OE1	2.41	0.41
13:N:38:ARG:NH2	50:8:142:U:OP1	2.46	0.41
14:O:44:SER:HG	48:5:2054:U:H6	1.63	0.41
17:R:79:GLY:O	48:5:3619:G:H4'	2.20	0.41
29:d:23:ARG:NH2	48:5:5058:A:H4'	2.35	0.41
48:5:756:G:O2'	48:5:757:G:H5'	2.20	0.41
48:5:914:U:O2'	48:5:915:A:C5'	2.69	0.41
48:5:1353:G:O2'	48:5:1503:A:N1	2.50	0.41
48:5:2488:C:C2'	48:5:2489:C:OP1	2.68	0.41
48:5:3784:A:O2'	48:5:3786:U:OP2	2.32	0.41
48:5:4065:G:P	48:5:4065:G:H8	2.44	0.41
48:5:4582:C:O2'	48:5:4583:C:H5'	2.20	0.41
49:7:108:G:O2'	49:7:109:U:H5'	2.21	0.41
51:9:103:A:C2	51:9:355:G:C6	3.09	0.41
51:9:547:G:N3	51:9:549:C:N4	2.68	0.41
51:9:805:U:OP2	74:WW:82:GLN:HG2	2.21	0.41
51:9:1439:A:H8	51:9:1439:A:O5'	2.03	0.41
52:AA:90:PHE:HD2	52:AA:179:ALA:HB2	1.77	0.41
56:EE:234:PRO:CG	56:EE:238:LEU:HD13	2.51	0.41
57:FF:178:ILE:O	57:FF:182:LYS:HG2	2.20	0.41
58:GG:233:ARG:HD3	58:GG:233:ARG:HA	1.90	0.41
60:II:65:PHE:O	60:II:109:TYR:OH	2.31	0.41
64:MM:89:VAL:CG1	64:MM:90:GLY:N	2.83	0.41
67:PP:57:LEU:HD21	67:PP:89:MET:HE2	2.02	0.41
67:PP:90:VAL:HG12	67:PP:91:GLY:N	2.35	0.41
76:YY:117:VAL:CG1	76:YY:121:ALA:HB3	2.49	0.41
84:gg:132:TRP:CD1	84:gg:132:TRP:N	2.88	0.41
87:jj:240:PHE:HB3	87:jj:243:PRO:HG3	2.03	0.41
4:D:289:ARG:NH1	4:D:289:ARG:CB	2.84	0.41
11:L:105:LYS:O	34:i:20:ASN:N	2.41	0.41
11:L:170:THR:CG2	11:L:171:GLU:N	2.83	0.41
12:M:123:ILE:O	12:M:127:VAL:HG23	2.20	0.41
13:N:95:ALA:O	48:5:300:A:H5'	2.20	0.41
16:Q:49:LYS:HG2	16:Q:53:MET:CE	2.50	0.41
16:Q:177:ALA:C	26:a:51:GLY:HA2	2.46	0.41
27:b:55:LYS:O	27:b:58:GLN:HG2	2.21	0.41
35:j:21:ARG:NH2	35:j:39:TYR:HA	2.36	0.41
46:2:67:G:C2	46:2:68:G:C8	3.08	0.41
47:3:50:A:C6	47:3:65:G:C6	3.09	0.41
48:5:1450:C:H2'	48:5:1451:G:O4'	2.20	0.41
48:5:4773:C:H2'	48:5:4774:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5065:U:H2'	48:5:5066:U:O4'	2.21	0.41
51:9:202:G:H5''	51:9:203:G:OP2	2.21	0.41
51:9:293:C:O2	51:9:293:C:H2'	2.21	0.41
51:9:385:G:O2'	60:II:10:LYS:NZ	2.54	0.41
51:9:875:A:O5'	51:9:875:A:H8	2.03	0.41
51:9:1477:U:OP2	69:RR:3:ARG:NH1	2.40	0.41
54:CC:135:GLY:HA2	54:CC:165:VAL:HB	2.02	0.41
55:DD:99:ILE:HG13	55:DD:100:ALA:N	2.36	0.41
56:EE:160:ILE:HD12	56:EE:162:ILE:HD11	2.03	0.41
58:GG:23:LYS:O	58:GG:26:THR:HG22	2.21	0.41
58:GG:126:ASP:C	58:GG:127:THR:HG1	2.19	0.41
58:GG:181:THR:O	58:GG:184:VAL:N	2.53	0.41
62:KK:15:LEU:O	62:KK:18:GLU:C	2.64	0.41
68:QQ:24:HIS:O	68:QQ:68:ILE:HA	2.21	0.41
68:QQ:101:ASP:OD1	68:QQ:101:ASP:C	2.63	0.41
87:jj:347:MET:SD	87:jj:347:MET:C	3.04	0.41
2:B:217:ILE:HD11	2:B:333:LEU:CD2	2.48	0.41
3:C:120:LYS:HD2	48:5:1374:G:OP1	2.20	0.41
3:C:159:GLU:HA	3:C:217:ILE:HB	2.03	0.41
3:C:221:PHE:CB	3:C:229:LEU:HD21	2.51	0.41
3:C:283:LYS:NZ	16:Q:22:ASP:OD2	2.50	0.41
6:F:36:PHE:CG	48:5:1272:C:H4'	2.56	0.41
8:H:80:MET:O	8:H:84:VAL:HG22	2.20	0.41
10:J:101:ASP:OD1	48:5:4248:A:H1'	2.21	0.41
17:R:3:MET:HE2	17:R:5:ARG:NH1	2.36	0.41
20:U:60:VAL:HG11	20:U:76:VAL:CG2	2.51	0.41
21:V:41:SER:OG	48:5:4507:A:O2'	2.34	0.41
22:W:9:SER:HA	22:W:52:THR:HG22	2.02	0.41
25:Z:72:VAL:O	25:Z:72:VAL:HG23	2.21	0.41
33:h:17:LEU:HD13	33:h:61:ILE:HG13	2.03	0.41
33:h:121:VAL:CG1	33:h:122:LYS:N	2.84	0.41
36:k:7:GLU:HB2	36:k:10:ASP:OD2	2.20	0.41
44:t:131:GLU:HA	44:t:152:ILE:HG21	2.02	0.41
47:3:76:A:C2	48:5:4370:OMG:H2'	2.56	0.41
48:5:409:G:H21	48:5:2329:U:H4'	1.86	0.41
48:5:658:C:N4	48:5:659:G:O6	2.54	0.41
48:5:674:G:H2'	48:5:675:C:C6	2.55	0.41
48:5:756:G:C6	48:5:908:G:C6	3.09	0.41
48:5:1173:G:C6	48:5:1174:G:C6	3.08	0.41
48:5:1195:G:C5	48:5:1196:G:N7	2.89	0.41
48:5:1445:U:H3'	48:5:1446:C:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1609:U:H2'	48:5:1610:C:O4'	2.20	0.41
48:5:1818:G:N3	48:5:1818:G:H2'	2.36	0.41
48:5:1895:G:H2'	48:5:1896:A:O4'	2.21	0.41
48:5:1981:G:H1'	86:ii:315:GLY:HA3	2.03	0.41
48:5:1994:C:H2'	48:5:1995:G:C8	2.56	0.41
48:5:2079:G:H2'	48:5:2080:U:C6	2.56	0.41
48:5:2306:G:H1'	48:5:2332:A:N6	2.36	0.41
48:5:2485:U:H2'	48:5:2486:G:C8	2.56	0.41
48:5:2491:C:H2'	48:5:2492:C:C4'	2.51	0.41
48:5:2517:A:N3	48:5:2539:C:O2'	2.52	0.41
48:5:2545:U:OP2	48:5:2546:G:H5''	2.21	0.41
48:5:2690:C:H2'	48:5:2691:U:O4'	2.21	0.41
48:5:3930:U:H2'	48:5:3931:C:C6	2.56	0.41
48:5:4100:C:C4	48:5:4101:C:N4	2.89	0.41
48:5:4236:G:H4'	48:5:4328:G:O2'	2.21	0.41
48:5:4492:U:O2'	48:5:4512:U:O2	2.27	0.41
48:5:4574:U:H3'	48:5:4575:G:C5'	2.48	0.41
48:5:4884:G:O2'	48:5:4885:U:OP1	2.39	0.41
50:8:88:A:H2'	50:8:89:U:O4'	2.21	0.41
50:8:108:A:H2'	50:8:109:C:O4'	2.20	0.41
51:9:304:C:O2'	51:9:309:G:C6	2.74	0.41
51:9:902:G:H2'	51:9:903:A:O5'	2.21	0.41
51:9:915:G:OP1	59:HH:120:ARG:NH1	2.41	0.41
51:9:931:C:H2'	51:9:932:G:C8	2.56	0.41
51:9:1059:G:C5	51:9:1060:A:C2	3.09	0.41
51:9:1097:G:O2'	51:9:1098:C:H5'	2.21	0.41
51:9:1287:A:OP2	83:ff:94:LYS:HD2	2.21	0.41
51:9:1579:A:H4'	51:9:1581:C:C5	2.55	0.41
52:AA:49:ILE:HG22	52:AA:50:ASN:N	2.36	0.41
53:BB:127:VAL:HG23	53:BB:177:GLN:HG3	2.03	0.41
53:BB:168:MET:O	53:BB:172:MET:CG	2.68	0.41
55:DD:221:THR:OG1	55:DD:222:PRO:HD2	2.19	0.41
56:EE:151:ASP:OD2	58:GG:212:LEU:HD21	2.21	0.41
57:FF:20:PHE:O	57:FF:20:PHE:HD1	2.03	0.41
58:GG:34:THR:HG23	58:GG:34:THR:O	2.19	0.41
59:HH:79:LEU:CD2	59:HH:83:LEU:HD13	2.51	0.41
60:II:149:TYR:O	60:II:153:LYS:NZ	2.54	0.41
62:KK:21:MET:SD	62:KK:49:MET:CE	3.09	0.41
67:PP:113:GLY:C	67:PP:114:HIS:ND1	2.79	0.41
69:RR:15:VAL:HG12	69:RR:19:LYS:NZ	2.35	0.41
70:SS:9:PHE:CE1	77:ZZ:49:LEU:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XX:105:PHE:HB2	75:XX:119:ARG:O	2.21	0.41
79:bb:33:MET:CE	79:bb:73:LEU:HD21	2.50	0.41
80:cc:28:THR:OG1	80:cc:50:VAL:HG22	2.20	0.41
84:gg:8:ARG:C	84:gg:309:VAL:HG13	2.46	0.41
86:ii:30:ASN:OD1	86:ii:30:ASN:N	2.53	0.41
86:ii:315:GLY:O	86:ii:414:ARG:NH1	2.54	0.41
86:ii:317:VAL:HG13	86:ii:387:ALA:HB2	2.03	0.41
87:jj:29:CYS:HA	91:jj:601:SF4:S2	2.61	0.41
87:jj:509:LEU:HD23	87:jj:510:HIS:HD2	1.86	0.41
1:A:104:VAL:HA	1:A:107:MET:SD	2.61	0.41
2:B:234:ARG:HD2	2:B:271:GLN:O	2.20	0.41
4:D:226:TYR:OH	49:7:48:G:OP1	2.37	0.41
6:F:106:LYS:O	6:F:110:LEU:HG	2.21	0.41
13:N:11:TRP:O	13:N:14:LYS:NZ	2.51	0.41
14:O:118:MET:SD	18:S:169:THR:HG22	2.61	0.41
19:T:4:THR:OG1	48:5:4208:U:OP2	2.35	0.41
28:c:81:LEU:HD21	28:c:94:LEU:HD23	2.03	0.41
43:s:187:LEU:O	43:s:188:ILE:HG13	2.21	0.41
47:3:35:U:H2'	47:3:36:U:O5'	2.22	0.41
48:5:664:G:H2'	48:5:665:C:C6	2.56	0.41
48:5:759:G:H2'	48:5:760:G:H5'	2.03	0.41
48:5:1183:C:H2'	48:5:1184:A:C8	2.56	0.41
48:5:1391:A:H2'	48:5:1392:A:O4'	2.21	0.41
48:5:1411(B):C:H6	48:5:1411(B):C:O5'	2.04	0.41
48:5:1764:G:C2'	48:5:1767:A:H62	2.34	0.41
48:5:1765:A:C4	48:5:1766:A:C8	3.08	0.41
48:5:2744:A:H2'	48:5:2745:A:C8	2.56	0.41
48:5:3662:A:O4'	48:5:3664:G:C8	2.74	0.41
48:5:3792:OMG:H1'	48:5:3792:OMG:HM23	1.84	0.41
48:5:3808:OMC:C5	48:5:3809:G:C6	3.09	0.41
48:5:3893:C:H2'	48:5:3894:A:C8	2.56	0.41
48:5:4071:U:H2'	48:5:4072:C:H6	1.86	0.41
48:5:4635:A:C8	48:5:5048:A:N6	2.86	0.41
51:9:879:C:H3'	51:9:880:G:H5''	2.02	0.41
51:9:1265:A:H5'	51:9:1326:OMU:HM21	2.03	0.41
51:9:1473:G:N2	51:9:1475:G:H3'	2.36	0.41
51:9:1624:U:O2	51:9:1624:U:O4'	2.38	0.41
51:9:1638:G:H5''	51:9:1639:G7M:OP1	2.21	0.41
51:9:1735:A:H2'	51:9:1736:G:O4'	2.21	0.41
55:DD:92:ALA:O	55:DD:93:THR:HG22	2.21	0.41
56:EE:59:ASP:O	56:EE:63:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:246:LEU:HD22	56:EE:251:GLU:OE1	2.21	0.41
58:GG:3:LEU:O	58:GG:15:LEU:HA	2.21	0.41
62:KK:18:GLU:C	62:KK:20:VAL:H	2.28	0.41
62:KK:43:LEU:O	62:KK:47:LYS:HG2	2.20	0.41
70:SS:5:ILE:O	70:SS:5:ILE:HG23	2.21	0.41
70:SS:33:ILE:HD13	70:SS:71:MET:HE1	2.02	0.41
71:TT:38:LYS:NZ	71:TT:43:LYS:O	2.48	0.41
72:UU:55:ARG:HG3	72:UU:55:ARG:HH11	1.85	0.41
74:WW:111:MET:SD	74:WW:115:GLU:HG2	2.61	0.41
76:YY:46:LYS:N	76:YY:46:LYS:HD3	2.35	0.41
79:bb:56:CYS:O	79:bb:57:VAL:C	2.64	0.41
82:ee:17:LEU:HD23	82:ee:17:LEU:N	2.35	0.41
84:gg:132:TRP:CZ3	84:gg:138:CYS:HB2	2.56	0.41
84:gg:146:SER:OG	84:gg:147:HIS:N	2.54	0.41
87:jj:256:ALA:HA	87:jj:282:LEU:CD1	2.51	0.41
87:jj:303:PHE:CE1	87:jj:311:ILE:HD13	2.56	0.41
3:C:69:THR:CG2	3:C:75:ARG:HD3	2.51	0.40
4:D:208:MET:HB3	4:D:208:MET:HE2	1.99	0.40
20:U:39:PHE:CE2	20:U:70:ILE:HD13	2.55	0.40
20:U:107:LYS:O	20:U:109:SER:N	2.53	0.40
21:V:30:ASP:HA	21:V:116:ALA:O	2.20	0.40
26:a:77:LYS:CE	48:5:1502:G:N2	2.76	0.40
43:s:28:PHE:HB3	43:s:189:ILE:CD1	2.51	0.40
48:5:223:G:H4'	48:5:225:G:C8	2.57	0.40
48:5:454:U:H2'	48:5:455:C:O4'	2.21	0.40
48:5:478:G:H2'	48:5:479:G:H8	1.85	0.40
48:5:960:A:H4'	48:5:961:G:OP2	2.21	0.40
48:5:1444:G:H2'	48:5:1445:U:C6	2.56	0.40
48:5:1942:A:H2'	48:5:1943:A:C8	2.56	0.40
48:5:2258:C:O2'	48:5:2259:G:P	2.79	0.40
48:5:2364:OMG:HM23	48:5:2364:OMG:H1'	1.80	0.40
48:5:2559:G:C6	48:5:2569:G:C6	3.09	0.40
48:5:4114:C:O2'	48:5:4115:G:O4'	2.38	0.40
48:5:4694:G:H2'	48:5:4694:G:N3	2.36	0.40
50:8:110:U:C2'	50:8:111:U:O4'	2.68	0.40
51:9:94:G:O2'	51:9:508:A:O2'	2.28	0.40
51:9:140:C:O2'	51:9:141:A:P	2.78	0.40
51:9:356:C:O2	51:9:356:C:H2'	2.20	0.40
51:9:449:A:O2'	51:9:452:G:N7	2.53	0.40
51:9:882:U:H6	51:9:882:U:O5'	2.03	0.40
51:9:1129:G:H2'	51:9:1130:G:N9	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1397:U:C3'	51:9:1398:G:C5'	2.99	0.40
51:9:1409:A:H61	51:9:1439:A:H1'	1.86	0.40
51:9:1440:C:O2'	51:9:1441:U:H5'	2.20	0.40
51:9:1456:G:C4	51:9:1457:U:C5	3.09	0.40
55:DD:123:LEU:HD21	55:DD:154:ASP:OD2	2.21	0.40
57:FF:68:ILE:HG12	57:FF:116:ILE:CD1	2.51	0.40
57:FF:104:THR:C	57:FF:106:GLU:H	2.29	0.40
60:II:34:ALA:CB	60:II:56:ARG:HD3	2.51	0.40
61:JJ:74:GLY:O	61:JJ:78:LEU:HG	2.20	0.40
62:KK:42:ASN:ND2	62:KK:46:MET:SD	2.94	0.40
67:PP:27:ASP:OD1	67:PP:27:ASP:C	2.64	0.40
68:QQ:41:MET:HE1	71:TT:8:ASP:O	2.21	0.40
69:RR:13:ALA:O	69:RR:17:ILE:HD13	2.21	0.40
70:SS:85:ASN:OD1	70:SS:85:ASN:C	2.63	0.40
71:TT:112:MET:O	71:TT:123:LEU:HD23	2.21	0.40
76:YY:88:LYS:HD3	76:YY:97:TYR:CE1	2.57	0.40
80:cc:16:LYS:HD3	80:cc:17:VAL:H	1.86	0.40
82:ee:36:MET:HE2	82:ee:36:MET:HB3	1.93	0.40
2:B:28:LYS:O	2:B:220:ILE:HG21	2.21	0.40
8:H:41:ILE:HG21	8:H:73:ILE:HD11	2.03	0.40
10:J:42:GLN:OE1	10:J:42:GLN:HA	2.22	0.40
23:X:87:MET:O	23:X:91:GLU:HG2	2.21	0.40
25:Z:88:ASP:O	25:Z:89:ILE:C	2.64	0.40
27:b:69:ALA:O	27:b:72:ILE:CG2	2.69	0.40
32:g:82:MET:HE3	32:g:82:MET:HB2	2.02	0.40
44:t:18:THR:HG21	44:t:61:LYS:HE2	2.02	0.40
48:5:231:U:C2'	48:5:232:G:OP1	2.70	0.40
48:5:3896:C:O2	48:5:4564:A:N1	2.54	0.40
50:8:44:A:H2'	50:8:45:C:O4'	2.21	0.40
50:8:124:U:H4'	50:8:125:C:O5'	2.20	0.40
50:8:133:G:O2'	50:8:134:G:H5'	2.21	0.40
51:9:64:A:OP1	58:GG:136:LYS:NZ	2.51	0.40
51:9:607:U:HO2'	51:9:608:C:P	2.39	0.40
51:9:608:C:O4'	82:ee:58:ASN:ND2	2.54	0.40
51:9:801:PSU:H5''	51:9:802:A:OP2	2.21	0.40
51:9:840:C:O2	76:YY:12:PHE:CE1	2.74	0.40
51:9:870:A:C4'	51:9:871:U:OP2	2.69	0.40
51:9:872:A:O2'	51:9:873:G:C5'	2.63	0.40
51:9:874:G:H2'	51:9:875:A:C8	2.56	0.40
51:9:1201:U:H2'	51:9:1202:U:C6	2.56	0.40
51:9:1287:A:C2	51:9:1313:A:N3	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1306:U:C3'	51:9:1307:U:H5''	2.51	0.40
51:9:1557:C:O2	51:9:1557:C:C2'	2.69	0.40
51:9:1772:C:O2'	51:9:1773:C:H5'	2.21	0.40
54:CC:252:THR:HG22	74:WW:99:PHE:CZ	2.57	0.40
55:DD:27:ARG:C	62:KK:61:GLN:NE2	2.79	0.40
55:DD:139:SER:O	55:DD:182:LEU:HD23	2.21	0.40
57:FF:42:LYS:HB3	57:FF:43:GLU:OE1	2.22	0.40
59:HH:26:ALA:HA	59:HH:29:GLU:OE1	2.21	0.40
61:JJ:160:SER:O	61:JJ:166:GLY:HA3	2.21	0.40
62:KK:66:HIS:O	62:KK:68:TYR:CE1	2.75	0.40
64:MM:18:LEU:HA	64:MM:21:VAL:HG12	2.04	0.40
64:MM:61:TYR:CE1	64:MM:65:VAL:HG21	2.56	0.40
65:NN:83:ASP:OD1	65:NN:84:LEU:N	2.54	0.40
66:OO:34:PHE:HB3	66:OO:41:PHE:HB2	2.02	0.40
70:SS:130:ARG:HD2	70:SS:134:GLN:HG3	2.03	0.40
84:gg:8:ARG:HA	84:gg:8:ARG:NE	2.33	0.40
84:gg:10:THR:HG22	84:gg:308:ARG:HG2	2.03	0.40
84:gg:77:PHE:CE1	84:gg:91:ASP:OD2	2.74	0.40
84:gg:210:GLY:CA	84:gg:239:LEU:HD11	2.50	0.40
87:jj:120:LEU:HD23	87:jj:120:LEU:HA	1.93	0.40
87:jj:253:LEU:HD13	87:jj:564:ILE:HD11	2.02	0.40
87:jj:360:PHE:C	87:jj:361:GLU:HG2	2.47	0.40
5:E:101:GLY:O	5:E:102:ASP:C	2.64	0.40
5:E:269:GLN:N	48:5:4931:G:OP1	2.44	0.40
11:L:25:TRP:CZ2	13:N:201:HIS:CE1	3.09	0.40
11:L:165:LYS:O	26:a:100:ILE:CD1	2.69	0.40
13:N:10:LEU:HD12	34:i:48:CYS:SG	2.61	0.40
13:N:114:ARG:HD2	13:N:137:PRO:HG3	2.03	0.40
13:N:146:PRO:HA	13:N:149:GLN:HG2	2.03	0.40
13:N:166:SER:O	13:N:170:LYS:HG2	2.21	0.40
14:O:171:LYS:NZ	48:5:4759:C:OP2	2.53	0.40
17:R:28:GLU:OE1	17:R:28:GLU:HA	2.22	0.40
20:U:19:LEU:HD11	20:U:77:PRO:HA	2.03	0.40
20:U:42:PHE:CG	20:U:90:TYR:HD2	2.39	0.40
32:g:26:PRO:HG3	48:5:2639:U:H1'	2.03	0.40
37:l:26:TRP:CE3	37:l:27:ILE:HD13	2.57	0.40
48:5:126:C:H2'	48:5:127:G:C8	2.55	0.40
48:5:216:C:O3'	48:5:217:C:H2'	2.21	0.40
48:5:424:U:H2'	48:5:425:U:C6	2.55	0.40
48:5:520:U:O4	48:5:641:G:O6	2.39	0.40
48:5:1834:U:O2	48:5:1834:U:O4'	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1905:U:H2'	48:5:1906:U:O4'	2.21	0.40
48:5:1987:C:P	48:5:1988:G:OP2	2.80	0.40
48:5:2414:G:O2'	48:5:2415:U:H5'	2.21	0.40
48:5:3907:G:O4'	48:5:4449:A:C5	2.74	0.40
48:5:4232:U:H4'	48:5:4233:A:O5'	2.20	0.40
48:5:5053:U:H3'	48:5:5054:C:O4'	2.21	0.40
49:7:28:C:H2'	49:7:29:C:H5'	2.03	0.40
50:8:49:G:H2'	50:8:50:C:O4'	2.22	0.40
51:9:173:A:H2'	51:9:174:OMC:O4'	2.22	0.40
51:9:488:U:O2'	51:9:489:A:P	2.79	0.40
51:9:886:A:H3'	51:9:887:U:C5'	2.51	0.40
51:9:1288:U:O4	51:9:1312:G:N2	2.53	0.40
51:9:1420:G:OP1	51:9:1420:G:C8	2.74	0.40
51:9:1573:G:H2'	51:9:1574:C:O4'	2.21	0.40
51:9:1601:A:H4'	51:9:1602:U:C6	2.57	0.40
51:9:1621:U:OP1	67:PP:40:ARG:HG2	2.22	0.40
57:FF:128:ILE:HG21	80:cc:68:LEU:HD12	2.04	0.40
59:HH:87:PHE:O	59:HH:88:SER:C	2.65	0.40
60:II:124:LYS:HB3	60:II:167:GLN:OE1	2.21	0.40
61:JJ:169:ARG:HE	61:JJ:169:ARG:HB3	1.81	0.40
62:KK:84:HIS:N	62:KK:84:HIS:CD2	2.87	0.40
64:MM:89:VAL:HG12	64:MM:90:GLY:N	2.36	0.40
67:PP:83:MET:HG3	67:PP:89:MET:HE1	2.03	0.40
70:SS:124:ARG:NH2	70:SS:129:LEU:HB3	2.36	0.40
71:TT:18:LEU:HD23	71:TT:58:ALA:CA	2.52	0.40
71:TT:28:LEU:O	71:TT:28:LEU:HG	2.21	0.40
75:XX:102:VAL:CG1	75:XX:120:PHE:HB3	2.52	0.40
76:YY:10:ARG:NH2	76:YY:24:VAL:HG11	2.36	0.40
84:gg:4:GLN:CG	84:gg:5:MET:N	2.84	0.40
84:gg:48:ASP:O	84:gg:51:ASN:O	2.39	0.40
84:gg:157:SER:OG	84:gg:164:ILE:HB	2.21	0.40
86:ii:252:LYS:HD3	86:ii:274:VAL:HG21	2.03	0.40
87:jj:452:GLU:H	87:jj:452:GLU:CD	2.29	0.40
1:A:186:TYR:HB2	1:A:196:TRP:CZ3	2.56	0.40
3:C:11:TYR:CZ	3:C:148:PRO:HB2	2.57	0.40
3:C:308:LYS:HD3	3:C:310:HIS:NE2	2.35	0.40
4:D:108:ARG:HG2	4:D:112:ARG:HH21	1.87	0.40
7:G:87:LEU:HD21	7:G:222:ILE:HD13	2.03	0.40
10:J:139:PHE:HA	10:J:151:ILE:HD11	2.02	0.40
13:N:49:ARG:NH2	48:5:152:U:OP2	2.54	0.40
15:P:94:MET:HE1	15:P:146:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:133:LYS:HG2	17:R:137:ILE:HD12	2.02	0.40
20:U:78:PHE:HE2	20:U:83:LEU:HD21	1.86	0.40
20:U:80:LYS:O	20:U:110:TYR:HE2	2.05	0.40
26:a:38:MET:HE2	26:a:53:PHE:CG	2.56	0.40
29:d:37:GLY:O	29:d:41:ARG:HG3	2.22	0.40
44:t:78:SER:HB3	44:t:117:ARG:HD2	2.02	0.40
46:2:20(A):U:C3'	46:2:21:A:C5'	3.00	0.40
48:5:44:A:O2'	48:5:94:A:N1	2.45	0.40
48:5:134:G:H4'	48:5:135:G:H5'	2.04	0.40
48:5:231:U:O2'	48:5:232:G:OP1	2.29	0.40
48:5:261:G:N1	48:5:262:G:C2	2.90	0.40
48:5:382:G:H4'	48:5:407:A:N1	2.35	0.40
48:5:654:C:C2	48:5:655:C:C6	3.09	0.40
48:5:757:G:C2	48:5:758:G:N7	2.90	0.40
48:5:913:U:HO2'	48:5:914:U:P	2.36	0.40
48:5:1991:A:O2'	48:5:1992:U:C5'	2.69	0.40
48:5:2415:U:H2'	48:5:2416:G:C8	2.56	0.40
48:5:2446:C:H2'	48:5:2447:U:C1'	2.52	0.40
48:5:2666:U:O2'	48:5:2668:G:N7	2.48	0.40
48:5:3604:A:H2'	48:5:3605:C:N1	2.37	0.40
48:5:4471:U:H2'	48:5:4472:G:C8	2.56	0.40
48:5:4538:G:H2'	48:5:4539:U:C6	2.57	0.40
51:9:85:A:H2'	51:9:86:C:C6	2.57	0.40
51:9:124:U:O4	51:9:338:G:N1	2.55	0.40
51:9:360:A:C2	51:9:362:C:H2'	2.57	0.40
51:9:690:G:C8	51:9:691:G:H1'	2.57	0.40
51:9:1134:G:H2'	51:9:1135:C:C6	2.56	0.40
51:9:1139:C:O2	51:9:1139:C:OP1	2.40	0.40
51:9:1315:U:O5'	62:KK:2:LEU:HB2	2.22	0.40
51:9:1442:OMU:H3'	51:9:1442:OMU:H6	2.04	0.40
51:9:1480:A:C2'	81:dd:56:ASP:OD1	2.66	0.40
51:9:1617:G:N2	51:9:1619:A:H3'	2.36	0.40
54:CC:233:LEU:HD23	54:CC:233:LEU:C	2.46	0.40
55:DD:105:LEU:HD22	55:DD:122:VAL:HG11	2.03	0.40
58:GG:32:MET:SD	58:GG:63:MET:HE2	2.62	0.40
59:HH:135:PHE:HB3	59:HH:136:PRO:HD3	2.03	0.40
59:HH:149:ASP:O	59:HH:149:ASP:OD1	2.40	0.40
65:NN:110:ASP:O	65:NN:114:ARG:HG2	2.20	0.40
68:QQ:57:LEU:HD21	68:QQ:115:TYR:HB2	2.03	0.40
84:gg:159:ASN:O	84:gg:160:SER:C	2.64	0.40
84:gg:259:TRP:HD1	84:gg:266:ILE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:62:ILE:HD12	87:jj:62:ILE:H	1.87	0.40
87:jj:105:VAL:N	87:jj:284:ASP:OD1	2.54	0.40
87:jj:292:VAL:HG23	87:jj:295:ALA:HB3	2.03	0.40
4:D:225:GLN:HB2	49:7:49:A:OP1	2.22	0.40
12:M:129:LYS:HD2	48:5:4894:A:OP1	2.22	0.40
21:V:112:MET:HE2	21:V:112:MET:HB3	1.99	0.40
37:l:29:MET:HE3	37:l:29:MET:HA	2.04	0.40
42:r:56:ASP:OD1	42:r:57:GLY:N	2.55	0.40
46:2:18:G:O4'	46:2:58:A:C2	2.75	0.40
48:5:716:C:H2'	48:5:717:U:O4'	2.22	0.40
48:5:969:C:H2'	48:5:2259:G:O6	2.21	0.40
48:5:4116:C:H4'	48:5:4117:U:OP2	2.22	0.40
48:5:4917:C:O5'	48:5:4917:C:H6	2.05	0.40
49:7:11:A:N1	49:7:66:G:O2'	2.42	0.40
51:9:201:C:H6	51:9:201:C:O5'	2.05	0.40
51:9:905:C:O3'	51:9:906:U:O4'	2.39	0.40
51:9:1060:A:O2'	51:9:1062:A:N7	2.48	0.40
51:9:1447:G:C2'	51:9:1448:A:H5'	2.52	0.40
52:AA:165:ASN:HA	52:AA:171:VAL:HG22	2.03	0.40
54:CC:125:LYS:HE2	54:CC:141:VAL:HG11	2.02	0.40
55:DD:32:ASP:HB2	55:DD:54:ARG:HB3	2.03	0.40
57:FF:179:ASN:HB2	57:FF:187:SER:HB2	2.03	0.40
58:GG:35:GLU:HB3	58:GG:49:VAL:HG12	2.04	0.40
61:JJ:134:HIS:O	61:JJ:159:PHE:HA	2.21	0.40
69:RR:105:MET:O	69:RR:109:LEU:HG	2.22	0.40
71:TT:31:PRO:O	71:TT:34:VAL:HG23	2.22	0.40
77:ZZ:62:VAL:N	77:ZZ:63:PRO:CD	2.85	0.40
84:gg:199:THR:HG21	84:gg:239:LEU:C	2.47	0.40
86:ii:332:VAL:HG12	86:ii:370:GLU:HG3	2.03	0.40
86:ii:359:ASP:O	86:ii:360:LYS:HB2	2.20	0.40
87:jj:82:GLU:O	87:jj:83:THR:C	2.64	0.40
87:jj:216:ASP:O	87:jj:217:LEU:HD22	2.21	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	242/257 (94%)	226 (93%)	16 (7%)	0	100	100
2	B	392/403 (97%)	376 (96%)	16 (4%)	0	100	100
3	C	360/413 (87%)	348 (97%)	12 (3%)	0	100	100
4	D	287/297 (97%)	270 (94%)	16 (6%)	1 (0%)	36	55
5	E	209/291 (72%)	189 (90%)	20 (10%)	0	100	100
6	F	223/247 (90%)	218 (98%)	5 (2%)	0	100	100
7	G	214/319 (67%)	202 (94%)	12 (6%)	0	100	100
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	200/214 (94%)	193 (96%)	7 (4%)	0	100	100
10	J	165/178 (93%)	151 (92%)	13 (8%)	1 (1%)	21	38
11	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
12	M	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
13	N	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
14	O	196/203 (97%)	187 (95%)	8 (4%)	1 (0%)	24	43
15	P	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
16	Q	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
17	R	177/196 (90%)	172 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
19	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
20	U	96/128 (75%)	88 (92%)	8 (8%)	0	100	100
21	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
22	W	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
23	X	114/156 (73%)	108 (95%)	6 (5%)	0	100	100
24	Y	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
25	Z	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
26	a	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	18	34
27	b	73/245 (30%)	70 (96%)	3 (4%)	0	100	100
28	c	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
29	d	96/125 (77%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	e	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
31	f	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
32	g	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
33	h	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
34	i	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
35	j	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
36	k	66/70 (94%)	60 (91%)	5 (8%)	1 (2%)	8	16
37	l	47/51 (92%)	45 (96%)	2 (4%)	0	100	100
38	m	49/93 (53%)	47 (96%)	2 (4%)	0	100	100
39	n	21/25 (84%)	21 (100%)	0	0	100	100
40	o	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
41	p	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
42	r	123/137 (90%)	113 (92%)	10 (8%)	0	100	100
43	s	188/318 (59%)	163 (87%)	25 (13%)	0	100	100
44	t	135/165 (82%)	113 (84%)	21 (16%)	1 (1%)	18	34
45	1	13/130 (10%)	11 (85%)	2 (15%)	0	100	100
52	AA	204/295 (69%)	189 (93%)	15 (7%)	0	100	100
53	BB	210/264 (80%)	200 (95%)	10 (5%)	0	100	100
54	CC	214/293 (73%)	202 (94%)	12 (6%)	0	100	100
55	DD	217/243 (89%)	196 (90%)	21 (10%)	0	100	100
56	EE	257/263 (98%)	231 (90%)	26 (10%)	0	100	100
57	FF	177/204 (87%)	163 (92%)	13 (7%)	1 (1%)	21	38
58	GG	235/249 (94%)	205 (87%)	29 (12%)	1 (0%)	30	49
59	HH	173/194 (89%)	146 (84%)	27 (16%)	0	100	100
60	II	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
61	JJ	183/194 (94%)	167 (91%)	16 (9%)	0	100	100
62	KK	84/165 (51%)	76 (90%)	8 (10%)	0	100	100
63	LL	132/158 (84%)	125 (95%)	7 (5%)	0	100	100
64	MM	120/132 (91%)	91 (76%)	29 (24%)	0	100	100
65	NN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
66	OO	125/168 (74%)	121 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	PP	115/145 (79%)	106 (92%)	9 (8%)	0	100	100
68	QQ	138/146 (94%)	128 (93%)	10 (7%)	0	100	100
69	RR	116/135 (86%)	106 (91%)	10 (9%)	0	100	100
70	SS	138/152 (91%)	130 (94%)	8 (6%)	0	100	100
71	TT	136/145 (94%)	124 (91%)	12 (9%)	0	100	100
72	UU	100/119 (84%)	89 (89%)	11 (11%)	0	100	100
73	VV	79/83 (95%)	71 (90%)	8 (10%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
76	YY	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
77	ZZ	70/125 (56%)	64 (91%)	6 (9%)	0	100	100
78	aa	96/115 (84%)	86 (90%)	10 (10%)	0	100	100
79	bb	75/84 (89%)	70 (93%)	5 (7%)	0	100	100
80	cc	59/69 (86%)	54 (92%)	5 (8%)	0	100	100
81	dd	51/56 (91%)	45 (88%)	6 (12%)	0	100	100
82	ee	43/133 (32%)	37 (86%)	6 (14%)	0	100	100
83	ff	59/156 (38%)	49 (83%)	10 (17%)	0	100	100
84	gg	300/317 (95%)	252 (84%)	48 (16%)	0	100	100
86	ii	414/459 (90%)	380 (92%)	33 (8%)	1 (0%)	43	63
87	jj	574/599 (96%)	529 (92%)	44 (8%)	1 (0%)	43	63
All	All	12249/14542 (84%)	11407 (93%)	832 (7%)	10 (0%)	49	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
58	GG	128	THR
57	FF	33	ILE
86	ii	180	HIS
26	a	15	VAL
10	J	173	ILE
14	O	187	LYS
4	D	235	MET
87	jj	96	ARG
36	k	61	PRO
44	t	32	ILE

