



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 07:49 PM EDT

PDB ID : 8VVT / pdb_00008vvt
EMDB ID : EMD-43568
Title : Mammalian ribosomes bound to Anisomycin in the rotated conformation
Authors : Loerch, S.; Petrossian, E.; Smith, P.R.; Campbell, Z.T.
Deposited on : 2024-01-31
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

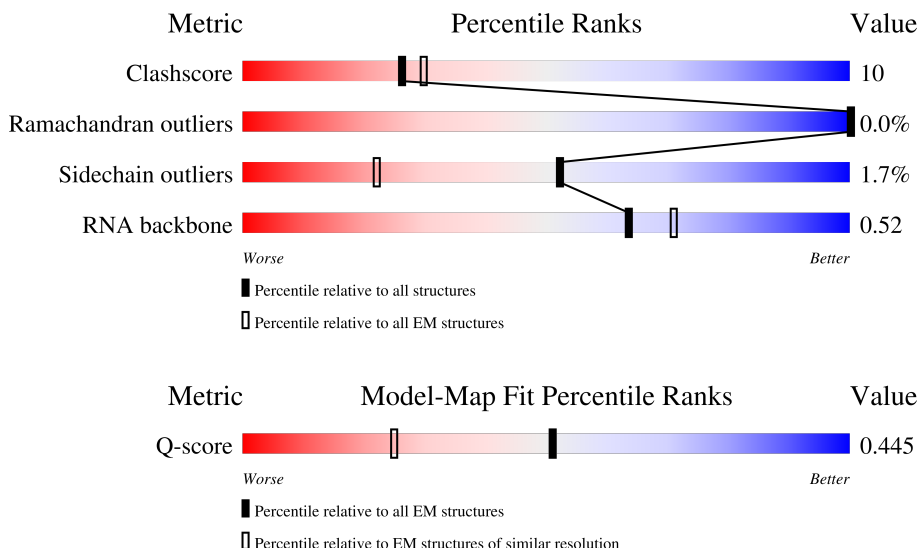
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



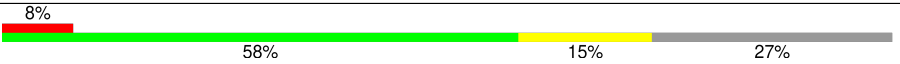
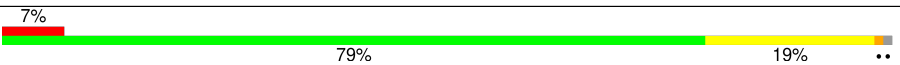
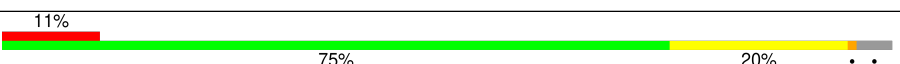
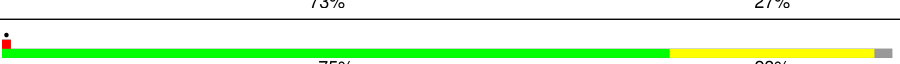
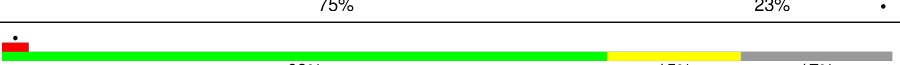
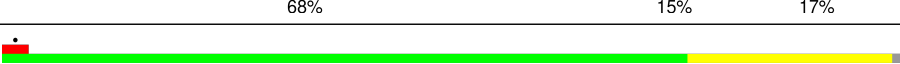
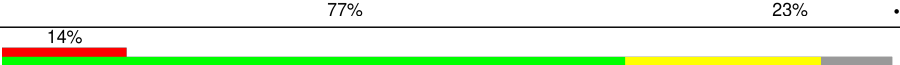
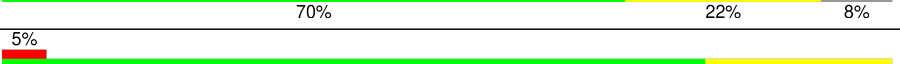
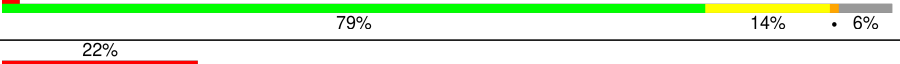
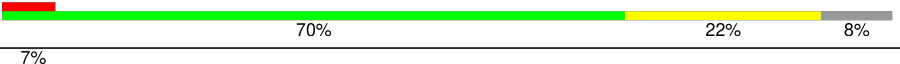
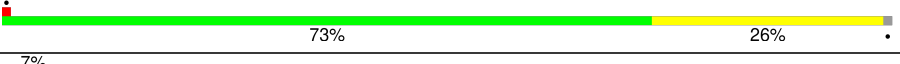
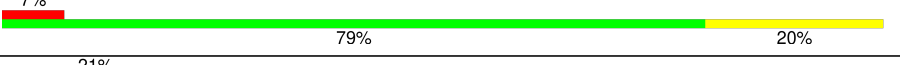
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	257	
2	B	403	
3	C	425	

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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	218	
12	M	204	
13	N	203	
14	O	184	
15	P	188	
16	Q	196	
17	R	176	
18	S	160	
19	T	128	
20	U	140	
21	V	157	
22	W	156	
23	X	145	
24	Y	136	
25	Z	148	
26	K	211	
27	AB	295	
28	BB	264	

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Mol	Chain	Length	Quality of chain
29	CB	293	
30	WA	3635	
31	XA	120	
32	YA	156	
33	AA	245	
34	BA	115	
35	CA	125	
36	DA	135	
37	EA	110	
38	FA	117	
39	GA	123	
40	HA	105	
41	IA	97	
42	JA	70	
43	KA	51	
44	LA	102	
45	MA	25	
46	NA	106	
47	OA	92	
48	PA	137	
49	QA	318	
50	RA	165	
51	v	839	
52	w	46	
53	ZA	1869	

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Mol	Chain	Length	Quality of chain
54	DB	243	
55	EB	263	
56	FB	204	
57	GB	249	
58	HB	194	
59	IB	208	
60	JB	194	
61	KB	165	
62	LB	158	
63	MB	132	
64	NB	151	
65	OB	168	
66	PB	145	
67	QB	146	
68	RB	135	
69	SB	152	
70	TB	145	
71	UB	119	
72	VB	83	
73	WB	130	
74	XB	143	
75	YB	130	
76	ZB	125	
77	AC	115	
78	BC	84	

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Mol	Chain	Length	Quality of chain
79	CC	69	
80	DC	56	
81	EC	133	
82	FC	156	
83	GC	317	
84	b	394	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 221459 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 L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2884	1813	577	480	14		

- Molecule 4 is a protein called L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 5 is a protein called L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1720	1109	327	281	3		

- Molecule 6 is a protein called uL30.

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 eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called L10.

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

- Molecule 10 is a protein called L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called L14.

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

- Molecule 12 is a protein called L15.

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

- Molecule 13 is a protein called uL13.

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

- Molecule 14 is a protein called uL22.

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

- Molecule 15 is a protein called eL18.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	4	ASP	ASN	conflict	UNP G1TFE0
P	14	ARG	TRP	conflict	UNP G1TFE0
P	53	MET	LEU	conflict	UNP G1TFE0
P	58	ARG	TRP	conflict	UNP G1TFE0
P	75	ARG	GLN	conflict	UNP G1TFE0
P	80	ALA	PRO	conflict	UNP G1TFE0
P	86	VAL	ILE	conflict	UNP G1TFE0
P	104	ARG	HIS	conflict	UNP G1TFE0
P	110	ARG	CYS	conflict	UNP G1TFE0
P	137	VAL	GLY	conflict	UNP G1TFE0
P	157	GLY	ARG	conflict	UNP G1TFE0
P	181	ARG	TRP	conflict	UNP G1TFE0

- Molecule 16 is a protein called eL19.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 17 is a protein called eL20.

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

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	THR	conflict	UNP G1TTY7
R	18	PRO	-	insertion	UNP G1TTY7
R	19	THR	-	insertion	UNP G1TTY7
R	20	PRO	SER	conflict	UNP G1TTY7
R	22	CYS	SER	conflict	UNP G1TTY7
R	23	ARG	PRO	conflict	UNP G1TTY7
R	24	THR	ALA	conflict	UNP G1TTY7
R	49	SER	LEU	conflict	UNP G1TTY7
R	50	GLN	GLU	conflict	UNP G1TTY7
R	95	ARG	HIS	conflict	UNP G1TTY7
R	101	THR	ILE	conflict	UNP G1TTY7
R	102	THR	MET	conflict	UNP G1TTY7
R	104	GLY	SER	conflict	UNP G1TTY7
R	126	ILE	VAL	conflict	UNP G1TTY7
R	132	ILE	MET	conflict	UNP G1TTY7
R	135	SER	ALA	conflict	UNP G1TTY7
R	136	LYS	ARG	conflict	UNP G1TTY7
R	138	ARG	PRO	conflict	UNP G1TTY7
R	149	LYS	ARG	conflict	UNP G1TTY7
R	151	LYS	ARG	conflict	UNP G1TTY7
R	168	THR	TYR	conflict	UNP G1TTY7
R	169	THR	ALA	conflict	UNP G1TTY7
R	176	PHE	-	insertion	UNP G1TTY7

- Molecule 18 is a protein called eL21.

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

- Molecule 19 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	18	LEU	VAL	conflict	UNP G1TSG1
T	32	GLY	ARG	conflict	UNP G1TSG1
T	36	ALA	GLU	conflict	UNP G1TSG1
T	39	PHE	SER	conflict	UNP G1TSG1
T	54	GLY	ARG	conflict	UNP G1TSG1
T	60	VAL	ALA	conflict	UNP G1TSG1
T	62	SER	THR	conflict	UNP G1TSG1
T	63	LEU	ILE	conflict	UNP G1TSG1
T	97	ARG	HIS	conflict	UNP G1TSG1
T	106	THR	SER	conflict	UNP G1TSG1
T	126	GLU	ASP	conflict	UNP G1TSG1

- Molecule 20 is a protein called L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 21 is a protein called L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	98	Total	C	N	O	S	0	0
			800	501	161	134	4		

- Molecule 22 is a protein called uL23.

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

- Molecule 23 is a protein called L26.

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

- Molecule 24 is a protein called L27.

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

- Molecule 25 is a protein called uL15.

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

- Molecule 26 is a protein called eL13.

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

There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 27 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AB	217	Total	C	N	O	S	0	0
			1712	1087	300	317	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 28 is a protein called S3A.

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

- Molecule 29 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CB	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 30 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	WA	3541	Total	C	N	O	P	0	0
			76047	33931	13901	24674	3541		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	XA	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
XA	2	U	N	conflict	GB X06789.1
XA	36	C	N	conflict	GB X06789.1
XA	102	U	N	conflict	GB X06789.1
XA	112	U	N	conflict	GB X06789.1
XA	114	U	N	conflict	GB X06789.1
XA	119	U	C	conflict	GB X06789.1
XA	120	U	N	conflict	GB X06789.1

- Molecule 32 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	YA	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 33 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AA	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 34 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 35 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CA	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 36 is a protein called eL32.

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

- Molecule 37 is a protein called eL33.

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

- Molecule 38 is a protein called eL34.

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

- Molecule 39 is a protein called uL29.

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

- Molecule 40 is a protein called L36.

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

- Molecule 41 is a protein called L37.

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

- Molecule 42 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 43 is a protein called eL39.

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

- Molecule 44 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LA	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 45 is a protein called eL41.

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

- Molecule 46 is a protein called eL42.

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

- Molecule 47 is a protein called eL43.

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

- Molecule 48 is a protein called eL28.

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

- Molecule 49 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QA	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 50 is a protein called uL3.

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

- Molecule 51 is a protein called eukaryotic elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	832	Total	C	N	O	S	0	0
			6489	4128	1111	1207	43		

- Molecule 52 is a protein called Serpine mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	w	46	Total	C	N	O	0	0
			366	219	76	71		

- Molecule 53 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ZA	1698	Total	C	N	O	P	0	0
			36263	16190	6509	11867	1697		

- Molecule 54 is a protein called uS3.

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

- Molecule 55 is a protein called eS4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 56 is a protein called S5.

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

- Molecule 57 is a protein called S6.

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

- Molecule 58 is a protein called S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HB	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 59 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 60 is a protein called S9.

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

- Molecule 61 is a protein called eS10.

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

- Molecule 62 is a protein called S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LB	138	Total	C	N	O	S	0	0
			1137	725	214	192	6		

- Molecule 63 is a protein called S12.

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

- Molecule 64 is a protein called uS15.

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

- Molecule 65 is a protein called uS11.

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

- Molecule 66 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PB	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 67 is a protein called S16.

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

- Molecule 68 is a protein called eS17.

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

- Molecule 69 is a protein called uS13.

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

- Molecule 70 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	TB	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 71 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	UB	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 72 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 73 is a protein called S15A.

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

- Molecule 74 is a protein called uS12.

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

- Molecule 75 is a protein called eS24.

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

- Molecule 76 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	ZB	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 77 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AC	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 78 is a protein called S27.

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

- Molecule 79 is a protein called S28.

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

- Molecule 80 is a protein called uS14.

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

- Molecule 81 is a protein called S30.

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

- Molecule 82 is a protein called S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	FC	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 83 is a protein called RACK1.

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

- Molecule 84 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	b	325	Total	C	N	O	S	0	0
			2422	1547	422	439	14		

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

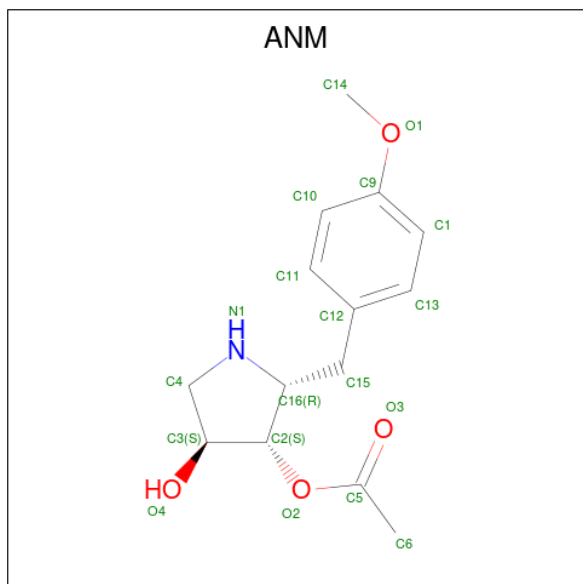
Mol	Chain	Residues	Atoms		AltConf
85	B	2	Total	Mg	0
			2	2	
85	I	1	Total	Mg	0
			1	1	
85	O	1	Total	Mg	0
			1	1	
85	U	1	Total	Mg	0
			1	1	
85	WA	110	Total	Mg	0
			110	110	
85	XA	4	Total	Mg	0
			4	4	
85	YA	1	Total	Mg	0
			1	1	
85	DA	1	Total	Mg	0
			1	1	
85	FA	1	Total	Mg	0
			1	1	
85	KA	1	Total	Mg	0
			1	1	
85	ZA	19	Total	Mg	0
			19	19	
85	TB	1	Total	Mg	0
			1	1	

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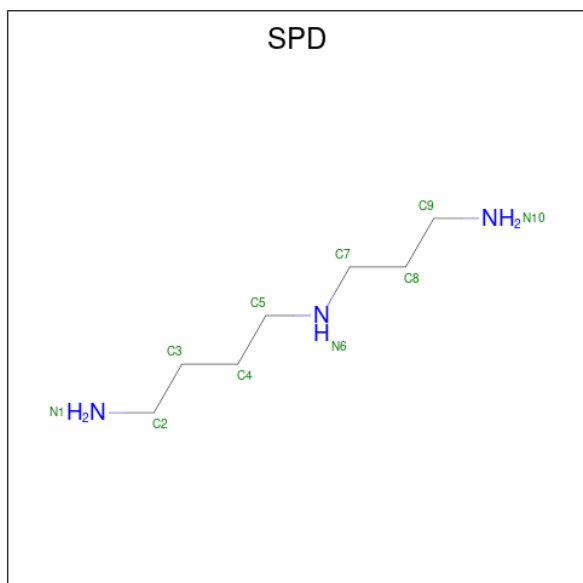
Mol	Chain	Residues	Atoms		AltConf
85	AC	1	Total	Mg	0
			1	1	

- Molecule 86 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



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

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

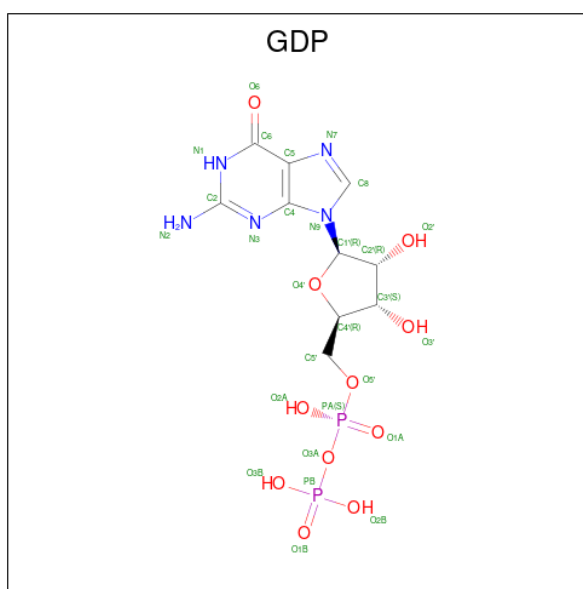


Mol	Chain	Residues	Atoms			AltConf
87	WA	1	Total	C	N	0
			10	7	3	

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 89 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

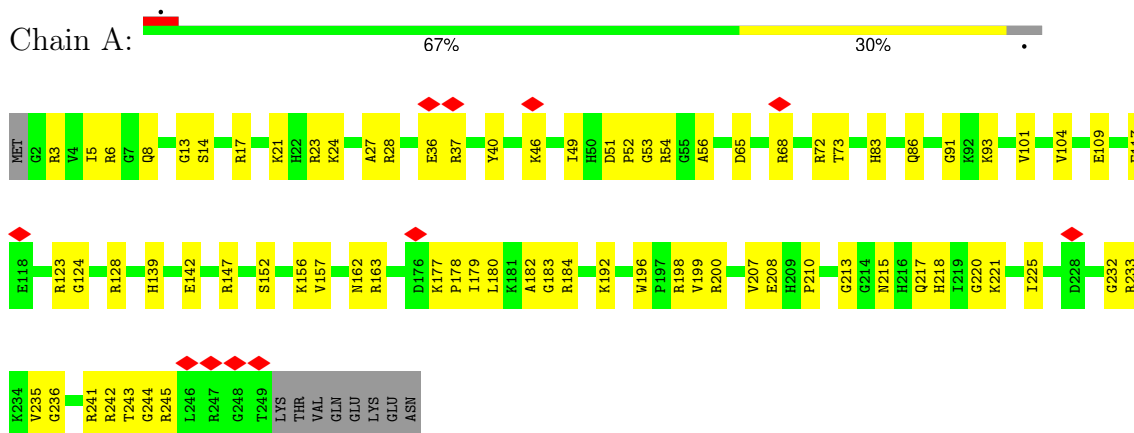


Mol	Chain	Residues	Atoms					AltConf
89	v	1	Total	C	N	O	P	0
			28	10	5	11	2	

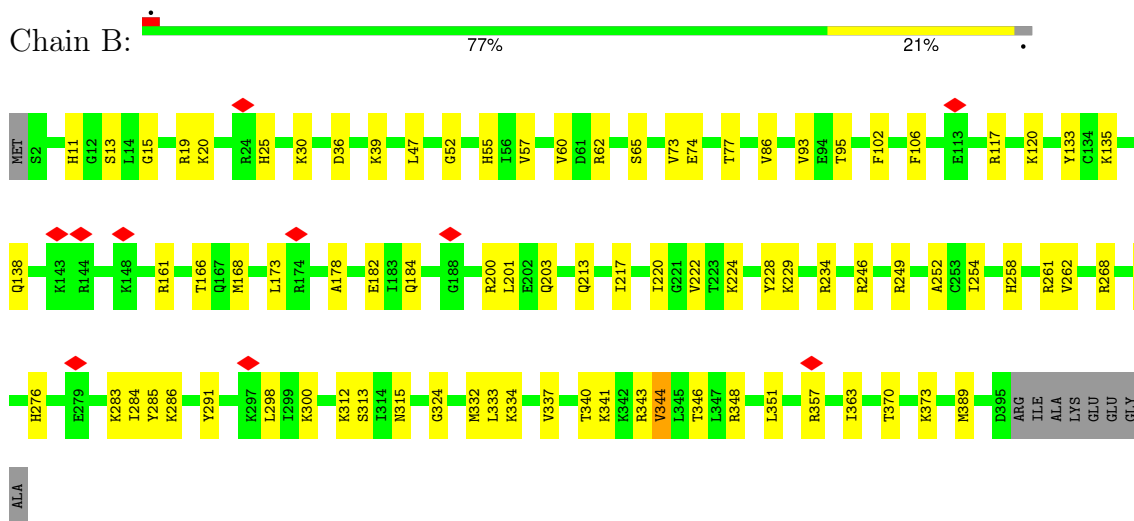
3 Residue-property plots

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

• Molecule 1: L8



• Molecule 2: uL3

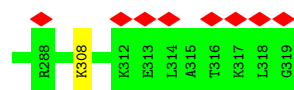
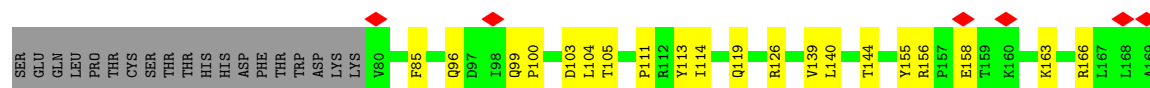
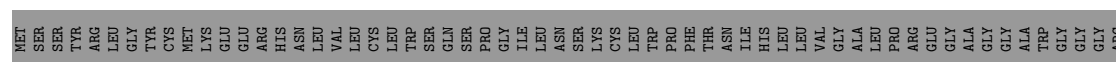


• Molecule 3: uL4

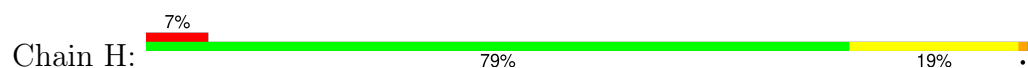




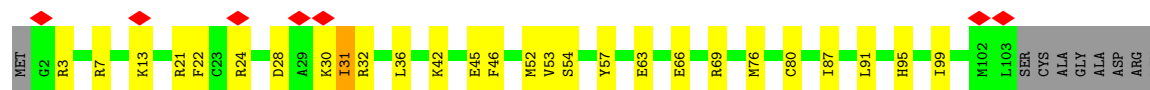
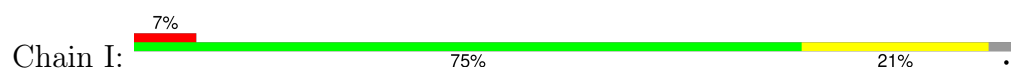
• Molecule 7: eL8



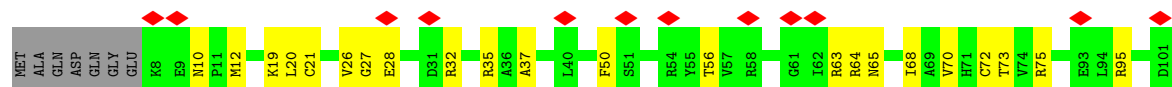
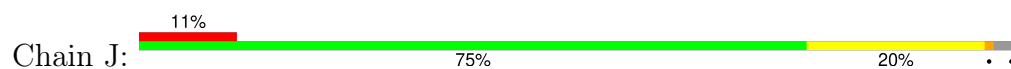
• Molecule 8: uL6



• Molecule 9: L10

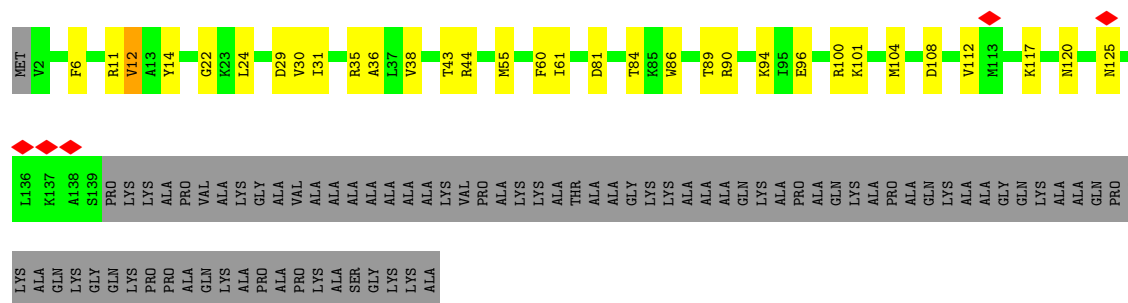


• Molecule 10: L11

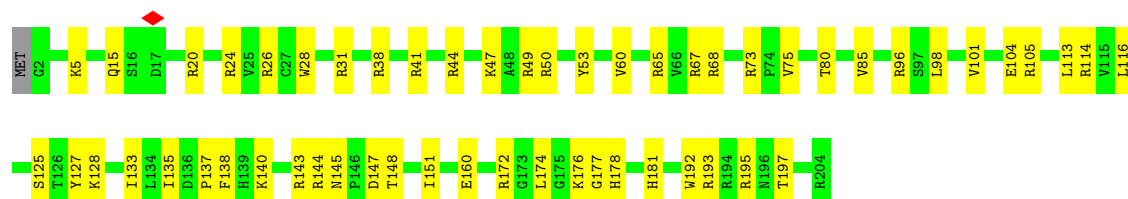




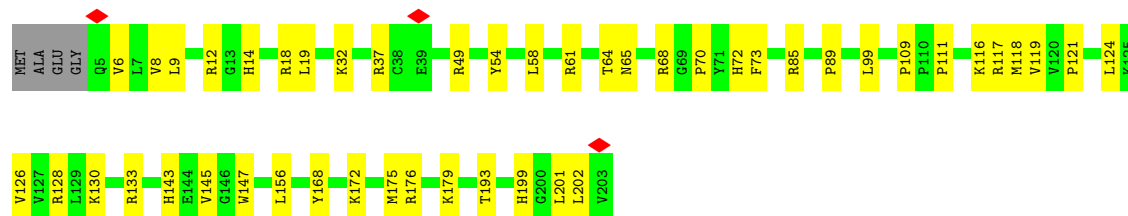
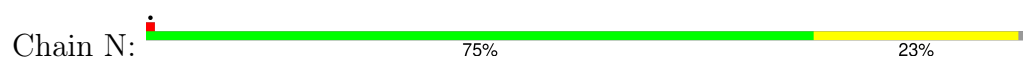
• Molecule 11: L14



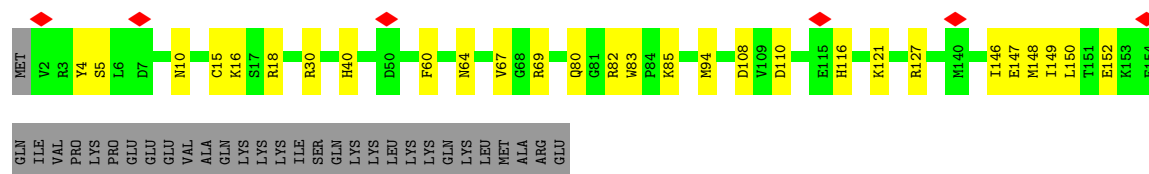
• Molecule 12: L15



• Molecule 13: uL13

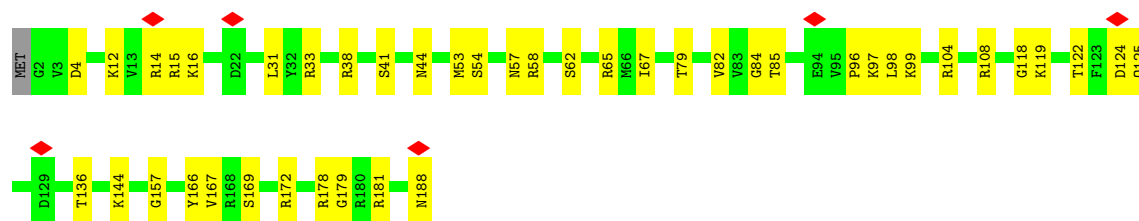


• Molecule 14: uL22



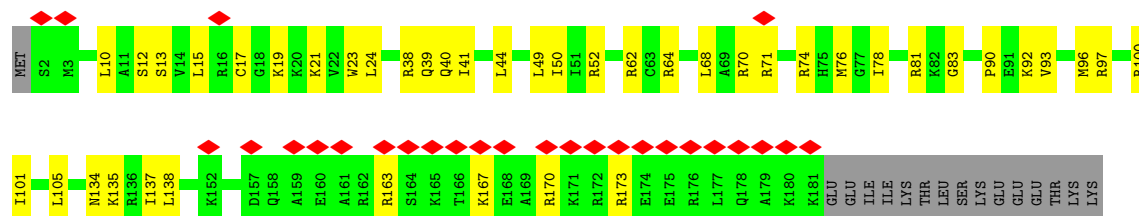
• Molecule 15: eL18

Chain P:  77% 23%



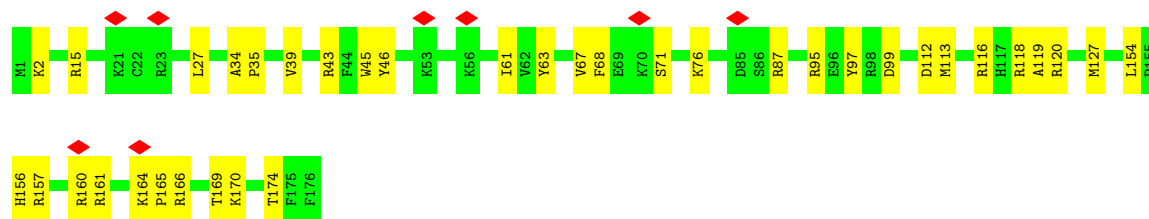
• Molecule 16: eL19

Chain Q:  14% 70% 22% 8%



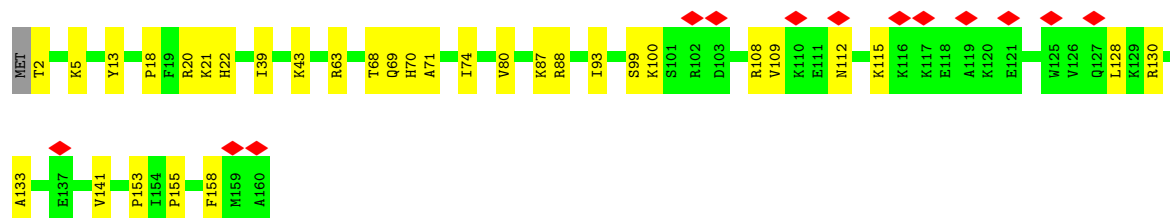
• Molecule 17: eL20

Chain R:  5% 79% 21%



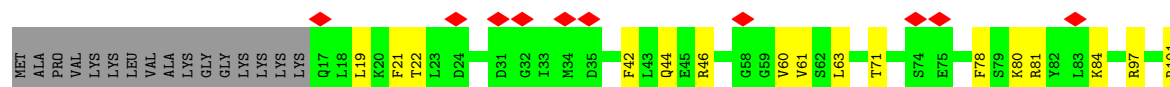
• Molecule 18: eL21

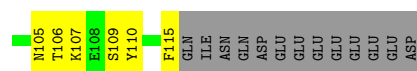
Chain S:  8% 79% 20%



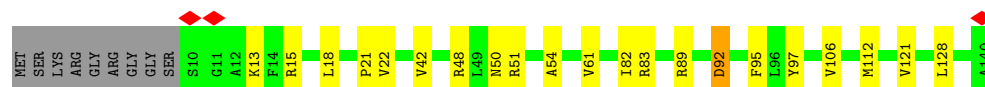
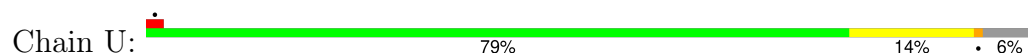
• Molecule 19: eL22

Chain T:  8% 60% 17% 23%

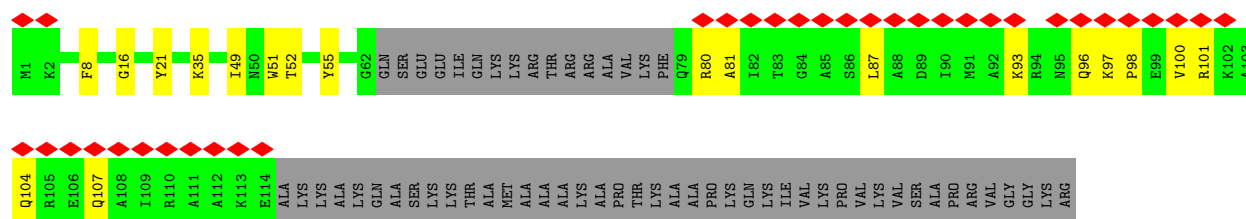




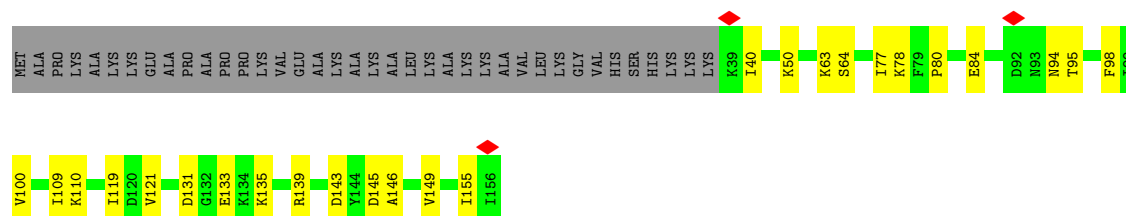
• Molecule 20: L23



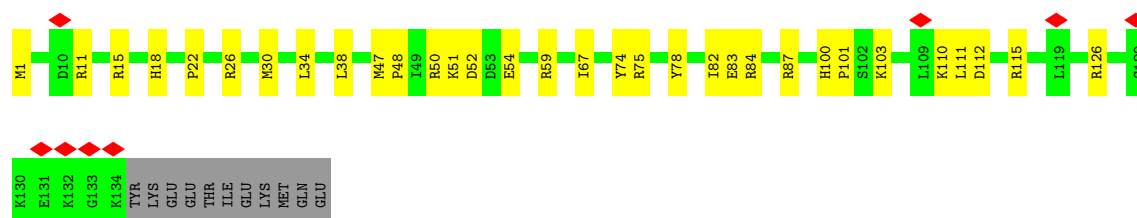
• Molecule 21: L24



• Molecule 22: uL23

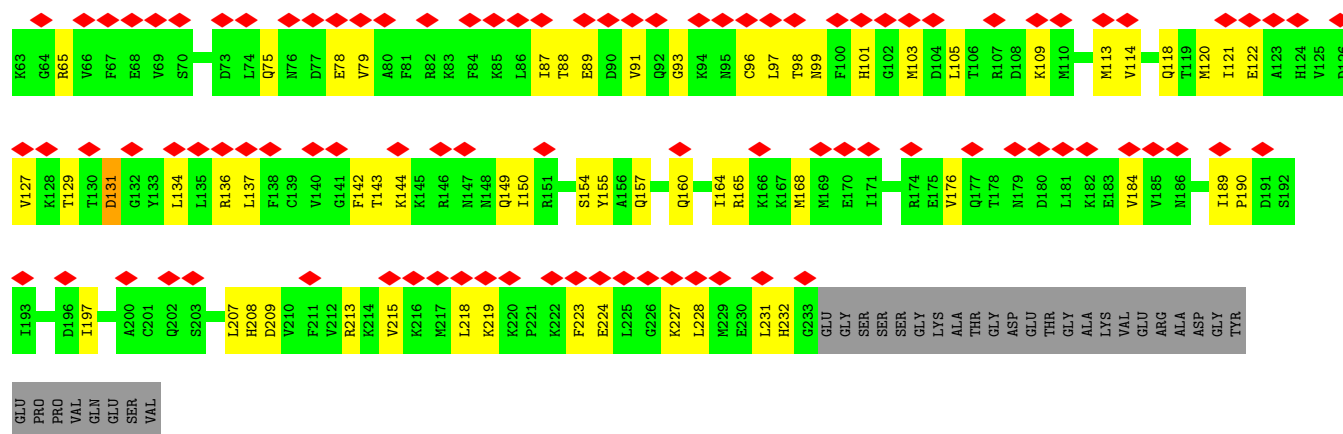


• Molecule 23: L26

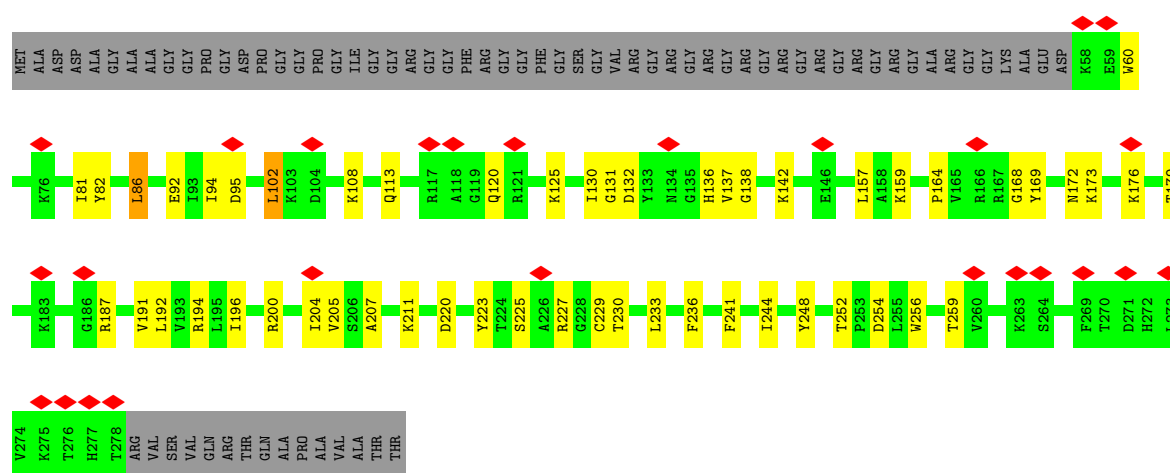


• Molecule 24: L27

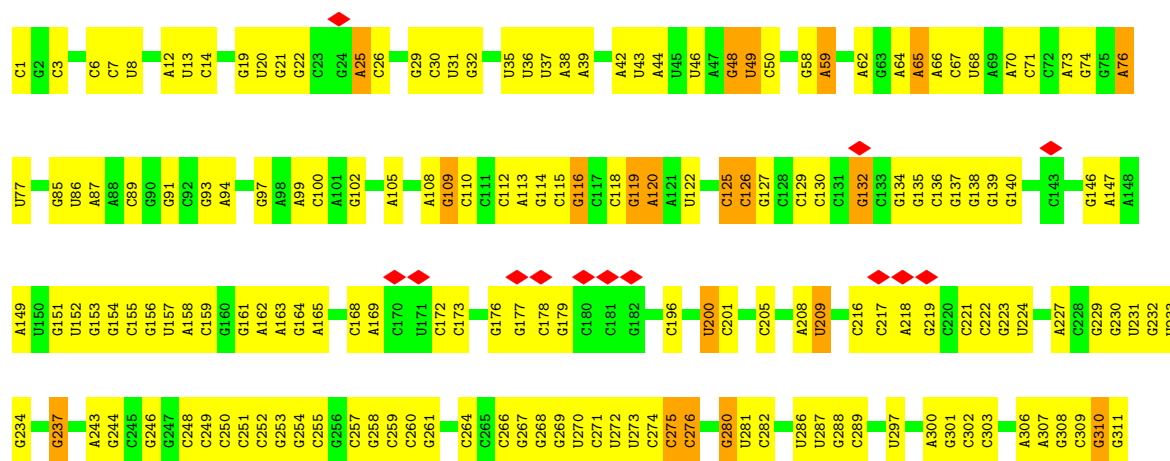




• Molecule 29: eS1



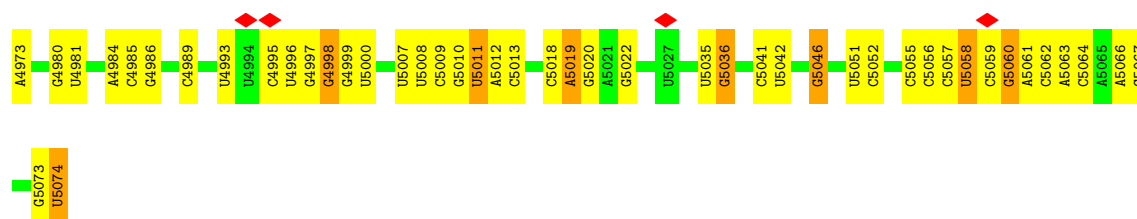
• Molecule 30: 28S rRNA



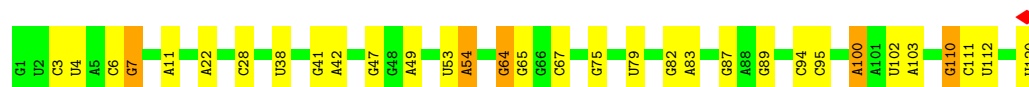
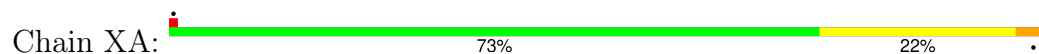