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	187/199 (94%)	186 (100%)	1 (0%)	81	92
2	B	336/348 (97%)	328 (98%)	8 (2%)	43	70
3	C	302/337 (90%)	295 (98%)	7 (2%)	44	72
4	D	245/250 (98%)	238 (97%)	7 (3%)	37	65
5	E	191/251 (76%)	183 (96%)	8 (4%)	26	52
6	F	196/215 (91%)	196 (100%)	0	100	100
7	G	189/272 (70%)	181 (96%)	8 (4%)	26	52
8	H	169/171 (99%)	168 (99%)	1 (1%)	78	91
9	I	174/181 (96%)	173 (99%)	1 (1%)	78	91
10	J	140/149 (94%)	134 (96%)	6 (4%)	26	51
11	L	175/176 (99%)	171 (98%)	4 (2%)	44	72
12	M	117/161 (73%)	116 (99%)	1 (1%)	70	87
13	N	171/172 (99%)	169 (99%)	2 (1%)	63	83
14	O	170/173 (98%)	166 (98%)	4 (2%)	43	70
15	P	134/163 (82%)	133 (99%)	1 (1%)	76	89
16	Q	164/165 (99%)	161 (98%)	3 (2%)	51	77
17	R	158/175 (90%)	155 (98%)	3 (2%)	50	76
18	S	157/157 (100%)	153 (98%)	4 (2%)	42	69
19	T	139/140 (99%)	139 (100%)	0	100	100
20	U	88/114 (77%)	85 (97%)	3 (3%)	32	60
21	V	100/107 (94%)	99 (99%)	1 (1%)	68	86
22	W	55/126 (44%)	55 (100%)	0	100	100
23	X	104/134 (78%)	103 (99%)	1 (1%)	68	86
24	Y	124/135 (92%)	123 (99%)	1 (1%)	73	88
25	Z	117/118 (99%)	113 (97%)	4 (3%)	32	60
26	a	119/120 (99%)	118 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	62/184 (34%)	62 (100%)	0	100	100
28	c	80/98 (82%)	76 (95%)	4 (5%)	22	44
29	d	91/110 (83%)	89 (98%)	2 (2%)	45	73
30	e	114/121 (94%)	114 (100%)	0	100	100
31	f	88/89 (99%)	87 (99%)	1 (1%)	65	84
32	g	98/100 (98%)	95 (97%)	3 (3%)	35	62
33	h	109/110 (99%)	106 (97%)	3 (3%)	38	66
34	i	86/89 (97%)	85 (99%)	1 (1%)	63	83
35	j	73/80 (91%)	68 (93%)	5 (7%)	14	31
36	k	63/65 (97%)	57 (90%)	6 (10%)	8	17
37	l	46/48 (96%)	46 (100%)	0	100	100
38	m	47/84 (56%)	46 (98%)	1 (2%)	47	74
39	n	22/24 (92%)	22 (100%)	0	100	100
40	o	91/94 (97%)	90 (99%)	1 (1%)	65	84
41	p	74/75 (99%)	72 (97%)	2 (3%)	39	67
42	r	109/121 (90%)	109 (100%)	0	100	100
43	s	159/258 (62%)	154 (97%)	5 (3%)	35	62
44	t	115/137 (84%)	112 (97%)	3 (3%)	40	68
45	1	13/102 (13%)	13 (100%)	0	100	100
52	AA	172/244 (70%)	165 (96%)	7 (4%)	27	53
53	BB	193/231 (84%)	192 (100%)	1 (0%)	81	92
54	CC	182/225 (81%)	172 (94%)	10 (6%)	19	40
55	DD	185/202 (92%)	177 (96%)	8 (4%)	26	51
56	EE	222/225 (99%)	217 (98%)	5 (2%)	44	72
57	FF	154/170 (91%)	145 (94%)	9 (6%)	18	38
58	GG	207/218 (95%)	200 (97%)	7 (3%)	32	60
59	HH	158/174 (91%)	151 (96%)	7 (4%)	25	50
60	II	178/180 (99%)	172 (97%)	6 (3%)	32	60
61	JJ	161/168 (96%)	157 (98%)	4 (2%)	42	69
62	KK	78/136 (57%)	76 (97%)	2 (3%)	40	68
63	LL	125/142 (88%)	121 (97%)	4 (3%)	34	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	MM	102/108 (94%)	99 (97%)	3 (3%)	37	65
65	NN	130/131 (99%)	128 (98%)	2 (2%)	57	80
66	OO	100/130 (77%)	94 (94%)	6 (6%)	17	36
67	PP	106/130 (82%)	104 (98%)	2 (2%)	50	76
68	QQ	116/121 (96%)	115 (99%)	1 (1%)	70	87
69	RR	107/121 (88%)	99 (92%)	8 (8%)	12	26
70	SS	122/132 (92%)	121 (99%)	1 (1%)	73	88
71	TT	109/115 (95%)	106 (97%)	3 (3%)	38	66
72	UU	93/107 (87%)	89 (96%)	4 (4%)	26	51
73	VV	65/67 (97%)	63 (97%)	2 (3%)	35	62
74	WW	112/113 (99%)	109 (97%)	3 (3%)	39	67
75	XX	113/115 (98%)	110 (97%)	3 (3%)	39	67
76	YY	107/112 (96%)	101 (94%)	6 (6%)	19	39
77	ZZ	64/103 (62%)	63 (98%)	1 (2%)	55	79
78	aa	85/98 (87%)	83 (98%)	2 (2%)	43	70
79	bb	72/76 (95%)	71 (99%)	1 (1%)	59	81
80	cc	54/62 (87%)	50 (93%)	4 (7%)	13	27
81	dd	47/49 (96%)	44 (94%)	3 (6%)	16	33
82	ee	39/106 (37%)	38 (97%)	1 (3%)	40	68
83	ff	59/140 (42%)	57 (97%)	2 (3%)	32	60
84	gg	263/275 (96%)	246 (94%)	17 (6%)	15	32
86	ii	358/394 (91%)	336 (94%)	22 (6%)	17	35
87	jj	508/526 (97%)	491 (97%)	17 (3%)	33	61
All	All	10707/12344 (87%)	10406 (97%)	301 (3%)	38	66

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ILE
2	B	38	SER
2	B	66	LYS
2	B	125	SER
2	B	136	LYS
2	B	138	GLN

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Mol	Chain	Res	Type
2	B	287	ILE
2	B	313	SER
2	B	317	LEU
3	C	150	LEU
3	C	153	VAL
3	C	204	ARG
3	C	227	ILE
3	C	259	LYS
3	C	285	LEU
3	C	308	LYS
4	D	154	THR
4	D	185	SER
4	D	224	SER
4	D	228	LYS
4	D	232	THR
4	D	235	MET
4	D	288	LEU
5	E	62	SER
5	E	66	SER
5	E	98	PRO
5	E	124	VAL
5	E	203	LYS
5	E	204	ILE
5	E	214	HIS
5	E	276	SER
7	G	43	GLN
7	G	53	ARG
7	G	86	VAL
7	G	98	LEU
7	G	150	LYS
7	G	164	ILE
7	G	229	ARG
7	G	250	ILE
8	H	94	SER
9	I	214	SER
10	J	49	VAL
10	J	52	LYS
10	J	81	GLU
10	J	132	VAL
10	J	158	SER
10	J	171	ASP
11	L	42	ARG

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Mol	Chain	Res	Type
11	L	122	SER
11	L	146	LEU
11	L	208	GLU
12	M	50	MET
13	N	36	LEU
13	N	67	ARG
14	O	16	LEU
14	O	61	ARG
14	O	173	GLN
14	O	201	LEU
15	P	14	SER
16	Q	42	THR
16	Q	128	LEU
16	Q	167	VAL
17	R	13	SER
17	R	29	THR
17	R	37	SER
18	S	21	LYS
18	S	71	SER
18	S	102	THR
18	S	138	ARG
20	U	60	VAL
20	U	101	ARG
20	U	102	VAL
21	V	139	ILE
23	X	53	ARG
24	Y	46	SER
25	Z	26	VAL
25	Z	43	VAL
25	Z	60	LYS
25	Z	96	VAL
26	a	95	THR
28	c	16	SER
28	c	75	SER
28	c	92	CYS
28	c	103	ASP
29	d	46	LEU
29	d	78	ARG
31	f	69	VAL
32	g	3	GLN
32	g	68	SER
32	g	87	VAL

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Mol	Chain	Res	Type
33	h	19	LYS
33	h	20	GLN
33	h	42	SER
34	i	17	VAL
35	j	10	LYS
35	j	33	THR
35	j	36	LYS
35	j	55	ARG
35	j	82	THR
36	k	8	ILE
36	k	14	THR
36	k	21	LYS
36	k	44	THR
36	k	48	THR
36	k	61	PRO
38	m	84	GLN
40	o	79	SER
41	p	45	THR
41	p	74	THR
43	s	11	SER
43	s	47	LEU
43	s	96	THR
43	s	136	SER
43	s	187	LEU
44	t	13	VAL
44	t	63	THR
44	t	71	ILE
52	AA	13	GLU
52	AA	14	ASP
52	AA	81	ASN
52	AA	89	LYS
52	AA	135	THR
52	AA	191	ARG
52	AA	193	HIS
53	BB	88	THR
54	CC	72	ASP
54	CC	73	MET
54	CC	77	SER
54	CC	121	ARG
54	CC	141	VAL
54	CC	184	VAL
54	CC	206	SER

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Mol	Chain	Res	Type
54	CC	259	THR
54	CC	263	LYS
54	CC	272	HIS
55	DD	5	ILE
55	DD	84	VAL
55	DD	93	THR
55	DD	99	ILE
55	DD	123	LEU
55	DD	124	ARG
55	DD	175	VAL
55	DD	221	THR
56	EE	140	VAL
56	EE	146	THR
56	EE	170	THR
56	EE	181	CYS
56	EE	236	ILE
57	FF	26	ASP
57	FF	30	ILE
57	FF	36	GLN
57	FF	66	CYS
57	FF	127	ARG
57	FF	140	ASP
57	FF	193	LYS
57	FF	196	LEU
57	FF	202	SER
58	GG	26	THR
58	GG	36	VAL
58	GG	53	SER
58	GG	67	VAL
58	GG	111	LEU
58	GG	139	SER
58	GG	217	MET
59	HH	23	ILE
59	HH	24	SER
59	HH	28	LEU
59	HH	83	LEU
59	HH	113	LYS
59	HH	167	GLU
59	HH	177	TYR
60	II	89	GLU
60	II	121	LEU
60	II	130	THR

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Mol	Chain	Res	Type
60	II	159	SER
60	II	191	GLU
60	II	205	ARG
61	JJ	23	SER
61	JJ	112	THR
61	JJ	128	VAL
61	JJ	161	LEU
62	KK	3	MET
62	KK	61	GLN
63	LL	20	LYS
63	LL	72	ILE
63	LL	116	CYS
63	LL	118	ARG
64	MM	65	VAL
64	MM	91	LEU
64	MM	109	VAL
65	NN	22	VAL
65	NN	145	THR
66	OO	45	THR
66	OO	48	SER
66	OO	81	VAL
66	OO	137	SER
66	OO	138	ASP
66	OO	151	LEU
67	PP	75	VAL
67	PP	108	LYS
68	QQ	7	LEU
69	RR	17	ILE
69	RR	22	THR
69	RR	40	ILE
69	RR	70	SER
69	RR	76	GLU
69	RR	89	SER
69	RR	105	MET
69	RR	116	ASN
70	SS	30	ILE
71	TT	49	ASP
71	TT	90	SER
71	TT	131	LEU
72	UU	20	ILE
72	UU	24	LEU
72	UU	65	THR

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Mol	Chain	Res	Type
72	UU	81	GLN
73	VV	65	SER
73	VV	69	ILE
74	WW	63	VAL
74	WW	66	THR
74	WW	121	THR
75	XX	90	CYS
75	XX	105	PHE
75	XX	130	LEU
76	YY	11	LYS
76	YY	16	ARG
76	YY	42	GLU
76	YY	50	THR
76	YY	116	LYS
76	YY	120	THR
77	ZZ	54	THR
78	aa	45	VAL
78	aa	69	VAL
79	bb	34	ASP
80	cc	9	ILE
80	cc	30	VAL
80	cc	62	GLU
80	cc	67	ARG
81	dd	33	LYS
81	dd	49	ASP
81	dd	53	ILE
82	ee	26	LYS
83	ff	125	VAL
83	ff	144	CYS
84	gg	5	MET
84	gg	43	TRP
84	gg	66	VAL
84	gg	67	SER
84	gg	69	VAL
84	gg	102	VAL
84	gg	110	SER
84	gg	113	PHE
84	gg	126	ASP
84	gg	133	ASN
84	gg	160	SER
84	gg	165	ILE
84	gg	182	CYS

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Mol	Chain	Res	Type
84	gg	184	LEU
84	gg	199	THR
84	gg	225	LYS
84	gg	285	GLN
86	ii	17	ILE
86	ii	30	ASN
86	ii	123	SER
86	ii	154	SER
86	ii	166	ARG
86	ii	173	THR
86	ii	177	PRO
86	ii	179	LYS
86	ii	189	ARG
86	ii	237	SER
86	ii	258	TYR
86	ii	274	VAL
86	ii	284	LYS
86	ii	322	VAL
86	ii	332	VAL
86	ii	342	LYS
86	ii	343	ILE
86	ii	367	GLU
86	ii	368	LEU
86	ii	393	THR
86	ii	394	ASP
86	ii	400	SER
87	jj	53	THR
87	jj	73	VAL
87	jj	104	GLU
87	jj	118	THR
87	jj	143	ILE
87	jj	152	LEU
87	jj	160	LEU
87	jj	284	ASP
87	jj	323	ARG
87	jj	370	THR
87	jj	445	VAL
87	jj	489	SER
87	jj	528	LEU
87	jj	536	ASP
87	jj	574	ARG
87	jj	576	ARG

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Mol	Chain	Res	Type
87	jj	584	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	203	GLN
3	C	38	ASN
3	C	43	ASN
3	C	61	GLN
3	C	245	HIS
3	C	329	ASN
4	D	39	GLN
4	D	45	ASN
4	D	57	ASN
4	D	138	GLN
4	D	244	HIS
5	E	185	ASN
6	F	79	ASN
6	F	238	GLN
7	G	141	ASN
8	H	8	GLN
9	I	92	HIS
9	I	100	ASN
11	L	87	HIS
11	L	175	ASN
12	M	125	ASN
13	N	8	GLN
14	O	167	HIS
15	P	21	ASN
15	P	137	ASN
16	Q	162	HIS
16	Q	188	ASN
20	U	50	ASN
22	W	17	HIS
22	W	50	ASN
22	W	59	HIS
23	X	93	ASN
24	Y	61	HIS
24	Y	72	GLN
27	b	6	ASN
30	e	23	HIS
30	e	80	HIS

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Mol	Chain	Res	Type
35	j	13	ASN
42	r	103	HIS
43	s	81	HIS
43	s	176	ASN
44	t	65	GLN
52	AA	9	GLN
52	AA	70	ASN
53	BB	124	HIS
53	BB	202	GLN
55	DD	165	ASN
55	DD	207	HIS
56	EE	216	ASN
57	FF	118	ASN
60	II	52	ASN
60	II	116	HIS
61	JJ	124	HIS
62	KK	61	GLN
63	LL	11	GLN
63	LL	18	GLN
64	MM	19	GLN
65	NN	90	HIS
68	QQ	142	GLN
70	SS	97	GLN
71	TT	51	ASN
74	WW	5	ASN
75	XX	31	HIS
78	aa	43	ASN
86	ii	61	ASN
86	ii	334	HIS
87	jj	453	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	0
47	3	72/75 (96%)	20 (27%)	0
48	5	3505/3543 (98%)	655 (18%)	72 (2%)
49	7	119/120 (99%)	11 (9%)	0
50	8	155/156 (99%)	29 (18%)	3 (1%)
51	9	1685/1869 (90%)	440 (26%)	36 (2%)
85	hh	10/197 (5%)	3 (30%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5620/6036 (93%)	1178 (20%)	111 (1%)

All (1178) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	7	G
46	2	8	U
46	2	9	A
46	2	15	G
46	2	19	G
46	2	20	U
46	2	31	C
46	2	47	U
46	2	49	C
46	2	58	A
46	2	61	C
46	2	62	C
46	2	65	G
46	2	67	G
46	2	68	G
46	2	70	A
46	2	73	A
46	2	74	C
46	2	75	C
46	2	76	A
47	3	11	C
47	3	13	C
47	3	16	C
47	3	19	G
47	3	21	A
47	3	22	G
47	3	23	A
47	3	31	A
47	3	34	U
47	3	46	G
47	3	47	U
47	3	49	C
47	3	50	A
47	3	56	C
47	3	58	A
47	3	63	C
47	3	65	G

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Mol	Chain	Res	Type
47	3	67	U
47	3	69	G
47	3	76	A
48	5	13	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	56	A
48	5	59	A
48	5	64	A
48	5	65	A
48	5	73	A
48	5	74	G
48	5	91	G
48	5	98	A
48	5	104	G
48	5	109	G
48	5	110	C
48	5	116	G
48	5	117	C
48	5	118	C
48	5	119	G
48	5	120	A
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	140	G
48	5	144	G
48	5	159	C
48	5	166	C
48	5	167	C
48	5	170	C
48	5	177	G
48	5	182	G
48	5	200	U
48	5	201	C
48	5	209	U
48	5	216	C
48	5	218	A
48	5	219	G
48	5	220	C

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Mol	Chain	Res	Type
48	5	224	U
48	5	232	G
48	5	233	U
48	5	234	G
48	5	238	C
48	5	246	G
48	5	253	G
48	5	256	G
48	5	260	C
48	5	265	C
48	5	266	C
48	5	267	G
48	5	268	G
48	5	271	C
48	5	276	C
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	315	G
48	5	316	U
48	5	326	C
48	5	334	A
48	5	340	C
48	5	350	C
48	5	354	U
48	5	386	A
48	5	387	G
48	5	403	G
48	5	407	A
48	5	409	G
48	5	412	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	462	G
48	5	463	A

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Mol	Chain	Res	Type
48	5	464	G
48	5	465	G
48	5	467	U
48	5	468	U
48	5	481	G
48	5	481(A)	C
48	5	482	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	492	U
48	5	493	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	521	C
48	5	639	U
48	5	642	G
48	5	657	C
48	5	658	C
48	5	660	G
48	5	666	G
48	5	670	G
48	5	685	C
48	5	686	A
48	5	687	U
48	5	694	C
48	5	697	G
48	5	703	G
48	5	704	C
48	5	705	G
48	5	730	G
48	5	731	G
48	5	733	A
48	5	738	C
48	5	742	G
48	5	744	G
48	5	746	A
48	5	747	A
48	5	758	G
48	5	910	G

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Mol	Chain	Res	Type
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	923	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	935(A)	G
48	5	936	C
48	5	943	A
48	5	945	U
48	5	959	G
48	5	960	A
48	5	961	G
48	5	966	A
48	5	967	C
48	5	969	C
48	5	972	C
48	5	973	G
48	5	983	C
48	5	1068	G
48	5	1070	G
48	5	1071	C
48	5	1072	C
48	5	1073	G
48	5	1079	C
48	5	1082	C
48	5	1094	G
48	5	1097	C
48	5	1169	G
48	5	1172	C
48	5	1174	G
48	5	1176	C
48	5	1179	U
48	5	1184	A
48	5	1195	G

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Mol	Chain	Res	Type
48	5	1200	G
48	5	1209	U
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1275	G
48	5	1277	G
48	5	1280	C
48	5	1284	G
48	5	1285	U
48	5	1287	G
48	5	1292	C
48	5	1293	G
48	5	1294	A
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1313	C
48	5	1326	A2M
48	5	1337	A
48	5	1354	A
48	5	1358	G
48	5	1359	G
48	5	1371	A
48	5	1377	G
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1406	G
48	5	1411(A)	G
48	5	1412	G
48	5	1414	C

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Mol	Chain	Res	Type
48	5	1415	G
48	5	1420	A
48	5	1437	C
48	5	1441	C
48	5	1442	C
48	5	1443	A
48	5	1445	U
48	5	1446	C
48	5	1456	C
48	5	1457	G
48	5	1477	C
48	5	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1514	U
48	5	1523	A
48	5	1534	A2M
48	5	1535	C
48	5	1547	A
48	5	1564	A
48	5	1566	C
48	5	1578	U
48	5	1591	U
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	OMG
48	5	1626	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1638	A
48	5	1641	G
48	5	1654	G
48	5	1661	C

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Mol	Chain	Res	Type
48	5	1676	C
48	5	1677	PSU
48	5	1694	C
48	5	1726	U
48	5	1731	C
48	5	1734	G
48	5	1735	U
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1754	U
48	5	1756	U
48	5	1757	U
48	5	1759	G
48	5	1760	G
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1780	A
48	5	1781	PSU
48	5	1787	A
48	5	1804	A
48	5	1805	A
48	5	1806	G
48	5	1809	C
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1892	A
48	5	1897	A
48	5	1918	U
48	5	1920	C

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Mol	Chain	Res	Type
48	5	1921	C
48	5	1922	G
48	5	1930	U
48	5	1931	C
48	5	1932	A
48	5	1940	G
48	5	1948	G
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1960	A
48	5	1961	G
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1971	C
48	5	1972	G
48	5	1974	U
48	5	1975	G
48	5	1976	G
48	5	1978	C
48	5	1979	A
48	5	1980	U
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1987	C
48	5	1988	G
48	5	1990	A
48	5	1991	A
48	5	1992	U
48	5	1997	U
48	5	1998	A
48	5	1999	A
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2009	A
48	5	2011	C
48	5	2025	A
48	5	2026	A

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Mol	Chain	Res	Type
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2069	A
48	5	2071	A
48	5	2084	U
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2267	U
48	5	2289	C
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2333	G
48	5	2348	G
48	5	2351	OMC
48	5	2360	A
48	5	2382	A
48	5	2395	A
48	5	2422	OMC
48	5	2424	OMG
48	5	2425	U

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Mol	Chain	Res	Type
48	5	2433	G
48	5	2441	C
48	5	2450	G
48	5	2453	A
48	5	2475	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2492	C
48	5	2494	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2511	A
48	5	2513	A
48	5	2529	A
48	5	2530	U
48	5	2544	G
48	5	2545	U
48	5	2546	G
48	5	2547	G
48	5	2554	U
48	5	2564	G
48	5	2565	A
48	5	2566	G
48	5	2569	G
48	5	2570	U
48	5	2583	C
48	5	2587	A
48	5	2588	C
48	5	2611	A
48	5	2628	U
48	5	2638	G
48	5	2640	G
48	5	2653	C
48	5	2658	G
48	5	2662	G
48	5	2669	C
48	5	2673	G
48	5	2687	U

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Mol	Chain	Res	Type
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2711	G
48	5	2716	C
48	5	2721	G
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2753	G
48	5	2754	G
48	5	2763	U
48	5	2764	A
48	5	2765	A
48	5	2769	U
48	5	2788	U
48	5	2790	U
48	5	2799	G
48	5	2826	U
48	5	2827	G
48	5	2829	U
48	5	2833	A
48	5	2842	G
48	5	2855	G
48	5	2869	U
48	5	3598	C
48	5	3602	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3616	U
48	5	3617	G
48	5	3618	C
48	5	3625	G
48	5	3626	G
48	5	3635	A
48	5	3644	U
48	5	3657	U
48	5	3662	A

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Mol	Chain	Res	Type
48	5	3673	C
48	5	3688	U
48	5	3710	G
48	5	3712	A
48	5	3713	U
48	5	3714	G
48	5	3743	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3760	A2M
48	5	3761	C
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3783	A
48	5	3784	A
48	5	3786	U
48	5	3788	C
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3814	U
48	5	3817	A
48	5	3818	UY1
48	5	3819	G
48	5	3822	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3897	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U

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Mol	Chain	Res	Type
48	5	3939	G
48	5	3943	A
48	5	3948	C
48	5	4066	U
48	5	4069	U
48	5	4076	G
48	5	4084	G
48	5	4096	C
48	5	4097	G
48	5	4119	C
48	5	4120	U
48	5	4122	G
48	5	4127	A
48	5	4134	C
48	5	4158	C
48	5	4161	G
48	5	4163	U
48	5	4170	A
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4203	A
48	5	4225	G
48	5	4229	U
48	5	4233	A
48	5	4251	A
48	5	4252	C
48	5	4254	G
48	5	4258	C
48	5	4266	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4304	A
48	5	4305	G
48	5	4314	C
48	5	4329	G
48	5	4330	G
48	5	4339	A
48	5	4349	C

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Mol	Chain	Res	Type
48	5	4364	G
48	5	4373	G
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4394	A
48	5	4395	U
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4430	G
48	5	4439	U
48	5	4440	G
48	5	4448	G
48	5	4449	A
48	5	4464	A
48	5	4475	G
48	5	4500	PSU
48	5	4512	U
48	5	4513	A
48	5	4519	C
48	5	4524	G
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4590	A
48	5	4606	G
48	5	4636	U
48	5	4637	OMG
48	5	4656	A
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4700	A

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Mol	Chain	Res	Type
48	5	4709	U
48	5	4720	C
48	5	4736	C
48	5	4740	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4769	G
48	5	4771	C
48	5	4772	C
48	5	4776	G
48	5	4860	G
48	5	4867	G
48	5	4870	G
48	5	4871	C
48	5	4873	G
48	5	4875	G
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4895	C
48	5	4896	G
48	5	4903	G
48	5	4904	G
48	5	4905	C
48	5	4906	C
48	5	4907	G
48	5	4908	G
48	5	4912	G
48	5	4914	G
48	5	4917	C
48	5	4921	C
48	5	4922	C
48	5	4923	U
48	5	4924	C
48	5	4926	C
48	5	4933	C
48	5	4934	A

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Mol	Chain	Res	Type
48	5	4944	C
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4960	G
48	5	4963	G
48	5	4964	C
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4993	G
48	5	5007	A
48	5	5014	A
48	5	5017	G
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5061	A
48	5	5062	G
49	7	10	C
49	7	25	G
49	7	33	U
49	7	40	U
49	7	42	A
49	7	53	U
49	7	64	G
49	7	89	G
49	7	100	A
49	7	110	G
49	7	120	U
50	8	2	G
50	8	34	U
50	8	35	C

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Mol	Chain	Res	Type
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	81	C
50	8	82	A
50	8	83	C
50	8	84	A
50	8	85	U
50	8	86	U
50	8	94	G
50	8	95	A
50	8	103	A
50	8	105	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	114	G
50	8	125	C
50	8	126	C
50	8	127	U
50	8	135	C
50	8	147	G
50	8	150	C
50	8	153	C
50	8	156	U
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	34	PSU
51	9	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	62	G
51	9	65	C

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Mol	Chain	Res	Type
51	9	67	C
51	9	68	A
51	9	71	G
51	9	72	C
51	9	73	C
51	9	74	G
51	9	75	G
51	9	76	U
51	9	78	C
51	9	79	A
51	9	99	A2M
51	9	103	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	124	U
51	9	126	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	162	C
51	9	163	U
51	9	166	A2M
51	9	171	A
51	9	172	OMU
51	9	173	A
51	9	180	G
51	9	182	C
51	9	184	G
51	9	187	G
51	9	188	C
51	9	189	U
51	9	190	G
51	9	192	C
51	9	197	U
51	9	202	G
51	9	207	G
51	9	209	A
51	9	211	G

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Mol	Chain	Res	Type
51	9	212	C
51	9	214	U
51	9	215	G
51	9	216	C
51	9	217	A
51	9	291	G
51	9	292	A
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	305	U
51	9	306	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	310	C
51	9	313	A
51	9	319	C
51	9	320	G
51	9	321	C
51	9	322	C
51	9	324	C
51	9	325	C
51	9	326	C
51	9	327	G
51	9	328	U
51	9	334	C
51	9	336	A
51	9	338	G
51	9	343	A
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	369	C
51	9	370	G
51	9	385	G
51	9	386	C
51	9	400	C

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Mol	Chain	Res	Type
51	9	408	A
51	9	409	C
51	9	418	A
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	465	A
51	9	466	G
51	9	471	G
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	489	A
51	9	492	C
51	9	508	A
51	9	525	A
51	9	532	C
51	9	533	A
51	9	535	G
51	9	536	A
51	9	537	C
51	9	542	U
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	552	G
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	564	A
51	9	568	C
51	9	571	U
51	9	576	A
51	9	580	U

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Mol	Chain	Res	Type
51	9	583	A
51	9	585	C
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	600	G
51	9	605	A
51	9	606	G
51	9	608	C
51	9	614	C
51	9	617	G
51	9	620	G
51	9	628	A
51	9	631	U
51	9	632	C
51	9	643	A
51	9	646	G
51	9	655	A
51	9	660	C
51	9	664	A
51	9	668	A2M
51	9	669	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	688	U
51	9	694	G
51	9	696	G
51	9	698	G
51	9	732	U
51	9	733	C
51	9	734	C
51	9	735	C
51	9	736	C
51	9	737	G
51	9	738	C
51	9	800	U
51	9	801	PSU
51	9	810	A
51	9	811	A

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Mol	Chain	Res	Type
51	9	812	A
51	9	821	G
51	9	822	PSU
51	9	823	U
51	9	827	A
51	9	830	A
51	9	834	C
51	9	836	G
51	9	837	A
51	9	838	G
51	9	839	C
51	9	840	C
51	9	841	G
51	9	844	U
51	9	847	A
51	9	865	A
51	9	870	A
51	9	871	U
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	879	C
51	9	880	G
51	9	881	G
51	9	882	U
51	9	887	U
51	9	888	U
51	9	890	U
51	9	895	G
51	9	896	U
51	9	897	U
51	9	898	U
51	9	899	U
51	9	902	G
51	9	903	A
51	9	906	U
51	9	909	G
51	9	910	G
51	9	913	A
51	9	914	U

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Mol	Chain	Res	Type
51	9	917	U
51	9	920	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	953	C
51	9	970	G
51	9	971	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1017	U
51	9	1023	A
51	9	1040	G
51	9	1044	G
51	9	1045	PSU
51	9	1049	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1077	A
51	9	1083	A
51	9	1085	C
51	9	1086	G
51	9	1089	G
51	9	1096	G
51	9	1110	G
51	9	1113	A
51	9	1115	U
51	9	1116	C
51	9	1120	U
51	9	1131	G
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1158	G
51	9	1171	G

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Mol	Chain	Res	Type
51	9	1181	A
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1209	A
51	9	1210	G
51	9	1211	G
51	9	1215	C
51	9	1224	G
51	9	1242	U
51	9	1243	U
51	9	1251	A
51	9	1253	A
51	9	1256	G
51	9	1257	G
51	9	1265	A
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1280	G
51	9	1281	G
51	9	1282	A
51	9	1283	C
51	9	1284	A
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1291	A
51	9	1292	C
51	9	1293	A
51	9	1294	G
51	9	1298	G
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1310	U
51	9	1311	C
51	9	1313	A

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Mol	Chain	Res	Type
51	9	1314	U
51	9	1315	U
51	9	1317	C
51	9	1319	U
51	9	1321	G
51	9	1333	U
51	9	1342	U
51	9	1345	G
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1401	A
51	9	1402	A
51	9	1407	U
51	9	1408	U
51	9	1409	A
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1416	C
51	9	1418	C
51	9	1419	C
51	9	1420	G
51	9	1423	C
51	9	1424	G
51	9	1426	U
51	9	1427	C
51	9	1429	G
51	9	1431	G
51	9	1432	U
51	9	1433	C
51	9	1434	C
51	9	1435	C
51	9	1436	C
51	9	1438	A
51	9	1439	A

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Mol	Chain	Res	Type
51	9	1440	C
51	9	1442	OMU
51	9	1447	G
51	9	1454	A
51	9	1455	A
51	9	1460	C
51	9	1462	U
51	9	1463	U
51	9	1464	C
51	9	1472	C
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1480	A
51	9	1489	A
51	9	1490	OMG
51	9	1496	U
51	9	1498	A
51	9	1502	C
51	9	1510	G
51	9	1512	C
51	9	1514	G
51	9	1519	U
51	9	1521	C
51	9	1522	A
51	9	1533	A
51	9	1544	C
51	9	1548	G
51	9	1552	G
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1558	C
51	9	1560	U
51	9	1567	G
51	9	1574	C
51	9	1575	G
51	9	1576	G
51	9	1579	A
51	9	1580	A
51	9	1581	C
51	9	1586	U

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Mol	Chain	Res	Type
51	9	1587	G
51	9	1588	A
51	9	1599	U
51	9	1604	G
51	9	1621	U
51	9	1623	A
51	9	1637	A
51	9	1638	G
51	9	1639	G7M
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1657	G
51	9	1664	A
51	9	1665	G
51	9	1669	G
51	9	1695	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1744	G
51	9	1753	C
51	9	1756	C
51	9	1759	G
51	9	1774	C
51	9	1775	U
51	9	1777	G
51	9	1783	C
51	9	1784	G
51	9	1786	U
51	9	1794	C
51	9	1797	U
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1861	G

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Mol	Chain	Res	Type
51	9	1862	G
51	9	1863	A
51	9	1864	U
51	9	1865	C
85	hh	43	A
85	hh	46	G
85	hh	49	U

All (111) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	42	A
48	5	125	C
48	5	133	C
48	5	134	G
48	5	217	C
48	5	231	U
48	5	245	C
48	5	265	C
48	5	267	G
48	5	275	C
48	5	278	G
48	5	385	A
48	5	406	C
48	5	449	C
48	5	480	C
48	5	485	C
48	5	504	G
48	5	922(B)	C
48	5	924	C
48	5	930	G
48	5	959	G
48	5	1072	C
48	5	1211	G
48	5	1236	C
48	5	1238	A
48	5	1291	G
48	5	1370	G
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1590	C

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Mol	Chain	Res	Type
48	5	1625	OMG
48	5	1633	G
48	5	1733	G
48	5	1818	G
48	5	1956	A
48	5	1975	G
48	5	1978	C
48	5	1982	G
48	5	1990	A
48	5	1991	A
48	5	2046	G
48	5	2068	C
48	5	2089	G
48	5	2104	A
48	5	2258	C
48	5	2266	C
48	5	2488	C
48	5	2502	A
48	5	2529	A
48	5	2587	A
48	5	2639	U
48	5	2695	A
48	5	2794	C
48	5	3603	G
48	5	3625	G
48	5	3672	G
48	5	3876	A
48	5	3888	G
48	5	4119	C
48	5	4232	U
48	5	4378	A
48	5	4394	A
48	5	4395	U
48	5	4448	G
48	5	4548	A
48	5	4699	U
48	5	4719	G
48	5	4884	G
48	5	4925	U
48	5	4932	U
48	5	4947	U
50	8	81	C

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Mol	Chain	Res	Type
50	8	94	G
50	8	124	U
51	9	72	C
51	9	102	A
51	9	110	U
51	9	140	C
51	9	208	G
51	9	213	G
51	9	215	G
51	9	291	G
51	9	327	G
51	9	369	C
51	9	407	G
51	9	417	C
51	9	434	G
51	9	465	A
51	9	532	C
51	9	563	G
51	9	642	U
51	9	840	C
51	9	869	A
51	9	870	A
51	9	1137	U
51	9	1281	G
51	9	1394	G
51	9	1395	C
51	9	1408	U
51	9	1418	C
51	9	1432	U
51	9	1463	U
51	9	1477	U
51	9	1490	OMG
51	9	1556	A
51	9	1637	A
51	9	1646	C
51	9	1647	A
51	9	1824	A
51	9	1835	A