G3630	G3631	C3638	G3639	G3640	G3641	G3642	U3646	A3651	C3655	A3656	A3657	A3658	C3663	G3664	G3665	G3666	A3667	A3668	G3669	G3670	G3677	G3678	G3689	G3690	G3691	A3692	U3693	G3694	U3695	G3696	U3697	U3698	U3700	C3701	U3702	G3703	C3704	C3705	C3706	U3712	C3713	U3714	G3715	A3716	A3717	U3720	C3721	A3722	A3723																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
U2831	G2832	U2833	U2834	G2835	G2836	A2837	A2838	C2839	A2840	A2841	U2842	G2843	U2844	G2847	U2848	A2849	A2850	G2853	G2860	C2861	A2862	A2863	C2866	C2880	G2881	A2884	C2890	U2891	U2892	U2893	G2902	G2903	A3604	G3605	C3610	U3611	U3612	A3613	G3614	A3615	A3616	G3620	C3623	G3624	G3625	A3626	C3627	C3628	A3629																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G2682	A2683	G2684	G2685	G2686	G2687	C2688	G2691	G2692	G2693	C2694	C2695	U2696	U2697	G2698	A2700	A2701	A2702	C2707	G2708	G2709	G2710	G2711	G2712	U2713	C2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2726	G2727	A2730	C2731	C2732	U2733	G2737	U2738	G2740	G2741	C2744	U2745	A2748	A2749	A2750	A2751	C2754																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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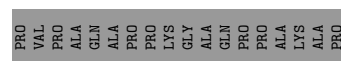
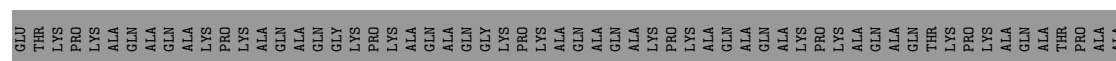
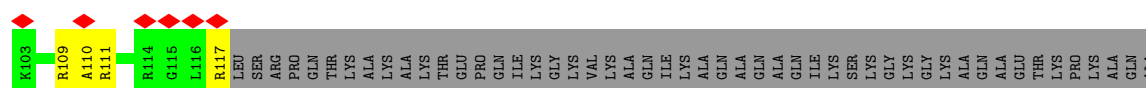
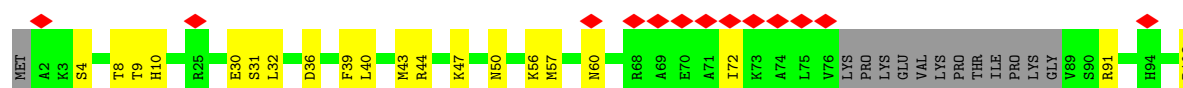
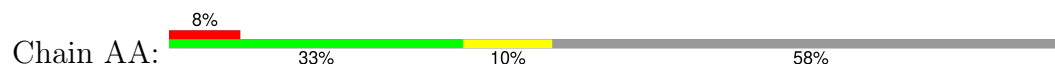
• Molecule 31: 5S rRNA



• Molecule 32: 5.8S rRNA

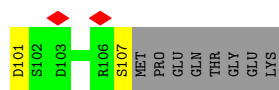


• Molecule 33: eL29

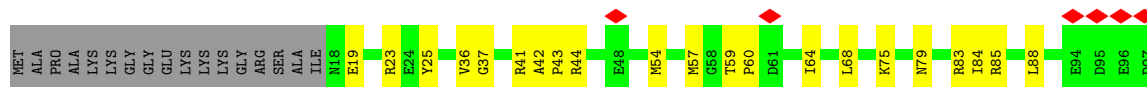


• Molecule 34: eL30

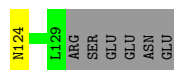
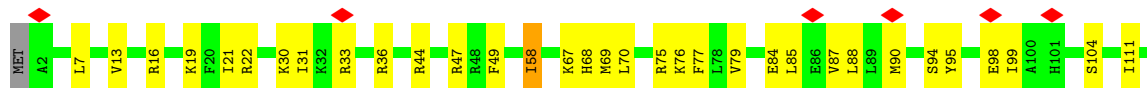




- Molecule 35: eL31



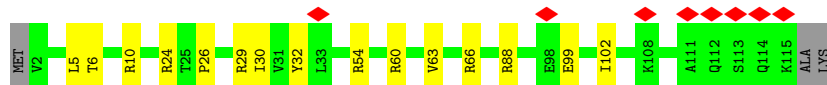
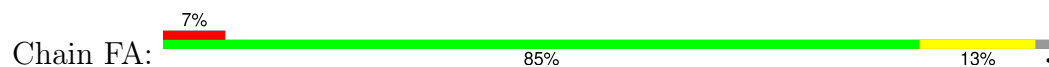
- Molecule 36: eL32



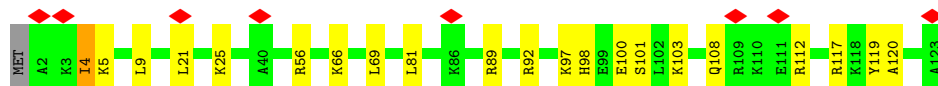
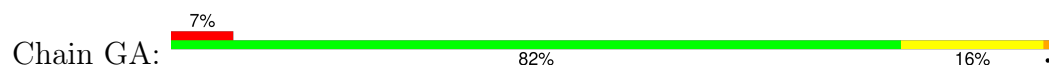
- Molecule 37: eL33



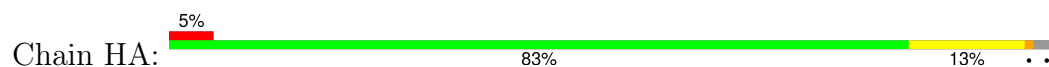
- Molecule 38: eL34



- Molecule 39: uL29



- Molecule 40: L36

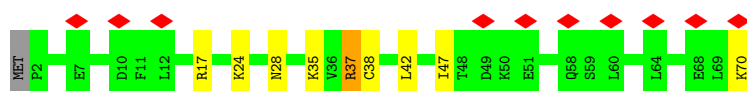




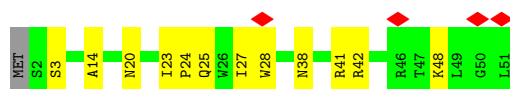
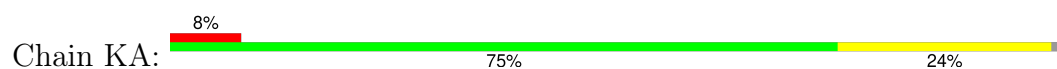
• Molecule 41: L37



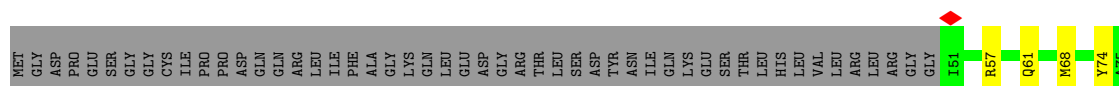
• Molecule 42: eL38



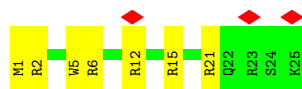
• Molecule 43: eL39



• Molecule 44: eL40



• Molecule 45: eL41

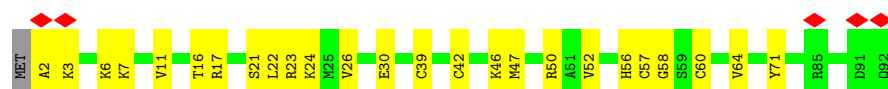
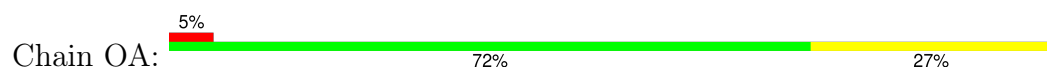


• Molecule 46: eL42

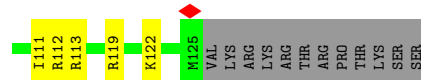
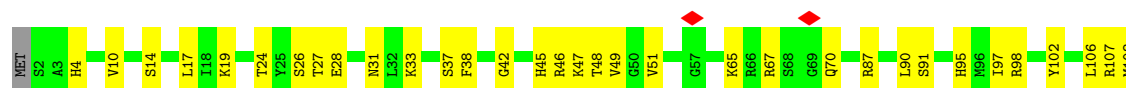




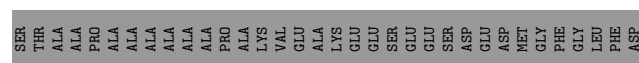
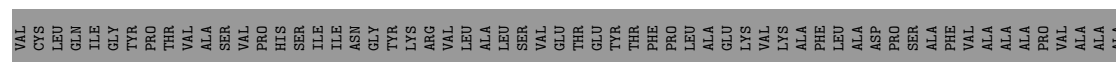
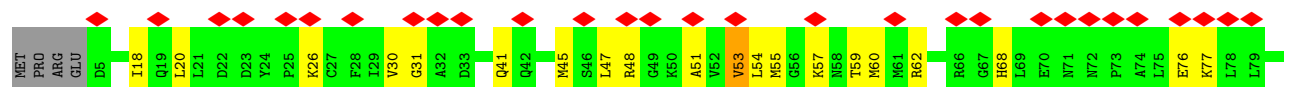
• Molecule 47: eL43



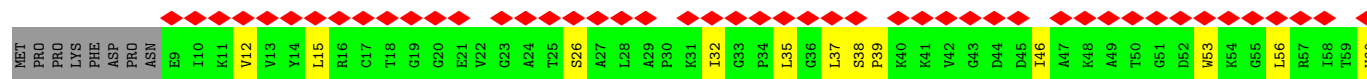
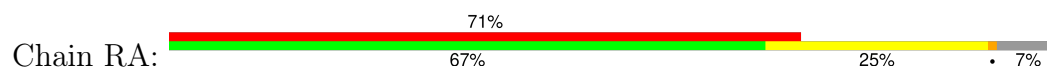
• Molecule 48: eL28



• Molecule 49: uL10

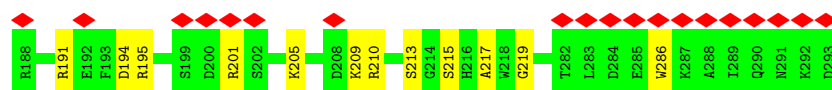
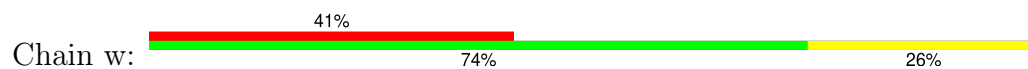