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

163 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
48	PSU	5	1862	48	17,20,22	1.11	1 (5%)	21,28,33	1.99	5 (23%)
51	4AC	9	1337	51	21,24,25	3.09	10 (47%)	28,34,37	1.03	1 (3%)
51	A2M	9	99	51,88	22,25,26	3.53	9 (40%)	30,36,39	2.60	10 (33%)
51	PSU	9	1177	51	17,20,22	1.08	1 (5%)	21,28,33	1.77	4 (19%)
48	5MC	5	4447	48,88	19,22,23	3.54	8 (42%)	26,32,35	1.14	2 (7%)
48	OMC	5	2824	48	19,22,23	2.84	8 (42%)	25,31,34	0.95	1 (4%)
51	OMC	9	174	51	19,22,23	2.91	8 (42%)	25,31,34	0.95	0
51	PSU	9	863	51	17,20,22	0.99	1 (5%)	21,28,33	1.93	3 (14%)
48	OMG	5	4228	48	23,26,27	2.30	7 (30%)	32,38,41	2.08	10 (31%)
48	OMG	5	4623	48	23,26,27	2.43	8 (34%)	32,38,41	2.17	9 (28%)
51	A2M	9	1031	51	22,25,26	3.51	10 (45%)	30,36,39	2.46	9 (30%)
51	MA6	9	1851	51	23,26,27	1.40	4 (17%)	33,38,41	4.48	13 (39%)
51	A2M	9	668	51,88	22,25,26	3.45	9 (40%)	30,36,39	2.75	13 (43%)
48	1MA	5	1322	48,88	21,25,26	2.66	6 (28%)	30,37,40	2.29	6 (20%)
48	OMG	5	3899	48,88	23,26,27	2.37	8 (34%)	32,38,41	2.16	10 (31%)
48	OMG	5	1625	48,88	23,26,27	2.46	7 (30%)	32,38,41	2.23	10 (31%)
48	OMU	5	4227	48	19,22,23	2.83	7 (36%)	25,31,34	1.85	5 (20%)
48	A2M	5	398	48	22,25,26	3.53	9 (40%)	30,36,39	2.68	11 (36%)
48	PSU	5	4628	48	17,20,22	1.22	2 (11%)	21,28,33	2.19	6 (28%)
48	A2M	5	3760	48,88	22,25,26	3.50	9 (40%)	30,36,39	2.67	11 (36%)
51	PSU	9	801	51	17,20,22	1.25	2 (11%)	21,28,33	1.67	4 (19%)
48	PSU	5	4361	48	17,20,22	1.11	1 (5%)	21,28,33	2.01	5 (23%)
51	PSU	9	1643	51	17,20,22	1.03	1 (5%)	21,28,33	2.08	4 (19%)
51	PSU	9	218	51	17,20,22	1.13	1 (5%)	21,28,33	2.28	7 (33%)
51	OMG	9	436	51	23,26,27	2.46	6 (26%)	32,38,41	2.09	9 (28%)
51	A2M	9	1678	51	22,25,26	3.45	9 (40%)	30,36,39	2.72	11 (36%)
51	MA6	9	1850	51	23,26,27	1.53	5 (21%)	33,38,41	3.96	14 (42%)
51	PSU	9	609	51	17,20,22	1.08	1 (5%)	21,28,33	2.01	4 (19%)
48	A2M	5	4571	48	22,25,26	3.60	10 (45%)	30,36,39	2.64	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	6MZ	5	4220	48	22,25,26	2.74	4 (18%)	29,36,39	2.17	9 (31%)
48	A2M	5	3724	48	22,25,26	3.54	9 (40%)	30,36,39	2.51	9 (30%)
51	A2M	9	166	51	22,25,26	3.45	9 (40%)	30,36,39	2.57	10 (33%)
48	B9B	5	237	48	25,28,29	1.79	6 (24%)	35,40,43	2.38	15 (42%)
48	PSU	5	4457	48	17,20,22	1.15	1 (5%)	21,28,33	1.77	3 (14%)
48	A2M	5	2363	48,88	22,25,26	3.53	10 (45%)	30,36,39	2.59	9 (30%)
48	PSU	5	4500	48	17,20,22	1.11	3 (17%)	21,28,33	2.07	5 (23%)
48	PSU	5	1677	48	17,20,22	1.25	2 (11%)	21,28,33	2.17	4 (19%)
51	OMU	9	116	51	19,22,23	2.80	6 (31%)	25,31,34	1.78	5 (20%)
48	A2M	5	1524	48	22,25,26	3.44	9 (40%)	30,36,39	2.67	12 (40%)
48	PSU	5	4532	48	17,20,22	1.12	1 (5%)	21,28,33	1.76	3 (14%)
51	PSU	9	822	51	17,20,22	1.23	3 (17%)	21,28,33	2.24	6 (28%)
48	OMU	5	4620	48	19,22,23	2.83	7 (36%)	25,31,34	1.87	5 (20%)
51	PSU	9	119	51	17,20,22	1.08	1 (5%)	21,28,33	2.02	5 (23%)
48	OMG	5	1522	48	23,26,27	2.37	9 (39%)	32,38,41	2.14	12 (37%)
48	OMC	5	3887	48	19,22,23	2.78	7 (36%)	25,31,34	0.77	1 (4%)
48	PSU	5	1782	48	17,20,22	1.10	1 (5%)	21,28,33	2.01	5 (23%)
48	OMU	5	2837	48	19,22,23	2.84	6 (31%)	25,31,34	2.02	6 (24%)
51	A2M	9	468	51	22,25,26	3.55	9 (40%)	30,36,39	2.60	10 (33%)
51	PSU	9	815	51	17,20,22	1.06	1 (5%)	21,28,33	2.17	5 (23%)
48	PSU	5	1781	48	17,20,22	1.13	2 (11%)	21,28,33	1.96	5 (23%)
51	PSU	9	1004	51	17,20,22	1.13	1 (5%)	21,28,33	1.99	4 (19%)
51	OMU	9	1326	51	19,22,23	2.81	7 (36%)	25,31,34	1.95	5 (20%)
48	PSU	5	3695	48	17,20,22	1.05	1 (5%)	21,28,33	1.97	4 (19%)
51	PSU	9	1244	51	17,20,22	1.17	1 (5%)	21,28,33	2.06	5 (23%)
48	OMG	5	373	48	23,26,27	2.41	7 (30%)	32,38,41	2.21	11 (34%)
51	PSU	9	109	51	17,20,22	1.20	1 (5%)	21,28,33	2.02	4 (19%)
48	A2M	5	400	48	22,25,26	3.43	9 (40%)	30,36,39	2.51	9 (30%)
48	A2M	5	1534	48,88	22,25,26	3.56	9 (40%)	30,36,39	2.64	11 (36%)
48	PSU	5	3762	48	17,20,22	1.14	1 (5%)	21,28,33	2.13	5 (23%)
48	PSU	5	1744	48,88	17,20,22	0.96	1 (5%)	21,28,33	2.01	4 (19%)
48	OMG	5	3627	48	23,26,27	2.38	8 (34%)	32,38,41	2.11	11 (34%)
51	PSU	9	649	51	17,20,22	1.06	1 (5%)	21,28,33	1.89	4 (19%)
51	PSU	9	686	51	17,20,22	1.02	2 (11%)	21,28,33	2.29	6 (28%)
48	OMG	5	3792	48	23,26,27	2.32	6 (26%)	32,38,41	2.00	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	A2M	9	512	51	22,25,26	3.50	9 (40%)	30,36,39	2.77	10 (33%)
48	PSU	5	4299	48	17,20,22	1.00	1 (5%)	21,28,33	1.94	3 (14%)
50	OMG	8	75	50	23,26,27	2.35	8 (34%)	32,38,41	2.11	11 (34%)
48	PSU	5	4296	48	17,20,22	1.20	2 (11%)	21,28,33	1.96	3 (14%)
51	G7M	9	1639	46,51	23,26,27	2.77	9 (39%)	34,39,42	1.74	9 (26%)
48	OMG	5	4196	46,48	23,26,27	2.42	7 (30%)	32,38,41	2.06	10 (31%)
48	2MG	5	1517	48	23,26,27	2.57	9 (39%)	33,38,41	2.53	13 (39%)
51	PSU	9	105	51	17,20,22	1.14	1 (5%)	21,28,33	2.00	4 (19%)
51	A2M	9	484	51	22,25,26	3.50	9 (40%)	30,36,39	2.69	10 (33%)
51	OMU	9	1442	51	19,22,23	2.84	6 (31%)	25,31,34	1.83	4 (16%)
48	A2M	5	3867	48	22,25,26	3.46	9 (40%)	30,36,39	2.57	8 (26%)
48	OMG	5	2876	48	23,26,27	2.40	7 (30%)	32,38,41	2.01	9 (28%)
48	OMC	5	2861	48	19,22,23	2.94	8 (42%)	25,31,34	0.84	1 (4%)
51	PSU	9	1445	51	17,20,22	1.05	1 (5%)	21,28,33	1.84	4 (19%)
51	OMC	9	1391	51	19,22,23	2.96	8 (42%)	25,31,34	0.97	1 (4%)
51	PSU	9	1174	51	17,20,22	1.11	1 (5%)	21,28,33	2.07	4 (19%)
51	OMC	9	1703	51	19,22,23	2.96	8 (42%)	25,31,34	0.80	0
51	PSU	9	1367	51	17,20,22	1.15	1 (5%)	21,28,33	1.90	4 (19%)
48	OMG	5	2364	48	23,26,27	2.34	8 (34%)	32,38,41	2.15	10 (31%)
51	OMG	9	644	51	23,26,27	2.37	7 (30%)	32,38,41	1.95	9 (28%)
51	PSU	9	814	51	17,20,22	1.08	1 (5%)	21,28,33	2.05	5 (23%)
48	5MC	5	3782	48,88	19,22,23	3.55	8 (42%)	26,32,35	1.14	2 (7%)
48	PSU	5	2508	48	17,20,22	1.07	1 (5%)	21,28,33	1.92	4 (19%)
51	OMG	9	1490	51,88	23,26,27	2.33	8 (34%)	32,38,41	2.22	8 (25%)
51	OMC	9	517	51	19,22,23	2.99	8 (42%)	25,31,34	0.82	0
48	PSU	5	3920	48	17,20,22	1.05	1 (5%)	21,28,33	2.18	5 (23%)
51	PSU	9	1238	51	17,20,22	1.22	2 (11%)	21,28,33	2.00	4 (19%)
48	OMG	5	1316	48	23,26,27	2.37	8 (34%)	32,38,41	2.17	10 (31%)
48	PSU	5	4442	48	17,20,22	1.09	1 (5%)	21,28,33	2.09	5 (23%)
51	PSU	9	34	51	17,20,22	1.16	1 (5%)	21,28,33	1.96	4 (19%)
51	OMG	9	509	51,88	23,26,27	2.40	7 (30%)	32,38,41	1.99	9 (28%)
48	OMC	5	3808	48	19,22,23	2.74	8 (42%)	25,31,34	0.65	0
48	PSU	5	4579	48	17,20,22	1.05	1 (5%)	21,28,33	1.89	4 (19%)
48	OMU	5	3925	48	19,22,23	2.81	7 (36%)	25,31,34	1.88	4 (16%)
48	OMC	5	3869	48	19,22,23	2.83	7 (36%)	25,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	4AC	9	1842	51	21,24,25	3.00	10 (47%)	28,34,37	1.08	2 (7%)
51	OMU	9	121	51	19,22,23	2.72	6 (31%)	25,31,34	1.90	6 (24%)
48	A2M	5	3785	48	22,25,26	3.33	10 (45%)	30,36,39	2.71	10 (33%)
48	OMC	5	4456	48	19,22,23	2.80	8 (42%)	25,31,34	0.77	0
51	OMU	9	428	51	19,22,23	2.87	7 (36%)	25,31,34	1.79	5 (20%)
51	PSU	9	1232	51	17,20,22	1.20	1 (5%)	21,28,33	1.93	3 (14%)
48	PSU	5	3639	48	17,20,22	1.16	1 (5%)	21,28,33	1.91	4 (19%)
48	OMG	5	4618	48	23,26,27	2.33	8 (34%)	32,38,41	2.12	11 (34%)
48	PSU	5	4423	48	17,20,22	1.00	1 (5%)	21,28,33	1.98	4 (19%)
51	PSU	9	1045	51	17,20,22	1.15	2 (11%)	21,28,33	2.14	5 (23%)
48	PSU	5	4353	48	17,20,22	1.12	2 (11%)	21,28,33	2.11	5 (23%)
48	PSU	5	2632	48	17,20,22	1.15	1 (5%)	21,28,33	1.97	4 (19%)
48	OMC	5	3701	48,88	19,22,23	2.76	8 (42%)	25,31,34	1.04	1 (4%)
48	OMC	5	2422	48,88	19,22,23	2.93	8 (42%)	25,31,34	0.72	0
48	PSU	5	1792	48	17,20,22	1.03	1 (5%)	21,28,33	1.89	3 (14%)
48	PSU	5	4521	48,88	17,20,22	1.24	2 (11%)	21,28,33	2.25	7 (33%)
51	PSU	9	1046	51	17,20,22	1.13	1 (5%)	21,28,33	1.92	5 (23%)
48	PSU	5	3851	48	17,20,22	1.09	2 (11%)	21,28,33	2.06	4 (19%)
51	OMG	9	1328	51	23,26,27	2.35	9 (39%)	32,38,41	2.08	9 (28%)
48	A2M	5	2815	48	22,25,26	3.44	9 (40%)	30,36,39	2.57	9 (30%)
48	PSU	5	3715	48	17,20,22	1.13	3 (17%)	21,28,33	2.10	6 (28%)
48	A2M	5	3830	48	22,25,26	3.42	9 (40%)	30,36,39	2.66	11 (36%)
48	OMG	5	4637	48	23,26,27	2.38	8 (34%)	32,38,41	2.14	10 (31%)
51	PSU	9	1692	51	17,20,22	1.14	1 (5%)	21,28,33	1.78	3 (14%)
48	OMG	5	4392	48	23,26,27	2.32	8 (34%)	32,38,41	2.14	9 (28%)
48	OMG	5	2424	48	23,26,27	2.35	8 (34%)	32,38,41	2.06	9 (28%)
48	OMC	5	2365	48	19,22,23	2.84	8 (42%)	25,31,34	0.67	0
48	PSU	5	4293	48	17,20,22	1.22	2 (11%)	21,28,33	1.88	4 (19%)
48	PSU	5	1860	48	17,20,22	1.03	1 (5%)	21,28,33	1.92	4 (19%)
48	UY1	5	3818	48,88	19,22,23	4.33	9 (47%)	21,31,34	2.11	5 (23%)
48	A2M	5	1326	48	22,25,26	3.50	9 (40%)	30,36,39	2.55	8 (26%)
48	OMC	5	2351	48	19,22,23	2.74	8 (42%)	25,31,34	0.82	0
48	OMU	5	4306	48	19,22,23	2.86	7 (36%)	25,31,34	1.85	4 (16%)
48	PSU	5	4403	48	17,20,22	1.10	1 (5%)	21,28,33	1.88	4 (19%)
48	OMC	5	1340	48	19,22,23	2.97	8 (42%)	25,31,34	1.01	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMG	5	4494	48	23,26,27	2.30	8 (34%)	32,38,41	2.03	10 (31%)
51	PSU	9	572	51	17,20,22	1.08	1 (5%)	21,28,33	1.95	4 (19%)
51	PSU	9	1081	51	17,20,22	1.14	1 (5%)	21,28,33	2.03	6 (28%)
51	B8N	9	1248	51	25,29,30	3.40	8 (32%)	28,42,45	2.31	7 (25%)
48	PSU	5	3764	48	17,20,22	1.18	1 (5%)	21,28,33	2.04	5 (23%)
48	OMG	5	4499	48	23,26,27	2.45	9 (39%)	32,38,41	2.05	9 (28%)
48	PSU	5	4420	48	17,20,22	1.13	1 (5%)	21,28,33	2.06	4 (19%)
48	OMC	5	4536	48	19,22,23	2.77	8 (42%)	25,31,34	0.86	0
48	PSU	5	4552	48	17,20,22	1.16	1 (5%)	21,28,33	1.93	4 (19%)
48	A2M	5	4523	48,88	22,25,26	3.48	9 (40%)	30,36,39	2.67	11 (36%)
48	PSU	5	3734	48	17,20,22	1.19	2 (11%)	21,28,33	1.93	5 (23%)
48	A2M	5	3825	48	22,25,26	3.48	9 (40%)	30,36,39	2.50	10 (33%)
48	A2M	5	1871	48,88	22,25,26	3.46	10 (45%)	30,36,39	2.50	10 (33%)
48	A2M	5	3718	48	22,25,26	3.55	10 (45%)	30,36,39	2.64	11 (36%)
48	OMC	5	3841	48	19,22,23	2.82	8 (42%)	25,31,34	0.90	0
51	OMU	9	172	51	19,22,23	2.85	7 (36%)	25,31,34	1.82	5 (20%)
51	A2M	9	1383	51	22,25,26	3.46	10 (45%)	30,36,39	2.69	11 (36%)
48	OMU	5	4498	48	19,22,23	2.81	8 (42%)	25,31,34	1.93	5 (20%)
48	PSU	5	3853	48	17,20,22	1.21	1 (5%)	21,28,33	2.19	5 (23%)
51	6MZ	9	1832	51,88	22,25,26	2.53	4 (18%)	29,36,39	2.22	10 (34%)
48	OMG	5	4370	48	23,26,27	2.36	8 (34%)	32,38,41	2.15	11 (34%)
48	OMC	5	2804	48	19,22,23	2.79	8 (42%)	25,31,34	0.72	0
48	UR3	5	4530	48	19,22,23	2.64	8 (42%)	26,32,35	1.50	4 (15%)
48	A2M	5	2787	48	22,25,26	3.42	9 (40%)	30,36,39	2.69	10 (33%)
48	PSU	5	1683	48,88	17,20,22	1.23	1 (5%)	21,28,33	2.02	4 (19%)
51	OMG	9	683	51	23,26,27	2.46	8 (34%)	32,38,41	2.21	11 (34%)
51	PSU	9	1347	51	17,20,22	1.08	1 (5%)	21,28,33	2.00	5 (23%)
51	A2M	9	159	51	22,25,26	3.56	9 (40%)	30,36,39	2.53	10 (33%)
51	A2M	9	27	51	22,25,26	3.43	9 (40%)	30,36,39	2.51	9 (30%)

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
48	PSU	5	1862	48	-	0/6/24/26	0/2/2/2
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
51	A2M	9	99	51,88	-	2/9/27/28	0/3/3/3
51	PSU	9	1177	51	-	0/6/24/26	0/2/2/2
48	5MC	5	4447	48,88	-	4/7/25/26	0/2/2/2
48	OMC	5	2824	48	-	0/9/27/28	0/2/2/2
51	OMC	9	174	51	-	0/9/27/28	0/2/2/2
51	PSU	9	863	51	-	2/6/24/26	0/2/2/2
48	OMG	5	4228	48	-	1/9/27/28	0/3/3/3
48	OMG	5	4623	48	-	0/9/27/28	0/3/3/3
51	A2M	9	1031	51	-	1/9/27/28	0/3/3/3
51	MA6	9	1851	51	-	3/11/29/30	0/3/3/3
51	A2M	9	668	51,88	-	3/9/27/28	0/3/3/3
48	1MA	5	1322	48,88	-	2/7/25/26	0/3/3/3
48	OMG	5	3899	48,88	-	0/9/27/28	0/3/3/3
48	OMG	5	1625	48,88	-	1/9/27/28	0/3/3/3
48	OMU	5	4227	48	-	0/9/27/28	0/2/2/2
48	A2M	5	398	48	-	0/9/27/28	0/3/3/3
48	PSU	5	4628	48	-	0/6/24/26	0/2/2/2
48	A2M	5	3760	48,88	-	3/9/27/28	0/3/3/3
51	PSU	9	801	51	-	2/6/24/26	0/2/2/2
48	PSU	5	4361	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1643	51	-	0/6/24/26	0/2/2/2
51	PSU	9	218	51	-	0/6/24/26	0/2/2/2
51	OMG	9	436	51	-	0/9/27/28	0/3/3/3
51	A2M	9	1678	51	-	0/9/27/28	0/3/3/3
51	MA6	9	1850	51	-	0/11/29/30	0/3/3/3
51	PSU	9	609	51	-	0/6/24/26	0/2/2/2
48	A2M	5	4571	48	-	0/9/27/28	0/3/3/3
48	6MZ	5	4220	48	-	0/9/27/28	0/3/3/3
48	A2M	5	3724	48	-	0/9/27/28	0/3/3/3
51	A2M	9	166	51	-	2/9/27/28	0/3/3/3
48	B9B	5	237	48	-	2/11/29/30	0/3/3/3
48	PSU	5	4457	48	-	0/6/24/26	0/2/2/2
48	A2M	5	2363	48,88	-	0/9/27/28	0/3/3/3
48	PSU	5	4500	48	-	2/6/24/26	0/2/2/2
48	PSU	5	1677	48	-	0/6/24/26	0/2/2/2
51	OMU	9	116	51	-	0/9/27/28	0/2/2/2
48	A2M	5	1524	48	-	1/9/27/28	0/3/3/3
48	PSU	5	4532	48	-	0/6/24/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PSU	9	822	51	-	2/6/24/26	0/2/2/2
48	OMU	5	4620	48	-	0/9/27/28	0/2/2/2
51	PSU	9	119	51	-	0/6/24/26	0/2/2/2
48	OMG	5	1522	48	-	0/9/27/28	0/3/3/3
48	OMC	5	3887	48	-	0/9/27/28	0/2/2/2
48	PSU	5	1782	48	-	0/6/24/26	0/2/2/2
48	OMU	5	2837	48	-	1/9/27/28	0/2/2/2
51	A2M	9	468	51	-	1/9/27/28	0/3/3/3
51	PSU	9	815	51	-	0/6/24/26	0/2/2/2
48	PSU	5	1781	48	-	2/6/24/26	0/2/2/2
51	PSU	9	1004	51	-	0/6/24/26	0/2/2/2
51	OMU	9	1326	51	-	0/9/27/28	0/2/2/2
48	PSU	5	3695	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1244	51	-	0/6/24/26	0/2/2/2
48	OMG	5	373	48	-	1/9/27/28	0/3/3/3
51	PSU	9	109	51	-	0/6/24/26	0/2/2/2
48	A2M	5	400	48	-	0/9/27/28	0/3/3/3
48	A2M	5	1534	48,88	-	2/9/27/28	0/3/3/3
48	PSU	5	3762	48	-	0/6/24/26	0/2/2/2
48	PSU	5	1744	48,88	-	0/6/24/26	0/2/2/2
48	OMG	5	3627	48	-	0/9/27/28	0/3/3/3
51	PSU	9	649	51	-	0/6/24/26	0/2/2/2
51	PSU	9	686	51	-	0/6/24/26	0/2/2/2
48	OMG	5	3792	48	-	2/9/27/28	0/3/3/3
51	A2M	9	512	51	-	1/9/27/28	0/3/3/3
48	PSU	5	4299	48	-	0/6/24/26	0/2/2/2
50	OMG	8	75	50	-	0/9/27/28	0/3/3/3
48	PSU	5	4296	48	-	0/6/24/26	0/2/2/2
51	G7M	9	1639	46,51	-	2/7/25/26	0/3/3/3
48	OMG	5	4196	46,48	-	0/9/27/28	0/3/3/3
48	2MG	5	1517	48	-	0/9/27/28	0/3/3/3
51	PSU	9	105	51	-	0/6/24/26	0/2/2/2
51	A2M	9	484	51	-	0/9/27/28	0/3/3/3
51	OMU	9	1442	51	-	2/9/27/28	0/2/2/2
48	A2M	5	3867	48	-	1/9/27/28	0/3/3/3
48	OMG	5	2876	48	-	0/9/27/28	0/3/3/3
48	OMC	5	2861	48	-	0/9/27/28	0/2/2/2
51	PSU	9	1445	51	-	1/6/24/26	0/2/2/2
51	OMC	9	1391	51	-	0/9/27/28	0/2/2/2
51	PSU	9	1174	51	-	0/6/24/26	0/2/2/2
51	OMC	9	1703	51	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PSU	9	1367	51	-	0/6/24/26	0/2/2/2
48	OMG	5	2364	48	-	3/9/27/28	0/3/3/3
51	OMG	9	644	51	-	1/9/27/28	0/3/3/3
51	PSU	9	814	51	-	0/6/24/26	0/2/2/2
48	5MC	5	3782	48,88	-	0/7/25/26	0/2/2/2
48	PSU	5	2508	48	-	0/6/24/26	0/2/2/2
51	OMG	9	1490	51,88	-	2/9/27/28	0/3/3/3
51	OMC	9	517	51	-	0/9/27/28	0/2/2/2
48	PSU	5	3920	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1238	51	-	0/6/24/26	0/2/2/2
48	OMG	5	1316	48	-	0/9/27/28	0/3/3/3
48	PSU	5	4442	48	-	0/6/24/26	0/2/2/2
51	PSU	9	34	51	-	4/6/24/26	0/2/2/2
51	OMG	9	509	51,88	-	0/9/27/28	0/3/3/3
48	OMC	5	3808	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4579	48	-	0/6/24/26	0/2/2/2
48	OMU	5	3925	48	-	0/9/27/28	0/2/2/2
48	OMC	5	3869	48	-	0/9/27/28	0/2/2/2
51	4AC	9	1842	51	-	0/11/29/30	0/2/2/2
51	OMU	9	121	51	-	1/9/27/28	0/2/2/2
48	A2M	5	3785	48	-	3/9/27/28	0/3/3/3
48	OMC	5	4456	48	-	0/9/27/28	0/2/2/2
51	OMU	9	428	51	-	4/9/27/28	0/2/2/2
51	PSU	9	1232	51	-	0/6/24/26	0/2/2/2
48	PSU	5	3639	48	-	0/6/24/26	0/2/2/2
48	OMG	5	4618	48	-	0/9/27/28	0/3/3/3
48	PSU	5	4423	48	-	0/6/24/26	0/2/2/2
51	PSU	9	1045	51	-	2/6/24/26	0/2/2/2
48	PSU	5	4353	48	-	0/6/24/26	0/2/2/2
48	PSU	5	2632	48	-	0/6/24/26	0/2/2/2
48	OMC	5	3701	48,88	-	4/9/27/28	0/2/2/2
48	OMC	5	2422	48,88	-	0/9/27/28	0/2/2/2
48	PSU	5	1792	48	-	0/6/24/26	0/2/2/2
48	PSU	5	4521	48,88	-	0/6/24/26	0/2/2/2
51	PSU	9	1046	51	-	0/6/24/26	0/2/2/2
48	PSU	5	3851	48	-	1/6/24/26	0/2/2/2
51	OMG	9	1328	51	-	1/9/27/28	0/3/3/3
48	A2M	5	2815	48	-	2/9/27/28	0/3/3/3
48	PSU	5	3715	48	-	0/6/24/26	0/2/2/2
48	A2M	5	3830	48	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMG	5	4637	48	-	0/9/27/28	0/3/3/3
51	PSU	9	1692	51	-	0/6/24/26	0/2/2/2
48	OMG	5	4392	48	-	0/9/27/28	0/3/3/3
48	OMG	5	2424	48	-	3/9/27/28	0/3/3/3
48	OMC	5	2365	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4293	48	-	0/6/24/26	0/2/2/2
48	PSU	5	1860	48	-	0/6/24/26	0/2/2/2
48	UY1	5	3818	48,88	-	3/9/27/28	0/2/2/2
48	A2M	5	1326	48	-	1/9/27/28	0/3/3/3
48	OMC	5	2351	48	-	1/9/27/28	0/2/2/2
48	OMU	5	4306	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4403	48	-	0/6/24/26	0/2/2/2
48	OMC	5	1340	48	-	0/9/27/28	0/2/2/2
48	OMG	5	4494	48	-	1/9/27/28	0/3/3/3
51	PSU	9	572	51	-	0/6/24/26	0/2/2/2
51	PSU	9	1081	51	-	0/6/24/26	0/2/2/2
51	B8N	9	1248	51	-	4/16/34/35	0/2/2/2
48	PSU	5	3764	48	-	0/6/24/26	0/2/2/2
48	OMG	5	4499	48	-	1/9/27/28	0/3/3/3
48	PSU	5	4420	48	-	0/6/24/26	0/2/2/2
48	OMC	5	4536	48	-	0/9/27/28	0/2/2/2
48	PSU	5	4552	48	-	0/6/24/26	0/2/2/2
48	A2M	5	4523	48,88	-	0/9/27/28	0/3/3/3
48	PSU	5	3734	48	-	0/6/24/26	0/2/2/2
48	A2M	5	3825	48	-	0/9/27/28	0/3/3/3
48	A2M	5	1871	48,88	-	0/9/27/28	0/3/3/3
48	A2M	5	3718	48	-	0/9/27/28	0/3/3/3
48	OMC	5	3841	48	-	0/9/27/28	0/2/2/2
51	OMU	9	172	51	-	2/9/27/28	0/2/2/2
51	A2M	9	1383	51	-	0/9/27/28	0/3/3/3
48	OMU	5	4498	48	-	0/9/27/28	0/2/2/2
48	PSU	5	3853	48	-	0/6/24/26	0/2/2/2
51	6MZ	9	1832	51,88	-	2/9/27/28	0/3/3/3
48	OMG	5	4370	48	-	0/9/27/28	0/3/3/3
48	OMC	5	2804	48	-	0/9/27/28	0/2/2/2
48	UR3	5	4530	48	-	0/7/25/26	0/2/2/2
48	A2M	5	2787	48	-	3/9/27/28	0/3/3/3
48	PSU	5	1683	48,88	-	0/6/24/26	0/2/2/2
51	OMG	9	683	51	-	3/9/27/28	0/3/3/3
51	PSU	9	1347	51	-	0/6/24/26	0/2/2/2
51	A2M	9	159	51	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A2M	9	27	51	-	0/9/27/28	0/3/3/3

All (881) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3818	UY1	C6-C5	11.34	1.47	1.35
48	5	4220	6MZ	C6-N6	11.33	1.47	1.34
51	9	1832	6MZ	C6-N6	10.55	1.46	1.34
48	5	3818	UY1	C2-N1	9.65	1.49	1.36
51	9	159	A2M	C2'-C1'	-9.32	1.30	1.53
51	9	468	A2M	C2'-C1'	-9.28	1.30	1.53
48	5	3782	5MC	C6-C5	9.13	1.49	1.34
48	5	3724	A2M	C2'-C1'	-9.12	1.30	1.53
48	5	2363	A2M	C2'-C1'	-9.12	1.30	1.53
48	5	4571	A2M	C2'-C1'	-9.08	1.30	1.53
51	9	1031	A2M	C2'-C1'	-9.07	1.30	1.53
51	9	512	A2M	C2'-C1'	-9.06	1.30	1.53
48	5	3718	A2M	C2'-C1'	-9.04	1.30	1.53
48	5	1326	A2M	C2'-C1'	-9.00	1.30	1.53
48	5	398	A2M	C2'-C1'	-8.98	1.31	1.53
51	9	99	A2M	C2'-C1'	-8.98	1.31	1.53
51	9	1383	A2M	O4'-C1'	8.97	1.62	1.42
48	5	1534	A2M	C2'-C1'	-8.94	1.31	1.53
48	5	3724	A2M	O4'-C1'	8.94	1.62	1.42
51	9	166	A2M	C2'-C1'	-8.93	1.31	1.53
51	9	99	A2M	O4'-C1'	8.92	1.62	1.42
48	5	398	A2M	O4'-C1'	8.92	1.62	1.42
48	5	3825	A2M	C2'-C1'	-8.90	1.31	1.53
48	5	4523	A2M	C2'-C1'	-8.88	1.31	1.53
51	9	159	A2M	O4'-C1'	8.88	1.62	1.42
48	5	3718	A2M	O4'-C1'	8.88	1.62	1.42
51	9	484	A2M	O4'-C1'	8.87	1.62	1.42
48	5	3760	A2M	C2'-C1'	-8.85	1.31	1.53
48	5	3867	A2M	C2'-C1'	-8.84	1.31	1.53
48	5	3760	A2M	O4'-C1'	8.83	1.62	1.42
48	5	2815	A2M	C2'-C1'	-8.76	1.31	1.53
51	9	484	A2M	C2'-C1'	-8.76	1.31	1.53
51	9	1383	A2M	C2'-C1'	-8.75	1.31	1.53
48	5	4571	A2M	O4'-C1'	8.74	1.62	1.42
51	9	468	A2M	O4'-C1'	8.73	1.62	1.42
48	5	4447	5MC	C6-C5	8.73	1.48	1.34
51	9	27	A2M	C2'-C1'	-8.72	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1031	A2M	O4'-C1'	8.72	1.62	1.42
51	9	512	A2M	O4'-C1'	8.71	1.62	1.42
48	5	1534	A2M	O4'-C1'	8.70	1.62	1.42
48	5	3785	A2M	C2'-C1'	-8.69	1.31	1.53
48	5	3825	A2M	O4'-C1'	8.69	1.62	1.42
48	5	3830	A2M	C2'-C1'	-8.67	1.31	1.53
48	5	2363	A2M	O4'-C1'	8.66	1.62	1.42
48	5	1871	A2M	C2'-C1'	-8.65	1.31	1.53
51	9	1678	A2M	O4'-C1'	8.62	1.61	1.42
48	5	1524	A2M	C2'-C1'	-8.58	1.32	1.53
51	9	1678	A2M	C2'-C1'	-8.58	1.32	1.53
48	5	2787	A2M	C2'-C1'	-8.56	1.32	1.53
48	5	400	A2M	C2'-C1'	-8.50	1.32	1.53
51	9	27	A2M	O4'-C1'	8.48	1.61	1.42
51	9	166	A2M	O4'-C1'	8.48	1.61	1.42
48	5	400	A2M	O4'-C1'	8.47	1.61	1.42
48	5	2815	A2M	O4'-C1'	8.43	1.61	1.42
48	5	1326	A2M	O4'-C1'	8.43	1.61	1.42
48	5	2787	A2M	O4'-C1'	8.41	1.61	1.42
48	5	4523	A2M	O4'-C1'	8.40	1.61	1.42
51	9	668	A2M	O4'-C1'	8.40	1.61	1.42
48	5	3830	A2M	O4'-C1'	8.39	1.61	1.42
48	5	3867	A2M	O4'-C1'	8.34	1.61	1.42
48	5	1871	A2M	O4'-C1'	8.33	1.61	1.42
51	9	668	A2M	C2'-C1'	-8.27	1.32	1.53
48	5	1524	A2M	O4'-C1'	8.18	1.60	1.42
48	5	3785	A2M	O4'-C1'	8.09	1.60	1.42
51	9	1248	B8N	C4-C5	8.03	1.65	1.47
48	5	1322	1MA	C2-N3	7.54	1.44	1.30
51	9	1248	B8N	C6-N1	7.54	1.54	1.36
51	9	1248	B8N	C4-N3	-7.46	1.27	1.40
51	9	1442	OMU	C2-N1	7.14	1.49	1.38
51	9	668	A2M	O4'-C4'	-7.11	1.29	1.45
48	5	2837	OMU	C2-N1	7.10	1.49	1.38
48	5	4530	UR3	C2-N1	7.04	1.48	1.38
48	5	3818	UY1	C2-N3	7.00	1.49	1.37
48	5	1524	A2M	O4'-C4'	-6.87	1.29	1.45
48	5	4620	OMU	C2-N1	6.84	1.49	1.38
48	5	4571	A2M	O4'-C4'	-6.83	1.29	1.45
48	5	1534	A2M	O4'-C4'	-6.78	1.29	1.45
51	9	428	OMU	C2-N1	6.74	1.49	1.38
48	5	4499	OMG	C4-N3	6.71	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	509	OMG	C4-N3	6.66	1.49	1.34
51	9	683	OMG	C4-N3	6.66	1.49	1.34
51	9	428	OMU	C2-N3	6.66	1.49	1.38
48	5	3867	A2M	O4'-C4'	-6.65	1.30	1.45
51	9	436	OMG	C4-N3	6.64	1.49	1.34
51	9	116	OMU	C2-N1	6.64	1.48	1.38
48	5	3925	OMU	C2-N1	6.63	1.48	1.38
51	9	1391	OMC	C2-N3	6.60	1.49	1.36
48	5	4306	OMU	C2-N1	6.60	1.48	1.38
48	5	2876	OMG	C4-N3	6.59	1.49	1.34
48	5	1517	2MG	C2-N3	6.59	1.44	1.32
48	5	4227	OMU	C2-N1	6.58	1.48	1.38
51	9	1248	B8N	C2-N1	6.57	1.58	1.39
48	5	4623	OMG	C4-N3	6.56	1.49	1.34
48	5	4637	OMG	C4-N3	6.55	1.49	1.34
48	5	400	A2M	O4'-C4'	-6.52	1.30	1.45
48	5	2815	A2M	O4'-C4'	-6.52	1.30	1.45
51	9	172	OMU	C2-N3	6.51	1.49	1.38
51	9	1639	G7M	C2-N2	6.50	1.49	1.34
48	5	1625	OMG	C4-N3	6.50	1.49	1.34
48	5	4196	OMG	C4-N3	6.50	1.49	1.34
48	5	2363	A2M	O4'-C4'	-6.49	1.30	1.45
48	5	1340	OMC	C2-N3	6.45	1.49	1.36
48	5	1326	A2M	O4'-C4'	-6.44	1.30	1.45
48	5	1871	A2M	O4'-C4'	-6.44	1.30	1.45
48	5	3760	A2M	O4'-C4'	-6.44	1.30	1.45
51	9	159	A2M	O4'-C4'	-6.43	1.30	1.45
48	5	3899	OMG	C4-N3	6.43	1.49	1.34
51	9	517	OMC	C2-N3	6.43	1.49	1.36
51	9	1031	A2M	O4'-C4'	-6.43	1.30	1.45
48	5	373	OMG	C4-N3	6.43	1.49	1.34
51	9	27	A2M	O4'-C4'	-6.40	1.30	1.45
48	5	3782	5MC	C5-C4	6.40	1.49	1.44
51	9	484	A2M	O4'-C4'	-6.39	1.30	1.45
51	9	172	OMU	C2-N1	6.38	1.48	1.38
48	5	3718	A2M	O4'-C4'	-6.38	1.30	1.45
51	9	644	OMG	C4-N3	6.37	1.48	1.34
48	5	2422	OMC	C2-N3	6.35	1.49	1.36
48	5	3887	OMC	C2-N3	6.35	1.48	1.36
51	9	468	A2M	O4'-C4'	-6.34	1.30	1.45
48	5	4498	OMU	C2-N1	6.34	1.48	1.38
51	9	1639	G7M	C4-N3	6.34	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4370	OMG	C4-N3	6.34	1.48	1.34
51	9	1326	OMU	C2-N1	6.33	1.48	1.38
48	5	398	A2M	O4'-C4'	-6.33	1.30	1.45
48	5	2787	A2M	O4'-C4'	-6.32	1.30	1.45
51	9	1337	4AC	C6-C5	6.31	1.49	1.35
48	5	1522	OMG	C4-N3	6.31	1.48	1.34
51	9	1703	OMC	C2-N3	6.31	1.48	1.36
48	5	4523	A2M	O4'-C4'	-6.31	1.31	1.45
51	9	121	OMU	C2-N1	6.29	1.48	1.38
48	5	3627	OMG	C4-N3	6.28	1.48	1.34
51	9	517	OMC	C6-C5	6.27	1.49	1.35
48	5	4228	OMG	C4-N3	6.27	1.48	1.34
48	5	2861	OMC	C2-N3	6.24	1.48	1.36
48	5	3830	A2M	O4'-C4'	-6.23	1.31	1.45
51	9	1328	OMG	C4-N3	6.23	1.48	1.34
51	9	1442	OMU	C2-N3	6.23	1.48	1.38
51	9	99	A2M	O4'-C4'	-6.20	1.31	1.45
48	5	2364	OMG	C4-N3	6.19	1.48	1.34
48	5	3792	OMG	C4-N3	6.19	1.48	1.34
51	9	512	A2M	O4'-C4'	-6.18	1.31	1.45
48	5	3825	A2M	O4'-C4'	-6.16	1.31	1.45
51	9	116	OMU	C2-N3	6.16	1.48	1.38
51	9	1678	A2M	O4'-C4'	-6.15	1.31	1.45
48	5	1316	OMG	C4-N3	6.15	1.48	1.34
48	5	4447	5MC	C4-N3	6.15	1.44	1.34
51	9	166	A2M	O4'-C4'	-6.14	1.31	1.45
51	9	1326	OMU	C2-N3	6.14	1.48	1.38
48	5	1340	OMC	C6-C5	6.14	1.49	1.35
51	9	121	OMU	C2-N3	6.14	1.48	1.38
48	5	2837	OMU	C2-N3	6.13	1.48	1.38
48	5	1322	1MA	C4-N3	6.13	1.48	1.35
48	5	3724	A2M	O4'-C4'	-6.11	1.31	1.45
48	5	2424	OMG	C4-N3	6.11	1.48	1.34
48	5	4498	OMU	C2-N3	6.10	1.48	1.38
48	5	4620	OMU	C2-N3	6.10	1.48	1.38
48	5	3785	A2M	O4'-C4'	-6.08	1.31	1.45
51	9	1490	OMG	C4-N3	6.07	1.48	1.34
51	9	174	OMC	C2-N3	6.06	1.48	1.36
48	5	4618	OMG	C4-N3	6.05	1.48	1.34
51	9	1383	A2M	O4'-C4'	-6.05	1.31	1.45
48	5	4392	OMG	C4-N3	6.04	1.48	1.34
50	8	75	OMG	C4-N3	6.04	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	174	OMC	C6-C5	6.04	1.49	1.35
48	5	2804	OMC	C2-N3	6.04	1.48	1.36
51	9	1391	OMC	C6-C5	6.03	1.49	1.35
48	5	4227	OMU	C2-N3	6.03	1.48	1.38
48	5	4536	OMC	C6-C5	6.01	1.49	1.35
48	5	2365	OMC	C2-N3	6.01	1.48	1.36
48	5	3925	OMU	C2-N3	6.01	1.48	1.38
48	5	3841	OMC	C2-N3	6.00	1.48	1.36
51	9	1337	4AC	C4-N3	5.97	1.42	1.32
51	9	1842	4AC	C4-N3	5.95	1.42	1.32
48	5	3869	OMC	C6-C5	5.94	1.48	1.35
48	5	4494	OMG	C4-N3	5.93	1.47	1.34
48	5	3841	OMC	C6-C5	5.92	1.48	1.35
48	5	4306	OMU	C6-C5	5.91	1.48	1.35
51	9	1703	OMC	C6-C5	5.90	1.48	1.35
48	5	2365	OMC	C6-C5	5.88	1.48	1.35
48	5	2861	OMC	C6-C5	5.88	1.48	1.35
48	5	4306	OMU	C2-N3	5.88	1.48	1.38
51	9	172	OMU	C6-C5	5.87	1.48	1.35
48	5	4456	OMC	C2-N3	5.87	1.48	1.36
48	5	2824	OMC	C2-N3	5.85	1.48	1.36
51	9	1842	4AC	C6-C5	5.84	1.48	1.35
48	5	2422	OMC	C6-C5	5.84	1.48	1.35
48	5	2351	OMC	C6-C5	5.80	1.48	1.35
48	5	3701	OMC	C6-C5	5.79	1.48	1.35
51	9	116	OMU	C6-C5	5.78	1.48	1.35
48	5	2824	OMC	C6-C5	5.77	1.48	1.35
48	5	4447	5MC	C2-N3	5.75	1.47	1.36
51	9	1326	OMU	C6-C5	5.74	1.48	1.35
48	5	3869	OMC	C2-N3	5.73	1.47	1.36
51	9	1248	B8N	C6-C5	5.70	1.43	1.35
48	5	3808	OMC	C2-N3	5.69	1.47	1.36
51	9	436	OMG	C2-N3	5.67	1.46	1.33
48	5	2804	OMC	C6-C5	5.66	1.48	1.35
48	5	4536	OMC	C2-N3	5.66	1.47	1.36
48	5	4456	OMC	C6-C5	5.65	1.48	1.35
48	5	4498	OMU	C6-C5	5.64	1.48	1.35
48	5	4227	OMU	C6-C5	5.64	1.48	1.35
48	5	3925	OMU	C6-C5	5.64	1.48	1.35
48	5	4620	OMU	C6-C5	5.62	1.48	1.35
48	5	3808	OMC	C6-C5	5.57	1.48	1.35
51	9	683	OMG	C2-N3	5.55	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3701	OMC	C2-N3	5.54	1.47	1.36
48	5	4530	UR3	C6-C5	5.52	1.47	1.35
51	9	428	OMU	C6-C5	5.52	1.47	1.35
48	5	2351	OMC	C2-N3	5.51	1.47	1.36
48	5	4196	OMG	C2-N3	5.49	1.46	1.33
51	9	1442	OMU	C6-C5	5.48	1.47	1.35
48	5	1625	OMG	C2-N3	5.44	1.46	1.33
48	5	237	B9B	C2-N2	5.40	1.44	1.33
48	5	4499	OMG	C2-N3	5.39	1.46	1.33
48	5	4447	5MC	C5-C4	5.38	1.48	1.44
48	5	3782	5MC	C4-N3	5.36	1.42	1.34
48	5	3887	OMC	C6-C5	5.35	1.47	1.35
48	5	3818	UY1	C1'-C5	-5.35	1.38	1.50
51	9	509	OMG	C2-N3	5.34	1.46	1.33
48	5	4623	OMG	C2-N3	5.31	1.46	1.33
48	5	2837	OMU	C6-C5	5.31	1.47	1.35
51	9	1337	4AC	C2-N3	5.29	1.46	1.36
51	9	1328	OMG	C2-N3	5.27	1.46	1.33
51	9	121	OMU	C6-C5	5.25	1.47	1.35
51	9	1639	G7M	C2-N3	5.20	1.45	1.33
48	5	3782	5MC	C2-N3	5.18	1.46	1.36
48	5	373	OMG	C2-N3	5.18	1.45	1.33
48	5	4637	OMG	C2-N3	5.15	1.45	1.33
48	5	2876	OMG	C2-N3	5.15	1.45	1.33
48	5	3627	OMG	C2-N3	5.10	1.45	1.33
48	5	4370	OMG	C2-N3	5.09	1.45	1.33
48	5	2364	OMG	C2-N3	5.08	1.45	1.33
51	9	644	OMG	C2-N3	5.08	1.45	1.33
51	9	1842	4AC	C2-N3	5.07	1.46	1.36
48	5	1517	2MG	C2-N2	5.07	1.44	1.33
48	5	2424	OMG	C2-N3	5.06	1.45	1.33
48	5	3899	OMG	C2-N3	5.05	1.45	1.33
48	5	1316	OMG	C2-N3	5.03	1.45	1.33
48	5	4392	OMG	C2-N3	5.02	1.45	1.33
50	8	75	OMG	C2-N3	5.01	1.45	1.33
48	5	3792	OMG	C2-N3	4.99	1.45	1.33
48	5	1340	OMC	C4-N4	4.97	1.45	1.33
51	9	1391	OMC	C4-N4	4.89	1.45	1.33
48	5	4618	OMG	C2-N3	4.89	1.45	1.33
48	5	1522	OMG	C2-N3	4.89	1.45	1.33
48	5	4494	OMG	C2-N3	4.88	1.45	1.33
48	5	1517	2MG	C4-N3	4.88	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1703	OMC	C2-N1	4.87	1.50	1.40
51	9	1337	4AC	C4-N4	4.84	1.47	1.39
51	9	1703	OMC	C4-N3	4.81	1.44	1.34
51	9	517	OMC	C4-N3	4.76	1.44	1.34
48	5	3887	OMC	C4-N3	4.73	1.43	1.34
51	9	174	OMC	C4-N3	4.71	1.43	1.34
48	5	4228	OMG	C2-N3	4.69	1.44	1.33
48	5	3818	UY1	C6-N1	4.67	1.44	1.36
48	5	2422	OMC	C4-N3	4.67	1.43	1.34
48	5	1625	OMG	C2-N2	4.64	1.45	1.34
51	9	1490	OMG	C2-N3	4.63	1.44	1.33
48	5	2861	OMC	C4-N3	4.62	1.43	1.34
51	9	166	A2M	C6-N6	4.61	1.46	1.34
51	9	1703	OMC	C4-N4	4.55	1.44	1.33
48	5	3869	OMC	C4-N4	4.53	1.44	1.33
48	5	2365	OMC	C4-N3	4.52	1.43	1.34
51	9	644	OMG	C2-N2	4.51	1.44	1.34
48	5	4196	OMG	C2-N2	4.50	1.44	1.34
48	5	3869	OMC	C4-N3	4.50	1.43	1.34
51	9	1639	G7M	C5-N7	-4.49	1.34	1.39
51	9	517	OMC	C4-N4	4.49	1.44	1.33
48	5	4456	OMC	C4-N3	4.48	1.43	1.34
48	5	2861	OMC	C2-N1	4.46	1.49	1.40
48	5	4456	OMC	C4-N4	4.46	1.44	1.33
48	5	2824	OMC	C4-N4	4.45	1.44	1.33
51	9	174	OMC	C4-N4	4.45	1.44	1.33
48	5	2422	OMC	C2-N1	4.44	1.49	1.40
48	5	4499	OMG	C2-N2	4.44	1.44	1.34
51	9	683	OMG	C2-N2	4.44	1.44	1.34
48	5	2861	OMC	C4-N4	4.44	1.44	1.33
51	9	1391	OMC	C4-N3	4.43	1.43	1.34
51	9	436	OMG	C2-N2	4.43	1.44	1.34
48	5	2365	OMC	C4-N4	4.42	1.44	1.33
48	5	4571	A2M	C6-N6	4.42	1.45	1.34
48	5	4623	OMG	C2-N2	4.42	1.44	1.34
51	9	517	OMC	C2-N1	4.41	1.49	1.40
48	5	4530	UR3	C2-N3	4.41	1.47	1.39
51	9	1678	A2M	C6-N6	4.40	1.45	1.34
48	5	2422	OMC	C4-N4	4.38	1.44	1.33
48	5	3825	A2M	C6-N6	4.38	1.45	1.34
48	5	2424	OMG	C2-N2	4.38	1.44	1.34
51	9	1842	4AC	C7-N4	4.37	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1490	OMG	C2-N2	4.37	1.44	1.34
48	5	3887	OMC	C4-N4	4.37	1.44	1.33
48	5	3701	OMC	C4-N3	4.36	1.43	1.34
48	5	3841	OMC	C4-N4	4.34	1.44	1.33
48	5	1340	OMC	C4-N3	4.34	1.43	1.34
50	8	75	OMG	C2-N2	4.34	1.44	1.34
48	5	2364	OMG	C2-N2	4.34	1.44	1.34
48	5	4447	5MC	C6-N1	4.34	1.45	1.38
48	5	373	OMG	C2-N2	4.32	1.44	1.34
51	9	509	OMG	C2-N2	4.32	1.44	1.34
51	9	1328	OMG	C2-N2	4.30	1.44	1.34
51	9	174	OMC	C2-N1	4.29	1.49	1.40
48	5	4370	OMG	C2-N2	4.29	1.44	1.34
48	5	2824	OMC	C2-N1	4.28	1.49	1.40
48	5	2804	OMC	C4-N4	4.28	1.44	1.33
48	5	398	A2M	C6-N6	4.27	1.45	1.34
48	5	3899	OMG	C2-N2	4.27	1.44	1.34
51	9	1391	OMC	C2-N1	4.27	1.49	1.40
48	5	3808	OMC	C2-N1	4.27	1.49	1.40
51	9	468	A2M	C6-N6	4.27	1.45	1.34
48	5	4536	OMC	C4-N4	4.26	1.44	1.33
48	5	2351	OMC	C4-N3	4.25	1.43	1.34
48	5	3841	OMC	C4-N3	4.24	1.42	1.34
48	5	4228	OMG	C2-N2	4.23	1.44	1.34
48	5	3701	OMC	C2-N1	4.23	1.48	1.40
48	5	3627	OMG	C2-N2	4.21	1.44	1.34
48	5	4618	OMG	C2-N2	4.20	1.44	1.34
48	5	2804	OMC	C4-N3	4.20	1.42	1.34
48	5	3724	A2M	C6-N6	4.20	1.44	1.34
48	5	2824	OMC	C4-N3	4.19	1.42	1.34
51	9	512	A2M	C6-N6	4.19	1.44	1.34
48	5	3808	OMC	C4-N3	4.18	1.42	1.34
48	5	3792	OMG	C2-N2	4.18	1.44	1.34
48	5	3782	5MC	C6-N1	4.17	1.45	1.38
48	5	4494	OMG	C2-N2	4.17	1.43	1.34
51	9	484	A2M	C6-N6	4.17	1.44	1.34
51	9	668	A2M	C6-N6	4.16	1.44	1.34
51	9	159	A2M	C6-N6	4.16	1.44	1.34
48	5	3760	A2M	C6-N6	4.16	1.44	1.34
48	5	3808	OMC	C4-N4	4.15	1.44	1.33
51	9	27	A2M	C6-N6	4.14	1.44	1.34
51	9	1842	4AC	C4-N4	4.11	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1524	A2M	C6-N6	4.10	1.44	1.34
51	9	1337	4AC	C7-N4	4.08	1.45	1.37
48	5	1522	OMG	C2-N2	4.08	1.43	1.34
48	5	2876	OMG	C2-N2	4.08	1.43	1.34
48	5	2351	OMC	C2-N1	4.07	1.48	1.40
48	5	3867	A2M	C6-N6	4.05	1.44	1.34
48	5	2351	OMC	C4-N4	4.05	1.43	1.33
48	5	3701	OMC	C4-N4	4.05	1.43	1.33
51	9	1383	A2M	C6-N6	4.04	1.44	1.34
48	5	4536	OMC	C2-N1	4.03	1.48	1.40
48	5	2787	A2M	C6-N6	4.02	1.44	1.34
48	5	4536	OMC	C4-N3	4.01	1.42	1.34
48	5	2804	OMC	C2-N1	4.01	1.48	1.40
48	5	1871	A2M	C6-N6	4.01	1.44	1.34
48	5	1316	OMG	C2-N2	4.01	1.43	1.34
48	5	1534	A2M	C6-N6	4.00	1.44	1.34
48	5	4447	5MC	C4-N4	3.99	1.44	1.34
48	5	3782	5MC	C4-N4	3.98	1.44	1.34
51	9	1031	A2M	C6-N6	3.98	1.44	1.34
48	5	4523	A2M	C6-N6	3.98	1.44	1.34
48	5	1340	OMC	C2-N1	3.97	1.48	1.40
48	5	400	A2M	C6-N6	3.97	1.44	1.34
48	5	4637	OMG	C2-N2	3.96	1.43	1.34
48	5	2363	A2M	C6-N6	3.94	1.44	1.34
48	5	3841	OMC	C2-N1	3.94	1.48	1.40
51	9	99	A2M	C6-N6	3.93	1.44	1.34
48	5	1326	A2M	C6-N6	3.93	1.44	1.34
48	5	2815	A2M	C6-N6	3.92	1.44	1.34
51	9	1842	4AC	C2-N1	3.92	1.48	1.40
48	5	3718	A2M	C6-N6	3.90	1.44	1.34
48	5	3785	A2M	C6-N6	3.88	1.44	1.34
51	9	1639	G7M	C5-C6	3.86	1.54	1.43
48	5	1322	1MA	C5-C6	3.85	1.54	1.43
48	5	4293	PSU	C6-C5	3.85	1.39	1.35
48	5	3734	PSU	C6-C5	3.85	1.39	1.35
48	5	2365	OMC	C2-N1	3.82	1.48	1.40
48	5	1517	2MG	C2-N1	3.82	1.42	1.36
48	5	3869	OMC	C2-N1	3.80	1.48	1.40
48	5	4392	OMG	C5-N7	-3.80	1.31	1.39
48	5	3887	OMC	C2-N1	3.80	1.48	1.40
48	5	4456	OMC	C2-N1	3.79	1.48	1.40
48	5	2876	OMG	C5-N7	-3.79	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1248	B8N	O4-C4	-3.76	1.15	1.23
48	5	4392	OMG	C2-N2	3.76	1.43	1.34
48	5	4306	OMU	O2-C2	-3.76	1.16	1.23
48	5	3830	A2M	C6-N6	3.75	1.43	1.34
48	5	373	OMG	C5-N7	-3.75	1.31	1.39
48	5	4637	OMG	C5-N7	-3.74	1.31	1.39
51	9	801	PSU	C6-C5	3.73	1.39	1.35
48	5	4447	5MC	C2-N1	3.72	1.47	1.40
48	5	1683	PSU	C6-C5	3.71	1.39	1.35
48	5	3782	5MC	C2-N1	3.70	1.47	1.40
51	9	484	A2M	C5-C4	-3.69	1.32	1.39
48	5	3899	OMG	C5-N7	-3.68	1.31	1.39
48	5	237	B9B	O6-C6	3.66	1.40	1.34
51	9	436	OMG	C5-N7	-3.66	1.31	1.39
51	9	99	A2M	C5-C4	-3.65	1.32	1.39
51	9	1337	4AC	C5-C4	3.65	1.49	1.41
51	9	1842	4AC	C5-C4	3.64	1.49	1.41
48	5	4456	OMC	O2-C2	-3.64	1.16	1.23
48	5	2824	OMC	O2-C2	-3.64	1.16	1.23
48	5	4420	PSU	C6-C5	3.63	1.39	1.35
51	9	644	OMG	C5-N7	-3.63	1.31	1.39
48	5	3853	PSU	C6-C5	3.62	1.39	1.35
48	5	2787	A2M	C5-C4	-3.62	1.32	1.39
48	5	3718	A2M	C5-C4	-3.61	1.32	1.39
48	5	4296	PSU	C6-C5	3.60	1.39	1.35
48	5	4196	OMG	C5-N7	-3.60	1.31	1.39
48	5	1862	PSU	C6-C5	3.58	1.39	1.35
48	5	4457	PSU	C6-C5	3.58	1.39	1.35
48	5	2861	OMC	O2-C2	-3.58	1.17	1.23
51	9	1238	PSU	C6-C5	3.57	1.39	1.35
48	5	400	A2M	C5-N7	-3.57	1.32	1.39
48	5	4306	OMU	O4-C4	-3.56	1.17	1.24
48	5	3792	OMG	C5-N7	-3.56	1.31	1.39
48	5	4628	PSU	C6-C5	3.56	1.39	1.35
48	5	1871	A2M	C5-C4	-3.56	1.32	1.39
48	5	1625	OMG	C5-N7	-3.55	1.32	1.39
51	9	1850	MA6	C5-C4	-3.55	1.32	1.39
51	9	109	PSU	C6-C5	3.55	1.39	1.35
51	9	822	PSU	C6-C5	3.54	1.39	1.35
51	9	34	PSU	C6-C5	3.54	1.39	1.35
48	5	3869	OMC	O2-C2	-3.53	1.17	1.23
48	5	1326	A2M	C5-N7	-3.53	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4536	OMC	O2-C2	-3.52	1.17	1.23
48	5	2632	PSU	C6-C5	3.52	1.39	1.35
51	9	1692	PSU	C6-C5	3.52	1.39	1.35
48	5	1534	A2M	C5-C4	-3.52	1.32	1.39
51	9	1244	PSU	C6-C5	3.51	1.39	1.35
48	5	1322	1MA	C2-N1	3.51	1.43	1.35
48	5	4571	A2M	C5-C4	-3.51	1.32	1.39
51	9	1367	PSU	C6-C5	3.51	1.39	1.35
48	5	4523	A2M	C5-N7	-3.50	1.32	1.39
48	5	4620	OMU	O2-C2	-3.47	1.16	1.23
48	5	4494	OMG	C5-N7	-3.47	1.32	1.39
48	5	1316	OMG	C5-N7	-3.46	1.32	1.39
48	5	3925	OMU	O4-C4	-3.46	1.17	1.24
48	5	4521	PSU	C6-C5	3.46	1.39	1.35
48	5	3701	OMC	O2-C2	-3.46	1.17	1.23
51	9	105	PSU	C6-C5	3.45	1.39	1.35
51	9	1232	PSU	C6-C5	3.45	1.39	1.35
48	5	2804	OMC	O2-C2	-3.45	1.17	1.23
51	9	1031	A2M	C5-C4	-3.44	1.32	1.39
51	9	1442	OMU	C4-N3	3.44	1.44	1.38
50	8	75	OMG	C5-N7	-3.43	1.32	1.39
48	5	3764	PSU	C6-C5	3.43	1.39	1.35
51	9	1851	MA6	C5-C4	-3.43	1.33	1.39
51	9	428	OMU	C4-N3	3.43	1.44	1.38
51	9	509	OMG	C5-N7	-3.42	1.32	1.39
48	5	373	OMG	O6-C6	-3.42	1.17	1.23
48	5	3925	OMU	O2-C2	-3.42	1.17	1.23
48	5	1782	PSU	C6-C5	3.41	1.39	1.35
48	5	2424	OMG	C5-N7	-3.40	1.32	1.39
48	5	2787	A2M	C5-N7	-3.40	1.32	1.39
51	9	1004	PSU	C6-C5	3.40	1.39	1.35
51	9	609	PSU	C6-C5	3.39	1.39	1.35
51	9	1326	OMU	C4-N3	3.39	1.44	1.38
48	5	4227	OMU	O2-C2	-3.39	1.17	1.23
48	5	1522	OMG	O6-C6	-3.38	1.17	1.23
51	9	683	OMG	C5-N7	-3.38	1.32	1.39
48	5	2837	OMU	O2-C2	-3.38	1.17	1.23
51	9	1174	PSU	C6-C5	3.38	1.39	1.35
51	9	1045	PSU	C6-C5	3.38	1.39	1.35
48	5	1340	OMC	O2-C2	-3.38	1.17	1.23
48	5	3627	OMG	C5-N7	-3.38	1.32	1.39
48	5	3841	OMC	O2-C2	-3.37	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1046	PSU	C6-C5	3.37	1.39	1.35
48	5	2365	OMC	O2-C2	-3.37	1.17	1.23
51	9	468	A2M	O3'-C3'	-3.37	1.34	1.43
51	9	1842	4AC	O2-C2	-3.37	1.17	1.23
51	9	218	PSU	C6-C5	3.37	1.39	1.35
51	9	1177	PSU	C6-C5	3.37	1.39	1.35
51	9	572	PSU	C6-C5	3.36	1.39	1.35
51	9	121	OMU	O4-C4	-3.36	1.18	1.24
48	5	3808	OMC	O2-C2	-3.35	1.17	1.23
48	5	4532	PSU	C6-C5	3.35	1.39	1.35
48	5	1524	A2M	C5-C4	-3.35	1.33	1.39
48	5	2815	A2M	C5-C4	-3.35	1.33	1.39
48	5	4618	OMG	C5-N7	-3.35	1.32	1.39
48	5	3782	5MC	O2-C2	-3.35	1.17	1.23
48	5	1522	OMG	C5-N7	-3.34	1.32	1.39
48	5	4499	OMG	C5-N7	-3.34	1.32	1.39
48	5	3830	A2M	C5-N7	-3.33	1.33	1.39
51	9	1337	4AC	O2-C2	-3.33	1.17	1.23
51	9	172	OMU	C4-N3	3.32	1.44	1.38
48	5	4618	OMG	O6-C6	-3.32	1.17	1.23
48	5	2363	A2M	C5-N7	-3.32	1.33	1.39
48	5	237	B9B	C5-C4	-3.32	1.33	1.39
48	5	2351	OMC	O2-C2	-3.32	1.17	1.23
51	9	1850	MA6	C5-N7	-3.32	1.33	1.39
48	5	4552	PSU	C6-C5	3.32	1.39	1.35
51	9	174	OMC	O2-C2	-3.32	1.17	1.23
48	5	3830	A2M	C5-C4	-3.31	1.33	1.39
48	5	3867	A2M	C5-C4	-3.31	1.33	1.39
48	5	1316	OMG	O6-C6	-3.31	1.17	1.23
51	9	1081	PSU	C6-C5	3.30	1.38	1.35
48	5	3825	A2M	C5-N7	-3.30	1.33	1.39
48	5	1871	A2M	C5-N7	-3.30	1.33	1.39
51	9	1326	OMU	O2-C2	-3.29	1.17	1.23
51	9	27	A2M	C5-N7	-3.29	1.33	1.39
48	5	4498	OMU	O4-C4	-3.29	1.18	1.24
48	5	3785	A2M	C5-C4	-3.29	1.33	1.39
48	5	3867	A2M	C5-N7	-3.29	1.33	1.39
51	9	1490	OMG	C5-N7	-3.28	1.32	1.39
51	9	1337	4AC	C6-N1	3.28	1.45	1.38
48	5	4623	OMG	C5-N7	-3.27	1.32	1.39
48	5	1534	A2M	C5-N7	-3.27	1.33	1.39
48	5	1677	PSU	C6-C5	3.27	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4370	OMG	C5-N7	-3.27	1.32	1.39
48	5	2363	A2M	C5-C4	-3.26	1.33	1.39
48	5	2422	OMC	O2-C2	-3.26	1.17	1.23
48	5	4498	OMU	C4-N3	3.26	1.44	1.38
51	9	1337	4AC	C2-N1	3.26	1.46	1.40
48	5	1322	1MA	C4-N9	-3.26	1.29	1.38
48	5	4498	OMU	O2-C2	-3.25	1.17	1.23
48	5	3718	A2M	C5-N7	-3.25	1.33	1.39
48	5	4196	OMG	O6-C6	-3.24	1.17	1.23
48	5	4392	OMG	O6-C6	-3.24	1.17	1.23
48	5	4620	OMU	O4-C4	-3.24	1.18	1.24
48	5	3762	PSU	C6-C5	3.24	1.38	1.35
51	9	1678	A2M	C5-C4	-3.23	1.33	1.39
51	9	668	A2M	C5-C4	-3.23	1.33	1.39
51	9	509	OMG	O6-C6	-3.23	1.17	1.23
51	9	649	PSU	C6-C5	3.23	1.38	1.35
51	9	512	A2M	O2'-C2'	3.22	1.50	1.42
48	5	1625	OMG	O6-C6	-3.22	1.17	1.23
48	5	3785	A2M	C5-N7	-3.22	1.33	1.39
48	5	3639	PSU	C6-C5	3.22	1.38	1.35
48	5	3869	OMC	C6-N1	3.21	1.45	1.38
51	9	1328	OMG	C5-N7	-3.21	1.32	1.39
48	5	4442	PSU	C6-C5	3.21	1.38	1.35
48	5	4494	OMG	O6-C6	-3.21	1.17	1.23
51	9	1678	A2M	O2'-C2'	3.21	1.50	1.42
48	5	1860	PSU	C6-C5	3.20	1.38	1.35
48	5	400	A2M	C5-C4	-3.20	1.33	1.39
48	5	398	A2M	C5-C4	-3.20	1.33	1.39
48	5	4228	OMG	C5-N7	-3.19	1.32	1.39
48	5	4361	PSU	C6-C5	3.19	1.38	1.35
51	9	815	PSU	C6-C5	3.18	1.38	1.35
48	5	2861	OMC	C6-N1	3.18	1.45	1.38
48	5	4447	5MC	O2-C2	-3.17	1.17	1.23
48	5	4623	OMG	O6-C6	-3.17	1.17	1.23
48	5	2422	OMC	C6-N1	3.17	1.45	1.38
48	5	1326	A2M	O2'-C2'	3.17	1.50	1.42
51	9	1391	OMC	C6-N1	3.17	1.45	1.38
48	5	1781	PSU	C6-C5	3.17	1.38	1.35
48	5	3724	A2M	C5-C4	-3.17	1.33	1.39
51	9	668	A2M	C5-N7	-3.16	1.33	1.39
48	5	2508	PSU	C6-C5	3.15	1.38	1.35
51	9	119	PSU	C6-C5	3.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4370	OMG	O6-C6	-3.13	1.17	1.23
48	5	1326	A2M	C5-C4	-3.13	1.33	1.39
48	5	2364	OMG	C5-N7	-3.13	1.32	1.39
48	5	2824	OMC	C6-N1	3.13	1.45	1.38
48	5	1517	2MG	C4-N9	-3.13	1.30	1.38
51	9	1643	PSU	C6-C5	3.12	1.38	1.35
51	9	517	OMC	C6-N1	3.12	1.45	1.38
48	5	3841	OMC	C6-N1	3.12	1.45	1.38
51	9	1850	MA6	C6-N6	3.12	1.45	1.36
48	5	4227	OMU	C4-N3	3.11	1.43	1.38
51	9	1445	PSU	C6-C5	3.11	1.38	1.35
48	5	4571	A2M	C5-N7	-3.11	1.33	1.39
48	5	4227	OMU	O4-C4	-3.11	1.18	1.24
51	9	1383	A2M	C5-C4	-3.11	1.33	1.39
48	5	1340	OMC	C6-N1	3.11	1.45	1.38
48	5	3760	A2M	C5-C4	-3.10	1.33	1.39
51	9	1347	PSU	C6-C5	3.10	1.38	1.35
48	5	2364	OMG	O6-C6	-3.10	1.17	1.23
48	5	2837	OMU	O4-C4	-3.10	1.18	1.24
48	5	1524	A2M	C5-N7	-3.09	1.33	1.39
48	5	4353	PSU	C6-C5	3.09	1.38	1.35
51	9	512	A2M	C5-N7	-3.09	1.33	1.39
51	9	116	OMU	C4-N3	3.09	1.43	1.38
48	5	3724	A2M	C5-N7	-3.09	1.33	1.39
48	5	2365	OMC	C6-N1	3.08	1.45	1.38
48	5	2351	OMC	C6-N1	3.08	1.45	1.38
48	5	4571	A2M	O3'-C3'	-3.07	1.35	1.43
48	5	4523	A2M	O3'-C3'	-3.07	1.35	1.43
48	5	4228	OMG	O6-C6	-3.07	1.17	1.23
51	9	159	A2M	C5-C4	-3.06	1.33	1.39
48	5	1677	PSU	O4'-C1'	-3.06	1.39	1.43
51	9	1678	A2M	C5-N7	-3.06	1.33	1.39
48	5	398	A2M	C5-N7	-3.05	1.33	1.39
51	9	468	A2M	C5-C4	-3.05	1.33	1.39
48	5	4637	OMG	O6-C6	-3.05	1.17	1.23
48	5	3718	A2M	O2'-C2'	3.04	1.50	1.42
51	9	1391	OMC	O2-C2	-3.04	1.18	1.23
51	9	1851	MA6	C6-N6	3.04	1.45	1.36
48	5	3887	OMC	O2-C2	-3.04	1.18	1.23
51	9	814	PSU	C6-C5	3.03	1.38	1.35
51	9	121	OMU	O2-C2	-3.03	1.17	1.23
51	9	1703	OMC	C6-N1	3.03	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	4571	A2M	O2'-C2'	3.03	1.50	1.42
51	9	99	A2M	C5-N7	-3.03	1.33	1.39
48	5	4523	A2M	C5-C4	-3.02	1.33	1.39
48	5	3627	OMG	O6-C6	-3.02	1.17	1.23
48	5	4403	PSU	C6-C5	3.02	1.38	1.35
48	5	2424	OMG	O6-C6	-3.02	1.17	1.23
51	9	436	OMG	O6-C6	-3.01	1.17	1.23
48	5	3701	OMC	C6-N1	3.01	1.45	1.38
51	9	159	A2M	O3'-C3'	-3.01	1.35	1.43
48	5	3792	OMG	O6-C6	-3.01	1.17	1.23
51	9	174	OMC	C6-N1	3.00	1.45	1.38
51	9	166	A2M	C5-C4	-3.00	1.33	1.39
48	5	3818	UY1	C4-N3	3.00	1.44	1.38
51	9	166	A2M	O3'-C3'	-3.00	1.35	1.43
51	9	512	A2M	C5-C4	-2.99	1.33	1.39
51	9	1383	A2M	O2'-C2'	2.99	1.50	1.42
51	9	517	OMC	O2-C2	-2.98	1.18	1.23
51	9	1383	A2M	C5-N7	-2.98	1.33	1.39
48	5	4500	PSU	C6-C5	2.97	1.38	1.35
48	5	2876	OMG	O6-C6	-2.97	1.17	1.23
48	5	2363	A2M	O2'-C2'	2.96	1.49	1.42
51	9	172	OMU	O2-C2	-2.96	1.17	1.23
51	9	1490	OMG	C4-N9	-2.95	1.30	1.38
48	5	2804	OMC	C6-N1	2.95	1.45	1.38
51	9	484	A2M	O2'-C2'	2.94	1.49	1.42
48	5	3808	OMC	C6-N1	2.93	1.45	1.38
48	5	3760	A2M	C5-N7	-2.93	1.33	1.39
48	5	1534	A2M	O2'-C2'	2.93	1.49	1.42
51	9	172	OMU	O4-C4	-2.93	1.18	1.24
51	9	428	OMU	O4-C4	-2.93	1.18	1.24
48	5	2815	A2M	C5-N7	-2.93	1.33	1.39
48	5	1326	A2M	O3'-C3'	-2.93	1.35	1.43
48	5	3825	A2M	C5-C4	-2.93	1.33	1.39
48	5	4523	A2M	C8-N9	-2.92	1.32	1.37
48	5	3760	A2M	O2'-C2'	2.92	1.49	1.42
48	5	2837	OMU	C4-N3	2.92	1.43	1.38
51	9	159	A2M	O2'-C2'	2.92	1.49	1.42
48	5	4536	OMC	C6-N1	2.92	1.45	1.38
48	5	4579	PSU	C6-C5	2.91	1.38	1.35
48	5	4499	OMG	O6-C6	-2.91	1.18	1.23
48	5	398	A2M	O3'-C3'	-2.91	1.35	1.43
51	9	116	OMU	O2-C2	-2.91	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	3899	OMG	O6-C6	-2.91	1.18	1.23
48	5	1524	A2M	O2'-C2'	2.90	1.49	1.42
48	5	1517	2MG	O6-C6	-2.90	1.18	1.23
51	9	512	A2M	O3'-C3'	-2.90	1.35	1.43
51	9	863	PSU	C6-C5	2.90	1.38	1.35
51	9	166	A2M	C5-N7	-2.89	1.33	1.39
51	9	1442	OMU	O4-C4	-2.89	1.18	1.24
48	5	1792	PSU	C6-C5	2.89	1.38	1.35
48	5	3760	A2M	O3'-C3'	-2.89	1.35	1.43
48	5	3851	PSU	C6-C5	2.88	1.38	1.35
48	5	3887	OMC	C6-N1	2.88	1.44	1.38
48	5	3830	A2M	O3'-C3'	-2.87	1.35	1.43
51	9	686	PSU	C6-C5	2.87	1.38	1.35
51	9	668	A2M	O3'-C3'	-2.87	1.35	1.43
48	5	1517	2MG	C5-N7	-2.86	1.33	1.39
51	9	1832	6MZ	C5-C4	-2.86	1.34	1.39
48	5	3724	A2M	O3'-C3'	-2.86	1.35	1.43
51	9	166	A2M	O2'-C2'	2.85	1.49	1.42
48	5	2363	A2M	O3'-C3'	-2.85	1.35	1.43
51	9	668	A2M	O2'-C2'	2.85	1.49	1.42
51	9	1490	OMG	O6-C6	-2.85	1.18	1.23
51	9	1031	A2M	C5-N7	-2.85	1.33	1.39
48	5	2815	A2M	O2'-C2'	2.85	1.49	1.42
48	5	3867	A2M	O3'-C3'	-2.85	1.35	1.43
48	5	1534	A2M	O3'-C3'	-2.84	1.35	1.43
50	8	75	OMG	O6-C6	-2.84	1.18	1.23
51	9	1328	OMG	O6-C6	-2.84	1.18	1.23
48	5	3818	UY1	O2-C2	-2.84	1.17	1.23
48	5	3825	A2M	O2'-C2'	2.84	1.49	1.42
51	9	1842	4AC	C6-N1	2.84	1.44	1.38
48	5	1322	1MA	C5-N7	-2.84	1.33	1.39
51	9	468	A2M	C5-N7	-2.83	1.33	1.39
51	9	1851	MA6	C5-N7	-2.82	1.33	1.39
48	5	3920	PSU	C6-C5	2.82	1.38	1.35
51	9	1703	OMC	O2-C2	-2.82	1.18	1.23
48	5	4220	6MZ	C5-N7	-2.82	1.33	1.39
51	9	121	OMU	C4-N3	2.82	1.43	1.38
48	5	2787	A2M	O2'-C2'	2.82	1.49	1.42
48	5	398	A2M	O2'-C2'	2.81	1.49	1.42
48	5	237	B9B	C5-N7	-2.81	1.34	1.39
48	5	4423	PSU	C6-C5	2.80	1.38	1.35
48	5	3830	A2M	O2'-C2'	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1326	OMU	O4-C4	-2.79	1.19	1.24
51	9	1383	A2M	O3'-C3'	-2.79	1.36	1.43
51	9	159	A2M	C5-N7	-2.79	1.34	1.39
51	9	1850	MA6	C8-N9	-2.79	1.32	1.37
51	9	683	OMG	O6-C6	-2.79	1.18	1.23
48	5	4523	A2M	O2'-C2'	2.78	1.49	1.42
51	9	116	OMU	O4-C4	-2.78	1.19	1.24
48	5	4220	6MZ	C5-C4	-2.78	1.34	1.39
48	5	2787	A2M	O3'-C3'	-2.77	1.36	1.43
48	5	4530	UR3	C6-N1	2.77	1.44	1.38
48	5	1744	PSU	C6-C5	2.76	1.38	1.35
48	5	3715	PSU	C6-C5	2.76	1.38	1.35
51	9	27	A2M	O2'-C2'	2.76	1.49	1.42
51	9	99	A2M	O2'-C2'	2.76	1.49	1.42
51	9	468	A2M	O2'-C2'	2.75	1.49	1.42
48	5	4456	OMC	C6-N1	2.75	1.44	1.38
51	9	1678	A2M	C8-N9	-2.74	1.32	1.37
48	5	3818	UY1	O4-C4	-2.74	1.18	1.23
51	9	1639	G7M	C2-N1	2.74	1.44	1.37
48	5	3695	PSU	C6-C5	2.73	1.38	1.35
51	9	484	A2M	C5-N7	-2.73	1.34	1.39
48	5	4299	PSU	C6-C5	2.73	1.38	1.35
48	5	1871	A2M	O2'-C2'	2.73	1.49	1.42
51	9	428	OMU	O2-C2	-2.72	1.18	1.23
48	5	400	A2M	O3'-C3'	-2.72	1.36	1.43
51	9	1639	G7M	C6-N1	2.71	1.43	1.38
48	5	3724	A2M	O2'-C2'	2.70	1.49	1.42
48	5	2815	A2M	O3'-C3'	-2.69	1.36	1.43
51	9	99	A2M	O3'-C3'	-2.69	1.36	1.43
48	5	3825	A2M	O3'-C3'	-2.69	1.36	1.43
48	5	4530	UR3	O2-C2	-2.69	1.17	1.22
48	5	4220	6MZ	C8-N9	-2.68	1.33	1.37
51	9	99	A2M	C8-N9	-2.68	1.33	1.37
48	5	400	A2M	O2'-C2'	2.68	1.49	1.42
48	5	3867	A2M	O2'-C2'	2.67	1.49	1.42
48	5	1871	A2M	O3'-C3'	-2.67	1.36	1.43
51	9	27	A2M	C5-C4	-2.67	1.34	1.39
51	9	1031	A2M	O3'-C3'	-2.66	1.36	1.43
48	5	1524	A2M	O3'-C3'	-2.66	1.36	1.43
48	5	3718	A2M	O3'-C3'	-2.65	1.36	1.43
51	9	27	A2M	O3'-C3'	-2.65	1.36	1.43
48	5	3724	A2M	C8-N9	-2.64	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1639	G7M	O6-C6	-2.64	1.18	1.23
48	5	3760	A2M	C8-N9	-2.64	1.33	1.37
51	9	1442	OMU	O2-C2	-2.62	1.18	1.23
51	9	644	OMG	C2-N1	2.62	1.44	1.37
48	5	1326	A2M	C8-N9	-2.62	1.33	1.37
51	9	1031	A2M	O2'-C2'	2.61	1.49	1.42
51	9	484	A2M	O3'-C3'	-2.61	1.36	1.43
51	9	468	A2M	C8-N9	-2.60	1.33	1.37
48	5	3785	A2M	O2'-C2'	2.60	1.49	1.42
48	5	237	B9B	C8-N9	-2.60	1.33	1.37
48	5	4499	OMG	C2-N1	2.60	1.43	1.37
51	9	1842	4AC	O7-C7	-2.59	1.17	1.23
48	5	4530	UR3	O4-C4	-2.58	1.18	1.23
48	5	3818	UY1	O4'-C1'	-2.57	1.40	1.43
48	5	1534	A2M	C8-N9	-2.57	1.33	1.37
48	5	2364	OMG	C5-C6	2.57	1.54	1.44
48	5	398	A2M	C8-N9	-2.56	1.33	1.37
48	5	1517	2MG	C6-N1	2.55	1.43	1.38
48	5	2363	A2M	C8-N9	-2.54	1.33	1.37
51	9	1248	B8N	C32-C33	2.52	1.58	1.53
48	5	3825	A2M	C8-N9	-2.51	1.33	1.37
51	9	644	OMG	O6-C6	-2.50	1.18	1.23
48	5	3627	OMG	C5-C6	2.50	1.53	1.44
48	5	2815	A2M	C8-N9	-2.50	1.33	1.37
51	9	1703	OMC	C5-C4	2.50	1.48	1.42
51	9	1678	A2M	O3'-C3'	-2.49	1.36	1.43
48	5	1316	OMG	C4-N9	-2.48	1.31	1.38
51	9	484	A2M	C8-N9	-2.48	1.33	1.37
51	9	668	A2M	C8-N9	-2.47	1.33	1.37
48	5	1316	OMG	C5-C6	2.47	1.53	1.44
48	5	1871	A2M	C8-N9	-2.46	1.33	1.37
51	9	1851	MA6	C8-N9	-2.45	1.33	1.37
48	5	4306	OMU	C4-N3	2.45	1.42	1.38
50	8	75	OMG	C4-N9	-2.45	1.31	1.38
50	8	75	OMG	C2-N1	2.45	1.43	1.37
48	5	4228	OMG	C5-C6	2.45	1.53	1.44
51	9	159	A2M	C8-N9	-2.44	1.33	1.37
51	9	517	OMC	C5-C4	2.44	1.48	1.42
48	5	1524	A2M	C8-N9	-2.44	1.33	1.37
51	9	1832	6MZ	C5-N7	-2.43	1.34	1.39
48	5	2365	OMC	C5-C4	2.43	1.48	1.42
51	9	1337	4AC	O7-C7	-2.43	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	27	A2M	C8-N9	-2.42	1.33	1.37
48	5	1522	OMG	C5-C6	2.42	1.53	1.44
48	5	4392	OMG	C5-C6	2.42	1.53	1.44
48	5	3925	OMU	C4-N3	2.41	1.42	1.38
48	5	4620	OMU	C4-N3	2.41	1.42	1.38
48	5	2364	OMG	C2-N1	2.41	1.43	1.37
48	5	2876	OMG	C2-N1	2.40	1.43	1.37
48	5	1871	A2M	C4-N9	-2.40	1.32	1.37
48	5	1522	OMG	C2-N1	2.40	1.43	1.37
48	5	4571	A2M	C8-N9	-2.39	1.33	1.37
48	5	1625	OMG	C6-N1	2.39	1.43	1.38
51	9	1031	A2M	C8-N9	-2.38	1.33	1.37
48	5	2787	A2M	C8-N9	-2.37	1.33	1.37
48	5	4392	OMG	C4-N9	-2.36	1.32	1.38
48	5	4623	OMG	C4-N9	-2.36	1.32	1.38
48	5	3792	OMG	C4-N9	-2.36	1.32	1.38
48	5	2876	OMG	C5-C6	2.36	1.53	1.44
51	9	644	OMG	C5-C6	2.36	1.53	1.44
48	5	400	A2M	C8-N9	-2.36	1.33	1.37
51	9	683	OMG	C5-C6	2.36	1.53	1.44
48	5	3830	A2M	C8-N9	-2.36	1.33	1.37
48	5	3718	A2M	C4-N9	-2.36	1.32	1.37
48	5	4494	OMG	C4-N9	-2.35	1.32	1.38
51	9	1328	OMG	C2-N1	2.34	1.43	1.37
51	9	683	OMG	C2-N1	2.33	1.43	1.37
48	5	4228	OMG	C2-N1	2.33	1.43	1.37
48	5	4456	OMC	C5-C4	2.33	1.48	1.42
51	9	436	OMG	C2-N1	2.32	1.43	1.37
48	5	4618	OMG	C5-C6	2.32	1.53	1.44
48	5	3715	PSU	C4-C5	-2.32	1.37	1.44
51	9	174	OMC	C5-C4	2.32	1.48	1.42
48	5	2824	OMC	C5-C4	2.31	1.48	1.42
50	8	75	OMG	C5-C6	2.30	1.53	1.44
48	5	1625	OMG	C2-N1	2.30	1.43	1.37
48	5	4637	OMG	C5-C6	2.29	1.53	1.44
51	9	801	PSU	O4'-C1'	-2.29	1.40	1.43
51	9	512	A2M	C8-N9	-2.29	1.33	1.37
48	5	1340	OMC	C5-C4	2.28	1.48	1.42
48	5	3627	OMG	C4-N9	-2.27	1.32	1.38
48	5	3899	OMG	C5-C6	2.27	1.52	1.44
48	5	4370	OMG	C5-C6	2.27	1.52	1.44
48	5	4618	OMG	C2-N1	2.27	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1490	OMG	C5-C6	2.26	1.52	1.44
48	5	1522	OMG	C4-N9	-2.26	1.32	1.38
48	5	4370	OMG	C2-N1	2.26	1.43	1.37
48	5	1316	OMG	C2-N1	2.25	1.43	1.37
51	9	1639	G7M	C8-N7	2.25	1.36	1.33
48	5	2424	OMG	C4-N9	-2.25	1.32	1.38
48	5	3627	OMG	C2-N1	2.25	1.43	1.37
48	5	4499	OMG	C4-N9	-2.24	1.32	1.38
48	5	2422	OMC	C5-C4	2.24	1.48	1.42
48	5	4370	OMG	C4-N9	-2.23	1.32	1.38
48	5	4494	OMG	C2-N1	2.23	1.43	1.37
48	5	2861	OMC	C5-C4	2.22	1.48	1.42
48	5	4500	PSU	O4'-C1'	-2.21	1.40	1.43
48	5	2424	OMG	C5-C6	2.21	1.52	1.44
48	5	373	OMG	C2-N1	2.21	1.43	1.37
48	5	3715	PSU	O4'-C1'	-2.21	1.40	1.43
48	5	3867	A2M	C8-N9	-2.20	1.33	1.37
48	5	4623	OMG	C5-C6	2.19	1.52	1.44
48	5	2804	OMC	C5-C4	2.19	1.48	1.42
51	9	1328	OMG	C4-N9	-2.19	1.32	1.38
48	5	4618	OMG	C4-N9	-2.19	1.32	1.38
48	5	4637	OMG	C4-N9	-2.18	1.32	1.38
48	5	1517	2MG	CM2-N2	2.18	1.49	1.45
48	5	4494	OMG	C5-C6	2.18	1.52	1.44
48	5	3841	OMC	C5-C4	2.18	1.48	1.42
48	5	373	OMG	C5-C6	2.18	1.52	1.44
48	5	4637	OMG	C2-N1	2.18	1.42	1.37
51	9	1238	PSU	C4-C5	-2.18	1.38	1.44
48	5	2351	OMC	C5-C4	2.17	1.48	1.42
51	9	1832	6MZ	C8-N9	-2.16	1.33	1.37
48	5	3701	OMC	C5-C4	2.15	1.47	1.42
48	5	4196	OMG	C5-C6	2.14	1.52	1.44
51	9	428	OMU	C6-N1	2.14	1.43	1.38
51	9	822	PSU	O4'-C1'	-2.14	1.40	1.43
48	5	2424	OMG	C2-N1	2.13	1.42	1.37
51	9	822	PSU	C4-C5	-2.13	1.38	1.44
48	5	3925	OMU	C5-C4	2.12	1.48	1.43
48	5	3785	A2M	O3'-C3'	-2.12	1.37	1.43
48	5	2364	OMG	C4-N9	-2.12	1.32	1.38
51	9	509	OMG	C2-N1	2.12	1.42	1.37
48	5	3851	PSU	O4'-C1'	-2.11	1.40	1.43
51	9	1031	A2M	C4-N9	-2.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1326	OMU	C5-C4	2.10	1.48	1.43
48	5	3808	OMC	C5-C4	2.10	1.47	1.42
51	9	172	OMU	C5-C4	2.10	1.48	1.43
48	5	3734	PSU	C4-C5	-2.09	1.38	1.44
48	5	4392	OMG	C2-N1	2.09	1.42	1.37
51	9	166	A2M	C8-N9	-2.09	1.34	1.37
51	9	1383	A2M	C8-N9	-2.09	1.34	1.37
48	5	237	B9B	C4-N9	-2.09	1.33	1.37
48	5	4499	OMG	C5-C6	2.09	1.52	1.44
51	9	1490	OMG	C6-N1	2.09	1.42	1.38
51	9	1328	OMG	C5-C6	2.08	1.52	1.44
48	5	2363	A2M	C4-N9	-2.08	1.33	1.37
51	9	1850	MA6	C5-C6	-2.08	1.36	1.41
51	9	509	OMG	C4-N9	-2.08	1.32	1.38
48	5	4530	UR3	C5-C4	2.08	1.49	1.43
48	5	3785	A2M	C4-N9	-2.07	1.33	1.37
48	5	4536	OMC	C5-C4	2.07	1.47	1.42
48	5	3899	OMG	C2-N1	2.07	1.42	1.37
48	5	4623	OMG	C2-N1	2.07	1.42	1.37
48	5	4530	UR3	C4-N3	2.06	1.44	1.40
48	5	4227	OMU	C5-C4	2.06	1.48	1.43
48	5	4306	OMU	C6-N1	2.05	1.43	1.38
51	9	1248	B8N	O35-C34	2.04	1.28	1.22
51	9	1391	OMC	C5-C4	2.04	1.47	1.42
48	5	4293	PSU	C4-C5	-2.04	1.38	1.44
48	5	1781	PSU	C4-C5	-2.04	1.38	1.44
48	5	4571	A2M	C4-N9	-2.04	1.33	1.37
48	5	4628	PSU	C4-C5	-2.04	1.38	1.44
48	5	1522	OMG	C6-N1	2.03	1.42	1.38
48	5	4353	PSU	C4-C5	-2.03	1.38	1.44
48	5	4521	PSU	O4'-C1'	-2.02	1.41	1.43
48	5	3718	A2M	C8-N9	-2.02	1.34	1.37
48	5	3785	A2M	C8-N9	-2.02	1.34	1.37
51	9	1328	OMG	C6-N1	2.02	1.42	1.38
48	5	4498	OMU	C5-C4	2.02	1.48	1.43
48	5	4620	OMU	C6-N1	2.02	1.42	1.38
48	5	4296	PSU	C4-C5	-2.02	1.38	1.44
48	5	4196	OMG	C2-N1	2.02	1.42	1.37
48	5	4499	OMG	C6-N1	2.02	1.42	1.38
51	9	686	PSU	C4-C5	-2.01	1.38	1.44
48	5	4500	PSU	C4-C5	-2.01	1.38	1.44
48	5	3899	OMG	C4-N9	-2.00	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	683	OMG	C6-N1	2.00	1.42	1.38
48	5	4498	OMU	C6-N1	2.00	1.42	1.38
51	9	1045	PSU	C4-C5	-2.00	1.38	1.44
51	9	1383	A2M	C4-N9	-2.00	1.33	1.37