• Molecule 50: uL3

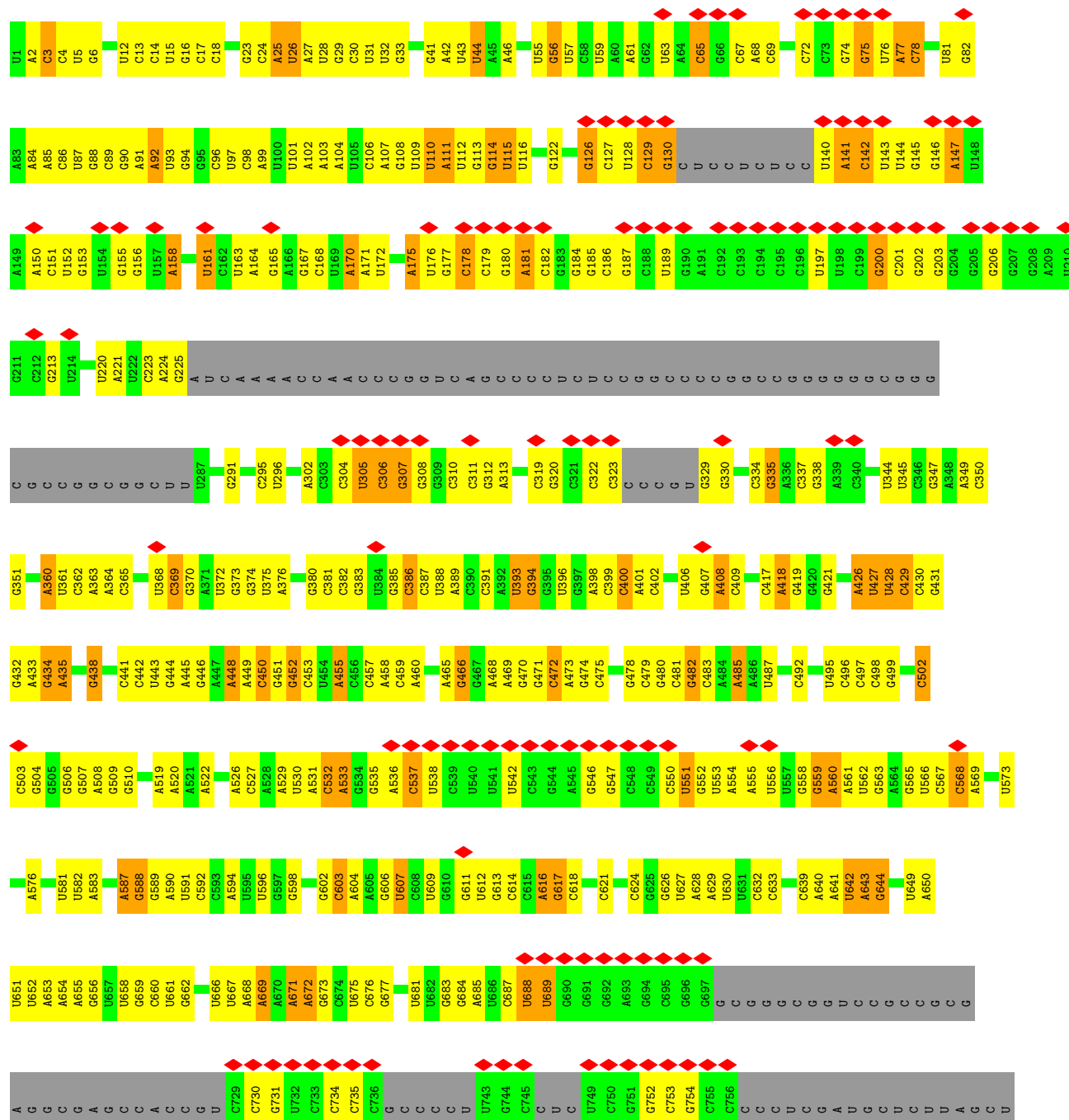


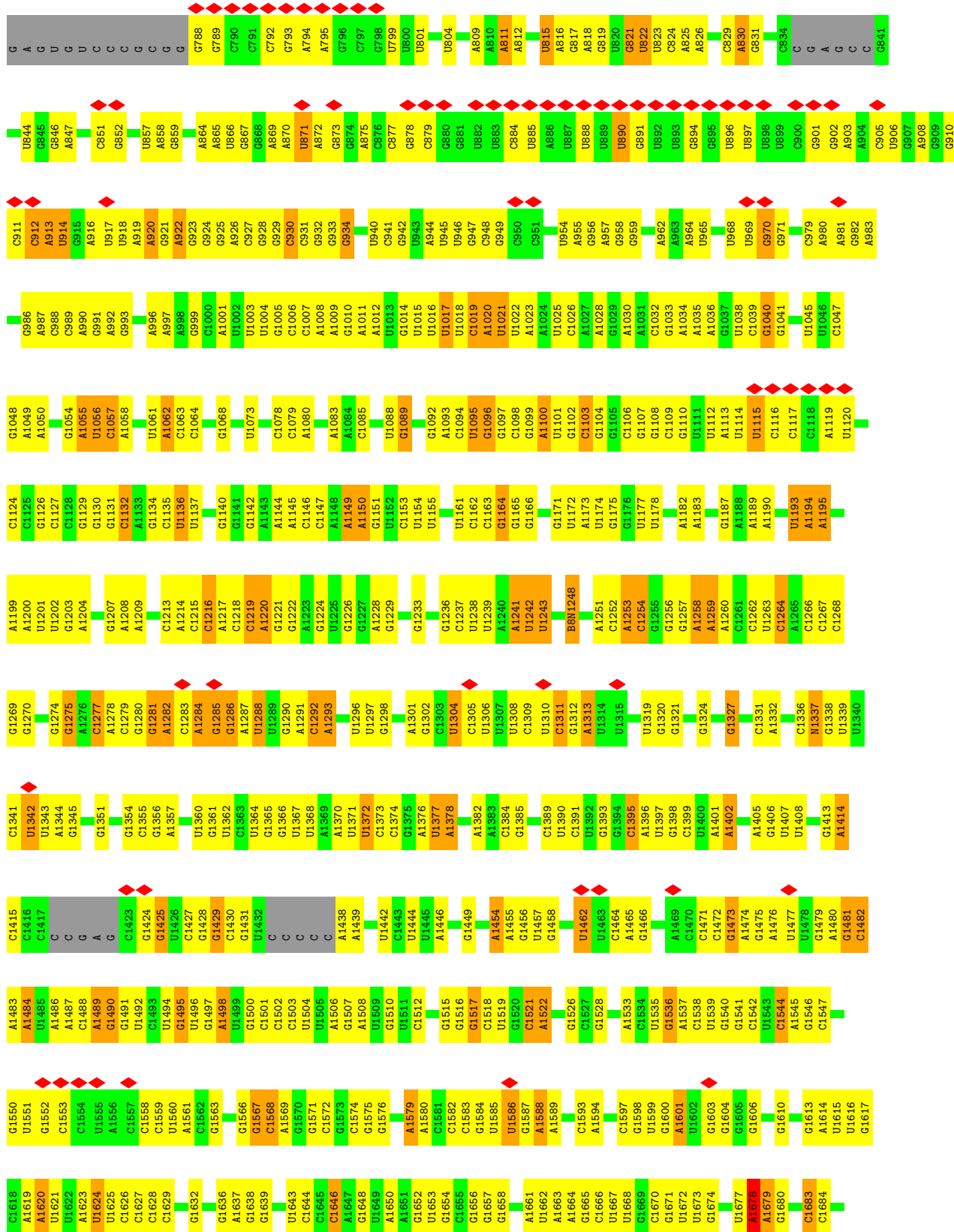


• Molecule 52: Serpine mRNA binding protein 1



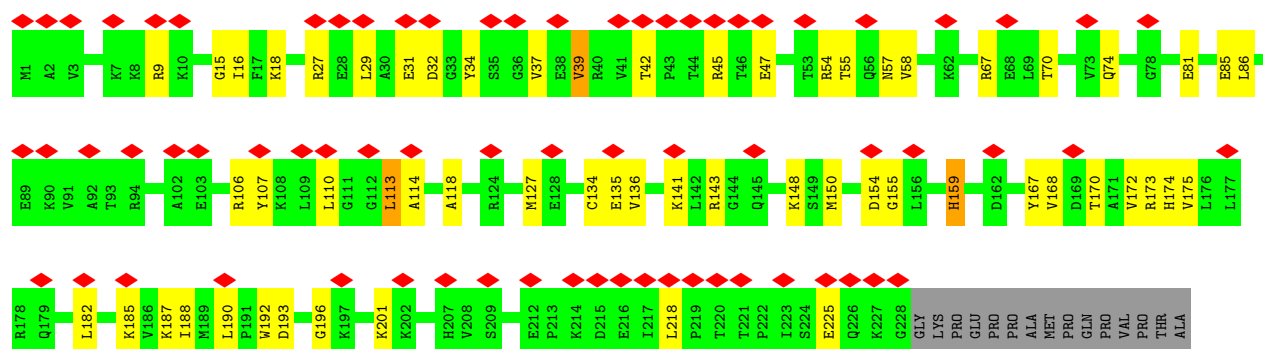
• Molecule 53: 18S rRNA



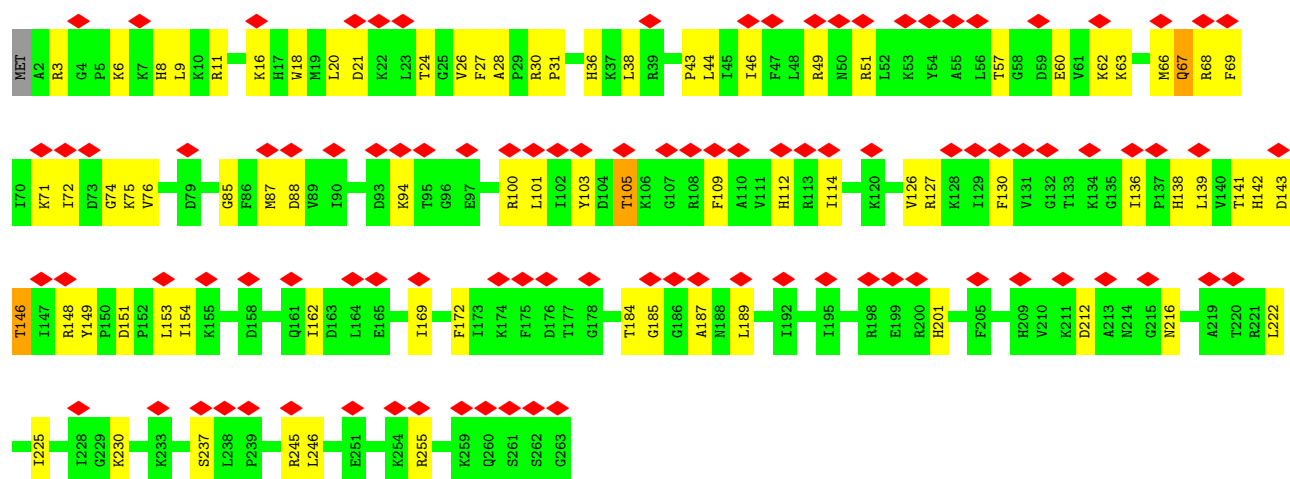
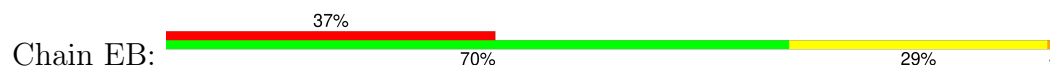




• Molecule 54: uS3

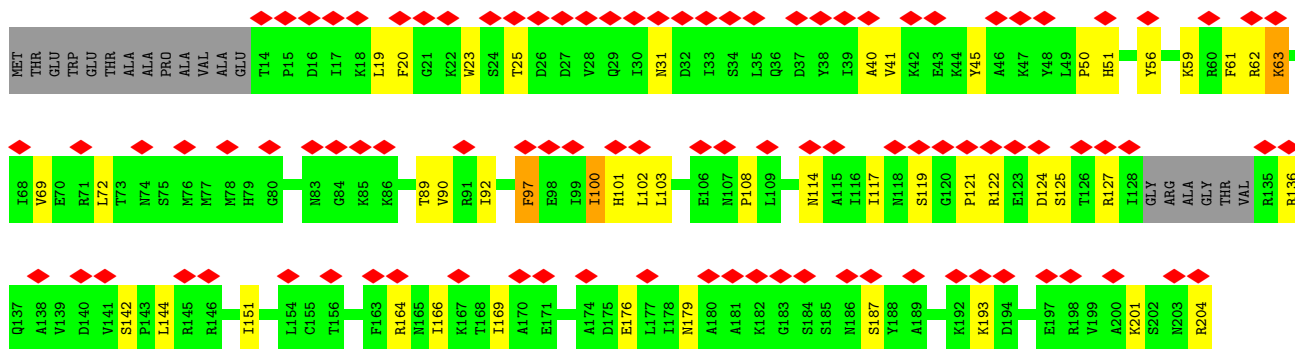


• Molecule 55: eS4

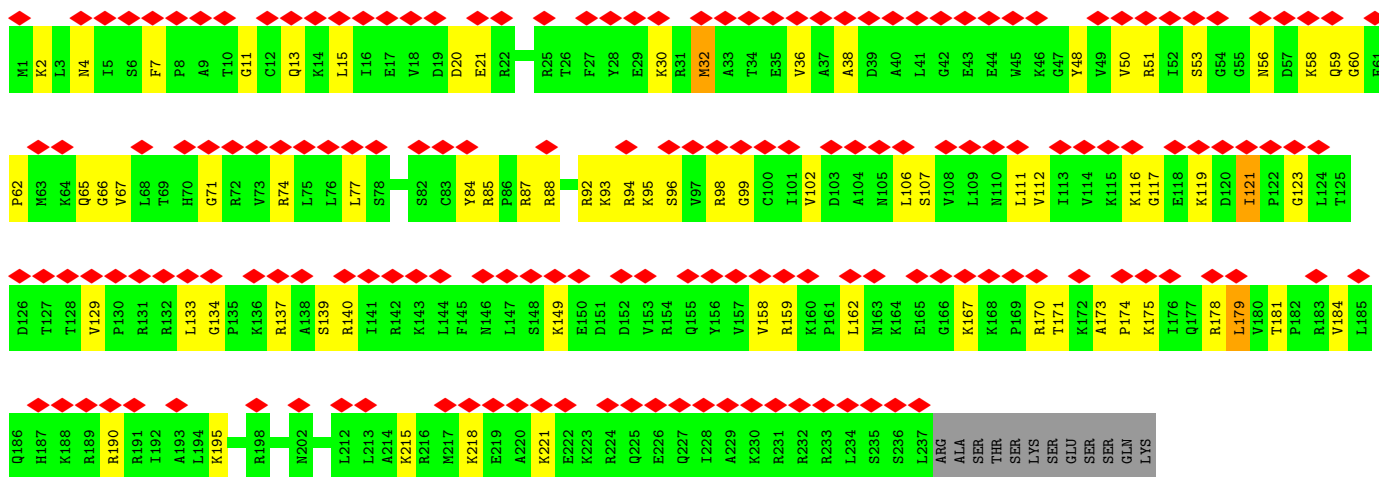


• Molecule 56: S5

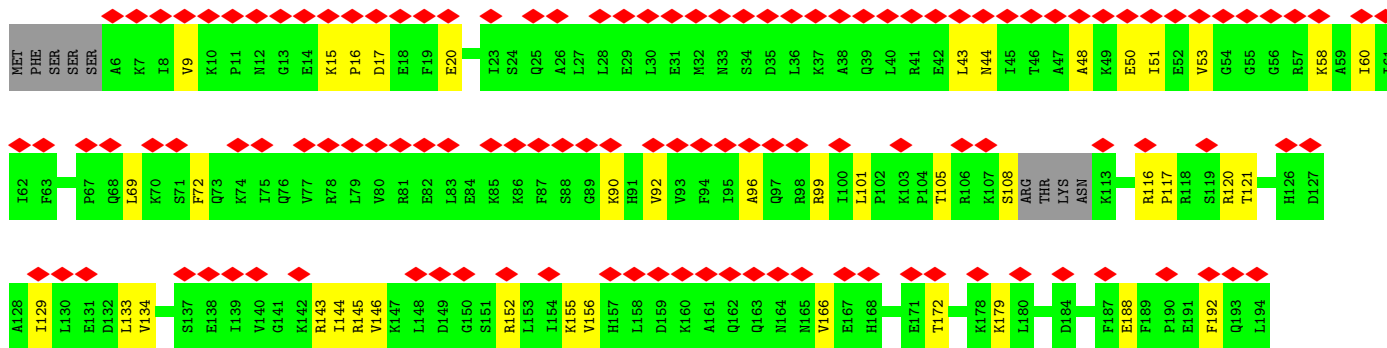
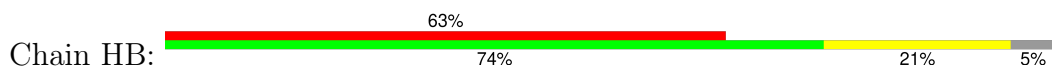




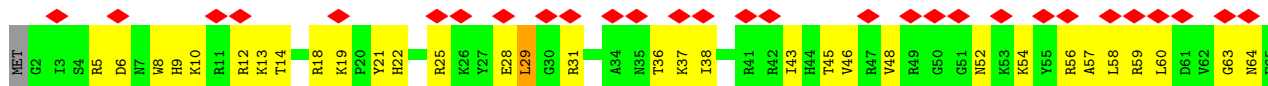
• Molecule 57: S6

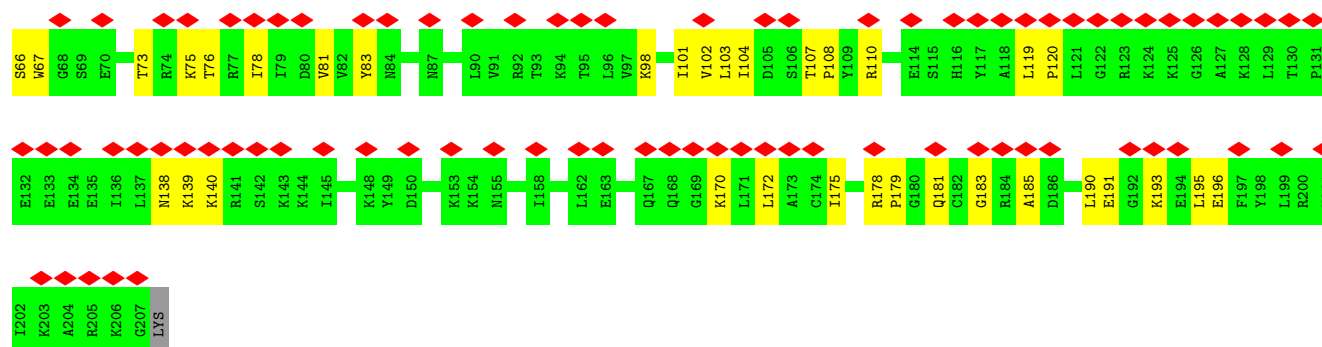


• Molecule 58: S7

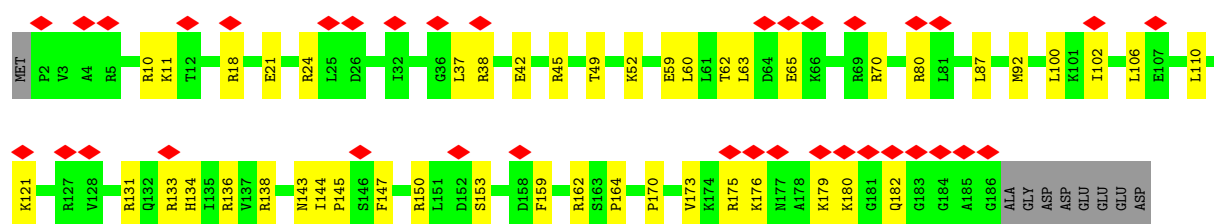
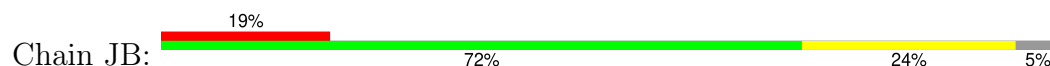


• Molecule 59: eS8

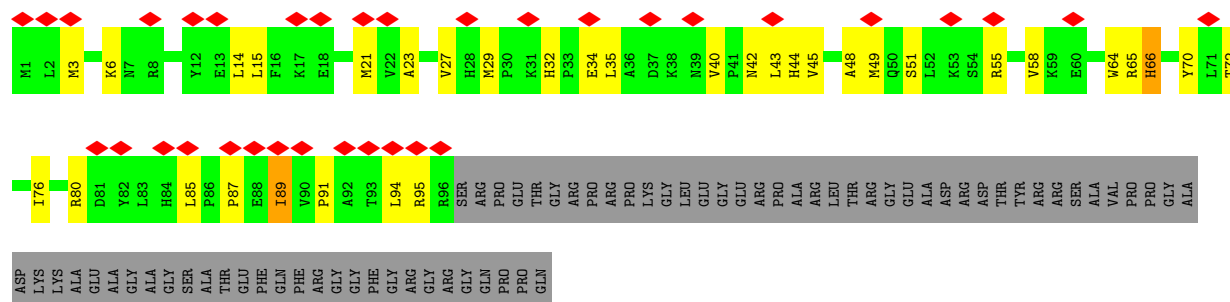




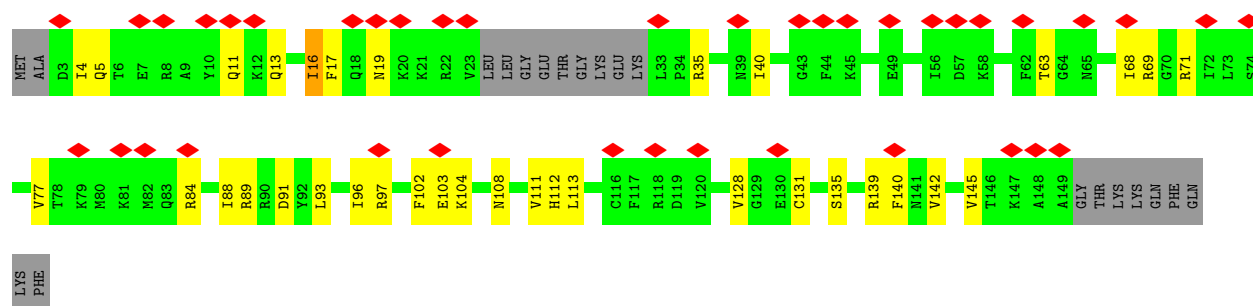
• Molecule 60: S9



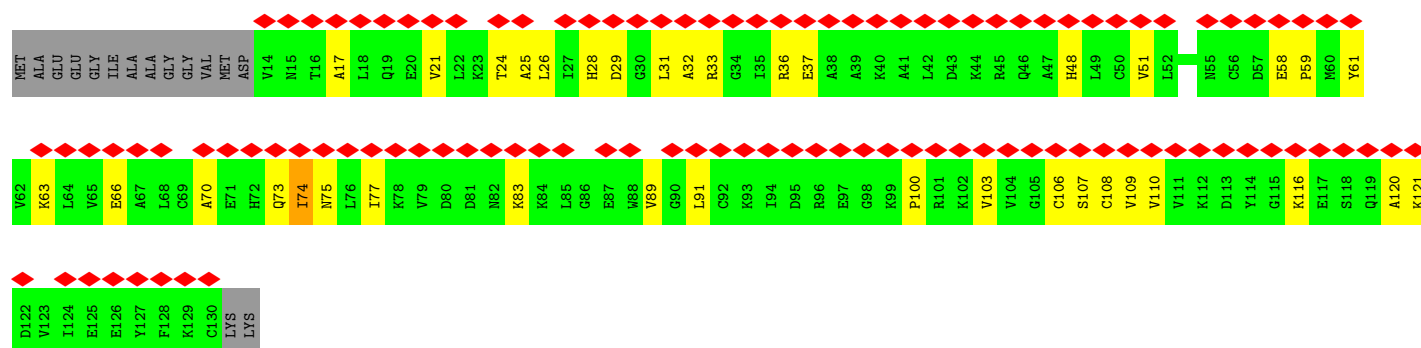
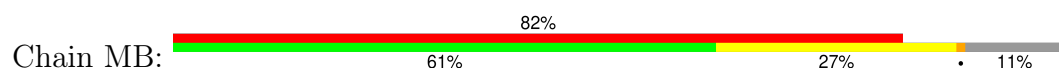
• Molecule 61: eS10



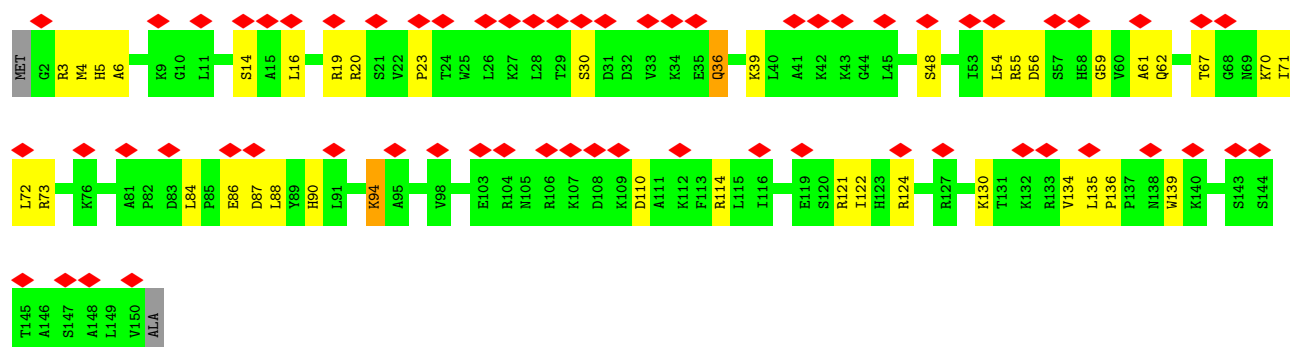
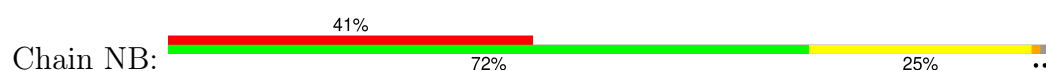
• Molecule 62: S11



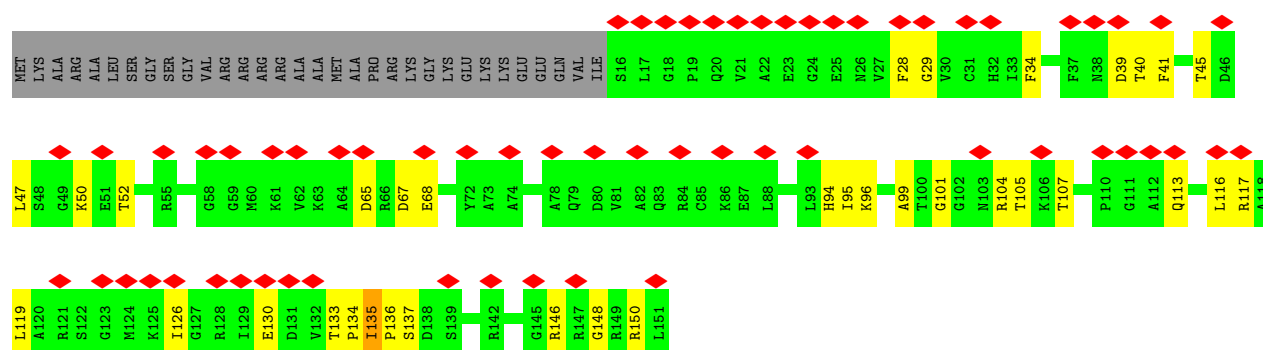
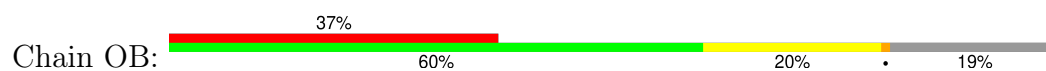
• Molecule 63: S12



• Molecule 64: uS15

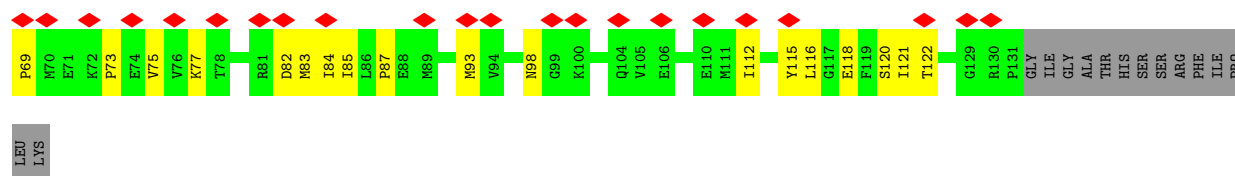


• Molecule 65: uS11

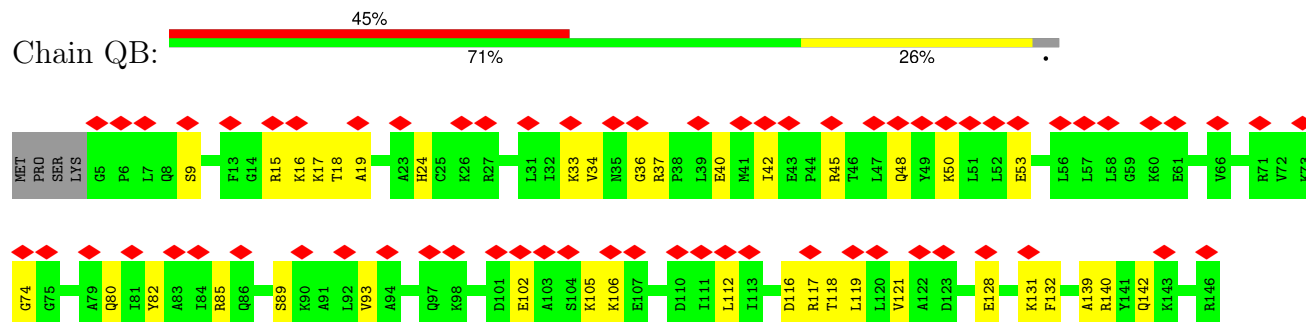


• Molecule 66: uS19

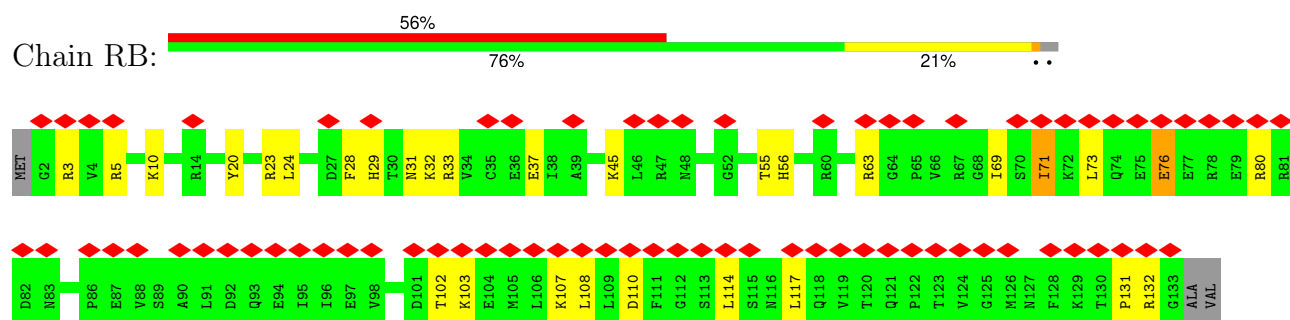




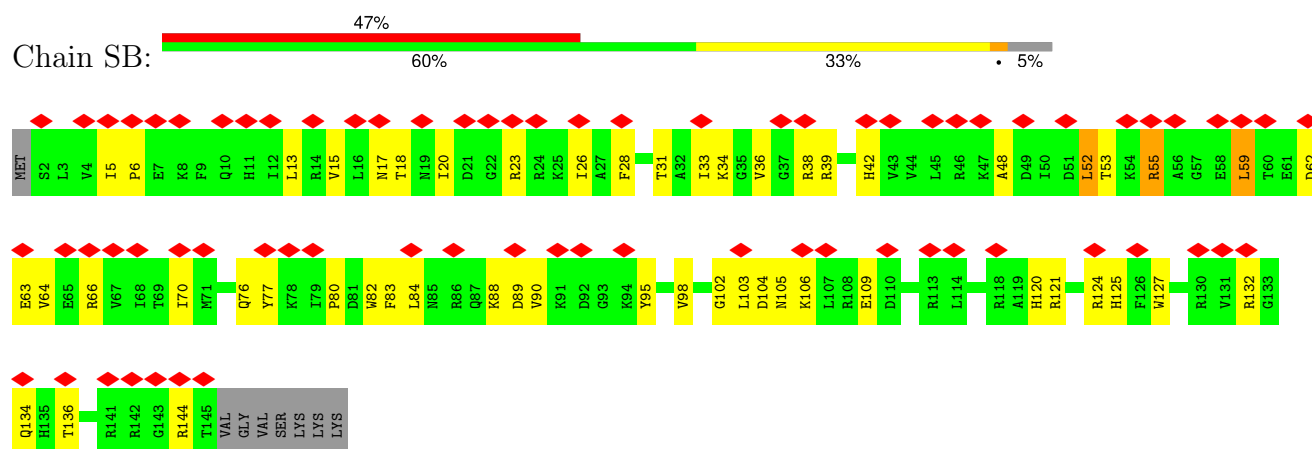
- Molecule 67: S16



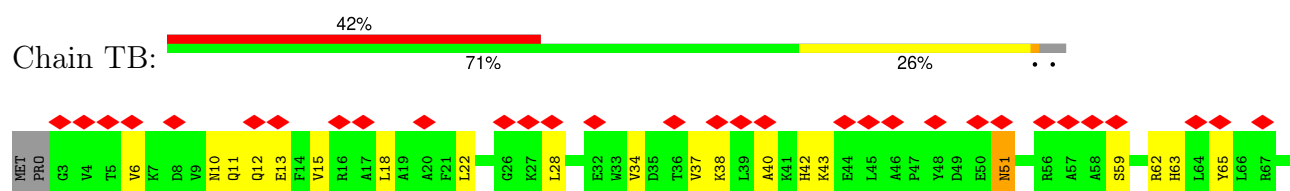
- Molecule 68: eS17



- Molecule 69: uS13

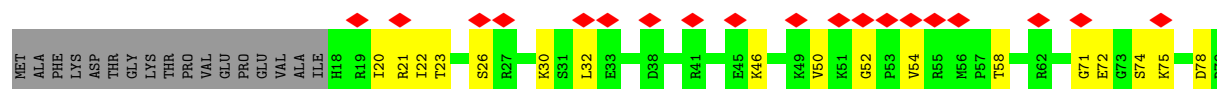
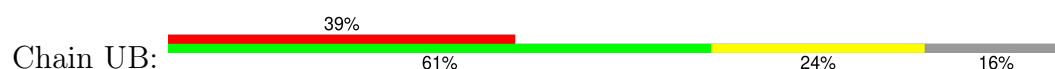


- Molecule 70: eS19

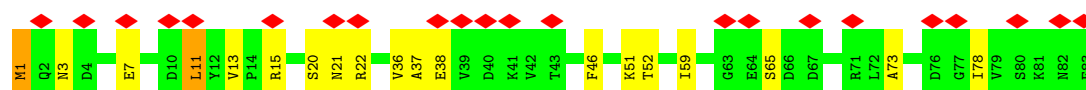
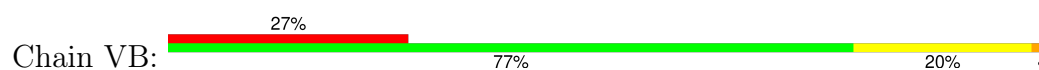




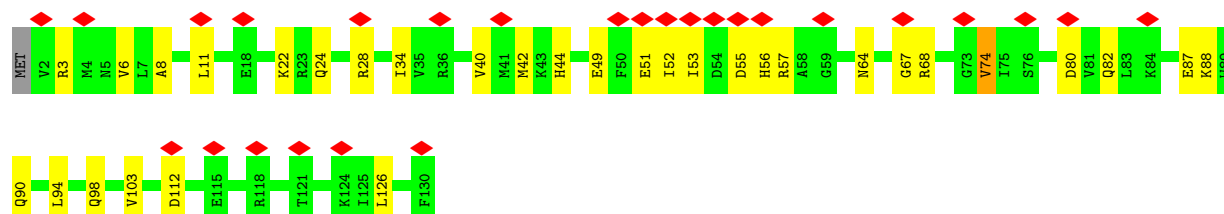
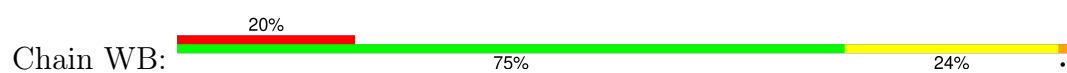
• Molecule 71: uS10



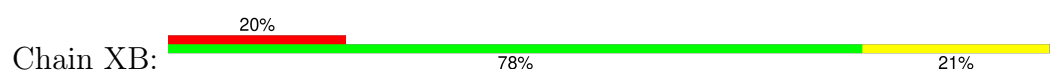
• Molecule 72: eS21



• Molecule 73: S15A

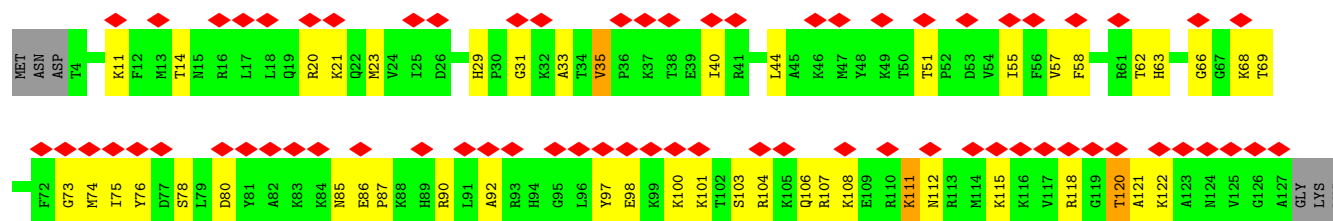


• Molecule 74: uS12

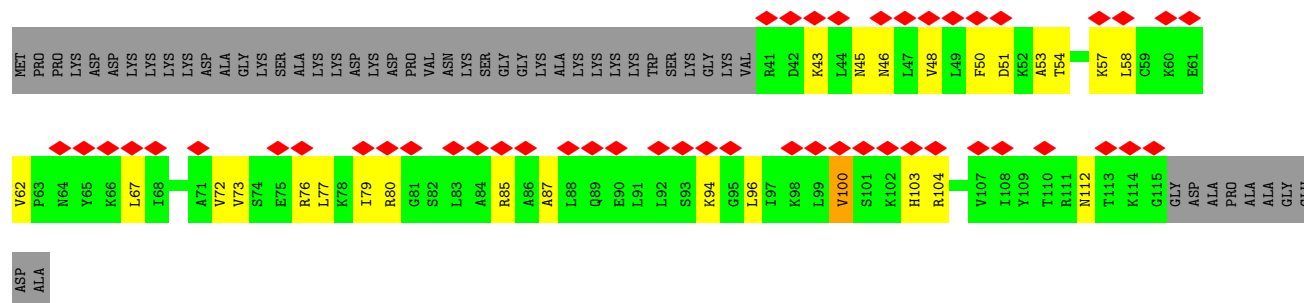


• Molecule 75: eS24

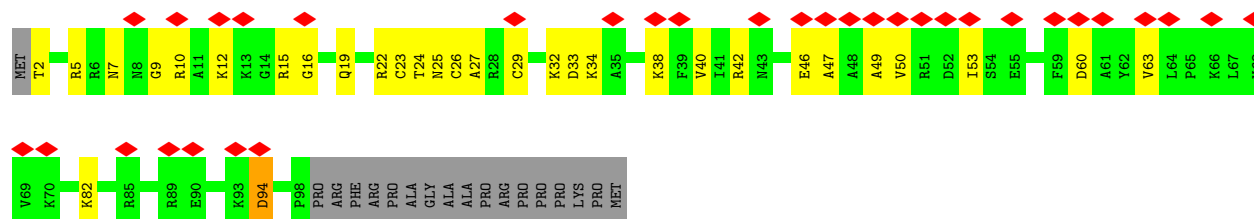




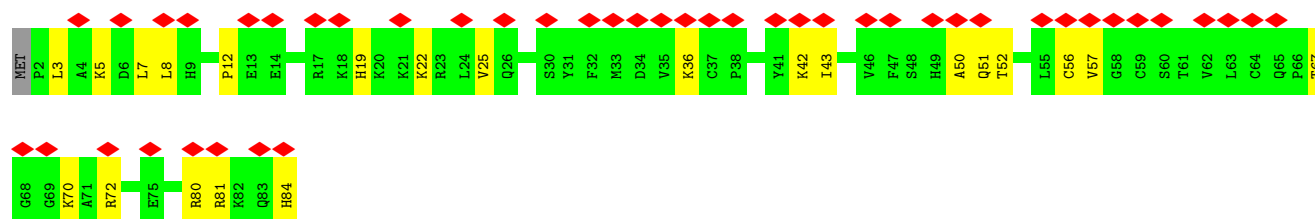
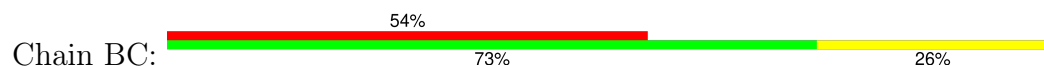
- Molecule 76: eS25



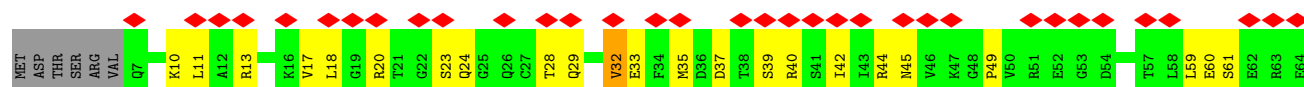
- Molecule 77: eS26

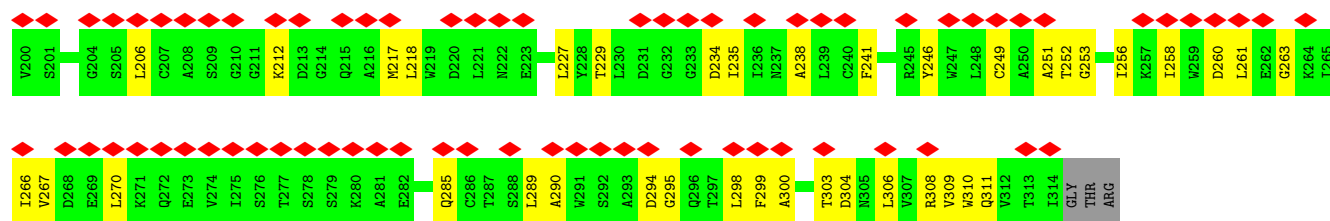


- Molecule 78: S27

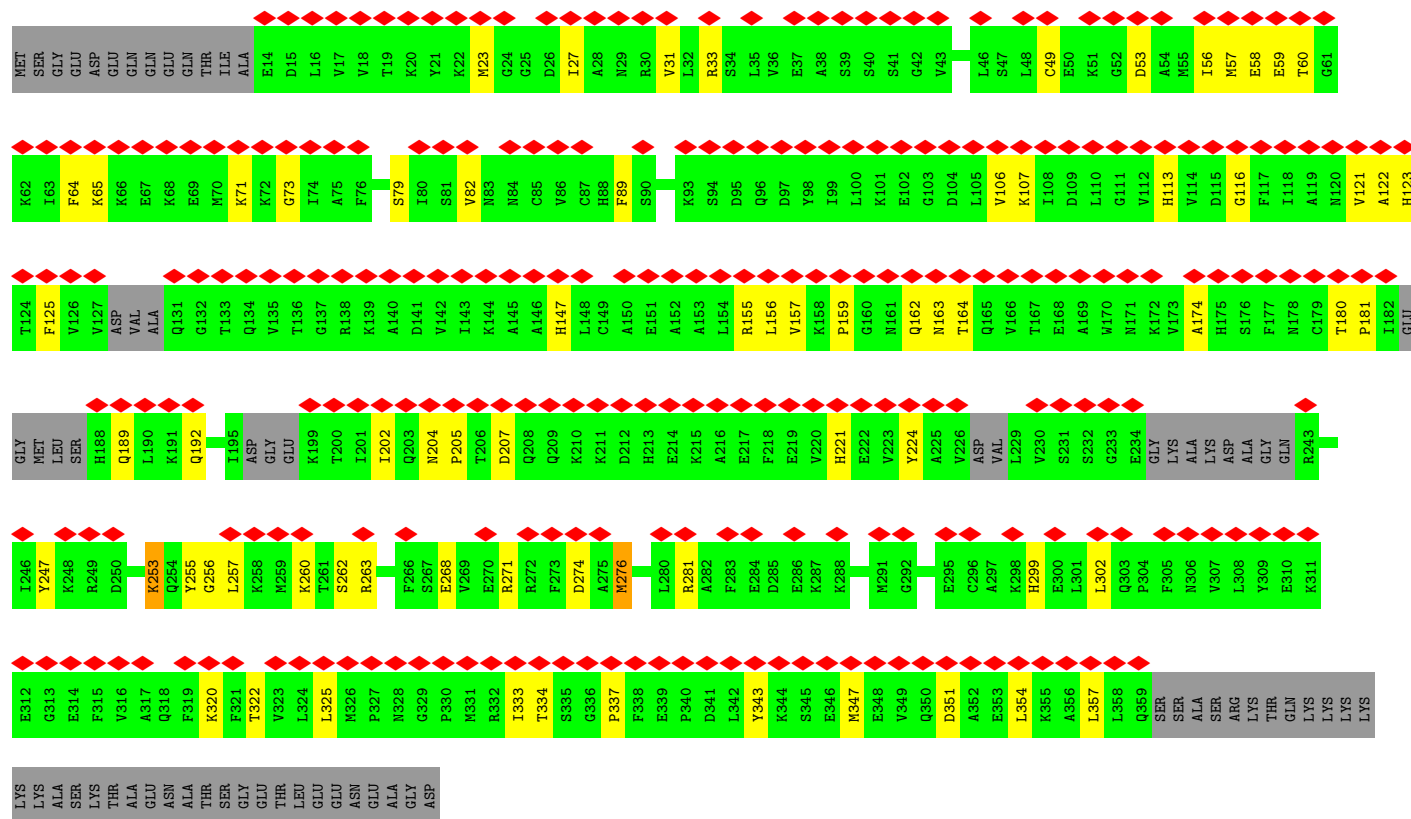


- Molecule 79: S28





• Molecule 84: Proliferation-associated protein 2G4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10568	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.231	Depositor
Minimum map value	-21.911	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.532	Depositor
Recommended contour level	6.3	Depositor
Map size (Å)	686.87994, 686.87994, 686.87994	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, I4U, 5MC, P4U, B8T, ZN, B9B, JMH, UR3, B8K, MLZ, 2MG, BGH, OMG, B8H, B9H, 1MA, MHG, SPD, M7A, A2M, PSU, OMU, P7G, OMC, B8W, 6MZ, B8N, 5MU, MG, 4AC, E7G, ANM, DDE, E6G, GDP