All (1007) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1851	MA6	N1-C6-N6	-15.95	97.42	116.86
51	9	1850	MA6	N1-C6-N6	-13.25	100.72	116.86
51	9	1851	MA6	C5-C6-N6	10.76	142.36	125.33
51	9	1850	MA6	C5-C6-N6	9.04	139.64	125.33
51	9	1851	MA6	C4-N9-C1'	-7.48	109.14	126.63
51	9	512	A2M	N6-C6-N1	-7.37	101.95	118.38
51	9	484	A2M	N6-C6-N1	-7.33	102.06	118.38
51	9	1678	A2M	N6-C6-N1	-7.25	102.23	118.38
48	5	1517	2MG	N1-C2-N2	7.24	123.96	116.56
48	5	3760	A2M	N6-C6-N1	-7.09	102.59	118.38
48	5	4571	A2M	N6-C6-N1	-7.09	102.59	118.38
48	5	2363	A2M	N6-C6-N1	-7.06	102.65	118.38
51	9	1383	A2M	N6-C6-N1	-7.02	102.74	118.38
48	5	4523	A2M	N6-C6-N1	-6.96	102.89	118.38
51	9	99	A2M	N6-C6-N1	-6.95	102.89	118.38
51	9	668	A2M	N6-C6-N1	-6.94	102.93	118.38
48	5	398	A2M	N6-C6-N1	-6.91	102.98	118.38
51	9	159	A2M	N6-C6-N1	-6.90	103.00	118.38
48	5	3718	A2M	N6-C6-N1	-6.79	103.26	118.38
51	9	1850	MA6	C4-N9-C1'	-6.76	110.83	126.63
48	5	2815	A2M	N6-C6-N1	-6.74	103.36	118.38
51	9	468	A2M	N6-C6-N1	-6.72	103.41	118.38
51	9	1851	MA6	C1'-N9-C8	6.71	141.99	127.09
51	9	27	A2M	N6-C6-N1	-6.70	103.44	118.38
48	5	3785	A2M	N6-C6-N1	-6.70	103.45	118.38
48	5	3867	A2M	N6-C6-N1	-6.66	103.54	118.38
48	5	3830	A2M	N6-C6-N1	-6.63	103.61	118.38
48	5	1524	A2M	N6-C6-N1	-6.57	103.74	118.38
48	5	1534	A2M	N6-C6-N1	-6.57	103.75	118.38
48	5	3724	A2M	N6-C6-N1	-6.51	103.88	118.38
48	5	1322	1MA	C1'-N9-C8	-6.50	108.26	126.73
51	9	1031	A2M	N6-C6-N1	-6.44	104.04	118.38
48	5	2787	A2M	N6-C6-N1	-6.43	104.06	118.38
48	5	1326	A2M	N6-C6-N1	-6.42	104.08	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	166	A2M	N6-C6-N1	-6.38	104.16	118.38
48	5	1517	2MG	C2-N3-C4	6.34	119.94	112.00
48	5	2876	OMG	C5-C4-N3	-6.31	118.35	128.39
51	9	166	A2M	N3-C2-N1	-6.26	119.11	128.58
48	5	237	B9B	C5-C4-N3	-6.18	120.67	127.18
51	9	512	A2M	C5-C6-N6	6.16	138.54	123.29
51	9	484	A2M	N3-C2-N1	-6.16	119.26	128.58
48	5	1871	A2M	N6-C6-N1	-6.13	104.72	118.38
48	5	4498	OMU	C4-N3-C2	-6.11	119.03	126.61
51	9	512	A2M	N3-C2-N1	-6.08	119.38	128.58
48	5	373	OMG	C5-C4-N3	-6.08	118.72	128.39
48	5	3830	A2M	N3-C2-N1	-6.06	119.41	128.58
48	5	1625	OMG	C5-C4-N3	-6.04	118.77	128.39
51	9	1326	OMU	C4-N3-C2	-6.04	119.11	126.61
51	9	1832	6MZ	N1-C2-N3	-6.02	119.46	128.58
48	5	3825	A2M	N6-C6-N1	-6.02	104.97	118.38
48	5	1871	A2M	N3-C2-N1	-6.01	119.48	128.58
51	9	484	A2M	C5-C6-N6	5.99	138.13	123.29
51	9	1248	B8N	C1'-C5-C4	5.99	126.70	117.61
48	5	2837	OMU	C4-N3-C2	-5.99	119.18	126.61
51	9	1490	OMG	C1'-N9-C4	-5.97	108.86	126.49
51	9	1031	A2M	N3-C2-N1	-5.95	119.58	128.58
48	5	4196	OMG	C5-C4-N3	-5.94	118.94	128.39
48	5	3867	A2M	N3-C2-N1	-5.89	119.67	128.58
51	9	1851	MA6	C5-C4-N3	-5.85	118.66	126.72
51	9	1851	MA6	N1-C2-N3	-5.85	119.73	128.58
51	9	1678	A2M	C5-C6-N6	5.84	137.75	123.29
48	5	1326	A2M	N3-C2-N1	-5.83	119.75	128.58
51	9	1383	A2M	N3-C2-N1	-5.83	119.76	128.58
48	5	4521	PSU	N1-C2-N3	5.82	121.31	115.17
48	5	3925	OMU	C4-N3-C2	-5.82	119.39	126.61
48	5	4571	A2M	N3-C2-N1	-5.81	119.78	128.58
48	5	2364	OMG	C5-C4-N3	-5.81	119.14	128.39
51	9	218	PSU	N1-C2-N3	5.80	121.29	115.17
48	5	2815	A2M	N3-C2-N1	-5.80	119.80	128.58
48	5	4392	OMG	C5-C4-N3	-5.80	119.16	128.39
48	5	4227	OMU	C4-N3-C2	-5.79	119.43	126.61
51	9	686	PSU	C4-N3-C2	-5.78	118.40	126.37
48	5	2787	A2M	C5-C4-N3	-5.77	118.78	126.72
51	9	468	A2M	N3-C2-N1	-5.77	119.85	128.58
48	5	4523	A2M	N3-C2-N1	-5.75	119.87	128.58
51	9	668	A2M	N3-C2-N1	-5.75	119.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	683	OMG	C5-C4-N3	-5.75	119.24	128.39
48	5	4523	A2M	C5-C6-N6	5.73	137.47	123.29
51	9	1490	OMG	C1'-N9-C8	5.72	142.98	126.73
48	5	4637	OMG	C5-C4-N3	-5.72	119.29	128.39
51	9	1850	MA6	C1'-N9-C8	5.71	139.77	127.09
48	5	1524	A2M	N3-C2-N1	-5.71	119.94	128.58
48	5	3718	A2M	N3-C2-N1	-5.68	119.99	128.58
48	5	3899	OMG	C5-C4-N3	-5.67	119.36	128.39
51	9	1383	A2M	C5-C6-N6	5.66	137.29	123.29
48	5	2363	A2M	C5-C6-N6	5.65	137.28	123.29
48	5	1534	A2M	N3-C2-N1	-5.65	120.03	128.58
48	5	400	A2M	N6-C6-N1	-5.65	105.79	118.38
48	5	4620	OMU	C4-N3-C2	-5.63	119.62	126.61
48	5	3760	A2M	C5-C6-N6	5.63	137.22	123.29
48	5	4571	A2M	C5-C6-N6	5.62	137.20	123.29
48	5	4306	OMU	C4-N3-C2	-5.62	119.64	126.61
48	5	4220	6MZ	N1-C2-N3	-5.61	120.09	128.58
51	9	27	A2M	N3-C2-N1	-5.60	120.10	128.58
51	9	27	A2M	C5-C6-N6	5.60	137.16	123.29
51	9	436	OMG	C5-C4-N3	-5.59	119.49	128.39
48	5	3762	PSU	C4-N3-C2	-5.59	118.67	126.37
48	5	3853	PSU	N1-C2-N3	5.58	121.05	115.17
51	9	218	PSU	C4-N3-C2	-5.58	118.69	126.37
48	5	4628	PSU	N1-C2-N3	5.56	121.03	115.17
51	9	172	OMU	C4-N3-C2	-5.56	119.71	126.61
51	9	159	A2M	C5-C6-N6	5.56	137.04	123.29
51	9	1678	A2M	N3-C2-N1	-5.55	120.17	128.58
51	9	668	A2M	C5-C6-N6	5.55	137.04	123.29
48	5	2787	A2M	N3-C2-N1	-5.54	120.19	128.58
51	9	1442	OMU	C4-N3-C2	-5.54	119.73	126.61
51	9	121	OMU	C4-N3-C2	-5.54	119.73	126.61
48	5	398	A2M	C5-C4-N3	-5.53	119.10	126.72
51	9	99	A2M	C5-C6-N6	5.51	136.92	123.29
48	5	3718	A2M	C5-C6-N6	5.50	136.90	123.29
48	5	3760	A2M	N3-C2-N1	-5.49	120.26	128.58
48	5	1677	PSU	N1-C2-N3	5.49	120.96	115.17
48	5	398	A2M	N3-C2-N1	-5.48	120.28	128.58
48	5	1524	A2M	C5-C6-N6	5.48	136.85	123.29
48	5	1677	PSU	C4-N3-C2	-5.46	118.85	126.37
48	5	1683	PSU	N1-C2-N3	5.46	120.92	115.17
51	9	1174	PSU	N1-C2-N3	5.46	120.92	115.17
48	5	1322	1MA	C1'-N9-C4	5.46	142.60	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2363	A2M	N3-C2-N1	-5.46	120.32	128.58
48	5	400	A2M	C5-C4-N3	-5.45	119.21	126.72
51	9	509	OMG	C5-C4-N3	-5.45	119.71	128.39
48	5	3785	A2M	N3-C2-N1	-5.45	120.33	128.58
51	9	822	PSU	N1-C2-N3	5.45	120.91	115.17
48	5	1534	A2M	C5-C6-N6	5.44	136.76	123.29
48	5	4442	PSU	N1-C2-N3	5.44	120.91	115.17
48	5	3724	A2M	N3-C2-N1	-5.44	120.35	128.58
51	9	1045	PSU	N1-C2-N3	5.44	120.90	115.17
48	5	3825	A2M	C5-C4-N3	-5.44	119.23	126.72
48	5	4353	PSU	N1-C2-N3	5.43	120.90	115.17
51	9	1643	PSU	C4-N3-C2	-5.43	118.89	126.37
48	5	4628	PSU	C4-N3-C2	-5.43	118.89	126.37
51	9	1248	B8N	C5-C4-N3	5.43	126.00	116.15
51	9	99	A2M	N3-C2-N1	-5.42	120.37	128.58
51	9	428	OMU	C4-N3-C2	-5.42	119.88	126.61
51	9	686	PSU	N1-C2-N3	5.41	120.87	115.17
51	9	166	A2M	C5-C6-N6	5.41	136.67	123.29
48	5	3851	PSU	N1-C2-N3	5.40	120.86	115.17
48	5	3830	A2M	C5-C6-N6	5.39	136.63	123.29
51	9	468	A2M	C5-C6-N6	5.38	136.62	123.29
48	5	2815	A2M	C5-C6-N6	5.38	136.61	123.29
48	5	3920	PSU	C4-N3-C2	-5.38	118.97	126.37
48	5	4370	OMG	C5-C4-N3	-5.37	119.84	128.39
48	5	1326	A2M	C5-C6-N6	5.37	136.58	123.29
48	5	3920	PSU	N1-C2-N3	5.36	120.83	115.17
51	9	109	PSU	N1-C2-N3	5.36	120.82	115.17
51	9	159	A2M	N3-C2-N1	-5.36	120.47	128.58
51	9	1850	MA6	N1-C2-N3	-5.35	120.48	128.58
48	5	398	A2M	C5-C6-N6	5.33	136.50	123.29
48	5	3760	A2M	C5-C4-N3	-5.33	119.37	126.72
51	9	1850	MA6	C5-C4-N3	-5.33	119.37	126.72
48	5	3867	A2M	C5-C6-N6	5.32	136.46	123.29
48	5	3762	PSU	N1-C2-N3	5.32	120.78	115.17
51	9	644	OMG	C5-C4-N3	-5.32	119.93	128.39
51	9	105	PSU	N1-C2-N3	5.32	120.78	115.17
51	9	1045	PSU	C4-N3-C2	-5.31	119.06	126.37
51	9	1643	PSU	N1-C2-N3	5.30	120.76	115.17
48	5	3724	A2M	C5-C4-N3	-5.30	119.42	126.72
48	5	4361	PSU	N1-C2-N3	5.29	120.75	115.17
51	9	116	OMU	C4-N3-C2	-5.29	120.04	126.61
51	9	1248	B8N	C4-N3-C2	-5.28	119.12	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	815	PSU	N1-C2-N3	5.27	120.73	115.17
48	5	4623	OMG	C5-C4-N3	-5.27	120.00	128.39
48	5	3764	PSU	N1-C2-N3	5.27	120.72	115.17
51	9	1244	PSU	C4-N3-C2	-5.27	119.12	126.37
48	5	4228	OMG	C5-C4-N3	-5.26	120.02	128.39
48	5	4494	OMG	C5-C4-N3	-5.26	120.02	128.39
51	9	1081	PSU	N1-C2-N3	5.26	120.71	115.17
48	5	3853	PSU	C4-N3-C2	-5.24	119.15	126.37
48	5	1871	A2M	C5-C6-N6	5.24	136.26	123.29
48	5	3785	A2M	C5-C6-N6	5.24	136.26	123.29
48	5	400	A2M	N3-C2-N1	-5.24	120.66	128.58
48	5	3792	OMG	C5-C4-N3	-5.23	120.07	128.39
48	5	3764	PSU	C4-N3-C2	-5.22	119.17	126.37
51	9	814	PSU	C4-N3-C2	-5.22	119.19	126.37
48	5	4423	PSU	C4-N3-C2	-5.20	119.20	126.37
51	9	34	PSU	N1-C2-N3	5.20	120.65	115.17
48	5	4361	PSU	C4-N3-C2	-5.19	119.23	126.37
51	9	822	PSU	C4-N3-C2	-5.19	119.23	126.37
51	9	109	PSU	C4-N3-C2	-5.18	119.23	126.37
51	9	815	PSU	C4-N3-C2	-5.18	119.23	126.37
48	5	4299	PSU	C4-N3-C2	-5.17	119.25	126.37
51	9	1031	A2M	C5-C6-N6	5.17	136.09	123.29
51	9	1850	MA6	C4-C5-C6	5.17	121.26	115.91
48	5	2424	OMG	C5-C4-N3	-5.17	120.16	128.39
51	9	1347	PSU	C4-N3-C2	-5.17	119.25	126.37
50	8	75	OMG	C5-C4-N3	-5.16	120.17	128.39
48	5	4296	PSU	N1-C2-N3	5.16	120.61	115.17
51	9	1004	PSU	N1-C2-N3	5.15	120.60	115.17
48	5	4552	PSU	C4-N3-C2	-5.15	119.28	126.37
51	9	1174	PSU	C4-N3-C2	-5.15	119.28	126.37
48	5	1683	PSU	C4-N3-C2	-5.15	119.28	126.37
51	9	814	PSU	N1-C2-N3	5.14	120.59	115.17
48	5	4420	PSU	N1-C2-N3	5.13	120.58	115.17
48	5	4499	OMG	C5-C4-N3	-5.12	120.23	128.39
48	5	2363	A2M	C5-C4-N3	-5.12	119.67	126.72
51	9	668	A2M	C5-C4-N3	-5.12	119.67	126.72
48	5	2632	PSU	N1-C2-N3	5.12	120.56	115.17
51	9	1244	PSU	N1-C2-N3	5.12	120.56	115.17
48	5	1782	PSU	N1-C2-N3	5.11	120.56	115.17
48	5	1522	OMG	C5-C4-N3	-5.11	120.25	128.39
48	5	3695	PSU	N1-C2-N3	5.11	120.56	115.17
48	5	4618	OMG	C5-C4-N3	-5.11	120.27	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	609	PSU	N1-C2-N3	5.10	120.55	115.17
48	5	3825	A2M	N3-C2-N1	-5.10	120.86	128.58
48	5	3785	A2M	C5-C4-N3	-5.09	119.70	126.72
48	5	3695	PSU	C4-N3-C2	-5.08	119.38	126.37
48	5	3851	PSU	C4-N3-C2	-5.08	119.38	126.37
48	5	3724	A2M	C5-C6-N6	5.06	135.82	123.29
48	5	1860	PSU	N1-C2-N3	5.06	120.51	115.17
51	9	119	PSU	C4-N3-C2	-5.06	119.41	126.37
51	9	1232	PSU	N1-C2-N3	5.05	120.50	115.17
51	9	99	A2M	C5-C4-N3	-5.05	119.76	126.72
48	5	3867	A2M	C5-C4-N3	-5.05	119.76	126.72
48	5	1322	1MA	N1-C2-N3	-5.04	120.00	126.00
48	5	1744	PSU	C4-N3-C2	-5.04	119.43	126.37
48	5	4423	PSU	N1-C2-N3	5.03	120.47	115.17
48	5	4442	PSU	C4-N3-C2	-5.03	119.44	126.37
48	5	1781	PSU	C4-N3-C2	-5.02	119.45	126.37
48	5	4521	PSU	C4-N3-C2	-5.02	119.45	126.37
48	5	4500	PSU	N1-C2-N3	5.02	120.46	115.17
51	9	119	PSU	N1-C2-N3	5.02	120.46	115.17
48	5	4353	PSU	C4-N3-C2	-5.02	119.46	126.37
48	5	4579	PSU	C4-N3-C2	-5.02	119.46	126.37
48	5	4523	A2M	C5-C4-N3	-5.01	119.81	126.72
51	9	649	PSU	C4-N3-C2	-5.01	119.47	126.37
48	5	4420	PSU	C4-N3-C2	-5.00	119.48	126.37
48	5	3825	A2M	C5-C6-N6	5.00	135.68	123.29
48	5	1862	PSU	N1-C2-N3	5.00	120.44	115.17
51	9	1238	PSU	C4-N3-C2	-5.00	119.49	126.37
51	9	27	A2M	C5-C4-N3	-4.99	119.84	126.72
48	5	1744	PSU	N1-C2-N3	4.99	120.44	115.17
51	9	1328	OMG	C5-C4-N3	-4.99	120.45	128.39
48	5	1625	OMG	C2-N3-C4	4.99	120.89	112.30
48	5	2787	A2M	C5-C6-N6	4.98	135.63	123.29
48	5	4293	PSU	C4-N3-C2	-4.98	119.52	126.37
48	5	1792	PSU	C4-N3-C2	-4.97	119.52	126.37
51	9	105	PSU	C4-N3-C2	-4.97	119.52	126.37
48	5	1782	PSU	C4-N3-C2	-4.97	119.52	126.37
51	9	1081	PSU	C4-N3-C2	-4.97	119.52	126.37
51	9	484	A2M	C5-C4-N3	-4.97	119.87	126.72
48	5	2632	PSU	C4-N3-C2	-4.96	119.53	126.37
51	9	1046	PSU	N1-C2-N3	4.96	120.40	115.17
48	5	1316	OMG	C5-C4-N3	-4.96	120.49	128.39
48	5	4403	PSU	C4-N3-C2	-4.96	119.54	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	609	PSU	C4-N3-C2	-4.96	119.55	126.37
51	9	1004	PSU	C4-N3-C2	-4.95	119.55	126.37
48	5	4457	PSU	C4-N3-C2	-4.94	119.56	126.37
51	9	863	PSU	C4-N3-C2	-4.94	119.57	126.37
48	5	3639	PSU	N1-C2-N3	4.92	120.36	115.17
48	5	4296	PSU	C4-N3-C2	-4.92	119.60	126.37
48	5	3734	PSU	N1-C2-N3	4.92	120.35	115.17
48	5	1862	PSU	C4-N3-C2	-4.91	119.61	126.37
48	5	4403	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	572	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	1238	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	1347	PSU	N1-C2-N3	4.90	120.34	115.17
51	9	1678	A2M	C5-C4-N3	-4.89	119.98	126.72
48	5	4552	PSU	N1-C2-N3	4.89	120.33	115.17
48	5	2508	PSU	C4-N3-C2	-4.89	119.63	126.37
48	5	4500	PSU	C4-N3-C2	-4.88	119.64	126.37
48	5	3639	PSU	C4-N3-C2	-4.88	119.65	126.37
48	5	4220	6MZ	C5-C4-N3	-4.87	120.01	126.72
48	5	2508	PSU	N1-C2-N3	4.87	120.30	115.17
51	9	1232	PSU	C4-N3-C2	-4.86	119.68	126.37
48	5	4532	PSU	C4-N3-C2	-4.85	119.69	126.37
51	9	1367	PSU	C4-N3-C2	-4.84	119.70	126.37
48	5	2364	OMG	C2-N3-C4	4.83	120.62	112.30
51	9	512	A2M	C5-C4-N3	-4.83	120.06	126.72
48	5	1534	A2M	C5-C4-N3	-4.83	120.07	126.72
48	5	2815	A2M	C5-C4-N3	-4.82	120.09	126.72
48	5	4299	PSU	N1-C2-N3	4.80	120.23	115.17
48	5	3818	UY1	N1-C2-N3	4.80	120.23	115.17
48	5	3830	A2M	C5-C4-N3	-4.80	120.11	126.72
48	5	4530	UR3	C4-N3-C2	-4.80	120.72	124.58
48	5	1316	OMG	C2-N3-C4	4.80	120.56	112.30
48	5	1781	PSU	N1-C2-N3	4.79	120.22	115.17
51	9	649	PSU	N1-C2-N3	4.78	120.21	115.17
51	9	1367	PSU	N1-C2-N3	4.78	120.21	115.17
48	5	1524	A2M	C5-C4-N3	-4.77	120.15	126.72
51	9	468	A2M	C5-C4-N3	-4.77	120.15	126.72
51	9	1832	6MZ	C5-C4-N3	-4.76	120.16	126.72
48	5	4579	PSU	N1-C2-N3	4.76	120.19	115.17
48	5	4196	OMG	C2-N3-C4	4.76	120.49	112.30
48	5	1860	PSU	C4-N3-C2	-4.75	119.83	126.37
48	5	1792	PSU	N1-C2-N3	4.74	120.17	115.17
51	9	1692	PSU	C4-N3-C2	-4.74	119.84	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4293	PSU	N1-C2-N3	4.74	120.17	115.17
48	5	3734	PSU	C4-N3-C2	-4.73	119.85	126.37
48	5	3818	UY1	C4-N3-C2	-4.73	119.86	126.37
48	5	4571	A2M	C5-C4-N3	-4.73	120.20	126.72
51	9	572	PSU	C4-N3-C2	-4.73	119.86	126.37
51	9	1046	PSU	C4-N3-C2	-4.72	119.87	126.37
48	5	1522	OMG	C2-N3-C4	4.71	120.42	112.30
48	5	3627	OMG	C5-C4-N3	-4.71	120.89	128.39
48	5	3899	OMG	C2-N3-C4	4.71	120.41	112.30
48	5	4392	OMG	C2-N3-C4	4.70	120.39	112.30
48	5	373	OMG	C2-N3-C4	4.69	120.38	112.30
48	5	1326	A2M	C5-C4-N3	-4.68	120.27	126.72
51	9	159	A2M	C5-C4-N3	-4.68	120.27	126.72
48	5	3715	PSU	N1-C2-N3	4.67	120.09	115.17
51	9	1851	MA6	C4-C5-C6	4.67	120.74	115.91
51	9	1851	MA6	N9-C8-N7	-4.66	107.33	113.94
51	9	1177	PSU	N1-C2-N3	4.65	120.07	115.17
51	9	34	PSU	C4-N3-C2	-4.64	119.98	126.37
48	5	4618	OMG	C2-N3-C4	4.64	120.29	112.30
51	9	1639	G7M	C2-N3-C4	4.61	120.24	112.30
48	5	400	A2M	C5-C6-N6	4.61	134.70	123.29
51	9	1445	PSU	N1-C2-N3	4.61	120.03	115.17
48	5	3718	A2M	C5-C4-N3	-4.61	120.38	126.72
51	9	863	PSU	N1-C2-N3	4.60	120.02	115.17
51	9	166	A2M	C5-C4-N3	-4.59	120.40	126.72
51	9	683	OMG	C2-N3-C4	4.59	120.20	112.30
50	8	75	OMG	C2-N3-C4	4.57	120.17	112.30
51	9	1177	PSU	C4-N3-C2	-4.57	120.08	126.37
51	9	1850	MA6	N9-C8-N7	-4.57	107.46	113.94
48	5	4228	OMG	C2-N3-C4	4.56	120.16	112.30
48	5	4623	OMG	C2-N3-C4	4.56	120.16	112.30
51	9	1692	PSU	N1-C2-N3	4.55	119.97	115.17
51	9	1850	MA6	N3-C4-N9	4.53	134.88	127.17
48	5	1625	OMG	N9-C4-N3	4.53	135.01	125.95
48	5	3715	PSU	C4-N3-C2	-4.50	120.17	126.37
48	5	4306	OMU	N3-C2-N1	4.50	120.75	114.89
48	5	4370	OMG	C2-N3-C4	4.49	120.04	112.30
51	9	1328	OMG	C1'-N9-C4	-4.48	113.26	126.49
51	9	1832	6MZ	N9-C8-N7	-4.46	107.60	113.94
48	5	3792	OMG	C2-N3-C4	4.46	119.98	112.30
48	5	4637	OMG	C2-N3-C4	4.46	119.97	112.30
48	5	3627	OMG	C1'-N9-C4	-4.45	113.33	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1383	A2M	C5-C4-N3	-4.43	120.61	126.72
51	9	1445	PSU	C4-N3-C2	-4.43	120.27	126.37
48	5	237	B9B	O6-C6-C5	4.40	122.55	116.73
48	5	1524	A2M	N9-C8-N7	-4.39	107.71	113.94
48	5	4494	OMG	C2-N3-C4	4.38	119.85	112.30
48	5	4571	A2M	N9-C8-N7	-4.37	107.74	113.94
48	5	2876	OMG	N9-C4-N3	4.35	134.66	125.95
51	9	1031	A2M	C5-C4-N3	-4.34	120.74	126.72
51	9	1326	OMU	N3-C2-N1	4.34	120.54	114.89
48	5	4532	PSU	N1-C2-N3	4.33	119.74	115.17
48	5	4623	OMG	C1'-N9-C4	-4.30	113.78	126.49
48	5	2876	OMG	C2-N3-C4	4.30	119.70	112.30
51	9	801	PSU	N1-C2-N3	4.29	119.70	115.17
48	5	2424	OMG	C2-N3-C4	4.29	119.69	112.30
48	5	4457	PSU	N1-C2-N3	4.29	119.69	115.17
48	5	4420	PSU	O2-C2-N1	-4.25	118.40	122.79
51	9	1851	MA6	N3-C4-N9	4.24	134.37	127.17
51	9	815	PSU	O2-C2-N1	-4.23	118.43	122.79
48	5	4499	OMG	C2-N3-C4	4.23	119.58	112.30
51	9	1678	A2M	N9-C8-N7	-4.22	107.94	113.94
51	9	801	PSU	C4-N3-C2	-4.21	120.57	126.37
48	5	3925	OMU	C5-C4-N3	4.20	120.68	114.80
48	5	237	B9B	N9-C8-N7	-4.19	108.00	113.94
51	9	1328	OMG	C1'-N9-C8	4.18	138.61	126.73
51	9	1328	OMG	C2-N3-C4	4.18	119.50	112.30
48	5	1534	A2M	N9-C8-N7	-4.17	108.02	113.94
48	5	3627	OMG	C2-N3-C4	4.17	119.48	112.30
48	5	4498	OMU	C5-C4-N3	4.17	120.64	114.80
51	9	644	OMG	C2-N3-C4	4.16	119.47	112.30
48	5	2787	A2M	N9-C8-N7	-4.15	108.05	113.94
51	9	1490	OMG	C5-C4-N3	-4.14	121.80	128.39
51	9	863	PSU	O2-C2-N1	-4.14	118.52	122.79
48	5	1517	2MG	C2-N1-C6	-4.14	119.55	124.55
51	9	116	OMU	N3-C2-N1	4.13	120.27	114.89
51	9	1490	OMG	C2-N3-C4	4.11	119.38	112.30
48	5	1316	OMG	C1'-N9-C4	-4.10	114.38	126.49
48	5	237	B9B	C4-C5-C6	4.10	119.24	115.22
48	5	1871	A2M	C5-C4-N3	-4.09	121.08	126.72
51	9	436	OMG	C2-N3-C4	4.09	119.35	112.30
51	9	436	OMG	N9-C4-N3	4.09	134.13	125.95
48	5	3853	PSU	O2-C2-N1	-4.08	118.58	122.79
48	5	4620	OMU	C5-C4-N3	4.08	120.51	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	8	75	OMG	C1'-N9-C4	-4.07	114.47	126.49
48	5	4220	6MZ	N9-C8-N7	-4.05	108.20	113.94
48	5	4227	OMU	C5-C4-N3	4.04	120.46	114.80
48	5	3627	OMG	C1'-N9-C8	4.04	138.20	126.73
48	5	3718	A2M	N9-C8-N7	-4.03	108.22	113.94
48	5	3715	PSU	O2-C2-N1	-4.03	118.64	122.79
48	5	1522	OMG	C1'-N9-C4	-4.02	114.62	126.49
48	5	3818	UY1	C6-C5-C4	4.01	120.88	118.17
48	5	4370	OMG	C1'-N9-C4	-4.01	114.65	126.49
48	5	4228	OMG	C1'-N9-C4	-4.01	114.65	126.49
48	5	3867	A2M	N9-C8-N7	-4.00	108.26	113.94
51	9	686	PSU	O2-C2-N1	-4.00	118.66	122.79
51	9	1442	OMU	N3-C2-N1	4.00	120.09	114.89
48	5	400	A2M	N3-C4-N9	3.98	133.94	127.17
48	5	4623	OMG	C1'-N9-C8	3.98	138.05	126.73
48	5	1871	A2M	N9-C8-N7	-3.98	108.29	113.94
48	5	3760	A2M	N9-C8-N7	-3.97	108.30	113.94
48	5	1517	2MG	C5-C4-N3	-3.96	122.09	128.39
51	9	512	A2M	N9-C8-N7	-3.96	108.32	113.94
48	5	4498	OMU	N3-C2-N1	3.95	120.04	114.89
48	5	2815	A2M	N9-C8-N7	-3.95	108.33	113.94
51	9	509	OMG	C2-N3-C4	3.95	119.11	112.30
48	5	398	A2M	N9-C8-N7	-3.94	108.35	113.94
48	5	3785	A2M	O4'-C1'-N9	3.94	115.65	108.09
51	9	1248	B8N	N3-C2-N1	3.93	121.52	116.72
51	9	428	OMU	C5-C4-N3	3.93	120.30	114.80
48	5	2837	OMU	C5-C4-N3	3.92	120.30	114.80
48	5	4523	A2M	N9-C8-N7	-3.92	108.37	113.94
51	9	1031	A2M	N9-C8-N7	-3.91	108.39	113.94
48	5	3899	OMG	C1'-N9-C4	-3.91	114.94	126.49
51	9	572	PSU	O2-C2-N1	-3.90	118.76	122.79
48	5	2424	OMG	C1'-N9-C4	-3.90	114.98	126.49
48	5	2837	OMU	N3-C2-N1	3.89	119.95	114.89
51	9	99	A2M	N9-C8-N7	-3.89	108.42	113.94
48	5	3830	A2M	N9-C8-N7	-3.89	108.42	113.94
51	9	683	OMG	N9-C4-N3	3.89	133.73	125.95
51	9	668	A2M	N9-C8-N7	-3.87	108.45	113.94
48	5	4637	OMG	N9-C4-N3	3.87	133.69	125.95
51	9	121	OMU	C5-C4-N3	3.86	120.21	114.80
48	5	373	OMG	N9-C4-N3	3.86	133.67	125.95
50	8	75	OMG	C1'-N9-C8	3.86	137.69	126.73
51	9	1639	G7M	C5-C4-N3	-3.85	120.86	128.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1643	PSU	O2-C2-N1	-3.85	118.82	122.79
48	5	237	B9B	N3-C2-N1	-3.85	119.59	125.48
48	5	2787	A2M	N3-C4-N9	3.84	133.70	127.17
48	5	4499	OMG	N9-C4-N3	3.83	133.61	125.95
48	5	4620	OMU	N3-C2-N1	3.82	119.87	114.89
51	9	468	A2M	N9-C8-N7	-3.81	108.53	113.94
51	9	166	A2M	N9-C8-N7	-3.81	108.53	113.94
48	5	3925	OMU	N3-C2-N1	3.81	119.85	114.89
51	9	1851	MA6	C2-N3-C4	3.80	121.12	111.83
51	9	509	OMG	N9-C4-N3	3.80	133.55	125.95
48	5	4227	OMU	N3-C2-N1	3.80	119.84	114.89
48	5	4392	OMG	C1'-N9-C4	-3.79	115.28	126.49
51	9	1383	A2M	N9-C8-N7	-3.78	108.57	113.94
48	5	4306	OMU	C5-C4-N3	3.77	120.07	114.80
51	9	1639	G7M	C5-C6-N1	3.76	119.62	111.84
48	5	1517	2MG	N9-C8-N7	-3.76	106.43	113.40
48	5	4220	6MZ	C4-C5-C6	3.74	119.89	116.78
51	9	609	PSU	O2-C2-N1	-3.74	118.93	122.79
48	5	4500	PSU	O2-C2-N1	-3.74	118.94	122.79
48	5	4228	OMG	C1'-N9-C8	3.74	137.34	126.73
51	9	159	A2M	N9-C8-N7	-3.73	108.65	113.94
48	5	1522	OMG	C1'-N9-C8	3.73	137.32	126.73
48	5	4392	OMG	C1'-N9-C8	3.72	137.29	126.73
51	9	172	OMU	C5-C4-N3	3.71	120.00	114.80
48	5	237	B9B	C2-N1-C6	3.71	121.12	115.96
48	5	1326	A2M	N9-C8-N7	-3.70	108.68	113.94
48	5	4196	OMG	N9-C4-N3	3.70	133.35	125.95
48	5	3715	PSU	C6-C5-C4	3.70	120.67	118.17
48	5	1316	OMG	C1'-N9-C8	3.69	137.20	126.73
48	5	2424	OMG	C1'-N9-C8	3.69	137.20	126.73
48	5	237	B9B	N2-C2-N3	3.69	122.75	117.22
48	5	3785	A2M	N9-C8-N7	-3.68	108.71	113.94
51	9	172	OMU	N3-C2-N1	3.68	119.68	114.89
48	5	4618	OMG	C1'-N9-C4	-3.67	115.64	126.49
48	5	2363	A2M	N9-C8-N7	-3.67	108.73	113.94
51	9	1326	OMU	C5-C4-N3	3.64	119.90	114.80
48	5	3899	OMG	C1'-N9-C8	3.63	137.04	126.73
51	9	1832	6MZ	C2-N3-C4	3.62	120.68	111.83
48	5	4521	PSU	C6-C5-C4	3.62	120.61	118.17
48	5	4499	OMG	C1'-N9-C4	-3.61	115.83	126.49
48	5	2787	A2M	C2-N3-C4	3.61	120.64	111.83
48	5	4637	OMG	C1'-N9-C4	-3.60	115.84	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4494	OMG	C1'-N9-C4	-3.60	115.85	126.49
51	9	484	A2M	C2-N3-C4	3.58	120.59	111.83
48	5	3825	A2M	N3-C4-N9	3.56	133.22	127.17
51	9	512	A2M	C2-N3-C4	3.56	120.52	111.83
51	9	668	A2M	C2-N3-C4	3.54	120.47	111.83
48	5	3792	OMG	C1'-N9-C4	-3.54	116.04	126.49
48	5	3782	5MC	C5-C6-N1	-3.53	119.47	123.31
48	5	4530	UR3	C5-C4-N3	3.53	119.69	115.04
48	5	1862	PSU	O2-C2-N1	-3.53	119.14	122.79
48	5	4628	PSU	O2-C2-N1	-3.53	119.15	122.79
48	5	3825	A2M	N9-C8-N7	-3.52	108.94	113.94
51	9	121	OMU	N3-C2-N1	3.52	119.48	114.89
48	5	3724	A2M	N3-C4-N9	3.51	133.15	127.17
51	9	428	OMU	O4-C4-C5	-3.51	119.11	125.16
48	5	3867	A2M	C2-N3-C4	3.51	120.40	111.83
48	5	2364	OMG	N9-C4-N3	3.51	132.96	125.95
48	5	400	A2M	N9-C8-N7	-3.50	108.97	113.94
51	9	509	OMG	C1'-N9-C4	-3.50	116.14	126.49
48	5	398	A2M	C2-N3-C4	3.50	120.38	111.83
48	5	3818	UY1	C6-N1-C2	-3.50	119.44	122.69
51	9	436	OMG	C1'-N9-C4	-3.49	116.17	126.49
48	5	4623	OMG	C2-N1-C6	-3.48	118.79	125.11
51	9	484	A2M	N9-C8-N7	-3.47	109.01	113.94
48	5	3899	OMG	N9-C4-N3	3.47	132.90	125.95
51	9	1850	MA6	C4-N9-C8	3.47	109.38	105.74
48	5	2815	A2M	C2-N3-C4	3.47	120.30	111.83
51	9	218	PSU	C6-C5-C4	3.46	120.51	118.17
48	5	4392	OMG	C2-N1-C6	-3.46	118.83	125.11
48	5	4370	OMG	C1'-N9-C8	3.46	136.57	126.73
48	5	4571	A2M	C2-N3-C4	3.46	120.27	111.83
48	5	3830	A2M	C2'-C1'-N9	-3.45	108.07	113.75
48	5	3792	OMG	N9-C4-N3	3.45	132.86	125.95
48	5	1677	PSU	O2-C2-N1	-3.45	119.23	122.79
48	5	1625	OMG	C2-N1-C6	-3.45	118.85	125.11
48	5	2364	OMG	C1'-N9-C4	-3.45	116.30	126.49
48	5	4447	5MC	C5-C6-N1	-3.45	119.57	123.31
48	5	1625	OMG	O6-C6-C5	-3.44	117.45	126.53
48	5	373	OMG	C1'-N9-C4	-3.44	116.32	126.49
51	9	644	OMG	C1'-N9-C4	-3.44	116.33	126.49
48	5	4494	OMG	C1'-N9-C8	3.44	136.49	126.73
51	9	116	OMU	C5-C4-N3	3.43	119.61	114.80
48	5	3762	PSU	O2-C2-N1	-3.42	119.26	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	398	A2M	N3-C4-N9	3.42	132.99	127.17
48	5	3724	A2M	N9-C8-N7	-3.42	109.09	113.94
48	5	1322	1MA	N9-C8-N7	-3.42	107.06	113.40
51	9	822	PSU	C6-C5-C4	3.42	120.48	118.17
48	5	3785	A2M	C2-N3-C4	3.41	120.17	111.83
48	5	3920	PSU	O2-C2-N1	-3.41	119.27	122.79
48	5	4523	A2M	N3-C4-N9	3.41	132.97	127.17
48	5	4521	PSU	O2-C2-N1	-3.41	119.27	122.79
51	9	1678	A2M	C2-N3-C4	3.40	120.14	111.83
51	9	1174	PSU	O2-C2-N1	-3.38	119.30	122.79
48	5	3760	A2M	C2-N3-C4	3.38	120.09	111.83
51	9	166	A2M	C2-N3-C4	3.38	120.09	111.83
48	5	2424	OMG	C2-N1-C6	-3.37	118.99	125.11
48	5	4392	OMG	N9-C4-N3	3.37	132.70	125.95
51	9	644	OMG	C1'-N9-C8	3.37	136.29	126.73
48	5	2876	OMG	C2-N1-C6	-3.36	119.01	125.11
51	9	99	A2M	C2-N3-C4	3.36	120.03	111.83
48	5	3724	A2M	C2-N3-C4	3.35	120.02	111.83
48	5	2363	A2M	C2-N3-C4	3.35	120.01	111.83
51	9	683	OMG	C2-N1-C6	-3.34	119.06	125.11
48	5	1517	2MG	N2-C2-N3	-3.33	116.26	120.51
48	5	3830	A2M	N3-C4-N9	3.33	132.82	127.17
51	9	1639	G7M	O6-C6-C5	-3.32	120.59	128.01
48	5	2364	OMG	C2-N1-C6	-3.32	119.08	125.11
51	9	468	A2M	C2-N3-C4	3.32	119.95	111.83
48	5	4370	OMG	N9-C8-N7	-3.32	107.24	113.40
48	5	1322	1MA	C2-N3-C4	3.32	119.03	112.53
51	9	436	OMG	C2-N1-C6	-3.31	119.11	125.11
48	5	3718	A2M	C2'-C1'-N9	-3.31	108.31	113.75
48	5	1524	A2M	C2-N3-C4	3.31	119.91	111.83
51	9	683	OMG	C1'-N9-C4	-3.30	116.74	126.49
48	5	4370	OMG	N9-C4-N3	3.30	132.55	125.95
48	5	3830	A2M	C2-N3-C4	3.29	119.88	111.83
48	5	4220	6MZ	C2-N3-C4	3.29	119.86	111.83
51	9	509	OMG	C1'-N9-C8	3.28	136.05	126.73
48	5	1744	PSU	O2-C2-N1	-3.28	119.41	122.79
48	5	4523	A2M	C2-N3-C4	3.27	119.81	111.83
48	5	4618	OMG	C1'-N9-C8	3.26	136.00	126.73
48	5	1534	A2M	C2-N3-C4	3.26	119.79	111.83
51	9	822	PSU	O2-C2-N1	-3.25	119.43	122.79
48	5	1782	PSU	O2-C2-N1	-3.25	119.43	122.79
51	9	1442	OMU	C5-C4-N3	3.25	119.35	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1326	A2M	C2-N3-C4	3.25	119.76	111.83
48	5	1792	PSU	O2-C2-N1	-3.24	119.45	122.79
51	9	1851	MA6	C5-N7-C8	3.24	108.54	103.45
51	9	119	PSU	O2-C2-N1	-3.24	119.45	122.79
48	5	3825	A2M	C2-N3-C4	3.24	119.74	111.83
48	5	2787	A2M	C5-N7-C8	3.24	108.54	103.45
48	5	4499	OMG	C2-N1-C6	-3.24	119.24	125.11
51	9	1850	MA6	C2-N1-C6	3.23	119.71	111.83
48	5	3627	OMG	N9-C8-N7	-3.23	107.42	113.40
48	5	4353	PSU	C6-C5-C4	3.22	120.34	118.17
50	8	75	OMG	C2-N1-C6	-3.21	119.28	125.11
48	5	3867	A2M	N3-C4-N9	3.21	132.62	127.17
51	9	1442	OMU	O4-C4-C5	-3.21	119.63	125.16
51	9	34	PSU	C6-N1-C2	-3.21	119.72	122.69
51	9	1031	A2M	C2-N3-C4	3.20	119.66	111.83
51	9	428	OMU	N3-C2-N1	3.20	119.06	114.89
48	5	4618	OMG	C2-N1-C6	-3.19	119.32	125.11
48	5	237	B9B	C5-C6-N1	-3.19	119.22	123.49
48	5	4637	OMG	N9-C8-N7	-3.19	107.48	113.40
51	9	1832	6MZ	C5-N7-C8	3.19	108.46	103.45
51	9	683	OMG	CM2-O2'-C2'	3.18	122.65	114.47
48	5	4623	OMG	N9-C4-N3	3.18	132.32	125.95
51	9	1383	A2M	C2-N3-C4	3.18	119.61	111.83
48	5	2363	A2M	N3-C4-N9	3.18	132.58	127.17
48	5	4637	OMG	C2-N1-C6	-3.18	119.35	125.11
51	9	27	A2M	C2-N3-C4	3.17	119.57	111.83
51	9	468	A2M	N3-C4-N9	3.17	132.55	127.17
51	9	1490	OMG	N9-C8-N7	-3.16	107.53	113.40
48	5	3760	A2M	N3-C4-N9	3.16	132.54	127.17
51	9	1851	MA6	C2-N1-C6	3.16	119.55	111.83
48	5	4370	OMG	C2-N1-C6	-3.16	119.38	125.11
51	9	1850	MA6	C2-N3-C4	3.16	119.55	111.83
48	5	3792	OMG	C1'-N9-C8	3.15	135.69	126.73
48	5	4423	PSU	O2-C2-N1	-3.15	119.54	122.79
48	5	3718	A2M	C2-N3-C4	3.14	119.49	111.83
51	9	1678	A2M	C5-N7-C8	3.13	108.37	103.45
48	5	4623	OMG	C5-C6-N1	3.13	121.22	113.25
48	5	4228	OMG	N9-C4-N3	3.13	132.21	125.95
48	5	1524	A2M	C5-N7-C8	3.12	108.36	103.45
51	9	159	A2M	C2-N3-C4	3.12	119.44	111.83
48	5	3760	A2M	C5-N7-C8	3.12	108.35	103.45
48	5	4618	OMG	N9-C8-N7	-3.12	107.62	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4637	OMG	C1'-N9-C8	3.12	135.58	126.73
48	5	237	B9B	N3-C4-N9	3.11	130.94	126.99
51	9	27	A2M	N9-C8-N7	-3.11	109.52	113.94
48	5	400	A2M	C6-C5-C4	3.11	121.43	117.18
48	5	2364	OMG	N9-C8-N7	-3.11	107.63	113.40
48	5	4196	OMG	C2-N1-C6	-3.11	119.47	125.11
48	5	373	OMG	C2-N1-C6	-3.11	119.47	125.11
48	5	373	OMG	C1'-N9-C8	3.10	135.53	126.73
51	9	644	OMG	N9-C4-N3	3.09	132.14	125.95
51	9	683	OMG	N9-C8-N7	-3.09	107.67	113.40
51	9	27	A2M	N3-C4-N9	3.09	132.42	127.17
48	5	1524	A2M	N3-C4-N9	3.09	132.42	127.17
48	5	1326	A2M	N3-C4-N9	3.09	132.41	127.17
48	5	400	A2M	C2-N3-C4	3.08	119.36	111.83
51	9	512	A2M	C5-N7-C8	3.08	108.29	103.45
51	9	1328	OMG	C2-N1-C6	-3.08	119.53	125.11
48	5	1316	OMG	N9-C8-N7	-3.07	107.71	113.40
51	9	509	OMG	C2-N1-C6	-3.06	119.55	125.11
51	9	686	PSU	C6-C5-C4	3.06	120.24	118.17
48	5	4494	OMG	N9-C4-N3	3.05	132.06	125.95
48	5	1522	OMG	C2-N1-C6	-3.05	119.58	125.11
48	5	4442	PSU	O2-C2-N1	-3.05	119.65	122.79
48	5	373	OMG	N9-C8-N7	-3.04	107.77	113.40
48	5	2364	OMG	C1'-N9-C8	3.03	135.35	126.73
48	5	3851	PSU	O2-C2-N1	-3.03	119.66	122.79
48	5	4618	OMG	N9-C4-N3	3.03	132.00	125.95
48	5	4494	OMG	C2-N1-C6	-3.02	119.63	125.11
51	9	218	PSU	O2-C2-N1	-3.02	119.67	122.79
48	5	3785	A2M	N3-C4-N9	3.02	132.30	127.17
48	5	1534	A2M	C5-N7-C8	3.01	108.19	103.45
48	5	4500	PSU	C6-C5-C4	3.01	120.21	118.17
51	9	1328	OMG	N9-C4-N3	3.00	131.96	125.95
48	5	1871	A2M	C2-N3-C4	3.00	119.17	111.83
48	5	4499	OMG	O6-C6-C5	-3.00	118.61	126.53
48	5	3899	OMG	N9-C8-N7	-3.00	107.84	113.40
48	5	4499	OMG	N9-C8-N7	-2.99	107.85	113.40
48	5	1625	OMG	C1'-N9-C4	-2.99	117.66	126.49
48	5	1625	OMG	N9-C8-N7	-2.98	107.88	113.40
48	5	1316	OMG	C2-N1-C6	-2.97	119.72	125.11
48	5	4220	6MZ	C5-N7-C8	2.97	108.12	103.45
48	5	3851	PSU	C6-N1-C2	-2.97	119.93	122.69
51	9	1248	B8N	O4-C4-N3	-2.96	115.18	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	644	OMG	C2-N1-C6	-2.96	119.75	125.11
51	9	1326	OMU	O2-C2-N1	-2.96	118.95	122.80
51	9	1445	PSU	C6-N1-C2	-2.95	119.95	122.69
51	9	668	A2M	C5-N7-C8	2.95	108.09	103.45
51	9	436	OMG	C1'-N9-C8	2.95	135.11	126.73
51	9	1851	MA6	C4-N9-C8	2.95	108.83	105.74
48	5	237	B9B	C5-N7-C8	2.95	108.08	103.45
48	5	4499	OMG	C1'-N9-C8	2.95	135.10	126.73
48	5	3920	PSU	C6-C5-C4	2.94	120.16	118.17
48	5	4228	OMG	N9-C8-N7	-2.94	107.95	113.40
48	5	3627	OMG	C2-N1-C6	-2.94	119.78	125.11
48	5	1860	PSU	O2-C2-N1	-2.93	119.77	122.79
51	9	668	A2M	O4'-C1'-N9	-2.92	102.47	108.09
51	9	436	OMG	O6-C6-C5	-2.92	118.82	126.53
48	5	2837	OMU	O2-C2-N1	-2.92	118.99	122.80
48	5	2424	OMG	N9-C4-N3	2.92	131.79	125.95
48	5	4523	A2M	C5-N7-C8	2.92	108.04	103.45
51	9	1850	MA6	C5-N7-C8	2.92	108.04	103.45
51	9	814	PSU	O2-C2-N1	-2.92	119.78	122.79
48	5	4196	OMG	C1'-N9-C4	-2.91	117.89	126.49
51	9	99	A2M	N3-C4-N9	2.90	132.10	127.17
48	5	4498	OMU	O4-C4-C5	-2.90	120.16	125.16
48	5	4196	OMG	C1'-N9-C8	2.90	134.97	126.73
51	9	1328	OMG	N9-C8-N7	-2.90	108.03	113.40
51	9	1045	PSU	O2-C2-N1	-2.90	119.80	122.79
48	5	1316	OMG	N9-C4-N3	2.89	131.73	125.95
48	5	398	A2M	C5-N7-C8	2.88	107.98	103.45
51	9	116	OMU	O2-C2-N1	-2.88	119.05	122.80
48	5	1625	OMG	C5-C6-N1	2.88	120.57	113.25
51	9	436	OMG	N9-C8-N7	-2.87	108.07	113.40
48	5	4571	A2M	C5-N7-C8	2.87	107.96	103.45
48	5	4623	OMG	N9-C8-N7	-2.87	108.08	113.40
51	9	1238	PSU	C6-C5-C4	2.87	120.11	118.17
48	5	1522	OMG	N9-C8-N7	-2.86	108.09	113.40
48	5	1522	OMG	N9-C4-N3	2.86	131.67	125.95
48	5	4499	OMG	C5-C6-N1	2.86	120.52	113.25
51	9	512	A2M	C4-C5-N7	-2.86	107.32	110.58
48	5	2815	A2M	C5-N7-C8	2.85	107.94	103.45
51	9	105	PSU	C6-N1-C2	-2.85	120.05	122.69
48	5	3792	OMG	O6-C6-C5	-2.85	119.01	126.53
48	5	2424	OMG	N9-C8-N7	-2.85	108.12	113.40
51	9	668	A2M	N3-C4-N9	2.85	132.01	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	512	A2M	C5-C4-N9	2.84	108.91	105.81
48	5	4637	OMG	O6-C6-C5	-2.84	119.03	126.53
48	5	1326	A2M	C5-N7-C8	2.84	107.91	103.45
48	5	2815	A2M	N3-C4-N9	2.84	131.99	127.17
51	9	1842	4AC	O2-C2-N3	-2.83	117.86	122.33
51	9	1004	PSU	O2-C2-N1	-2.83	119.87	122.79
48	5	3825	A2M	C6-C5-C4	2.83	121.04	117.18
48	5	4228	OMG	C2-N1-C6	-2.82	119.99	125.11
50	8	75	OMG	N9-C4-N3	2.82	131.59	125.95
48	5	1534	A2M	N3-C4-N9	2.82	131.96	127.17
51	9	1244	PSU	O2-C2-N1	-2.81	119.89	122.79
48	5	4498	OMU	O2-C2-N1	-2.81	119.14	122.80
51	9	436	OMG	C5-C6-N1	2.81	120.41	113.25
51	9	683	OMG	C1'-N9-C8	2.81	134.71	126.73
51	9	1639	G7M	C2-N1-C6	-2.80	120.03	125.11
51	9	1045	PSU	C6-C5-C4	2.80	120.06	118.17
50	8	75	OMG	N9-C8-N7	-2.80	108.21	113.40
51	9	1678	A2M	N3-C4-N9	2.80	131.93	127.17
48	5	4196	OMG	C5-C6-N1	2.80	120.37	113.25
51	9	683	OMG	C5-C6-N1	2.79	120.36	113.25
48	5	1316	OMG	C5-C6-N1	2.79	120.36	113.25
48	5	2837	OMU	C2'-C1'-N1	-2.79	108.94	114.24
48	5	4579	PSU	O2-C2-N1	-2.79	119.91	122.79
48	5	4623	OMG	O6-C6-C5	-2.79	119.17	126.53
48	5	2424	OMG	O6-C6-C5	-2.79	119.17	126.53
51	9	649	PSU	O2-C2-N1	-2.79	119.91	122.79
48	5	3853	PSU	C6-N1-C2	-2.78	120.11	122.69
51	9	822	PSU	C6-N1-C2	-2.78	120.11	122.69
51	9	1326	OMU	O4-C4-C5	-2.78	120.37	125.16
51	9	121	OMU	O4-C4-C5	-2.77	120.39	125.16
48	5	4392	OMG	C5-C6-N1	2.76	120.29	113.25
51	9	815	PSU	C6-N1-C2	-2.76	120.13	122.69
48	5	2837	OMU	O4-C4-C5	-2.76	120.40	125.16
48	5	3639	PSU	O2-C2-N1	-2.76	119.95	122.79
48	5	1683	PSU	C6-N1-C2	-2.75	120.14	122.69
51	9	509	OMG	C5-C6-N1	2.74	120.22	113.25
51	9	34	PSU	O2-C2-N1	-2.73	119.97	122.79
48	5	4370	OMG	C5-C6-N1	2.72	120.19	113.25
48	5	4353	PSU	C6-N1-C2	-2.72	120.17	122.69
48	5	1683	PSU	O2-C2-N1	-2.72	119.98	122.79
51	9	1832	6MZ	N3-C4-N9	2.71	131.78	127.17
48	5	3792	OMG	N9-C8-N7	-2.71	108.38	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4220	6MZ	C4-C5-N7	-2.70	107.49	110.58
48	5	3718	A2M	N3-C4-N9	2.70	131.76	127.17
48	5	3899	OMG	C2-N1-C6	-2.70	120.22	125.11
48	5	4618	OMG	C5-C6-N1	2.70	120.11	113.25
50	8	75	OMG	C5-C6-N1	2.69	120.11	113.25
51	9	509	OMG	O6-C6-C5	-2.68	119.45	126.53
51	9	1232	PSU	C6-N1-C2	-2.68	120.20	122.69
51	9	166	A2M	C5-N7-C8	2.68	107.66	103.45
48	5	3830	A2M	C5-N7-C8	2.68	107.66	103.45
48	5	1522	OMG	C5-C6-N1	2.68	120.07	113.25
48	5	1781	PSU	O2-C2-N1	-2.68	120.03	122.79
48	5	2632	PSU	C6-N1-C2	-2.68	120.21	122.69
48	5	3825	A2M	C5-N7-C8	2.67	107.65	103.45
48	5	2632	PSU	O2-C2-N1	-2.67	120.03	122.79
51	9	1046	PSU	O2-C2-N1	-2.67	120.04	122.79
48	5	1517	2MG	C5-C6-N1	2.67	120.04	113.25
48	5	2424	OMG	C5-C6-N1	2.66	120.03	113.25
48	5	3785	A2M	C5-N7-C8	2.66	107.63	103.45
51	9	1832	6MZ	C4-C5-C6	2.66	118.99	116.78
48	5	4637	OMG	C5-C6-N1	2.66	120.02	113.25
51	9	109	PSU	C6-N1-C2	-2.66	120.22	122.69
51	9	1244	PSU	C6-C5-C4	2.65	119.97	118.17
48	5	3867	A2M	C5-N7-C8	2.65	107.62	103.45
48	5	4392	OMG	N9-C8-N7	-2.65	108.49	113.40
51	9	1174	PSU	C6-N1-C2	-2.65	120.23	122.69
51	9	1328	OMG	O6-C6-C5	-2.65	119.55	126.53
48	5	4521	PSU	C6-N1-C2	-2.64	120.24	122.69
48	5	4628	PSU	C6-C5-C4	2.64	119.96	118.17
48	5	4494	OMG	N9-C8-N7	-2.64	108.50	113.40
48	5	1517	2MG	O6-C6-C5	-2.64	119.55	126.53
48	5	373	OMG	C5-C6-N1	2.64	119.98	113.25
48	5	237	B9B	C4-C5-N7	-2.64	107.56	110.58
48	5	1871	A2M	C2'-C1'-N9	-2.64	109.41	113.75
51	9	121	OMU	CM2-O2'-C2'	2.64	121.24	114.47
48	5	2787	A2M	C6-C5-C4	2.64	120.78	117.18
48	5	2364	OMG	C5-C6-N1	2.63	119.96	113.25
48	5	4442	PSU	C6-C5-C4	2.63	119.95	118.17
48	5	3792	OMG	C2-N1-C6	-2.63	120.35	125.11
48	5	1322	1MA	C5-C4-N3	-2.62	123.41	127.27
48	5	4220	6MZ	N3-C4-N9	2.62	131.63	127.17
51	9	484	A2M	N3-C4-N9	2.62	131.62	127.17
48	5	2363	A2M	C5-N7-C8	2.61	107.56	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	468	A2M	C5-N7-C8	2.61	107.55	103.45
51	9	1490	OMG	O6-C6-C5	-2.61	119.65	126.53
48	5	3627	OMG	C5-C6-N1	2.60	119.88	113.25
48	5	3764	PSU	O2-C2-N1	-2.60	120.11	122.79
51	9	1328	OMG	C5-C6-N1	2.60	119.87	113.25
48	5	1524	A2M	C4'-O4'-C1'	-2.60	103.72	109.47
48	5	3760	A2M	C4-C5-N7	-2.60	107.61	110.58
48	5	3925	OMU	O4-C4-C5	-2.59	120.70	125.16
51	9	1678	A2M	C4-C5-N7	-2.59	107.63	110.58
51	9	1046	PSU	C6-N1-C2	-2.59	120.29	122.69
51	9	159	A2M	N3-C4-N9	2.58	131.56	127.17
48	5	1860	PSU	C6-N1-C2	-2.58	120.30	122.69
48	5	4571	A2M	N3-C4-N9	2.58	131.55	127.17
48	5	4530	UR3	C6-N1-C2	-2.58	119.69	121.80
51	9	1639	G7M	N9-C4-N3	2.57	131.10	125.95
48	5	1871	A2M	N3-C4-N9	2.56	131.53	127.17
51	9	1383	A2M	C5-N7-C8	2.56	107.48	103.45
51	9	1639	G7M	CN7-N7-C5	2.56	129.99	126.80
48	5	3695	PSU	C6-N1-C2	-2.56	120.31	122.69
48	5	1517	2MG	C8-N7-C5	2.56	108.81	104.26
48	5	1782	PSU	C6-C5-C4	2.56	119.90	118.17
48	5	4361	PSU	O2-C2-N1	-2.55	120.15	122.79
51	9	99	A2M	C5-N7-C8	2.55	107.46	103.45
51	9	1850	MA6	C6-C5-N7	-2.55	129.37	133.43
51	9	1832	6MZ	C4-C5-N7	-2.55	107.67	110.58
51	9	1031	A2M	N3-C4-N9	2.55	131.50	127.17
51	9	644	OMG	N9-C8-N7	-2.55	108.68	113.40
51	9	484	A2M	C5-N7-C8	2.54	107.45	103.45
48	5	4442	PSU	C6-N1-C2	-2.54	120.33	122.69
51	9	572	PSU	C6-N1-C2	-2.54	120.33	122.69
48	5	4392	OMG	O6-C6-C5	-2.54	119.84	126.53
48	5	4620	OMU	O4-C4-C5	-2.53	120.79	125.16
48	5	4618	OMG	O6-C6-C5	-2.53	119.85	126.53
48	5	2876	OMG	N9-C8-N7	-2.53	108.71	113.40
51	9	1347	PSU	O2-C2-N1	-2.52	120.19	122.79
48	5	3627	OMG	N9-C4-N3	2.52	131.00	125.95
51	9	159	A2M	C5-N7-C8	2.52	107.41	103.45
48	5	4500	PSU	C6-N1-C2	-2.52	120.36	122.69
48	5	4299	PSU	O2-C2-N1	-2.52	120.19	122.79
48	5	1625	OMG	C1'-N9-C8	2.52	133.88	126.73
51	9	1367	PSU	C6-N1-C2	-2.51	120.36	122.69
48	5	4227	OMU	O4-C4-C5	-2.51	120.84	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	172	OMU	O4-C4-C5	-2.51	120.84	125.16
51	9	428	OMU	O2-C2-N1	-2.50	119.54	122.80
51	9	815	PSU	C6-C5-C4	2.50	119.86	118.17
48	5	1871	A2M	C5-N7-C8	2.50	107.37	103.45
48	5	1524	A2M	C4-N9-C8	2.49	108.35	105.74
48	5	2364	OMG	C8-N7-C5	2.49	108.69	104.26
51	9	801	PSU	C6-N1-C2	-2.49	120.38	122.69
48	5	1522	OMG	C2'-C1'-N9	-2.49	109.52	114.24
48	5	4494	OMG	C5-C6-N1	2.49	119.58	113.25
48	5	237	B9B	C2-N3-C4	2.48	120.16	113.51
51	9	1445	PSU	O2-C2-N1	-2.48	120.23	122.79
51	9	172	OMU	O2-C2-N1	-2.48	119.57	122.80
48	5	2824	OMC	O2-C2-N3	-2.48	118.42	122.33
51	9	1177	PSU	C6-N1-C2	-2.48	120.39	122.69
48	5	373	OMG	C8-N7-C5	2.48	108.67	104.26
51	9	468	A2M	C5'-C4'-C3'	-2.47	106.31	115.21
48	5	4370	OMG	C8-N7-C5	2.47	108.66	104.26
48	5	4353	PSU	O2-C2-N1	-2.47	120.24	122.79
51	9	484	A2M	C5-C4-N9	2.47	108.50	105.81
51	9	1692	PSU	O2-C2-N1	-2.46	120.25	122.79
51	9	116	OMU	O4-C4-C5	-2.46	120.92	125.16
48	5	4552	PSU	O2-C2-N1	-2.46	120.25	122.79
48	5	4196	OMG	N9-C8-N7	-2.46	108.84	113.40
48	5	4227	OMU	O2-C2-N1	-2.46	119.60	122.80
48	5	400	A2M	C5-N7-C8	2.46	107.31	103.45
48	5	3899	OMG	C5-C6-N1	2.46	119.51	113.25
48	5	3792	OMG	C5-C6-N1	2.45	119.50	113.25
51	9	668	A2M	C4-C5-N7	-2.45	107.78	110.58
51	9	801	PSU	O2-C2-N1	-2.45	120.26	122.79
51	9	1248	B8N	C31-N3-C4	2.45	120.64	117.18
51	9	683	OMG	C8-N7-C5	2.45	108.62	104.26
48	5	4228	OMG	C5-C6-N1	2.44	119.46	113.25
48	5	4447	5MC	CM5-C5-C6	-2.44	119.55	122.85
51	9	166	A2M	N3-C4-N9	2.44	131.31	127.17
48	5	3715	PSU	C6-N1-C2	-2.43	120.43	122.69
48	5	3627	OMG	C8-N7-C5	2.43	108.58	104.26
48	5	4420	PSU	C6-N1-C2	-2.42	120.44	122.69
51	9	1081	PSU	C6-C5-C4	2.42	119.81	118.17
48	5	3899	OMG	C8-N7-C5	2.42	108.57	104.26
51	9	1383	A2M	N3-C4-N9	2.42	131.28	127.17
50	8	75	OMG	O6-C6-C5	-2.41	120.16	126.53
48	5	3718	A2M	C5-N7-C8	2.41	107.24	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1517	2MG	C4-C5-N7	-2.41	106.85	110.67
51	9	609	PSU	C6-N1-C2	-2.41	120.46	122.69
51	9	1004	PSU	C6-N1-C2	-2.40	120.46	122.69
48	5	4296	PSU	C6-N1-C2	-2.40	120.47	122.69
51	9	644	OMG	C5-C6-N1	2.39	119.34	113.25
48	5	3734	PSU	C6-C5-C4	2.39	119.78	118.17
48	5	4196	OMG	O6-C6-C5	-2.38	120.24	126.53
51	9	119	PSU	C6-N1-C2	-2.38	120.49	122.69
51	9	1367	PSU	O2-C2-N1	-2.37	120.34	122.79
48	5	4637	OMG	C8-N7-C5	2.37	108.48	104.26
51	9	1045	PSU	C6-N1-C2	-2.37	120.49	122.69
48	5	237	B9B	C5-C4-N9	2.36	108.38	105.81
48	5	4494	OMG	O6-C6-C5	-2.36	120.31	126.53
48	5	4293	PSU	C6-N1-C2	-2.36	120.50	122.69
51	9	1031	A2M	C5-N7-C8	2.35	107.15	103.45
51	9	1832	6MZ	C4-N9-C8	2.35	108.20	105.74
48	5	3764	PSU	C6-N1-C2	-2.35	120.52	122.69
51	9	1347	PSU	C6-N1-C2	-2.35	120.52	122.69
48	5	1316	OMG	C8-N7-C5	2.34	108.43	104.26
48	5	4220	6MZ	C5-C4-N9	2.34	108.36	105.81
48	5	4457	PSU	O2-C2-N1	-2.34	120.38	122.79
48	5	1517	2MG	C6-C5-N7	2.34	134.54	130.29
48	5	3734	PSU	C6-N1-C2	-2.33	120.53	122.69
48	5	1340	OMC	C5-C4-N3	-2.33	117.39	121.32
48	5	2876	OMG	C5-C6-N1	2.33	119.19	113.25
48	5	3760	A2M	C6-C5-C4	2.33	120.36	117.18
48	5	1781	PSU	C6-C5-C4	2.32	119.74	118.17
48	5	398	A2M	C6-C5-C4	2.32	120.35	117.18
51	9	822	PSU	O4'-C1'-C2'	2.32	108.36	105.15
48	5	4618	OMG	C8-N7-C5	2.32	108.39	104.26
48	5	1517	2MG	N1-C2-N3	-2.32	119.78	123.68
48	5	3695	PSU	O2-C2-N1	-2.31	120.40	122.79
51	9	509	OMG	N9-C8-N7	-2.31	109.12	113.40
48	5	4370	OMG	O6-C6-C5	-2.31	120.44	126.53
51	9	668	A2M	C5-C4-N9	2.31	108.32	105.81
51	9	814	PSU	C6-N1-C2	-2.31	120.55	122.69
48	5	3724	A2M	C6-C5-C4	2.30	120.32	117.18
48	5	1534	A2M	C6-C5-C4	2.30	120.32	117.18
48	5	3899	OMG	O6-C6-C5	-2.30	120.46	126.53
48	5	3718	A2M	O4'-C1'-N9	2.30	112.50	108.09
48	5	3762	PSU	C6-N1-C2	-2.30	120.56	122.69
51	9	1490	OMG	C2-N1-C6	-2.30	120.95	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3724	A2M	C5-N7-C8	2.29	107.05	103.45
48	5	3701	OMC	O2-C2-N3	-2.29	118.72	122.33
51	9	468	A2M	C4-N9-C8	2.29	108.14	105.74
48	5	3734	PSU	O2-C2-N1	-2.29	120.43	122.79
51	9	27	A2M	C5-N7-C8	2.28	107.04	103.45
51	9	683	OMG	O6-C6-C5	-2.28	120.51	126.53
48	5	1522	OMG	O6-C6-C5	-2.28	120.52	126.53
48	5	2364	OMG	O6-C6-C5	-2.28	120.52	126.53
48	5	373	OMG	O6-C6-C5	-2.28	120.52	126.53
48	5	2876	OMG	C8-N7-C5	2.27	108.31	104.26
51	9	1081	PSU	O4'-C1'-C2'	2.27	108.29	105.15
48	5	1871	A2M	C4-N9-C8	2.27	108.12	105.74
51	9	512	A2M	N3-C4-N9	2.27	131.03	127.17
51	9	166	A2M	C5-C4-N9	2.27	108.28	105.81
48	5	4228	OMG	O6-C6-C5	-2.26	120.56	126.53
51	9	1081	PSU	O2-C2-N1	-2.26	120.45	122.79
51	9	1177	PSU	O2-C2-N1	-2.26	120.46	122.79
48	5	2508	PSU	O2-C2-N1	-2.26	120.46	122.79
48	5	1862	PSU	C6-C5-C4	2.26	119.70	118.17
51	9	1383	A2M	C2'-C3'-C4'	-2.26	97.14	101.99
51	9	814	PSU	C6-C5-C4	2.25	119.69	118.17
48	5	3715	PSU	O4'-C1'-C2'	2.25	108.26	105.15
51	9	1383	A2M	C2'-C1'-N9	-2.25	110.06	113.75
51	9	1081	PSU	C6-N1-C2	-2.24	120.61	122.69
48	5	4523	A2M	C4-N9-C8	2.24	108.09	105.74
51	9	218	PSU	C5-C6-N1	-2.24	119.03	122.14
51	9	218	PSU	C6-N1-C2	-2.24	120.61	122.69
51	9	1490	OMG	C5-C6-N1	2.24	118.95	113.25
48	5	4571	A2M	C5-C4-N9	2.24	108.25	105.81
48	5	1534	A2M	C4-C5-N7	-2.23	108.03	110.58
48	5	1517	2MG	C1'-N9-C8	-2.22	120.41	126.73
48	5	3627	OMG	O6-C6-C5	-2.22	120.67	126.53
48	5	2508	PSU	C6-N1-C2	-2.22	120.63	122.69
51	9	27	A2M	C6-C5-C4	2.22	120.21	117.18
48	5	4618	OMG	N2-C2-N1	2.21	121.44	116.76
48	5	2815	A2M	C4-C5-N7	-2.21	108.06	110.58
51	9	1238	PSU	C5-C6-N1	-2.20	119.09	122.14
48	5	2876	OMG	O6-C6-C5	-2.20	120.73	126.53
48	5	3818	UY1	O4'-C1'-C2'	2.20	108.41	104.56
48	5	4571	A2M	C4-C5-N7	-2.19	108.07	110.58
48	5	1534	A2M	C2'-C1'-N9	2.19	117.36	113.75
51	9	484	A2M	C4-C5-N7	-2.19	108.08	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4628	PSU	C6-N1-C2	-2.19	120.66	122.69
51	9	1639	G7M	N2-C2-N1	2.19	121.38	116.76
48	5	4228	OMG	C8-N7-C5	2.18	108.15	104.26
51	9	99	A2M	C6-C5-C4	2.18	120.16	117.18
48	5	2876	OMG	C6-C5-C4	2.18	122.11	118.83
48	5	398	A2M	C4-C5-N7	-2.18	108.09	110.58
51	9	119	PSU	C6-C5-C4	2.18	119.64	118.17
51	9	1248	B8N	O4-C4-C5	-2.18	118.81	122.58
48	5	3639	PSU	C6-N1-C2	-2.18	120.67	122.69
51	9	649	PSU	C6-N1-C2	-2.18	120.67	122.69
48	5	3920	PSU	C6-N1-C2	-2.18	120.67	122.69
48	5	4306	OMU	O2-C2-N1	-2.18	119.96	122.80
51	9	668	A2M	C2'-C1'-N9	2.17	117.33	113.75
48	5	4494	OMG	N2-C2-N1	2.17	121.35	116.76
51	9	159	A2M	C5-C4-N9	2.16	108.17	105.81
48	5	3782	5MC	CM5-C5-C6	-2.16	119.92	122.85
51	9	1031	A2M	C4-N9-C8	2.16	108.01	105.74
51	9	109	PSU	O2-C2-N1	-2.16	120.56	122.79
50	8	75	OMG	C8-N7-C5	2.16	108.11	104.26
48	5	1316	OMG	O6-C6-C5	-2.16	120.83	126.53
51	9	1244	PSU	C6-N1-C2	-2.16	120.69	122.69
51	9	159	A2M	C4-C5-N7	-2.15	108.12	110.58
48	5	237	B9B	C61-O6-C6	2.15	121.41	117.66
48	5	4579	PSU	C6-N1-C2	-2.15	120.69	122.69
48	5	1522	OMG	C8-N7-C5	2.15	108.09	104.26
48	5	3825	A2M	C2'-C1'-N9	-2.15	110.21	113.75
48	5	1524	A2M	C6-C5-C4	2.15	120.11	117.18
51	9	1643	PSU	C6-N1-C2	-2.14	120.70	122.69
48	5	1524	A2M	C4-C5-N7	-2.14	108.13	110.58
48	5	1744	PSU	C6-N1-C2	-2.14	120.71	122.69
48	5	1782	PSU	C6-N1-C2	-2.13	120.71	122.69
51	9	166	A2M	C4-C5-N7	-2.13	108.15	110.58
48	5	4571	A2M	C4-N9-C8	2.13	107.97	105.74
48	5	237	B9B	C4-N9-C8	2.13	107.97	105.74
51	9	99	A2M	C5-C4-N9	2.13	108.13	105.81
48	5	4552	PSU	C6-N1-C2	-2.13	120.72	122.69
48	5	1625	OMG	C8-N7-C5	2.13	108.05	104.26
51	9	668	A2M	C3'-C2'-C1'	2.13	106.88	102.81
48	5	398	A2M	C2'-C1'-N9	-2.12	110.26	113.75
48	5	373	OMG	C2'-C1'-N9	-2.12	110.22	114.24
50	8	75	OMG	N2-C2-N1	2.12	121.23	116.76
51	9	1678	A2M	C4-N9-C8	2.11	107.95	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2861	OMC	O2-C2-N3	-2.11	119.01	122.33
48	5	4423	PSU	C6-N1-C2	-2.10	120.74	122.69
51	9	1383	A2M	C5-C4-N9	2.10	108.10	105.81
51	9	1391	OMC	O2-C2-N3	-2.10	119.02	122.33
48	5	1677	PSU	C6-C5-C4	2.10	119.59	118.17
48	5	1522	OMG	N2-C2-N1	2.10	121.19	116.76
51	9	1678	A2M	C5-C4-N9	2.10	108.10	105.81
51	9	1347	PSU	O4-C4-C5	-2.10	118.80	124.01
48	5	4361	PSU	C6-N1-C2	-2.09	120.75	122.69
51	9	1046	PSU	O4'-C1'-C2'	2.09	108.05	105.15
48	5	3760	A2M	C5-C4-N9	2.08	108.08	105.81
51	9	105	PSU	O2-C2-N1	-2.08	120.64	122.79
48	5	4530	UR3	C1'-N1-C2	2.08	120.44	117.04
48	5	4403	PSU	C6-N1-C2	-2.07	120.77	122.69
51	9	121	OMU	C1'-N1-C2	2.07	121.32	117.59
48	5	4403	PSU	O4'-C1'-C2'	2.07	108.02	105.15
51	9	1832	6MZ	C5-C4-N9	2.07	108.06	105.81
48	5	4293	PSU	O4-C4-C5	-2.07	118.87	124.01
48	5	4521	PSU	C5-C6-N1	-2.06	119.28	122.14
48	5	4521	PSU	O4'-C1'-C2'	2.06	108.01	105.15
48	5	4628	PSU	O4'-C1'-C2'	2.06	108.00	105.15
51	9	1337	4AC	C5-C4-N4	2.06	126.41	122.94
51	9	644	OMG	C8-N7-C5	2.06	107.92	104.26
48	5	3830	A2M	C4-N9-C8	2.06	107.90	105.74
48	5	4196	OMG	C8-N7-C5	2.05	107.92	104.26
51	9	1639	G7M	N9-C8-N7	-2.05	107.50	112.48
48	5	3887	OMC	C2'-C1'-N1	-2.05	110.34	114.24
51	9	686	PSU	O4-C4-C5	-2.05	118.91	124.01
48	5	1862	PSU	C6-N1-C2	-2.05	120.79	122.69
48	5	4523	A2M	C6-C5-C4	2.05	119.98	117.18
48	5	2787	A2M	C4-C5-N7	-2.04	108.25	110.58
48	5	2363	A2M	C6-C5-C4	2.04	119.96	117.18
48	5	4532	PSU	O2-C2-N1	-2.04	120.69	122.79
48	5	1340	OMC	C6-C5-C4	2.04	120.87	117.53
51	9	1842	4AC	C6-C5-C4	2.04	119.45	117.00
48	5	3762	PSU	C6-C5-C4	2.03	119.54	118.17
48	5	4361	PSU	C6-C5-C4	2.03	119.54	118.17
48	5	3718	A2M	C6-C5-C4	2.03	119.95	117.18
48	5	1781	PSU	C6-N1-C2	-2.03	120.81	122.69
48	5	3853	PSU	O4'-C1'-C2'	2.02	107.95	105.15
48	5	3627	OMG	C4-C5-N7	-2.02	107.47	110.67
48	5	4370	OMG	N2-C2-N1	2.02	121.02	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4523	A2M	C4-C5-N7	-2.02	108.28	110.58
51	9	686	PSU	C6-N1-C2	-2.02	120.82	122.69
51	9	218	PSU	O4'-C1'-C2'	2.01	107.94	105.15
48	5	3830	A2M	C6-C5-C4	2.01	119.92	117.18
48	5	3764	PSU	C6-C5-C4	2.01	119.53	118.17
48	5	4620	OMU	O2-C2-N1	-2.00	120.19	122.80
48	5	3785	A2M	C5-C4-N9	2.00	107.99	105.81

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	5	237	B9B	C5-C6-O6-C61
48	5	237	B9B	N1-C6-O6-C61
48	5	1781	PSU	C3'-C4'-C5'-O5'
48	5	2424	OMG	O4'-C4'-C5'-O5'
48	5	2424	OMG	C1'-C2'-O2'-CM2
48	5	3701	OMC	C2'-C1'-N1-C2
48	5	3701	OMC	C2'-C1'-N1-C6
48	5	4228	OMG	C3'-C2'-O2'-CM2
48	5	4500	PSU	O4'-C4'-C5'-O5'
51	9	34	PSU	O4'-C4'-C5'-O5'
51	9	121	OMU	C1'-C2'-O2'-CM2
51	9	166	A2M	C3'-C4'-C5'-O5'
51	9	683	OMG	C1'-C2'-O2'-CM2
51	9	1248	B8N	C31-C32-C33-N34
51	9	1328	OMG	C1'-C2'-O2'-CM2
51	9	1851	MA6	O4'-C4'-C5'-O5'
48	5	2364	OMG	O4'-C4'-C5'-O5'
48	5	4500	PSU	C3'-C4'-C5'-O5'
51	9	99	A2M	O4'-C4'-C5'-O5'
51	9	166	A2M	O4'-C4'-C5'-O5'
51	9	801	PSU	C3'-C4'-C5'-O5'
51	9	822	PSU	C3'-C4'-C5'-O5'
48	5	1781	PSU	O4'-C4'-C5'-O5'
48	5	2424	OMG	C3'-C4'-C5'-O5'
48	5	2815	A2M	O4'-C4'-C5'-O5'
48	5	3760	A2M	C3'-C4'-C5'-O5'
51	9	34	PSU	C3'-C4'-C5'-O5'
51	9	822	PSU	O4'-C4'-C5'-O5'
51	9	1045	PSU	C3'-C4'-C5'-O5'
51	9	1442	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
51	9	1639	G7M	O4'-C4'-C5'-O5'
51	9	1639	G7M	C3'-C4'-C5'-O5'
51	9	1703	OMC	O4'-C4'-C5'-O5'
48	5	3818	UY1	O4'-C4'-C5'-O5'
51	9	668	A2M	O4'-C4'-C5'-O5'
51	9	668	A2M	C3'-C4'-C5'-O5'
51	9	1045	PSU	O4'-C4'-C5'-O5'
51	9	1851	MA6	C3'-C4'-C5'-O5'
48	5	3760	A2M	O4'-C4'-C5'-O5'
48	5	3785	A2M	O4'-C4'-C5'-O5'
48	5	3785	A2M	C3'-C4'-C5'-O5'
48	5	3818	UY1	C3'-C4'-C5'-O5'
51	9	99	A2M	C3'-C4'-C5'-O5'
51	9	172	OMU	O4'-C4'-C5'-O5'
51	9	801	PSU	O4'-C4'-C5'-O5'
48	5	4447	5MC	C2'-C1'-N1-C6
51	9	428	OMU	C2'-C1'-N1-C6
48	5	2364	OMG	C3'-C4'-C5'-O5'
51	9	172	OMU	C3'-C4'-C5'-O5'
51	9	1442	OMU	C3'-C4'-C5'-O5'
51	9	1490	OMG	O4'-C4'-C5'-O5'
48	5	2787	A2M	C2'-C1'-N9-C4
48	5	2787	A2M	C2'-C1'-N9-C8
48	5	3818	UY1	C4'-C5'-O5'-P
48	5	1625	OMG	C3'-C2'-O2'-CM2
48	5	2815	A2M	C3'-C4'-C5'-O5'
51	9	512	A2M	O4'-C4'-C5'-O5'
51	9	1248	B8N	C32-C33-C34-O35
48	5	1534	A2M	C4'-C5'-O5'-P
51	9	668	A2M	C2'-C1'-N9-C8
51	9	1832	6MZ	N1-C6-N6-C9
48	5	4447	5MC	O4'-C1'-N1-C6
48	5	3792	OMG	C3'-C4'-C5'-O5'
51	9	683	OMG	C3'-C4'-C5'-O5'
51	9	1248	B8N	N3-C31-C32-C33
51	9	1832	6MZ	C5-C6-N6-C9
51	9	1248	B8N	C32-C33-C34-O36
51	9	428	OMU	O4'-C1'-N1-C6
51	9	1490	OMG	C4'-C5'-O5'-P
48	5	4447	5MC	O4'-C1'-N1-C2
48	5	4447	5MC	C2'-C1'-N1-C2
48	5	1524	A2M	C3'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
51	9	1031	A2M	C3'-C2'-O2'-CM'
48	5	1326	A2M	C4'-C5'-O5'-P
51	9	34	PSU	O4'-C1'-C5-C4
51	9	1445	PSU	O4'-C1'-C5-C4
51	9	468	A2M	C3'-C4'-C5'-O5'
48	5	3701	OMC	O4'-C1'-N1-C6
48	5	3792	OMG	O4'-C4'-C5'-O5'
51	9	644	OMG	C4'-C5'-O5'-P
48	5	3851	PSU	C3'-C4'-C5'-O5'
48	5	4499	OMG	C3'-C2'-O2'-CM2
48	5	1322	1MA	C2'-C1'-N9-C4
51	9	1851	MA6	C4'-C5'-O5'-P
51	9	428	OMU	C2'-C1'-N1-C2
48	5	3701	OMC	O4'-C1'-N1-C2
48	5	2364	OMG	C1'-C2'-O2'-CM2
48	5	2837	OMU	C3'-C4'-C5'-O5'
51	9	863	PSU	C3'-C4'-C5'-O5'
51	9	1703	OMC	C3'-C4'-C5'-O5'
51	9	34	PSU	O4'-C1'-C5-C6
51	9	428	OMU	O4'-C1'-N1-C2
48	5	2787	A2M	O4'-C1'-N9-C8
48	5	3867	A2M	C3'-C4'-C5'-O5'
48	5	1322	1MA	C2'-C1'-N9-C8
48	5	3760	A2M	C3'-C2'-O2'-CM'
48	5	4494	OMG	C3'-C2'-O2'-CM2
48	5	1534	A2M	O4'-C4'-C5'-O5'
51	9	683	OMG	O4'-C4'-C5'-O5'
51	9	863	PSU	O4'-C4'-C5'-O5'
48	5	3785	A2M	C2'-C1'-N9-C8
48	5	373	OMG	C4'-C5'-O5'-P
48	5	2351	OMC	C2'-C1'-N1-C2