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	0.12	0/1936	0.27	0/2596
2	B	0.11	0/3240	0.24	0/4339
3	C	0.11	0/2927	0.22	0/3932
4	D	0.10	0/2437	0.22	0/3264
5	E	0.10	0/1753	0.23	0/2351
6	F	0.11	0/1911	0.23	0/2549
7	G	0.09	0/1910	0.22	0/2569
8	H	0.11	0/1535	0.23	0/2063
9	I	0.11	0/1702	0.21	0/2272
10	J	0.09	0/1385	0.22	0/1852
11	L	0.10	0/1158	0.22	0/1547
12	M	0.11	0/1746	0.23	0/2338
13	N	0.10	0/1662	0.23	0/2222
14	O	0.10	0/1268	0.23	0/1700
15	P	0.12	0/1539	0.24	0/2054
16	Q	0.08	0/1524	0.20	0/2013
17	R	0.11	0/1501	0.23	0/2012
18	S	0.10	0/1326	0.22	0/1770
19	T	0.09	0/823	0.24	0/1104
20	U	0.11	0/993	0.24	0/1332
21	V	0.09	0/813	0.22	0/1080
22	W	0.09	0/984	0.22	0/1323
23	X	0.10	0/1132	0.23	0/1504
24	Y	0.09	0/1130	0.24	0/1507
25	Z	0.11	0/1191	0.23	0/1590
26	K	0.10	0/1733	0.22	0/2316
27	AB	0.09	0/1749	0.22	0/2377
28	BB	0.08	0/1756	0.23	0/2350
29	CB	0.09	0/1753	0.24	0/2369
30	WA	0.14	0/82492	0.24	0/128582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	XA	0.11	0/2858	0.19	0/4455
32	YA	0.13	0/3559	0.21	0/5543
33	AA	0.08	0/861	0.20	0/1138
34	BA	0.09	0/771	0.19	0/1034
35	CA	0.11	0/903	0.25	0/1216
36	DA	0.11	0/1071	0.25	0/1429
37	EA	0.11	0/895	0.25	0/1198
38	FA	0.10	0/916	0.21	0/1220
39	GA	0.08	0/1021	0.19	0/1348
40	HA	0.09	0/841	0.21	0/1112
41	IA	0.11	0/720	0.25	0/952
42	JA	0.09	0/575	0.21	0/761
43	KA	0.11	0/459	0.26	0/608
44	LA	0.10	0/425	0.24	0/561
45	MA	0.08	0/240	0.21	0/305
46	NA	0.10	0/855	0.23	0/1128
47	OA	0.10	0/718	0.21	0/953
48	PA	0.09	0/1010	0.24	0/1354
49	QA	0.08	0/1530	0.21	0/2064
50	RA	0.08	0/1174	0.23	0/1582
51	v	0.10	0/6596	0.26	0/8909
52	w	0.09	0/372	0.25	0/492
53	ZA	0.10	0/40393	0.23	0/62941
54	DB	0.10	0/1796	0.25	0/2417
55	EB	0.09	0/2118	0.24	0/2849
56	FB	0.08	0/1492	0.23	0/2005
57	GB	0.08	0/1946	0.22	0/2590
58	HB	0.08	0/1510	0.21	0/2022
59	IB	0.09	0/1715	0.24	0/2287
60	JB	0.08	0/1550	0.20	0/2069
61	KB	0.09	0/834	0.26	0/1125
62	LB	0.09	0/1157	0.21	0/1549
63	MB	0.08	0/918	0.24	0/1233
64	NB	0.07	0/1226	0.20	0/1649
65	OB	0.08	0/1029	0.22	0/1380
66	PB	0.08	0/1017	0.21	0/1358
67	QB	0.09	0/1146	0.24	0/1534
68	RB	0.08	0/1082	0.20	0/1452
69	SB	0.09	0/1208	0.23	0/1618
70	TB	0.11	0/1115	0.23	0/1493
71	UB	0.08	0/805	0.21	0/1081
72	VB	0.08	0/643	0.22	0/860
73	WB	0.10	0/1051	0.24	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XB	0.09	0/1116	0.22	0/1490
75	YB	0.07	0/1028	0.22	0/1366
76	ZB	0.08	0/604	0.21	0/810
77	AC	0.10	0/786	0.23	0/1053
78	BC	0.09	0/665	0.24	0/891
79	CC	0.09	0/490	0.23	0/656
80	DC	0.09	0/470	0.22	0/623
81	EC	0.07	0/447	0.19	0/587
82	FC	0.07	0/567	0.20	0/753
83	GC	0.09	0/2493	0.24	0/3394
84	b	0.08	0/2462	0.22	0/3321
All	All	0.11	0/234258	0.23	0/342101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	65	0
2	B	3172	0	3310	68	0
3	C	2884	0	3053	54	0
4	D	2391	0	2424	44	0
5	E	1720	0	1874	36	0
6	F	1875	0	1995	39	0
7	G	1879	0	2027	38	0
8	H	1516	0	1597	23	0
9	I	1664	0	1712	29	0
10	J	1362	0	1399	26	0
11	L	1137	0	1211	22	0
12	M	1701	0	1749	43	0
13	N	1630	0	1778	37	0
14	O	1242	0	1274	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	1515	0	1633	37	0
16	Q	1508	0	1664	31	0
17	R	1462	0	1508	36	0
18	S	1298	0	1366	28	0
19	T	809	0	833	16	0
20	U	979	0	1039	16	0
21	V	800	0	833	14	0
22	W	967	0	1040	18	0
23	X	1115	0	1205	26	0
24	Y	1107	0	1182	27	0
25	Z	1162	0	1209	36	0
26	K	1702	0	1820	39	0
27	AB	1712	0	1713	35	0
28	BB	1729	0	1803	46	0
29	CB	1716	0	1806	34	0
30	WA	76047	0	38173	1359	0
31	XA	2558	0	1296	25	0
32	YA	3209	0	1631	74	0
33	AA	848	0	920	19	0
34	BA	761	0	794	14	0
35	CA	888	0	929	19	0
36	DA	1053	0	1147	26	0
37	EA	876	0	912	24	0
38	FA	906	0	998	12	0
39	GA	1013	0	1147	16	0
40	HA	830	0	916	13	0
41	IA	705	0	737	22	0
42	JA	569	0	637	6	0
43	KA	447	0	480	9	0
44	LA	430	0	465	6	0
45	MA	239	0	289	7	0
46	NA	842	0	912	21	0
47	OA	708	0	756	16	0
48	PA	994	0	1051	27	0
49	QA	1507	0	1564	32	0
50	RA	1160	0	1218	30	0
51	v	6489	0	6573	139	0
52	w	366	0	342	13	0
53	ZA	36263	0	18294	796	0
54	DB	1768	0	1866	41	0
55	EB	2076	0	2177	54	0
56	FB	1471	0	1522	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	GB	1923	0	2089	63	0
58	HB	1488	0	1582	27	0
59	IB	1686	0	1772	47	0
60	JB	1525	0	1640	34	0
61	KB	810	0	836	24	0
62	LB	1137	0	1200	24	0
63	MB	908	0	939	21	0
64	NB	1202	0	1289	36	0
65	OB	1016	0	1039	27	0
66	PB	997	0	1045	29	0
67	QB	1128	0	1195	32	0
68	RB	1068	0	1121	21	0
69	SB	1190	0	1249	38	0
70	TB	1097	0	1130	28	0
71	UB	795	0	862	20	0
72	VB	636	0	637	12	0
73	WB	1034	0	1080	28	0
74	XB	1098	0	1167	23	0
75	YB	1011	0	1083	35	0
76	ZB	598	0	656	19	0
77	AC	774	0	822	25	0
78	BC	651	0	672	19	0
79	CC	488	0	514	15	0
80	DC	459	0	448	15	0
81	EC	443	0	492	9	0
82	FC	555	0	566	14	0
83	GC	2436	0	2393	64	0
84	b	2422	0	2340	41	0
85	AC	1	0	0	0	0
85	B	2	0	0	0	0
85	DA	1	0	0	0	0
85	FA	1	0	0	0	0
85	I	1	0	0	0	0
85	KA	1	0	0	0	0
85	O	1	0	0	0	0
85	TB	1	0	0	0	0
85	U	1	0	0	0	0
85	WA	110	0	0	0	0
85	XA	4	0	0	0	0
85	YA	1	0	0	0	0
85	ZA	19	0	0	0	0
86	WA	19	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	WA	10	0	19	0	0
88	AC	1	0	0	0	0
88	DC	1	0	0	0	0
88	FA	1	0	0	0	0
88	FC	1	0	0	0	0
88	IA	1	0	0	0	0
88	LA	1	0	0	0	0
88	NA	1	0	0	0	0
88	OA	1	0	0	0	0
89	v	28	0	12	2	0
All	All	221459	0	167704	3842	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 10.