There are no ring outliers.

55 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	9	1337	4AC	1	0
48	5	4447	5MC	1	0
51	9	174	OMC	1	0
51	9	863	PSU	3	0
48	5	1322	1MA	1	0
48	5	3899	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	9	801	PSU	1	0
51	9	218	PSU	3	0
51	9	1850	MA6	1	0
51	9	166	A2M	1	0
51	9	116	OMU	2	0
51	9	1326	OMU	1	0
51	9	1244	PSU	1	0
48	5	373	OMG	1	0
51	9	109	PSU	2	0
48	5	400	A2M	2	0
51	9	686	PSU	1	0
48	5	3792	OMG	2	0
50	8	75	OMG	2	0
51	9	1639	G7M	1	0
48	5	4196	OMG	1	0
51	9	105	PSU	2	0
51	9	484	A2M	1	0
51	9	1442	OMU	3	0
48	5	3867	A2M	2	0
48	5	2876	OMG	1	0
51	9	1445	PSU	2	0
51	9	1391	OMC	1	0
51	9	1703	OMC	1	0
51	9	1367	PSU	1	0
48	5	2364	OMG	2	0
51	9	1490	OMG	2	0
48	5	1316	OMG	1	0
51	9	34	PSU	2	0
48	5	3808	OMC	2	0
51	9	1842	4AC	2	0
51	9	121	OMU	1	0
48	5	4456	OMC	1	0
51	9	1232	PSU	2	0
48	5	3701	OMC	1	0
51	9	1328	OMG	1	0
48	5	4637	OMG	1	0
51	9	1692	PSU	2	0
48	5	2424	OMG	1	0
48	5	3818	UY1	2	0
48	5	2351	OMC	2	0
48	5	1340	OMC	1	0
48	5	4420	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	5	1871	A2M	1	0
48	5	3718	A2M	1	0
51	9	172	OMU	2	0
48	5	4370	OMG	1	0
51	9	1347	PSU	1	0
51	9	159	A2M	1	0
51	9	27	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 323 ligands modelled in this entry, 320 are monoatomic - leaving 3 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	$\# Z > 2$
91	SF4	jj	601	87	0,12,12	-	-	-		
90	ZVM	ii	501	88	30,31,31	4.96	21 (70%)	32,46,46	3.11	7 (21%)
91	SF4	jj	602	87	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	SF4	jj	601	87	-	-	0/6/5/5
90	ZVM	ii	501	88	2/2/8/8	0/4/50/50	0/3/5/5
91	SF4	jj	602	87	-	-	0/6/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	ii	501	ZVM	O01-C01	12.83	1.39	1.22
90	ii	501	ZVM	O02-C15	9.69	1.39	1.22
90	ii	501	ZVM	C13-C14	8.13	1.52	1.38
90	ii	501	ZVM	C10-C09	7.54	1.53	1.39
90	ii	501	ZVM	C03-N01	7.44	1.38	1.27
90	ii	501	ZVM	C12-C11	6.49	1.52	1.38
90	ii	501	ZVM	C04-N02	-5.99	1.42	1.47
90	ii	501	ZVM	C03-N03	5.42	1.47	1.37
90	ii	501	ZVM	C05-C04	5.30	1.59	1.54
90	ii	501	ZVM	C02-C03	-4.97	1.40	1.52
90	ii	501	ZVM	C08-C05	-4.27	1.45	1.54
90	ii	501	ZVM	C17-N03	4.25	1.49	1.40
90	ii	501	ZVM	C11-C10	-4.19	1.31	1.38
90	ii	501	ZVM	C14-C09	-4.16	1.31	1.39
90	ii	501	ZVM	C21-C22	-4.06	1.33	1.39
90	ii	501	ZVM	C06-C05	-3.93	1.45	1.54
90	ii	501	ZVM	C12-C13	-2.98	1.31	1.38
90	ii	501	ZVM	C15-N02	2.98	1.40	1.36
90	ii	501	ZVM	C02-C01	-2.56	1.46	1.51
90	ii	501	ZVM	C07-C06	2.18	1.65	1.53
90	ii	501	ZVM	C07-C08	2.12	1.65	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	ii	501	ZVM	C05-C04-N01	11.95	121.33	109.91
90	ii	501	ZVM	O01-C01-C02	-9.29	118.89	126.79
90	ii	501	ZVM	C05-C04-N02	4.49	119.42	111.94
90	ii	501	ZVM	N02-C04-N01	4.29	119.25	113.37
90	ii	501	ZVM	C21-C22-C17	2.77	121.99	118.81
90	ii	501	ZVM	C22-C01-C02	2.70	120.36	116.72
90	ii	501	ZVM	C02-C15-N02	2.48	119.16	116.89

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
90	ii	501	ZVM	C04
90	ii	501	ZVM	C02

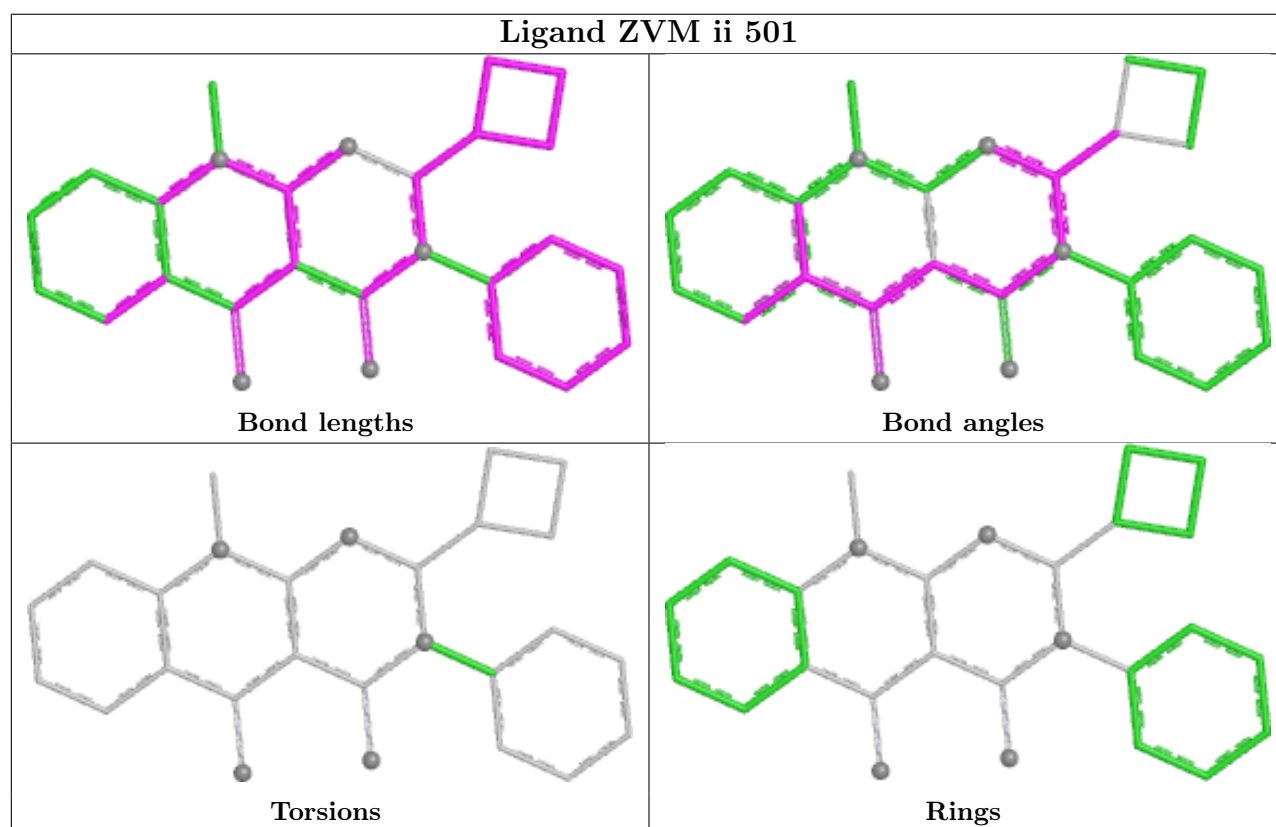
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	jj	601	SF4	4	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	23
51	9	3
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.98
1	5	1219:G	O3'	1233:G	P	19.96
1	5	1406(C):G	O3'	1411:C	P	16.99
1	5	1696:C	O3'	1720:C	P	16.41
1	5	990:C	O3'	1064:G	P	15.53
1	5	523:C	O3'	638:G	P	15.09
1	5	4138:C	O3'	4146:G	P	15.05
1	5	1364:U	O3'	1368:A	P	14.32
1	5	4777:C	O3'	4859:C	P	14.25
1	5	4101:C	O3'	4107:G	P	13.97
1	5	5022:U	O3'	5028:G	P	13.74
1	5	182:G	O3'	189:G	P	13.69
1	5	760:G	O3'	904:C	P	13.62
1	5	2901:G	O3'	3597:G	P	12.67
1	5	3948:C	O3'	4065:G	P	12.45
1	9	890:U	O3'	894:G	P	12.31
1	5	1180:C	O3'	1183:C	P	9.35
1	5	4729:A	O3'	4735:G	P	8.97
1	5	1980:U	O3'	1981:G	P	7.17
1	5	1981:G	O3'	1982:G	P	6.96
1	5	512:U	O3'	515:C	P	6.64
1	5	4740:G	O3'	4743:G	P	6.62
1	5	500:G	O3'	504:G	P	6.28
1	3	19:G	O3'	20:U	P	5.95
1	3	16:C	O3'	18:U	P	5.54
1	2	16:C	O3'	18:G	P	5.42
1	5	1100:U	O3'	1168:G	P	4.14
1	9	873:G	O3'	874:G	P	3.50
1	9	900:C	O3'	901:G	P	3.23

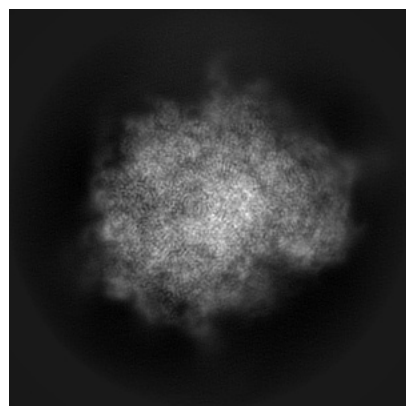
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40344. These allow visual inspection of the internal detail of the map and identification of artifacts.

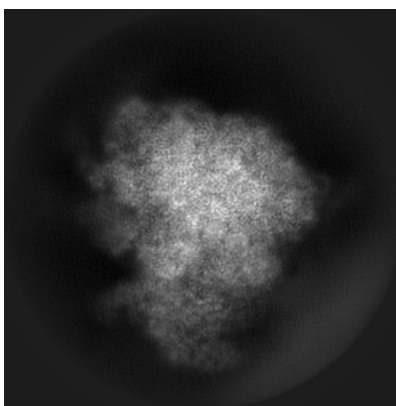
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

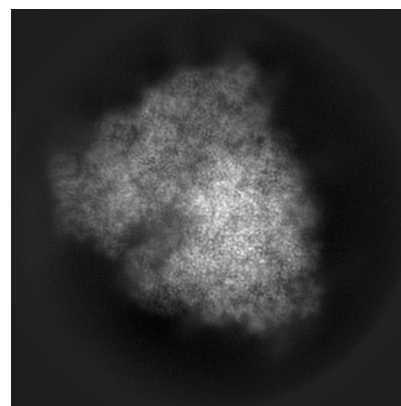
6.1.1 Primary map



X

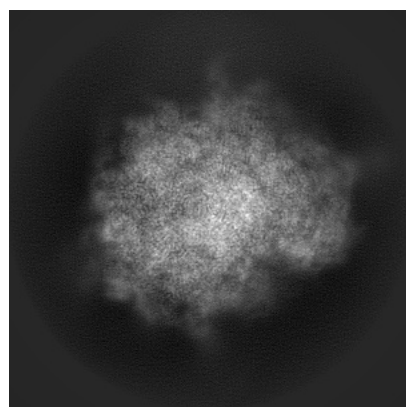


Y

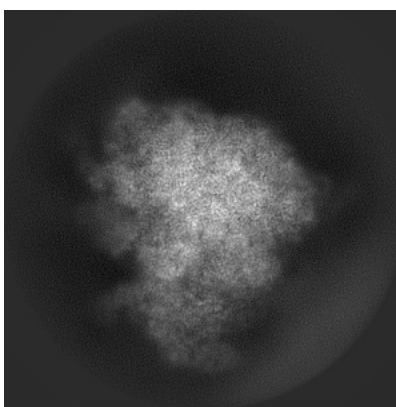


Z

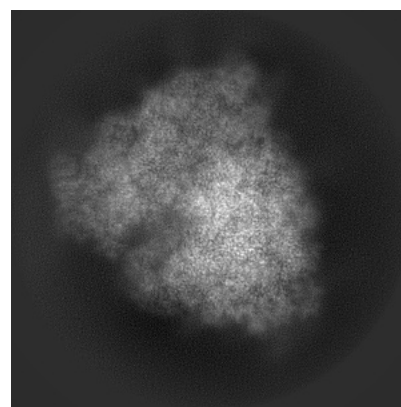
6.1.2 Raw map



X



Y

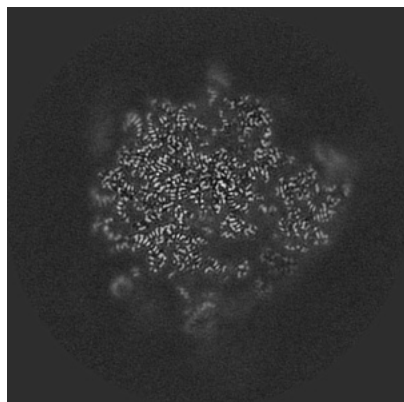


Z

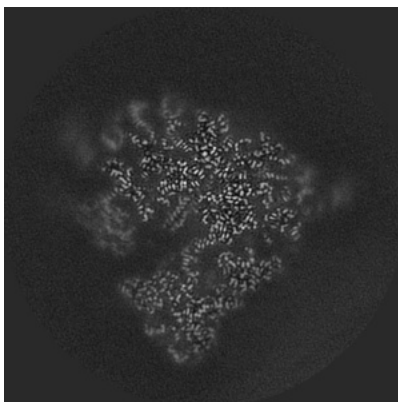
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

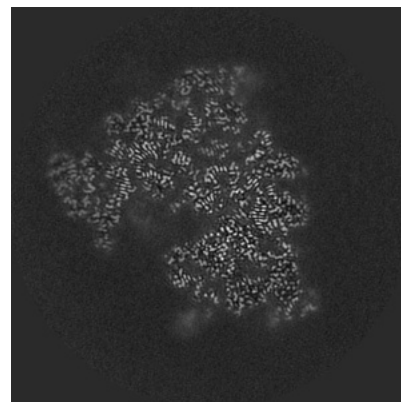
6.2.1 Primary map



X Index: 240

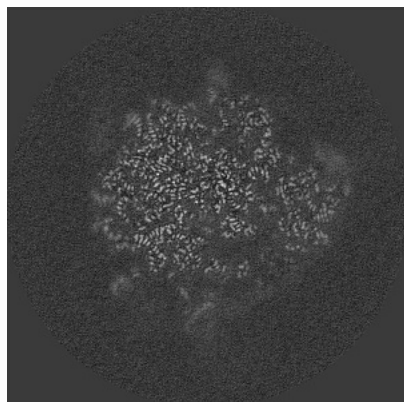


Y Index: 240

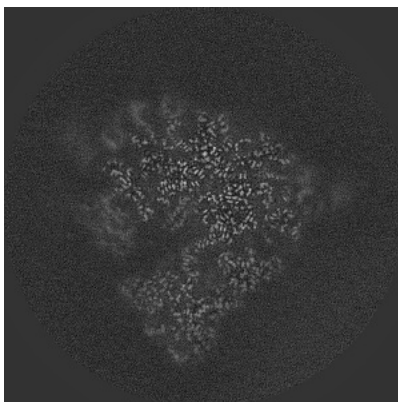


Z Index: 240

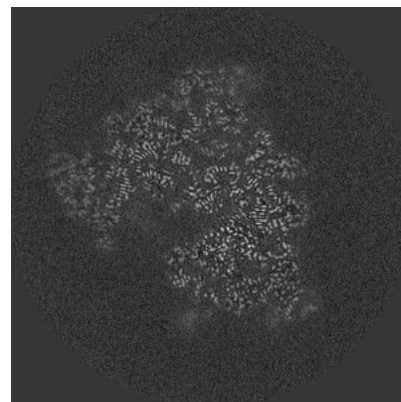
6.2.2 Raw map



X Index: 240



Y Index: 240

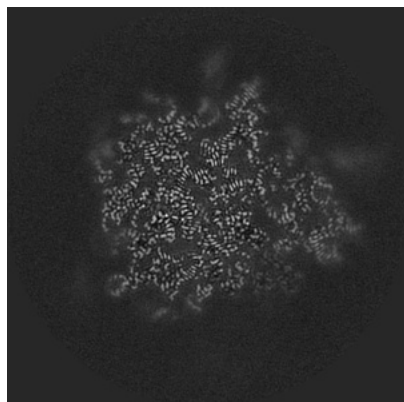


Z Index: 240

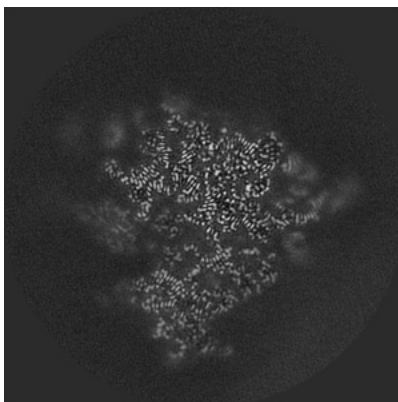
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

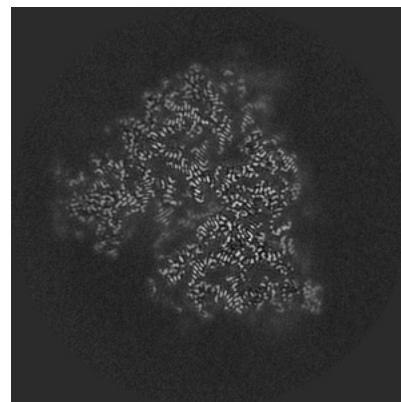
6.3.1 Primary map



X Index: 261

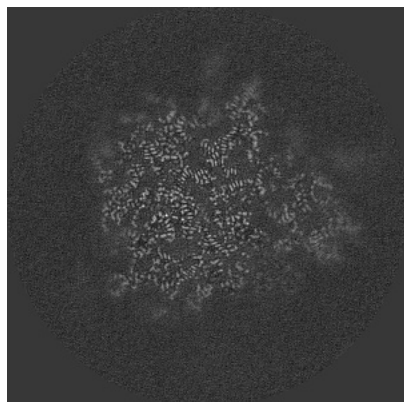


Y Index: 250

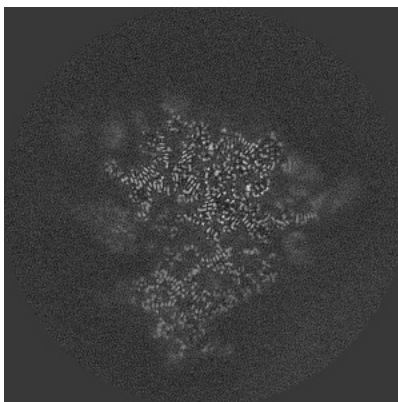


Z Index: 227

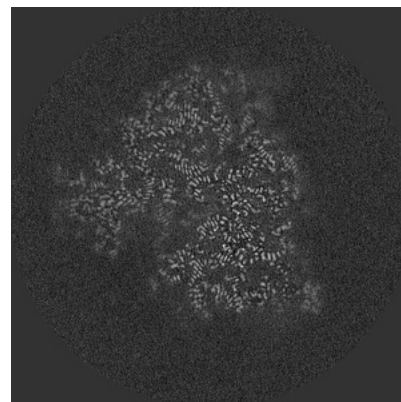
6.3.2 Raw map



X Index: 261



Y Index: 250

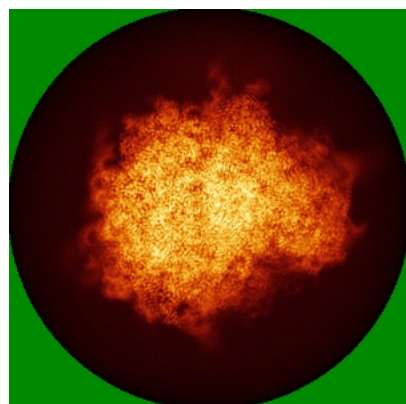


Z Index: 228

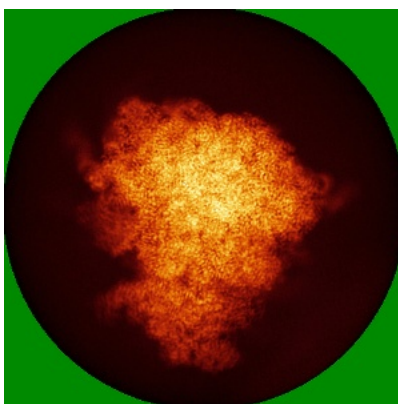
The images above show the largest variance slices of the map in three orthogonal directions.

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

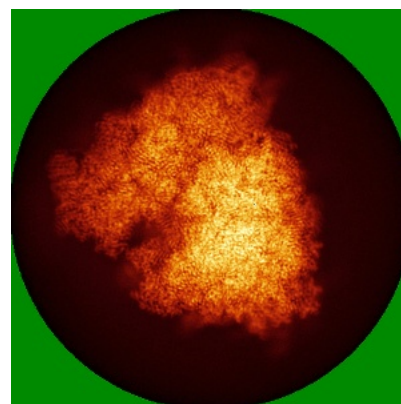
6.4.1 Primary map



X

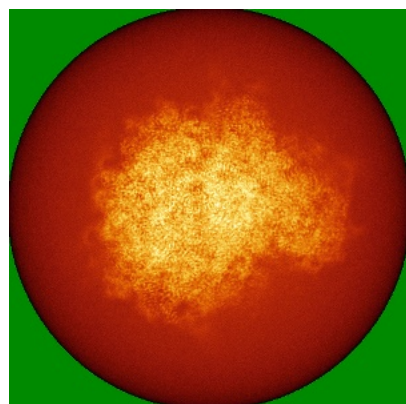


Y

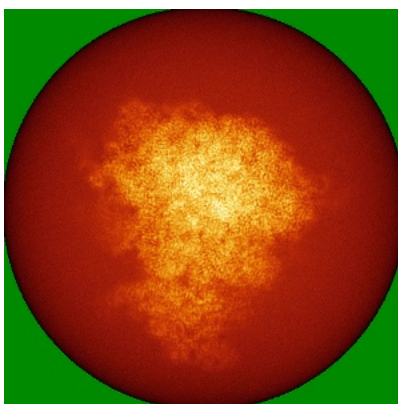


Z

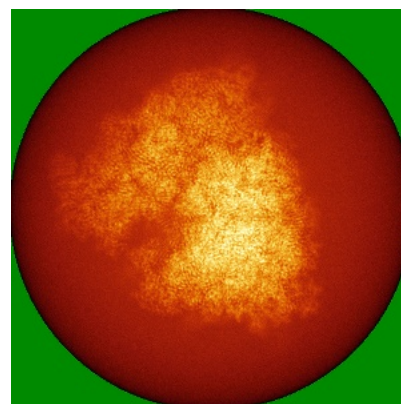
6.4.2 Raw map



X



Y

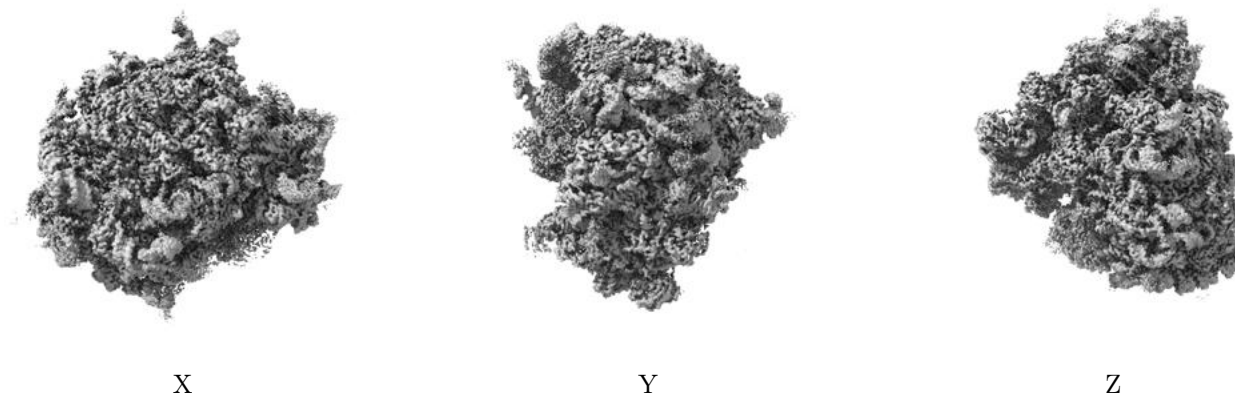


Z

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.

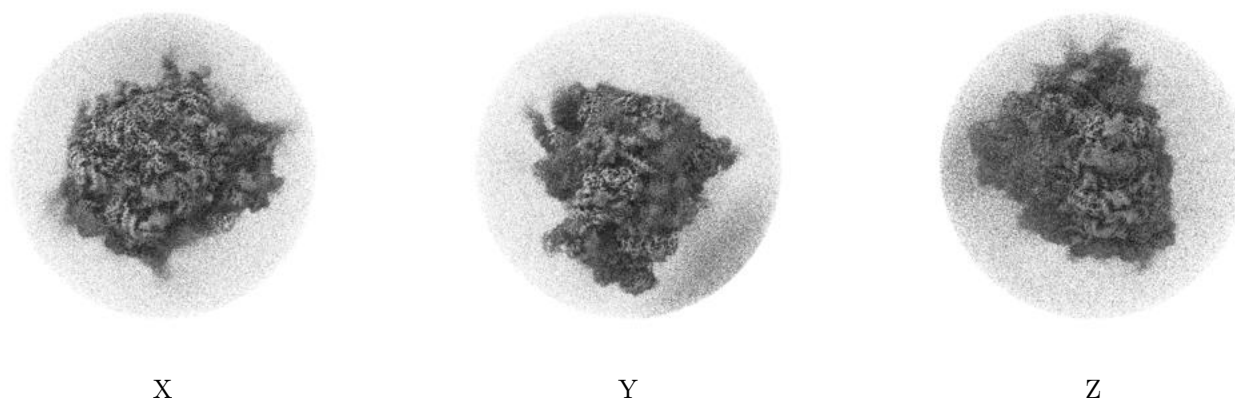
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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



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.

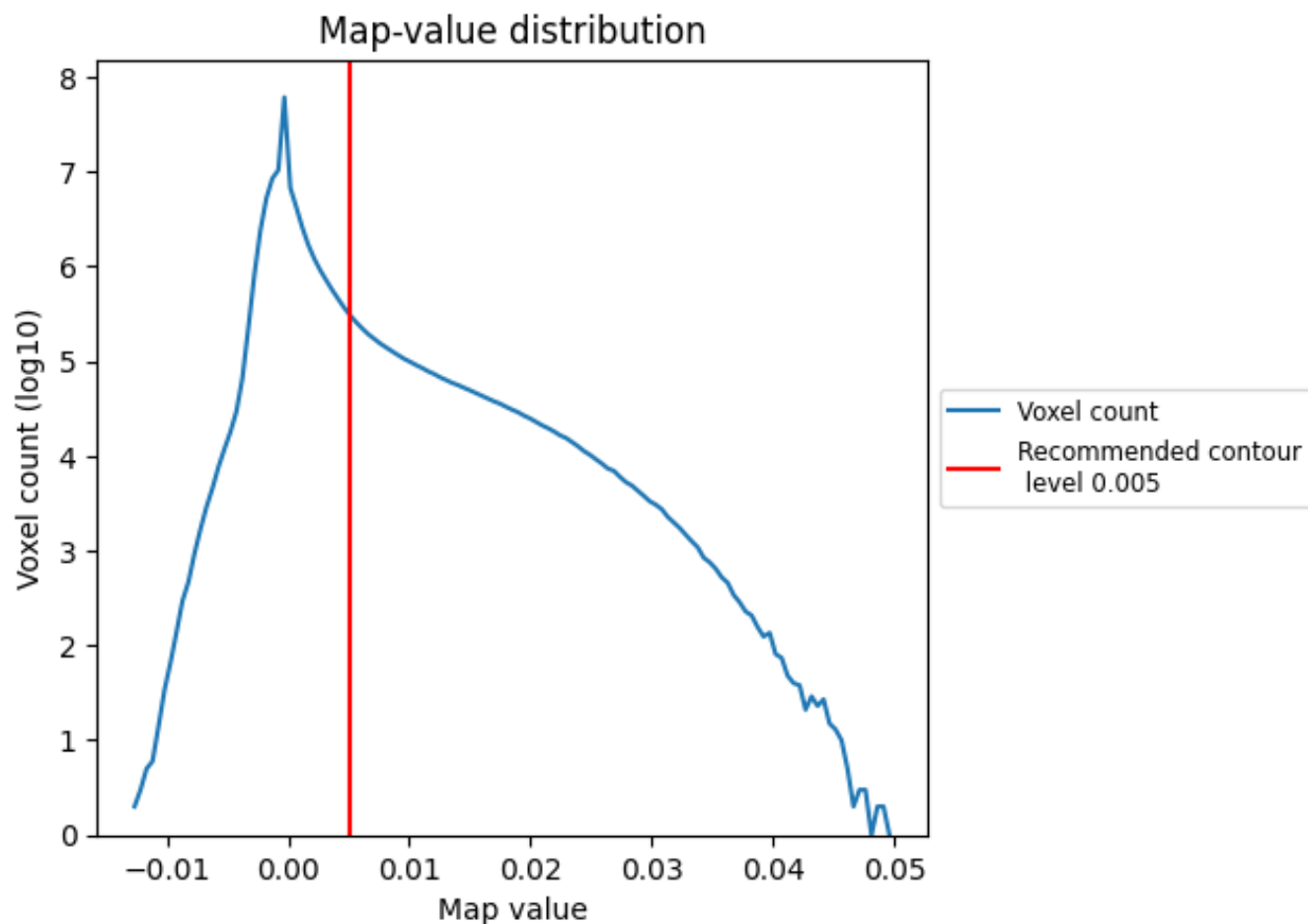
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

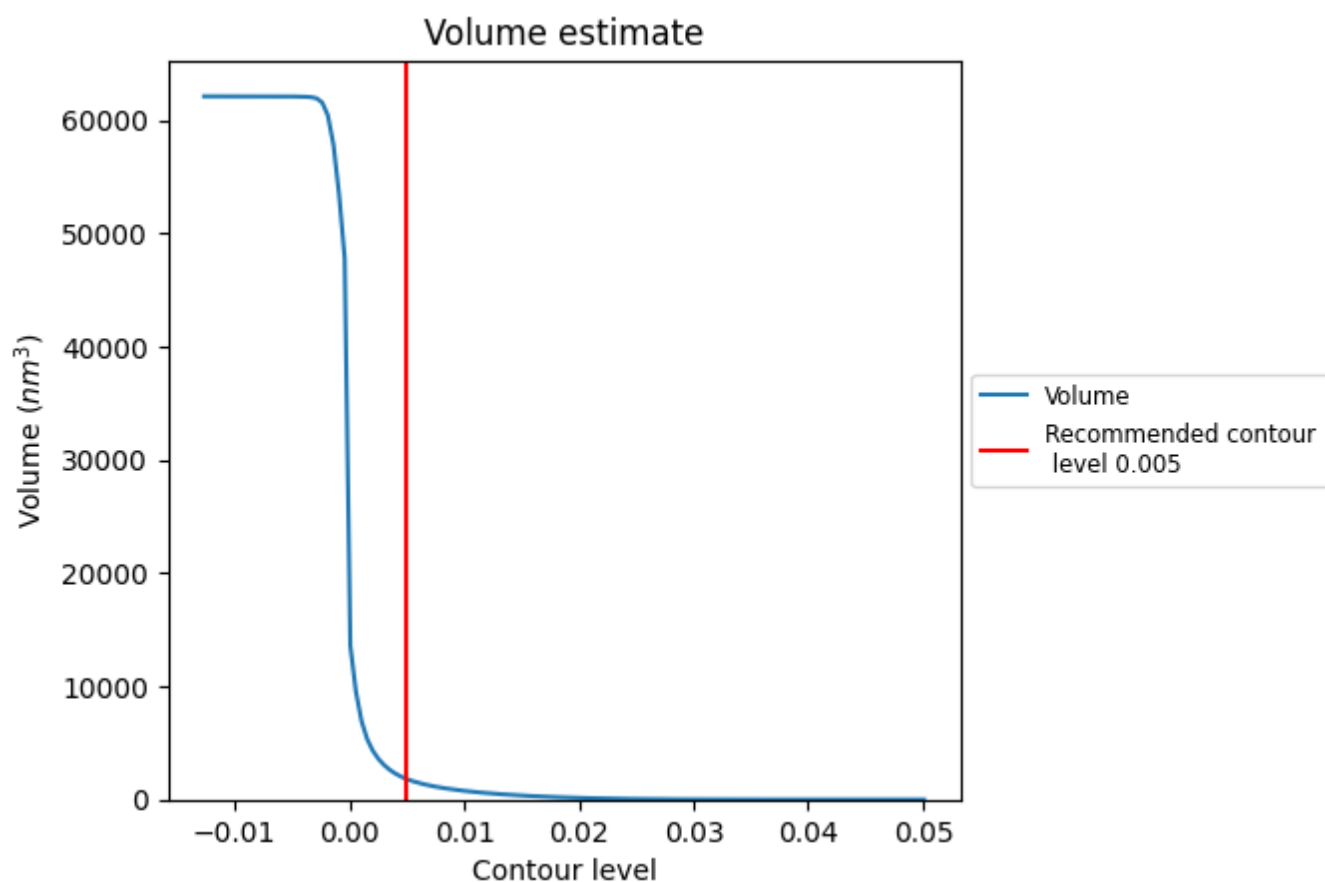
This section contains the results of statistical analysis of the map.

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.

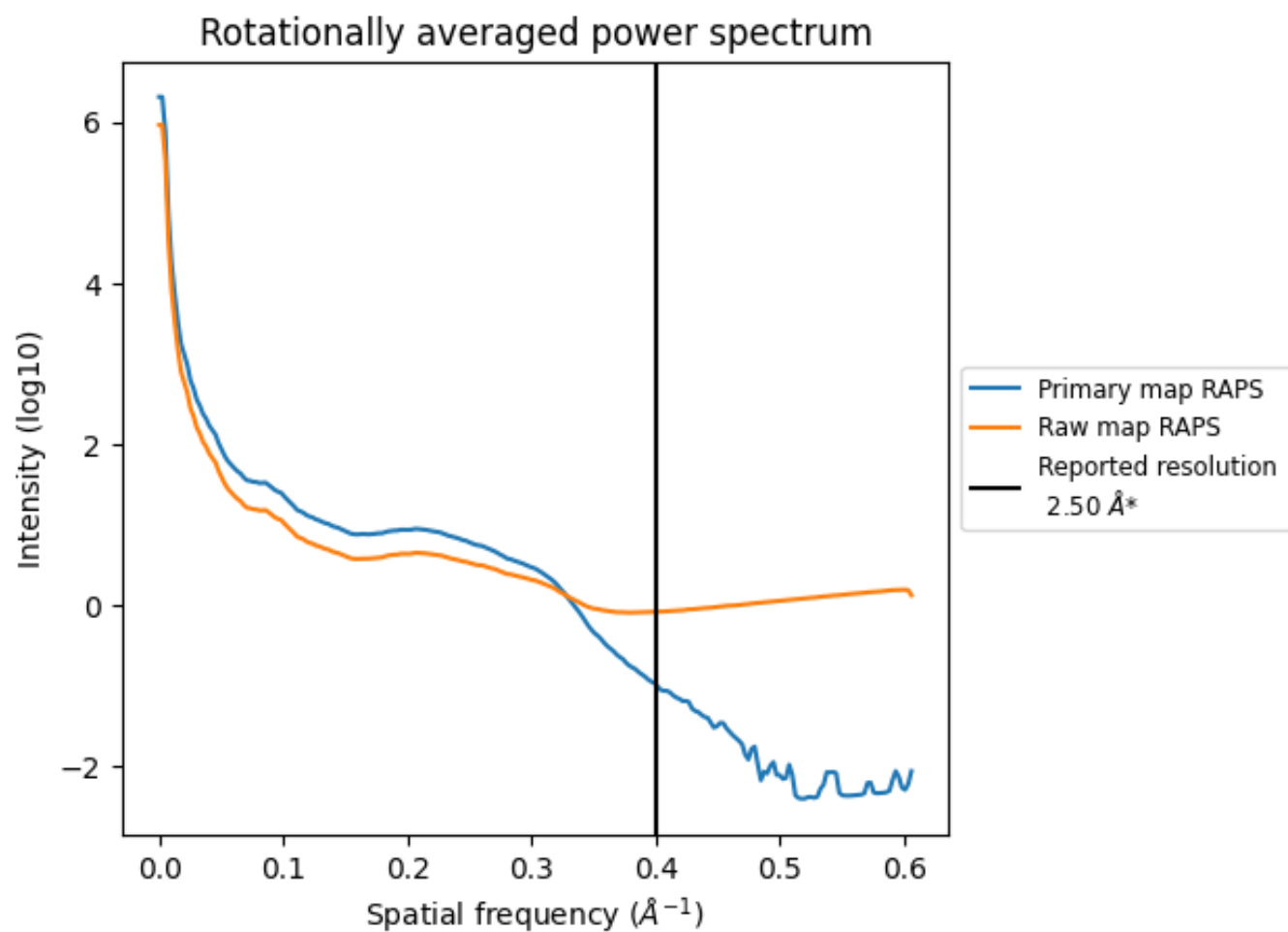
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1812 nm³; this corresponds to an approximate mass of 1637 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 ⓘ

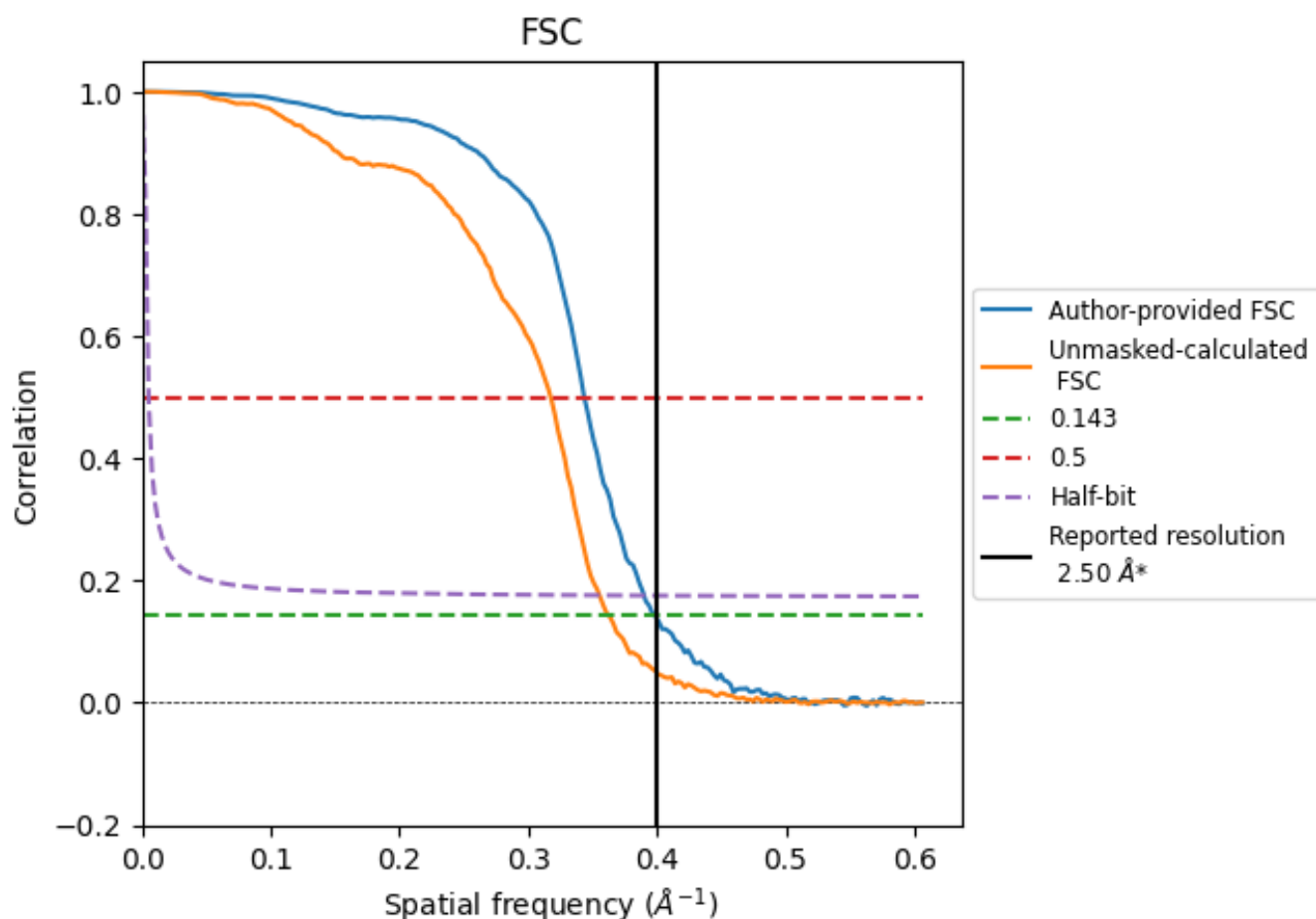


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

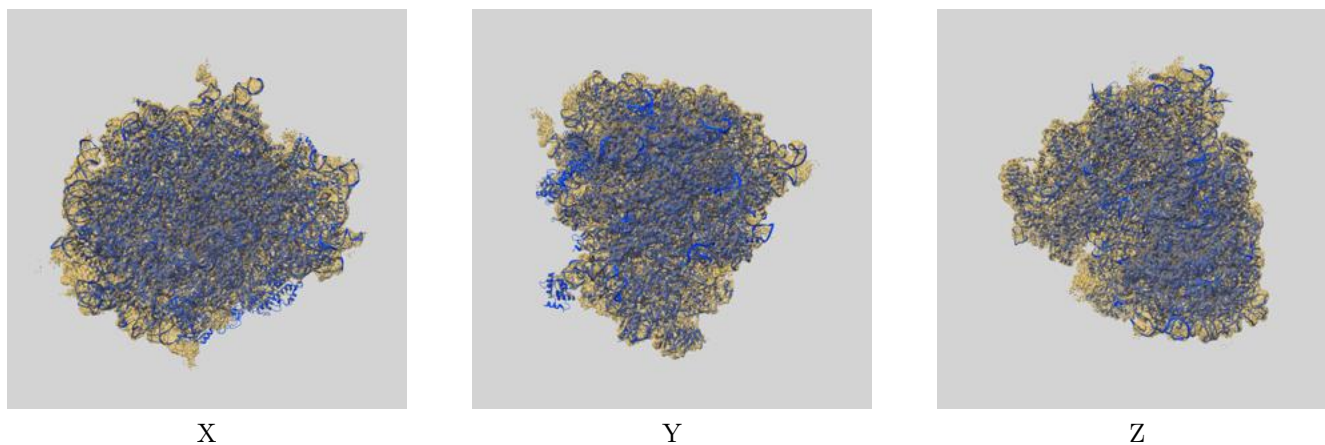
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.91	2.56
Unmasked-calculated*	2.76	3.15	2.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

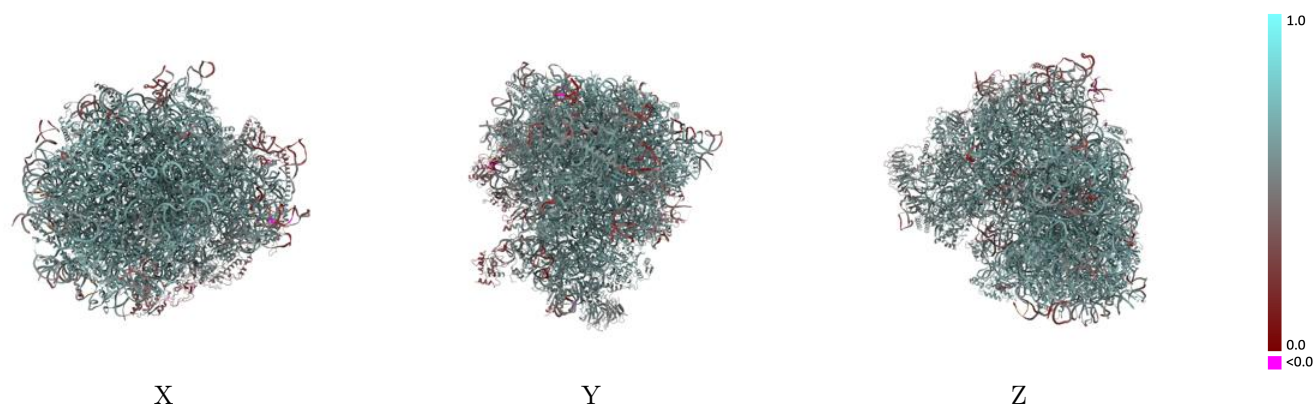
This section contains information regarding the fit between EMDB map EMD-40344 and PDB model 8SCB. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



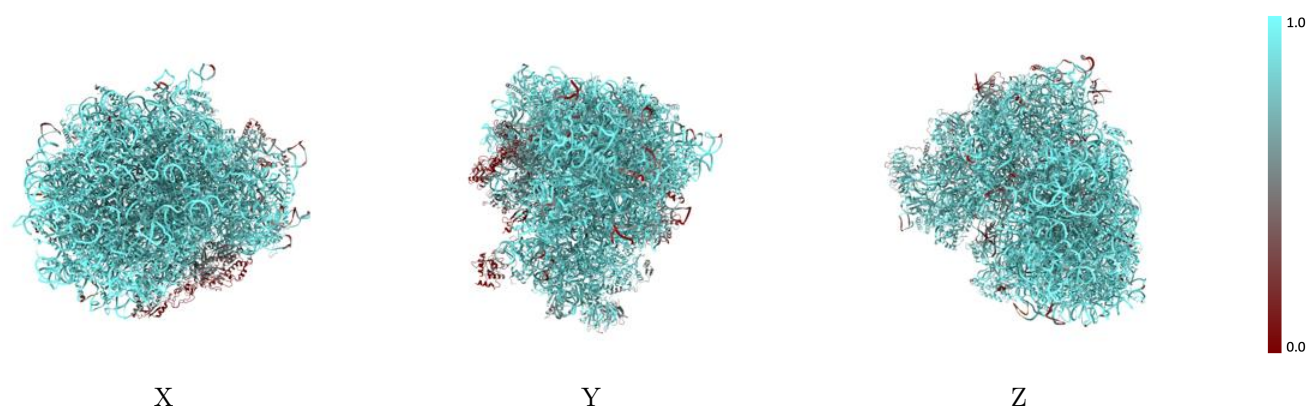
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



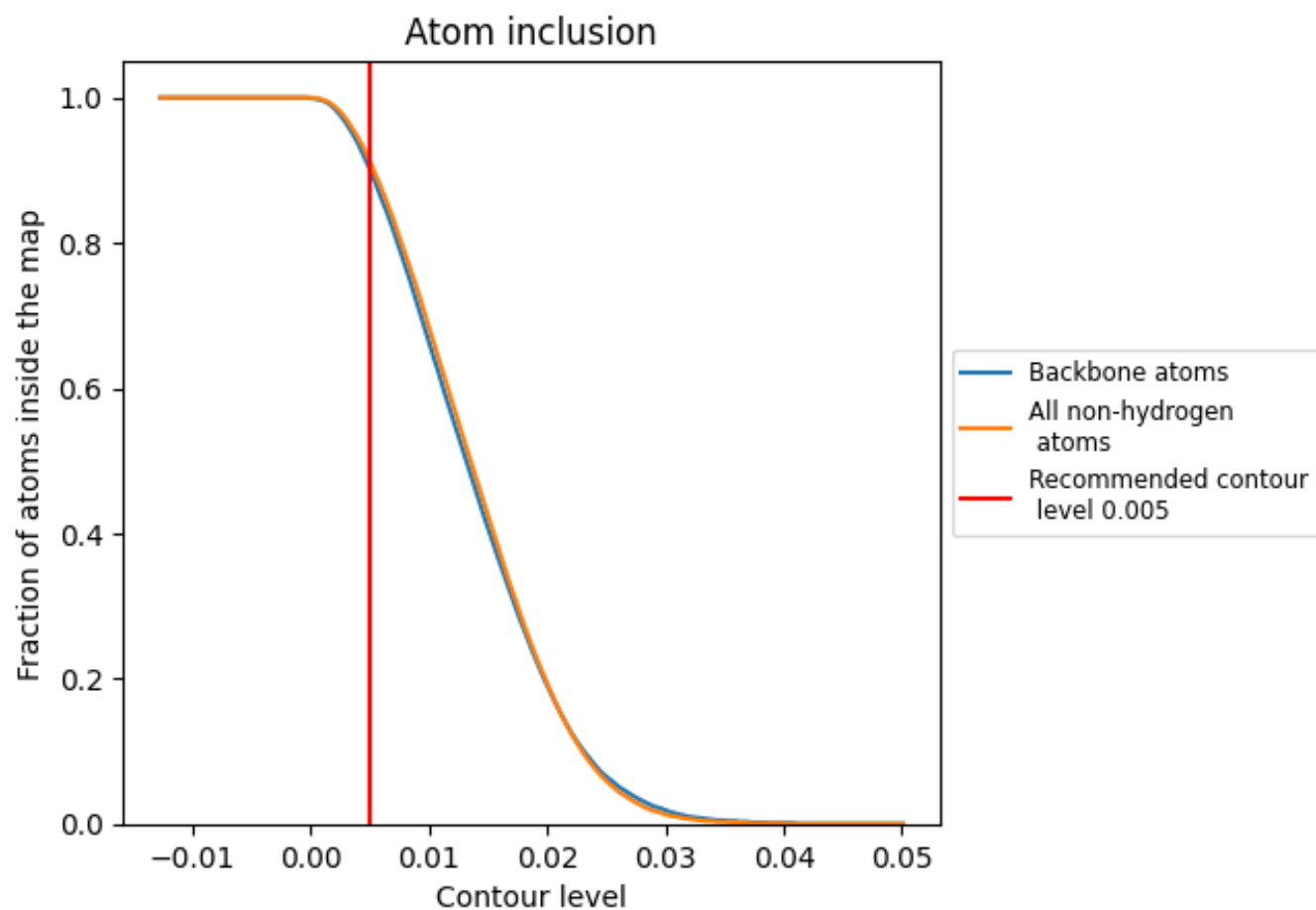
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.5890
1	 0.9590	 0.6230
2	 0.9490	 0.5410
3	 0.5710	 0.3940
5	 0.9750	 0.6070
7	 0.9950	 0.6350
8	 0.9630	 0.6010
9	 0.9380	 0.5680
A	 0.9860	 0.6570
AA	 0.8810	 0.5860
B	 0.9700	 0.6410
BB	 0.9000	 0.5920
C	 0.9670	 0.6410
CC	 0.9270	 0.6040
D	 0.9380	 0.6090
DD	 0.8180	 0.5420
E	 0.9520	 0.6100
EE	 0.9280	 0.5870
F	 0.9690	 0.6450
FF	 0.9060	 0.5780
G	 0.9140	 0.5970
GG	 0.7990	 0.5030
H	 0.9330	 0.6160
HH	 0.5830	 0.4750
I	 0.9590	 0.6300
II	 0.8730	 0.5680
J	 0.9180	 0.5910
JJ	 0.9020	 0.5760
KK	 0.8390	 0.5400
L	 0.9210	 0.6130
LL	 0.9440	 0.6250
M	 0.9470	 0.6130
MM	 0.1120	 0.3190
N	 0.9900	 0.6560
NN	 0.9280	 0.6010



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Chain	Atom inclusion	Q-score
O	 0.9690	 0.6370
OO	 0.9570	 0.6170
P	 0.9640	 0.6460
PP	 0.8780	 0.5590
Q	 0.9730	 0.6490
QQ	 0.9080	 0.5780
R	 0.9000	 0.6030
RR	 0.7450	 0.5440
S	 0.9760	 0.6450
SS	 0.8830	 0.5660
T	 0.9440	 0.6210
TT	 0.9120	 0.5790
U	 0.8820	 0.5490
UU	 0.7490	 0.5170
V	 0.9730	 0.6440
VV	 0.8760	 0.5780
W	 0.9490	 0.6300
WW	 0.9550	 0.6150
X	 0.9530	 0.6240
XX	 0.9590	 0.6230
Y	 0.9390	 0.6220
YY	 0.8960	 0.5620
Z	 0.9460	 0.6140
ZZ	 0.8430	 0.5540
a	 0.9660	 0.6480
aa	 0.9420	 0.6160
b	 0.8450	 0.5830
bb	 0.8470	 0.5730
c	 0.9440	 0.6220
cc	 0.8400	 0.5680
d	 0.9650	 0.6330
dd	 0.9490	 0.5990
e	 0.9830	 0.6530
ee	 0.9060	 0.5680
f	 0.9790	 0.6560
ff	 0.2530	 0.3490
g	 0.9350	 0.6170
gg	 0.7550	 0.5030
h	 0.9380	 0.6160
hh	 0.9920	 0.6100
i	 0.9210	 0.6070
ii	 0.7390	 0.5290

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Chain	Atom inclusion	Q-score
j	 0.9940	 0.6520
jj	 0.4420	 0.5120
k	 0.8460	 0.5750
l	 0.9860	 0.6370
m	 0.9490	 0.6270
n	 0.9750	 0.6320
o	 0.9610	 0.6380
p	 0.9580	 0.6370
r	 0.9660	 0.6340
s	 0.1770	 0.2900
t	 0.4670	 0.3450