All (3842) 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)
30:WA:4088:5MU:C4	30:WA:4088:5MU:C5	1.82	1.60
30:WA:4088:5MU:C6	30:WA:4088:5MU:N1	1.68	1.58
30:WA:4301:B8H:C5	30:WA:4301:B8H:C4	1.83	1.57
30:WA:3767:B8H:C4	30:WA:3767:B8H:C5	1.83	1.54
30:WA:1865:B8H:C4	30:WA:1865:B8H:C5	1.83	1.54
30:WA:1865:B8H:C6	30:WA:1865:B8H:N1	1.68	1.53
30:WA:4301:B8H:N1	30:WA:4301:B8H:C6	1.67	1.53
30:WA:3767:B8H:C6	30:WA:3767:B8H:N1	1.68	1.50
30:WA:3904:BGH:C4'	30:WA:3904:BGH:O4'	1.66	1.15
30:WA:3697:A:N6	30:WA:3828:G:H21	1.46	1.11
30:WA:3697:A:H62	30:WA:3828:G:N2	1.47	1.10
53:ZA:1288:U:H3	53:ZA:1311:C:N4	1.50	1.07
53:ZA:1472:C:N4	53:ZA:1476:A:H62	1.58	0.99
53:ZA:1472:C:H42	53:ZA:1476:A:N6	1.64	0.96
30:WA:2562:G:H1	30:WA:2575:U:H3	1.14	0.96
53:ZA:1351:G:H1	53:ZA:1360:U:H3	1.08	0.95
53:ZA:1656:G:H1	53:ZA:1668:U:H3	1.18	0.89
53:ZA:925:G:H1	53:ZA:1017:U:H3	1.22	0.86
53:ZA:1737:G:H1	53:ZA:1797:U:H3	1.24	0.86
30:WA:4301:B8H:C5	30:WA:4301:B8H:N1	2.36	0.84
30:WA:1551:C:H42	30:WA:1617:G:H22	1.24	0.84
53:ZA:304:C:H5''	53:ZA:305:U:H5'	1.61	0.82
30:WA:1:C:H42	32:YA:156:U:H3	1.22	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:102:G:HO2'	30:WA:1387:U:HO2'	1.26	0.81
30:WA:2850:A:H61	30:WA:3848:C:H42	1.24	0.81
30:WA:4742:G:H5'	30:WA:5074:U:H3'	1.60	0.81
30:WA:1404:A:H62	30:WA:1425:G:H21	1.29	0.81
30:WA:4088:5MU:C6	30:WA:4088:5MU:C2	2.66	0.80
30:WA:1:C:N4	32:YA:156:U:H3	1.79	0.80
30:WA:1609:G:H2'	30:WA:1610:7MG:H82	1.64	0.80
53:ZA:1729:U:H3	53:ZA:1805:G:H1	1.31	0.78
30:WA:3767:B8H:C5	30:WA:3767:B8H:N1	2.37	0.78
30:WA:3:C:O2	32:YA:154:G:N2	2.14	0.78
53:ZA:1266:C:N3	53:ZA:1517:G:N2	2.32	0.78
51:v:505:VAL:HG22	51:v:797:THR:HG21	1.66	0.78
55:EB:185:GLY:H	55:EB:189:LEU:HD13	1.49	0.78
32:YA:122:G:H1	32:YA:128:C:H41	1.30	0.77
62:LB:13:GLN:HE22	62:LB:35:ARG:HG3	1.48	0.77
20:U:22:VAL:HG21	30:WA:4499:OMG:HM21	1.66	0.77
57:GB:38:ALA:HB2	57:GB:50:VAL:HB	1.64	0.77
3:C:78:ARG:HB3	3:C:88:GLY:HA2	1.66	0.77
53:ZA:890:U:H5'	53:ZA:891:G:H5''	1.66	0.76
60:JB:170:PRO:O	60:JB:175:ARG:NH1	2.18	0.76
83:GC:7:LEU:HD11	83:GC:308:ARG:HB3	1.65	0.76
30:WA:1079:G:H1	30:WA:1244:A:H2	1.32	0.76
83:GC:87:LEU:HB2	83:GC:101:PHE:HB2	1.68	0.76
30:WA:4954:G:H4'	30:WA:4955:U:H5'	1.68	0.75
6:F:65:ARG:HH22	30:WA:1216:C:H41	1.31	0.75
30:WA:1312:C:H2'	30:WA:1313:A:H8	1.51	0.75
29:CB:196:ILE:HB	29:CB:223:TYR:HB2	1.66	0.75
53:ZA:43:U:OP2	53:ZA:485:A:N6	2.19	0.75
30:WA:132:G:O6	30:WA:137:G:N2	2.20	0.75
65:OB:99:ALA:H	65:OB:133:THR:HG22	1.50	0.75
30:WA:308:G:OP2	30:WA:308:G:N2	2.20	0.74
50:RA:73:VAL:HG13	50:RA:75:PRO:HD3	1.69	0.74
53:ZA:551:U:H2'	53:ZA:552:G:C8	2.22	0.74
30:WA:3722:A:H2'	30:WA:3723:A2M:H8	1.69	0.74
53:ZA:186:C:H42	53:ZA:213:G:H22	1.34	0.74
53:ZA:1472:C:H42	53:ZA:1476:A:H62	0.82	0.74
53:ZA:181:A:H3'	53:ZA:182:C:H2'	1.70	0.74
54:DB:225:GLU:HB2	83:GC:187:ASN:HB2	1.70	0.73
53:ZA:551:U:H2'	53:ZA:552:G:H8	1.53	0.73
30:WA:2850:A:H61	30:WA:3848:C:N4	1.86	0.73
30:WA:1764:G:H1	30:WA:1778:U:H3	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1351:G:O6	53:ZA:1360:U:O4	2.06	0.73
53:ZA:822:U:H3	53:ZA:826:A:H62	1.36	0.73
53:ZA:1259:A:N6	53:ZA:1519:U:OP1	2.21	0.73
54:DB:16:ILE:HD11	80:DC:36:LEU:HD23	1.71	0.73
57:GB:32:MET:SD	57:GB:65:GLN:NE2	2.62	0.73
30:WA:14:C:O2	32:YA:143:G:N2	2.16	0.72
30:WA:2643:G:H4'	38:FA:24:ARG:HD3	1.69	0.72
15:P:166:TYR:HB3	26:K:8:MET:HG3	1.71	0.72
30:WA:2525:C:O2	30:WA:2645:G:N2	2.22	0.72
30:WA:1205:G:H2'	30:WA:1206:G:H8	1.55	0.72
53:ZA:1475:G:N2	53:ZA:1475:G:OP2	2.22	0.72
61:KB:35:LEU:HG	61:KB:40:VAL:HG11	1.72	0.72
11:L:38:VAL:HG11	11:L:55:MET:HE1	1.72	0.72
51:v:435:THR:HG21	51:v:492:HIS:HA	1.71	0.72
79:CC:44:ARG:NH2	79:CC:60:GLU:O	2.22	0.72
2:B:268:ARG:NH2	30:WA:3901:C:O2'	2.22	0.72
53:ZA:15:U:O2'	53:ZA:669:A:N6	2.22	0.72
20:U:50:ASN:ND2	30:WA:4462:U:OP1	2.22	0.71
49:QA:135:THR:HG21	51:v:187:VAL:HG21	1.70	0.71
53:ZA:442:C:H42	53:ZA:449:A:H62	1.37	0.71
59:IB:178:ARG:HE	59:IB:181:GLN:HG3	1.55	0.71
30:WA:3949:G:H1	30:WA:4074:U:H3	1.36	0.71
30:WA:4088:5MU:C6	30:WA:4088:5MU:C1'	2.74	0.71
53:ZA:1286:G:N2	53:ZA:1312:G:O2'	2.18	0.71
57:GB:121:ILE:HG12	57:GB:123:GLY:H	1.56	0.71
30:WA:2606:A:N6	30:WA:2749:A:OP2	2.23	0.71
53:ZA:804:U:H3	53:ZA:859:G:H1	1.36	0.71
17:R:67:VAL:HA	30:WA:730:2MG:HN1	1.55	0.71
26:K:56:ARG:O	26:K:116:ARG:NH1	2.24	0.71
30:WA:1865:B8H:C6	30:WA:1865:B8H:C2	2.67	0.71
6:F:241:ARG:NH2	30:WA:945:C:OP1	2.24	0.70
53:ZA:877:C:H2'	53:ZA:878:G:H8	1.56	0.70
30:WA:4453:G:H5''	30:WA:4454:A:H5'	1.71	0.70
51:v:105:SER:HB2	51:v:115:VAL:HG22	1.72	0.70
30:WA:909:C:H2'	30:WA:910:G:H8	1.55	0.70
30:WA:2462:G:H21	30:WA:3677:G:H21	1.36	0.70
32:YA:65:A:OP1	39:GA:56:ARG:NH1	2.25	0.70
68:RB:71:ILE:HD13	68:RB:73:LEU:HB3	1.72	0.70
30:WA:1875:C:H2'	30:WA:1876:A2M:H8	1.74	0.70
32:YA:8:U:H2'	32:YA:9:A:H8	1.55	0.70
51:v:749:ILE:HD13	51:v:759:ILE:HG12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1854:U:H2'	53:ZA:1855:G:H8	1.55	0.70
30:WA:373:OMG:HM21	30:WA:1650:C:H4'	1.74	0.70
53:ZA:1396:A:O2'	53:ZA:1398:G:N7	2.24	0.70
30:WA:4277:G:N2	30:WA:4277:G:OP2	2.24	0.69
8:H:128:MET:SD	8:H:157:SER:OG	2.50	0.69
28:BB:35:ALA:HB2	28:BB:44:ILE:HD11	1.73	0.69
53:ZA:1144:A:H5'	53:ZA:1355:C:H41	1.57	0.69
53:ZA:65:C:N4	57:GB:134:GLY:O	2.24	0.69
1:A:220:GLY:O	30:WA:3754:C:O2'	2.11	0.69
30:WA:680:C:H2'	30:WA:681:G:H8	1.57	0.69
53:ZA:1488:C:H3'	53:ZA:1489:A:H4'	1.74	0.69
3:C:33:ARG:NH1	30:WA:1357:G:OP1	2.26	0.69
36:DA:44:ARG:HG3	36:DA:49:PHE:HD2	1.56	0.69
52:w:205:LYS:HD2	53:ZA:1698:C:H5'	1.75	0.69
53:ZA:75:G:N2	53:ZA:78:C:OP1	2.23	0.69
53:ZA:122:G:H21	55:EB:146:THR:HG21	1.58	0.69
30:WA:3767:B8H:C6	30:WA:3767:B8H:C2	2.66	0.69
53:ZA:1620:A:O2'	53:ZA:1624:U:OP2	2.10	0.69
2:B:246:ARG:NH1	30:WA:4530:C:OP1	2.26	0.69
21:V:80:ARG:NH1	57:GB:129:VAL:O	2.26	0.69
53:ZA:980:A:H2'	53:ZA:981:A:H8	1.58	0.69
15:P:157:GLY:O	15:P:188:ASN:ND2	2.26	0.69
30:WA:4766:G:H2'	30:WA:4767:A:H8	1.57	0.69
53:ZA:1545:A:H4'	67:QB:74:GLY:HA2	1.74	0.69
30:WA:4301:B8H:C6	30:WA:4301:B8H:C2	2.66	0.69
70:TB:40:ALA:HB3	70:TB:43:LYS:HG2	1.74	0.69
71:UB:78:ASP:OD2	80:DC:44:ARG:NH1	2.25	0.69
30:WA:1865:B8H:C6	30:WA:1865:B8H:CN1	2.70	0.68
7:G:139:VAL:HG21	7:G:238:LYS:HG3	1.73	0.68
57:GB:58:LYS:HA	57:GB:107:SER:HB2	1.74	0.68
58:HB:144:ILE:HG21	58:HB:152:ARG:HH21	1.58	0.68
15:P:108:ARG:NH2	30:WA:1361:G:OP1	2.26	0.68
55:EB:100:ARG:HB2	55:EB:114:ILE:HD13	1.76	0.68
62:LB:135:SER:O	62:LB:139:ARG:NH1	2.26	0.68
4:D:52:ILE:HD13	31:XA:6:C:H4'	1.74	0.68
30:WA:754:G:H1	30:WA:913:U:H3	1.41	0.68
53:ZA:363:A:N6	53:ZA:400:C:O2	2.27	0.68
53:ZA:1617:G:O6	66:PB:43:ARG:NH1	2.26	0.68
6:F:28:LYS:NZ	30:WA:970:G:N7	2.40	0.68
51:v:396:MET:HG3	51:v:485:ILE:HB	1.74	0.68
51:v:587:SER:HB2	51:v:605:LYS:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1545:A:H2	53:ZA:1671:G:H1'	1.58	0.68
12:M:68:ARG:NH2	30:WA:303:C:OP2	2.26	0.68
30:WA:4082:A:N1	30:WA:4176:C:N4	2.41	0.68
1:A:27:ALA:O	1:A:128:ARG:NH2	2.26	0.68
20:U:15:ARG:HB2	30:WA:4623:G:H5''	1.75	0.68
23:X:50:ARG:HB2	23:X:115:ARG:HH22	1.59	0.68
23:X:54:GLU:HB3	23:X:67:ILE:HD11	1.74	0.68
30:WA:3737:A:H2'	30:WA:3738:A:H8	1.58	0.68
59:IB:13:LYS:NZ	62:LB:108:ASN:O	2.27	0.68
30:WA:2412:G:N2	30:WA:2412:G:OP2	2.26	0.68
53:ZA:877:C:H2'	53:ZA:878:G:C8	2.29	0.68
30:WA:1666:C:OP1	36:DA:36:ARG:NH1	2.27	0.68
30:WA:3767:B8H:C6	30:WA:3767:B8H:CN1	2.69	0.68
51:v:412:ALA:HB3	51:v:472:LEU:HB2	1.76	0.68
8:H:12:ILE:HD13	8:H:18:ILE:HG21	1.76	0.67
45:MA:1:MET:HB2	53:ZA:1706:G:H5'	1.76	0.67
18:S:18:PRO:HB2	18:S:21:LYS:HG3	1.75	0.67
30:WA:1:C:N4	32:YA:156:U:N3	2.37	0.67
84:b:71:LYS:NZ	84:b:274:ASP:OD2	2.28	0.67
26:K:46:ILE:HB	26:K:49:ARG:HB2	1.77	0.67
30:WA:3697:A:H62	30:WA:3828:G:H21	0.72	0.67
49:QA:121:VAL:HB	49:QA:161:ILE:HB	1.75	0.67
53:ZA:153:G:N3	57:GB:13:GLN:NE2	2.41	0.67
3:C:2:ALA:N	30:WA:668:A:N7	2.43	0.67
5:E:141:ARG:NH1	5:E:172:SER:O	2.28	0.67
14:O:80:GLN:OE1	30:WA:3897:U:O2'	2.10	0.67
30:WA:2073:C:OP1	37:EA:15:LYS:NZ	2.26	0.67
51:v:581:GLU:HB3	51:v:697:MET:HG2	1.76	0.67
24:Y:57:MET:HE3	24:Y:62:ILE:HG22	1.77	0.67
83:GC:47:ARG:NE	83:GC:47:ARG:O	2.25	0.67
30:WA:4477:B8W:O2'	44:LA:74:TYR:O	2.13	0.67
13:N:130:LYS:HB2	13:N:133:ARG:HG2	1.77	0.67
30:WA:4575:G:H2'	30:WA:4576:A2M:H8	1.75	0.67
53:ZA:617:G:O2'	53:ZA:633:C:OP1	2.13	0.67
56:FB:50:PRO:HB3	56:FB:69:VAL:HG22	1.77	0.67
58:HB:9:VAL:H	58:HB:44:ASN:HD21	1.41	0.67
69:SB:127:TRP:O	69:SB:144:ARG:NH1	2.26	0.67
12:M:192:TRP:NE1	30:WA:48:G:OP1	2.28	0.66
24:Y:111:ARG:NH1	30:WA:2582:C:OP1	2.27	0.66
47:OA:3:LYS:HE3	47:OA:6:LYS:HA	1.76	0.66
59:IB:81:VAL:HG22	59:IB:102:VAL:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:94:LYS:NZ	30:WA:4877:2MG:OP2	2.28	0.66
20:U:48:ARG:NH1	30:WA:4626:C:OP1	2.29	0.66
53:ZA:981:A:H2'	53:ZA:982:G:C8	2.29	0.66
18:S:100:LYS:HB2	30:WA:1735:U:H4'	1.76	0.66
23:X:18:HIS:O	23:X:78:TYR:OH	2.14	0.66
84:b:351:ASP:HB3	84:b:354:LEU:HB3	1.76	0.66
1:A:147:ARG:HG2	1:A:157:VAL:HG22	1.77	0.66
30:WA:1338:C:H2'	30:WA:1339:A:H8	1.61	0.66
30:WA:1744:G:N3	30:WA:1747:A:N6	2.44	0.66
4:D:120:GLU:O	4:D:248:ARG:NH2	2.27	0.66
30:WA:2416:C:O2'	30:WA:2531:C:O2	2.14	0.66
53:ZA:1140:G:O2'	53:ZA:1151:G:O2'	2.14	0.66
22:W:84:GLU:OE2	30:WA:2531:C:N4	2.28	0.66
30:WA:308:G:H3'	40:HA:33:LEU:HB2	1.77	0.66
51:v:160:MET:HE1	51:v:214:PHE:HB3	1.77	0.66
53:ZA:1401:A:H4'	71:UB:52:GLY:HA3	1.76	0.66
84:b:221:HIS:H	84:b:325:LEU:HD22	1.60	0.66
17:R:87:ARG:HH21	30:WA:2039:G:H5'	1.60	0.66
30:WA:4647:U:H2'	30:WA:4648:G:H8	1.61	0.66
38:FA:5:LEU:HD21	38:FA:30:ILE:HG22	1.76	0.66
51:v:362:VAL:O	51:v:366:LYS:NZ	2.28	0.66
12:M:98:LEU:HD12	12:M:128:LYS:HE2	1.78	0.66
30:WA:2323:G:N2	30:WA:2326:G:OP2	2.26	0.66
53:ZA:1674:G:OP1	56:FB:51:HIS:NE2	2.29	0.66
5:E:180:GLY:HA3	5:E:187:VAL:HG23	1.78	0.66
6:F:229:GLY:HA3	17:R:2:LYS:HD3	1.78	0.66
30:WA:1865:B8H:C5	30:WA:1865:B8H:N1	2.36	0.66
30:WA:4301:B8H:C6	30:WA:4301:B8H:CN1	2.69	0.66
53:ZA:1644:C:H4'	67:QB:140:ARG:HB2	1.76	0.66
56:FB:122:ARG:HB3	79:CC:59:LEU:HD11	1.78	0.66
57:GB:74:ARG:HG2	57:GB:96:SER:HB3	1.77	0.66
30:WA:1332:A2M:OP2	30:WA:4450:U:O2'	2.12	0.65
53:ZA:818:A:OP1	60:JB:80:ARG:NH1	2.29	0.65
53:ZA:948:C:H2'	53:ZA:949:G:H8	1.60	0.65
54:DB:31:GLU:O	54:DB:54:ARG:NH2	2.28	0.65
69:SB:55:ARG:HE	69:SB:55:ARG:H	1.44	0.65
47:OA:39:CYS:HB3	47:OA:42:CYS:SG	2.35	0.65
53:ZA:932:G:H1	53:ZA:1009:A:H61	1.44	0.65
53:ZA:1310:U:H5'	82:FC:130:VAL:HG22	1.78	0.65
31:XA:28:C:H1'	31:XA:54:A:H61	1.60	0.65
53:ZA:1490:G:N2	71:UB:72:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4972:A:H2'	30:WA:4973:A:H8	1.61	0.65
3:C:223:ASN:ND2	30:WA:223:G:N3	2.45	0.65
84:b:82:VAL:HG12	84:b:106:VAL:HG12	1.78	0.65
1:A:243:THR:H	30:WA:3750:U:HO2'	1.44	0.65
6:F:231:ASP:OD1	6:F:235:ARG:NH1	2.29	0.65
25:Z:76:ASP:HB3	25:Z:115:GLY:HA3	1.79	0.65
30:WA:2837:A:H2'	30:WA:2838:A:H8	1.62	0.65
53:ZA:1650:A:H5''	67:QB:139:ALA:HB2	1.78	0.65
82:FC:123:SER:OG	82:FC:126:CYS:SG	2.55	0.65
84:b:276:MET:SD	84:b:276:MET:N	2.69	0.65
2:B:13:SER:HB2	30:WA:4627:A:H4'	1.79	0.65
5:E:181:PRO:O	5:E:184:LEU:N	2.29	0.65
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.79	0.65
11:L:35:ARG:NH2	17:R:99:ASP:OD1	2.28	0.65
15:P:108:ARG:HH21	30:WA:1360:A:H5'	1.62	0.65
30:WA:419:A:N3	30:WA:1338:C:O2'	2.30	0.65
53:ZA:1465:A:OP1	68:RB:56:HIS:NE2	2.25	0.65
53:ZA:1550:G:H3'	53:ZA:1579:A:H61	1.62	0.65
2:B:300:LYS:HG2	2:B:313:SER:HB3	1.79	0.65
30:WA:2500:U:H2'	30:WA:2501:G:H8	1.61	0.65
45:MA:2:ARG:NH2	53:ZA:1841:C:OP2	2.29	0.65
7:G:96:GLN:O	30:WA:4129:G:N2	2.30	0.65
13:N:176:ARG:HE	30:WA:4774:G:H5'	1.61	0.65
51:v:428:ARG:NH1	51:v:434:TYR:OH	2.30	0.65
53:ZA:482:G:N1	53:ZA:485:A:OP2	2.30	0.65
23:X:112:ASP:H	23:X:115:ARG:HB3	1.62	0.64
30:WA:1546:C:H1'	30:WA:2453:G:H21	1.62	0.64
30:WA:2850:A:N6	30:WA:3848:C:H42	1.93	0.64
53:ZA:89:C:H2'	53:ZA:90:G:C8	2.32	0.64
53:ZA:380:G:OP1	59:IB:56:ARG:NH2	2.29	0.64
53:ZA:1563:G:H5''	70:TB:121:ARG:HH12	1.63	0.64
2:B:249:ARG:NH1	30:WA:2842:U:OP1	2.30	0.64
9:I:13:LYS:NZ	30:WA:1872:A:OP1	2.29	0.64
19:T:101:ARG:NH1	30:WA:2628:A:OP1	2.30	0.64
41:IA:33:THR:HG22	41:IA:40:PRO:HG2	1.79	0.64
53:ZA:857:U:H2'	53:ZA:858:A:H8	1.61	0.64
53:ZA:1444:U:OP2	67:QB:15:ARG:NH2	2.30	0.64
13:N:117:ARG:NH2	30:WA:4765:G:OP1	2.30	0.64
30:WA:2709:C:H2'	30:WA:2710:G:H8	1.63	0.64
32:YA:67:U:H2'	32:YA:68:G:H8	1.63	0.64
53:ZA:1597:C:OP2	76:ZB:85:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:EB:63:LYS:O	55:EB:67:GLN:NE2	2.30	0.64
5:E:115:MET:O	48:PA:87:ARG:NH1	2.30	0.64
14:O:67:VAL:O	14:O:80:GLN:NE2	2.30	0.64
25:Z:59:ARG:NH1	30:WA:89:C:OP1	2.31	0.64
30:WA:2340:C:H2'	30:WA:2341:G:H8	1.63	0.64
53:ZA:28:U:H2'	53:ZA:29:G:H8	1.62	0.64
53:ZA:170:A:H5'	57:GB:137:ARG:HB2	1.79	0.64
53:ZA:172:U:H3	53:ZA:337:C:HO2'	1.44	0.64
53:ZA:934:G:O6	53:ZA:1008:A:N1	2.30	0.64
30:WA:4532:G:N2	30:WA:4532:G:OP2	2.31	0.64
53:ZA:380:G:N1	53:ZA:383:G:OP2	2.29	0.64
75:YB:44:LEU:HD11	75:YB:55:ILE:HD13	1.79	0.64
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.80	0.64
51:v:687:THR:HA	51:v:697:MET:HE2	1.80	0.64
55:EB:11:ARG:HD2	55:EB:20:LEU:HB3	1.80	0.64
67:QB:50:LYS:HE3	67:QB:85:ARG:HH12	1.63	0.64
1:A:215:ASN:ND2	30:WA:4551:A:N7	2.46	0.64
30:WA:2327:G:OP1	36:DA:36:ARG:NH2	2.30	0.64
30:WA:2525:C:H2'	30:WA:2526:G:H8	1.62	0.64
30:WA:2593:C:OP1	30:WA:2773:C:O2'	2.15	0.64
48:PA:42:GLY:HA2	48:PA:48:THR:HG21	1.79	0.64
53:ZA:640:A:H2'	53:ZA:641:A:H8	1.62	0.64
75:YB:87:PRO:HG2	75:YB:90:ARG:HH21	1.63	0.64
7:G:231:GLY:O	7:G:276:ARG:NH2	2.30	0.64
30:WA:1745:C:O2	30:WA:1791:A:N6	2.31	0.64
53:ZA:69:C:OP2	57:GB:167:LYS:NZ	2.31	0.64
53:ZA:959:G:OP1	65:OB:104:ARG:NH1	2.30	0.64
53:ZA:1292:C:N3	82:FC:138:ARG:NH2	2.45	0.64
2:B:213:GLN:NE2	2:B:285:TYR:O	2.30	0.63
11:L:24:LEU:HB2	11:L:43:THR:HG21	1.80	0.63
29:CB:207:ALA:HB2	53:ZA:4:C:H4'	1.80	0.63
30:WA:1392:C:O2'	30:WA:1507:G:N2	2.31	0.63
35:CA:23:ARG:O	35:CA:88:LEU:N	2.30	0.63
55:EB:11:ARG:NH1	55:EB:24:THR:OG1	2.31	0.63
62:LB:4:ILE:HG22	62:LB:5:GLN:HG2	1.80	0.63
65:OB:45:THR:HA	65:OB:52:THR:HA	1.80	0.63
30:WA:3801:U:O2'	53:ZA:1720:U:O2'	2.16	0.63
30:WA:4599:U:H2'	30:WA:4600:G:H8	1.61	0.63
53:ZA:980:A:H2'	53:ZA:981:A:C8	2.33	0.63
53:ZA:1286:G:H21	53:ZA:1313:A:H62	1.45	0.63
1:A:183:GLY:HA2	30:WA:1618:A:H5''	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:40:GLN:HE22	84:b:256:GLY:HA3	1.63	0.63
29:CB:192:LEU:HB3	29:CB:227:ARG:HB3	1.79	0.63
30:WA:2548:A:N7	30:WA:2551:G:N1	2.47	0.63
46:NA:63:THR:O	46:NA:87:ARG:NH1	2.32	0.63
53:ZA:1199:A:H5''	77:AC:2:THR:HG22	1.81	0.63
60:JB:176:LYS:HG3	60:JB:179:LYS:HE2	1.81	0.63
4:D:28:THR:O	30:WA:4285:A:N6	2.31	0.63
24:Y:84:ARG:NH1	38:FA:99:GLU:OE1	2.31	0.63
53:ZA:958:G:H3'	53:ZA:959:G:H8	1.64	0.63
50:RA:61:LYS:HB2	50:RA:72:GLU:HB3	1.79	0.63
53:ZA:1228:A:H2'	53:ZA:1229:G:C8	2.34	0.63
56:FB:201:LYS:O	56:FB:204:ARG:NH1	2.31	0.63
5:E:117:ARG:N	30:WA:458:C:OP1	2.30	0.63
60:JB:18:ARG:O	60:JB:24:ARG:NH2	2.31	0.63
83:GC:17:TRP:HB2	83:GC:303:THR:HA	1.79	0.63
83:GC:246:TYR:HB3	83:GC:261:LEU:HB2	1.79	0.63
2:B:252:ALA:HB1	30:WA:4529:G:C2	2.33	0.63
13:N:72:HIS:N	30:WA:4591:G:OP1	2.30	0.63
16:Q:62:ARG:NH2	30:WA:4653:A:OP1	2.31	0.63
26:K:18:TRP:NE1	30:WA:1521:G:O2'	2.32	0.63
53:ZA:99:A:H61	53:ZA:433:A:H1'	1.64	0.63
53:ZA:495:U:O2'	55:EB:27:PHE:O	2.17	0.63
53:ZA:982:G:H2'	53:ZA:983:A:H8	1.64	0.63
53:ZA:1165:G:OP2	53:ZA:1165:G:N2	2.30	0.63
53:ZA:1310:U:OP1	63:MB:36:ARG:NH1	2.32	0.63
63:MB:32:ALA:HB1	63:MB:37:GLU:HB3	1.79	0.63
12:M:114:ARG:NH1	12:M:151:ILE:O	2.31	0.63
27:AB:84:GLN:HG3	27:AB:100:ALA:HB1	1.81	0.63
30:WA:996:U:O2	30:WA:1070:G:O6	2.17	0.63
46:NA:36:GLN:OE1	46:NA:39:ARG:NH2	2.32	0.63
53:ZA:809:A:OP1	55:EB:187:ALA:N	2.31	0.63
53:ZA:1354:G:N2	53:ZA:1357:A:OP2	2.22	0.63
55:EB:162:ILE:HG12	55:EB:169:ILE:HG22	1.79	0.63
62:LB:5:GLN:NE2	62:LB:11:GLN:O	2.28	0.63
1:A:179:ILE:HG23	1:A:184:ARG:HB2	1.81	0.63
30:WA:1551:C:O2	30:WA:1617:G:O6	2.16	0.63
51:v:506:ARG:HG3	51:v:575:PRO:HG3	1.80	0.63
53:ZA:530:U:H2'	53:ZA:531:A:C8	2.33	0.63
53:ZA:885:U:O2	53:ZA:901:G:O6	2.17	0.63
16:Q:92:LYS:NZ	30:WA:1578:G:OP1	2.30	0.62
30:WA:113:A:OP2	30:WA:156:G:N2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:1947:A:H2'	30:WA:1948:A:C8	2.34	0.62
30:WA:4624:U:H2'	30:WA:4625:OMU:H6	1.81	0.62
55:EB:18:TRP:HB3	55:EB:20:LEU:HD13	1.80	0.62
15:P:62:SER:OG	30:WA:1507:G:OP2	2.17	0.62
30:WA:62:A:N3	30:WA:77:U:O2'	2.27	0.62
30:WA:1304:C:H2'	30:WA:1305:G:C8	2.33	0.62
30:WA:1557:G:O2'	30:WA:1579:B9B:N2	2.32	0.62
30:WA:1766:G:O6	30:WA:1777:C:N4	2.31	0.62
30:WA:2001:C:OP1	50:RA:123:ARG:NE	2.30	0.62
30:WA:2267:G:OP2	48:PA:98:ARG:NH2	2.32	0.62
36:DA:90:MET:HG2	48:PA:33:LYS:HG2	1.80	0.62
60:JB:179:LYS:HA	60:JB:182:GLN:HG2	1.81	0.62
26:K:34:ARG:NH2	32:YA:30:U:OP1	2.33	0.62
30:WA:2300:C:H2'	30:WA:2301:G:H8	1.64	0.62
30:WA:2490:U:H3	30:WA:2498:G:H1	1.46	0.62
49:QA:62:ARG:NH2	49:QA:82:ILE:O	2.31	0.62
53:ZA:831:G:O6	75:YB:11:LYS:NZ	2.33	0.62
53:ZA:1025:U:O3'	53:ZA:1089:G:N2	2.32	0.62
53:ZA:1341:C:OP2	53:ZA:1687:C:O2'	2.17	0.62
30:WA:955:G:H2'	30:WA:956:G:H8	1.64	0.62
30:WA:1568:A:N6	53:ZA:1028:A:N1	2.47	0.62
53:ZA:1004:U:H2'	53:ZA:1005:G:H8	1.64	0.62
53:ZA:1498:A:OP1	54:DB:27:ARG:NH2	2.32	0.62
53:ZA:1593:C:H4'	67:QB:45:ARG:HH21	1.64	0.62
65:OB:96:LYS:NZ	65:OB:130:GLU:OE2	2.32	0.62
16:Q:81:ARG:NH1	30:WA:3612:U:OP1	2.30	0.62
28:BB:120:MET:HG3	28:BB:142:PHE:HE1	1.63	0.62
53:ZA:75:G:N2	53:ZA:77:A:OP2	2.33	0.62
53:ZA:902:G:H2'	53:ZA:903:A:H8	1.64	0.62
62:LB:96:ILE:HD12	74:XB:10:ALA:HB1	1.81	0.62
83:GC:256:ILE:HB	83:GC:270:LEU:HB2	1.82	0.62
9:I:116:ARG:NH2	30:WA:4199:I4U:O2'	2.32	0.62
28:BB:105:LEU:HD13	28:BB:213:ARG:HA	1.81	0.62
30:WA:2314:G:H1	30:WA:2334:U:H3	1.48	0.62
30:WA:4279:A:H2'	30:WA:4280:G:C8	2.34	0.62
51:v:507:VAL:HG21	51:v:558:LEU:HD11	1.80	0.62
15:P:16:LYS:O	15:P:33:ARG:NH2	2.32	0.62
16:Q:39:GLN:NE2	30:WA:2716:G:OP2	2.32	0.62
28:BB:33:VAL:HA	28:BB:96:CYS:HB2	1.82	0.62
52:w:210:ARG:NH2	53:ZA:624:C:O2'	2.33	0.62
84:b:49:CYS:SG	84:b:281:ARG:NH1	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:139:ARG:NH1	30:WA:2538:C:OP1	2.33	0.62
51:v:150:ARG:NH1	51:v:367:TYR:O	2.32	0.62
62:LB:111:VAL:HG12	62:LB:140:PHE:HB2	1.82	0.62
2:B:95:THR:HG22	30:WA:4915:A:H4'	1.82	0.62
10:J:28:GLU:OE2	10:J:32:ARG:NH1	2.31	0.62
20:U:21:PRO:HA	20:U:54:ALA:HA	1.82	0.62
28:BB:88:THR:HG22	28:BB:98:THR:HG22	1.80	0.62
30:WA:2103:G:O2'	30:WA:2104:C:O4'	2.17	0.62
48:PA:38:PHE:O	48:PA:45:HIS:NE2	2.27	0.62
9:I:36:LEU:HD11	9:I:69:ARG:HH11	1.65	0.62
30:WA:1205:G:H2'	30:WA:1206:G:C8	2.34	0.62
53:ZA:306:C:O2	53:ZA:308:G:N1	2.32	0.62
53:ZA:659:G:O2'	53:ZA:662:G:O2'	2.17	0.62
55:EB:88:ASP:HB2	55:EB:101:LEU:HD12	1.81	0.62
30:WA:4953:C:H2'	30:WA:4954:G:H21	1.65	0.61
32:YA:8:U:H2'	32:YA:9:A:C8	2.35	0.61
51:v:89:ILE:HG22	51:v:356:ILE:HA	1.82	0.61
53:ZA:829:C:H5''	55:EB:21:ASP:HB3	1.82	0.61
55:EB:130:PHE:HB3	55:EB:138:HIS:HB2	1.81	0.61
2:B:324:GLY:HA2	30:WA:5056:C:H4'	1.81	0.61
55:EB:11:ARG:NH1	55:EB:21:ASP:O	2.32	0.61
83:GC:67:SER:N	83:GC:81:GLY:O	2.31	0.61
30:WA:4279:A:H2'	30:WA:4280:G:H8	1.64	0.61
30:WA:4685:G:H2'	30:WA:4686:A:C8	2.34	0.61
51:v:266:PHE:HB2	51:v:288:THR:HG22	1.81	0.61
1:A:36:GLU:OE1	1:A:163:ARG:NH1	2.33	0.61
19:T:81:ARG:NH2	30:WA:2638:U:O4	2.33	0.61
30:WA:4323:C:H4'	46:NA:17:LYS:HA	1.82	0.61
56:FB:56:TYR:HB3	56:FB:63:LYS:HA	1.82	0.61
84:b:121:VAL:HG11	84:b:334:THR:HB	1.82	0.61
1:A:200:ARG:NH1	30:WA:3656:A:OP2	2.34	0.61
30:WA:711:G:H2'	30:WA:712:A:H8	1.65	0.61
30:WA:2497:C:H2'	30:WA:2498:G:H8	1.65	0.61
30:WA:3658:A:C2	30:WA:3697:A:H4'	2.36	0.61
40:HA:29:ARG:NH1	40:HA:29:ARG:O	2.34	0.61
43:KA:23:ILE:HG13	43:KA:38:ASN:HB2	1.83	0.61
53:ZA:1262:C:O2	80:DC:17:GLY:N	2.33	0.61
2:B:246:ARG:NH2	30:WA:4563:U:OP2	2.33	0.61
4:D:17:GLN:O	30:WA:4270:U:N3	2.28	0.61
15:P:178:ARG:H	25:Z:51:GLY:HA2	1.66	0.61
30:WA:2652:A:H62	30:WA:2691:G:H8	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1601:A:OP2	53:ZA:1636:G:N2	2.33	0.61
66:PB:25:LEU:HG	66:PB:87:PRO:HG3	1.83	0.61
2:B:220:ILE:HB	2:B:346:THR:HB	1.82	0.61
2:B:224:LYS:NZ	30:WA:4672:C:OP1	2.32	0.61
2:B:258:HIS:NE2	30:WA:3883:C:N3	2.46	0.61
11:L:104:MET:HE2	13:N:199:HIS:HB3	1.81	0.61
18:S:109:VAL:HA	18:S:112:ASN:ND2	2.15	0.61
28:BB:224:GLU:HG3	28:BB:227:LYS:HE2	1.81	0.61
30:WA:1650:C:H2'	30:WA:1651:A:C8	2.35	0.61
34:BA:50:ASN:ND2	34:BA:75:SER:O	2.33	0.61
53:ZA:633:C:H1'	81:EC:89:THR:HG21	1.82	0.61
53:ZA:1566:G:N2	53:ZA:1569:A:OP2	2.32	0.61
58:HB:117:PRO:HG2	58:HB:120:ARG:HB2	1.82	0.61
6:F:30:LYS:HD3	30:WA:1444:U:H5''	1.82	0.61
6:F:93:ARG:HE	6:F:108:LEU:HD13	1.66	0.61
17:R:45:TRP:HE1	17:R:61:ILE:HD11	1.65	0.61
30:WA:3668:A:N6	30:WA:4173:G:O2'	2.34	0.61
30:WA:3853:U:H2'	30:WA:3854:A:H8	1.64	0.61
30:WA:4744:C:H2'	30:WA:4745:G:H4'	1.81	0.61
53:ZA:613:G:N2	53:ZA:626:G:OP1	2.33	0.61
53:ZA:913:A:OP1	58:HB:99:ARG:NH2	2.34	0.61
57:GB:215:LYS:HA	57:GB:218:LYS:HE2	1.83	0.61
67:QB:128:GLU:OE2	67:QB:131:LYS:NZ	2.33	0.61
83:GC:212:LYS:HA	83:GC:235:ILE:HG23	1.82	0.61
6:F:104:VAL:HG13	6:F:135:VAL:HG12	1.81	0.61
16:Q:74:ARG:NE	30:WA:2896:U:OP2	2.33	0.61
30:WA:369:G:N2	30:WA:372:A:OP2	2.29	0.61
51:v:27:HIS:HB2	51:v:139:THR:HG23	1.83	0.61
73:WB:11:LEU:HD12	73:WB:74:VAL:HB	1.83	0.61
12:M:53:TYR:HB2	12:M:133:ILE:HD13	1.81	0.61
30:WA:3804:A:N3	30:WA:4511:C:O2'	2.33	0.61
50:RA:12:VAL:HG22	50:RA:63:THR:HG22	1.83	0.61
66:PB:53:GLN:HB3	66:PB:83:MET:HE1	1.83	0.61
24:Y:5:MET:O	24:Y:28:ASN:ND2	2.34	0.60
30:WA:4542:C:H2'	30:WA:4543:G:H8	1.64	0.60
58:HB:69:LEU:HD22	58:HB:96:ALA:HB2	1.83	0.60
30:WA:1338:C:H2'	30:WA:1339:A:C8	2.37	0.60
30:WA:1485:C:O2'	30:WA:1487:G:OP2	2.13	0.60
30:WA:1823:G:OP2	30:WA:1823:G:N2	2.26	0.60
30:WA:1999:C:H2'	30:WA:2000:G:H8	1.65	0.60
30:WA:2268:A:OP1	48:PA:107:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4134:B8W:O6	30:WA:4161:G:N2	2.33	0.60
30:WA:4972:A:H2'	30:WA:4973:A:C8	2.36	0.60
53:ZA:90:G:OP1	53:ZA:445:A:N6	2.30	0.60
53:ZA:1079:C:O2'	53:ZA:1182:A:N1	2.31	0.60
1:A:14:SER:OG	30:WA:1633:C:OP1	2.16	0.60
30:WA:307:A:N3	30:WA:310:G:O2'	2.33	0.60
30:WA:3765:A:H62	53:ZA:1826:G:H5'	1.65	0.60
51:v:20:ARG:NH2	51:v:91:GLN:OE1	2.34	0.60
51:v:670:GLN:HE21	53:ZA:1327:G:H21	1.49	0.60
57:GB:30:LYS:HE3	57:GB:36:VAL:HG13	1.83	0.60
64:NB:36:GLN:OE1	64:NB:39:LYS:NZ	2.34	0.60
30:WA:2750:A:H2'	30:WA:2751:A:H8	1.65	0.60
30:WA:4193:U:H2'	30:WA:4194:U:C6	2.37	0.60
30:WA:4960:A:H2'	30:WA:4961:A:C8	2.36	0.60
53:ZA:109:U:O2	62:LB:71:ARG:NH2	2.34	0.60
60:JB:110:LEU:HB2	60:JB:147:PHE:HB3	1.83	0.60
65:OB:65:ASP:HA	65:OB:68:GLU:HG3	1.83	0.60
26:K:35:ARG:NH1	30:WA:105:A:O2'	2.35	0.60
27:AB:121:LEU:HD21	27:AB:145:ILE:HD13	1.83	0.60
30:WA:2308:C:H5''	36:DA:104:SER:HB2	1.83	0.60
30:WA:4237:U:H4'	30:WA:4238:A:O5'	2.02	0.60
53:ZA:1241:A:H8	53:ZA:1267:C:H1'	1.67	0.60
53:ZA:1616:U:OP2	66:PB:43:ARG:NH2	2.34	0.60
84:b:162:GLN:NE2	84:b:163:ASN:OD1	2.35	0.60
30:WA:1508:A:H4'	30:WA:1509:G:H5'	1.83	0.60
30:WA:1528:A:N3	30:WA:4394:C:O2'	2.35	0.60
24:Y:84:ARG:HH22	38:FA:102:ILE:HG21	1.66	0.60
30:WA:2778:OMG:HM22	30:WA:2779:C:H5'	1.84	0.60
32:YA:11:C:H2'	32:YA:12:G:H8	1.67	0.60
52:w:215:SER:O	54:DB:143:ARG:NH2	2.35	0.60
53:ZA:819:G:O2'	55:EB:255:ARG:NH2	2.31	0.60
53:ZA:1209:A:H5''	77:AC:82:LYS:HE2	1.83	0.60
83:GC:43:TRP:HA	83:GC:55:PRO:HA	1.83	0.60
30:WA:173:C:H1'	39:GA:112:ARG:HG2	1.84	0.60
30:WA:4298:PSU:O2'	46:NA:81:ARG:NH2	2.35	0.60
49:QA:31:GLY:HA2	49:QA:86:VAL:HA	1.83	0.60
53:ZA:1829:G:H1'	53:ZA:1850:A:H2	1.65	0.60
59:IB:37:LYS:N	59:IB:58:LEU:O	2.31	0.60
83:GC:217:MET:HG2	83:GC:229:THR:HG22	1.82	0.60
30:WA:1748:A:N1	30:WA:1794:C:O2'	2.33	0.60
53:ZA:1839:U:H2'	53:ZA:1840:U:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DB:29:LEU:HB2	54:DB:34:TYR:HB2	1.84	0.60
63:MB:48:HIS:O	63:MB:75:ASN:ND2	2.29	0.60
2:B:220:ILE:HD11	2:B:348:ARG:HE	1.67	0.60
8:H:59:LYS:HE2	8:H:66:GLU:HB3	1.84	0.60
30:WA:20:U:H3'	30:WA:21:G:H8	1.67	0.60
30:WA:1986:G:H21	51:v:773:GLU:HG2	1.67	0.60
30:WA:4996:U:H2'	30:WA:4997:G:H8	1.67	0.60
53:ZA:170:A:OP2	57:GB:140:ARG:NH1	2.35	0.60
73:WB:22:LYS:HD3	78:BC:3:LEU:HD12	1.83	0.60
8:H:91:LYS:HG2	8:H:145:VAL:HG12	1.83	0.59
30:WA:1183:U:H2'	30:WA:1184:G:H8	1.66	0.59
30:WA:1220:C:OP2	33:AA:91:ARG:NH1	2.35	0.59
30:WA:1807:A:O2'	30:WA:1842:A:OP1	2.20	0.59
30:WA:3791:U:OP1	30:WA:4555:7MG:O2'	2.17	0.59
30:WA:4243:G:H2'	30:WA:4244:A:H8	1.65	0.59
30:WA:4546:G:N2	30:WA:4549:A:OP2	2.28	0.59
53:ZA:649:U:H2'	53:ZA:650:A:H8	1.68	0.59
53:ZA:1001:A:N7	77:AC:19:GLN:NE2	2.50	0.59
53:ZA:1619:A:O2'	66:PB:82:ASP:OD2	2.20	0.59
65:OB:39:ASP:OD1	65:OB:40:THR:N	2.35	0.59
66:PB:73:PRO:HG2	66:PB:93:MET:HG2	1.85	0.59
84:b:347:MET:N	84:b:347:MET:SD	2.75	0.59
3:C:312:ARG:NH2	30:WA:2080:G:OP1	2.35	0.59
28:BB:114:VAL:O	53:ZA:1869:A:N6	2.34	0.59
29:CB:204:ILE:O	29:CB:211:LYS:NZ	2.35	0.59
35:CA:23:ARG:NH1	35:CA:25:TYR:OH	2.35	0.59
53:ZA:1598:G:H3'	76:ZB:80:ARG:HH11	1.67	0.59
64:NB:86:GLU:O	64:NB:90:HIS:ND1	2.32	0.59
67:QB:33:LYS:HD3	67:QB:36:GLY:HA2	1.83	0.59
83:GC:234:ASP:HB2	83:GC:252:THR:HG22	1.84	0.59
1:A:3:ARG:HD3	30:WA:1633:C:H42	1.66	0.59
11:L:112:VAL:HG11	13:N:201:LEU:HD12	1.83	0.59
14:O:18:ARG:NH1	14:O:147:GLU:OE2	2.35	0.59
30:WA:3:C:N3	32:YA:154:G:N1	2.46	0.59
30:WA:271:C:H2'	30:WA:272:U:C6	2.38	0.59
30:WA:4088:5MU:C5	30:WA:4088:5MU:C2	2.84	0.59
36:DA:30:LYS:HG3	36:DA:31:ILE:HD12	1.82	0.59
53:ZA:469:A:OP1	57:GB:95:LYS:NZ	2.36	0.59
18:S:70:HIS:NE2	30:WA:4332:C:OP1	2.35	0.59
30:WA:1800:A:N3	31:XA:79:U:O2'	2.35	0.59
30:WA:3666:G:H4'	30:WA:3667:A:H5'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:431:GLY:O	51:v:493:ASN:ND2	2.35	0.59
53:ZA:654:A:OP2	53:ZA:655:A:O2'	2.16	0.59
55:EB:87:MET:SD	55:EB:100:ARG:NH1	2.76	0.59
2:B:252:ALA:HB3	30:WA:4462:U:H1'	1.84	0.59
28:BB:113:MET:HB3	28:BB:142:PHE:HE2	1.67	0.59
30:WA:85:G:O2'	30:WA:97:G:O6	2.19	0.59
51:v:654:PRO:HD2	51:v:658:GLY:HA3	1.84	0.59
51:v:660:ASN:HD21	51:v:697:MET:HB2	1.67	0.59
53:ZA:642:U:O2'	53:ZA:643:A:O5'	2.16	0.59
3:C:80:ARG:NH2	30:WA:1650:C:OP1	2.35	0.59
6:F:176:ARG:NH1	30:WA:2106:A:N1	2.50	0.59
8:H:9:THR:HG21	8:H:54:ARG:HH21	1.66	0.59
30:WA:462:G:H2'	30:WA:463:A:C8	2.37	0.59
30:WA:2084:G:H2'	30:WA:2085:U:C6	2.38	0.59
51:v:369:CYS:SG	51:v:370:GLU:N	2.76	0.59
51:v:742:GLU:OE1	51:v:791:ASN:ND2	2.35	0.59
53:ZA:1033:G:N1	53:ZA:1080:A:O2'	2.29	0.59
53:ZA:1737:G:OP1	57:GB:94:ARG:NH2	2.35	0.59
83:GC:290:ALA:N	83:GC:299:PHE:O	2.32	0.59
1:A:179:ILE:O	30:WA:3658:A:O2'	2.16	0.59
10:J:95:ARG:NH2	10:J:177:GLY:O	2.35	0.59
18:S:88:ARG:NH2	33:AA:30:GLU:OE2	2.36	0.59
30:WA:2104:C:H4'	30:WA:2105:G:O5'	2.02	0.59
30:WA:4527:G:O2'	30:WA:4530:C:OP2	2.20	0.59
53:ZA:1546:G:N2	53:ZA:1670:C:O2	2.34	0.59
53:ZA:1779:G:H2'	53:ZA:1780:G:C4	2.37	0.59
64:NB:136:PRO:HG2	64:NB:139:TRP:HB2	1.83	0.59
83:GC:131:LEU:HD12	83:GC:140:TYR:HB3	1.83	0.59
22:W:78:LYS:NZ	22:W:133:GLU:OE1	2.34	0.59
49:QA:53:VAL:HB	49:QA:89:VAL:HG12	1.84	0.59
53:ZA:1228:A:H2'	53:ZA:1229:G:H8	1.66	0.59
75:YB:21:LYS:HG3	75:YB:75:ILE:HB	1.85	0.59
16:Q:15:LEU:HD13	16:Q:52:ARG:HB3	1.85	0.59
23:X:15:ARG:NH1	30:WA:230:G:OP1	2.36	0.59
30:WA:1302:G:O2'	30:WA:1303:U:O5'	2.21	0.59
56:FB:102:LEU:HD11	76:ZB:100:VAL:HG11	1.84	0.59
72:VB:11:LEU:HD23	72:VB:11:LEU:H	1.67	0.59
1:A:236:GLY:N	30:WA:3692:A:O2'	2.36	0.59
7:G:158:GLU:OE1	7:G:166:ARG:NH1	2.36	0.59
18:S:108:ARG:NH2	30:WA:1842:A:OP1	2.36	0.59
19:T:22:THR:HG22	19:T:71:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:909:C:H2'	30:WA:910:G:C8	2.36	0.59
30:WA:961:A:H1'	30:WA:2081:G:H5''	1.85	0.59
30:WA:4483:G:O2'	30:WA:4607:A:N1	2.36	0.59
53:ZA:144:U:OP2	57:GB:139:SER:OG	2.21	0.59
53:ZA:1016:U:H5''	64:NB:14:SER:HB2	1.85	0.59
53:ZA:1216:C:N4	53:ZA:1342:U:OP1	2.36	0.59
53:ZA:1277:C:H5'	61:KB:55:ARG:HH11	1.68	0.59
69:SB:105:ASN:ND2	69:SB:109:GLU:OE2	2.36	0.59
74:XB:91:LEU:HB3	81:EC:82:VAL:HG21	1.84	0.59
7:G:170:ARG:NH2	30:WA:119:G:O6	2.36	0.58
28:BB:49:VAL:HG21	28:BB:62:LEU:HD13	1.85	0.58
30:WA:102:G:O2'	30:WA:1387:U:O2'	2.08	0.58
53:ZA:1019:C:H5'	64:NB:72:LEU:HD23	1.85	0.58
53:ZA:1291:A:O2'	82:FC:140:TYR:OH	2.18	0.58
59:IB:103:LEU:HD13	59:IB:170:LYS:HD2	1.83	0.58
63:MB:70:ALA:O	63:MB:73:GLN:NE2	2.36	0.58
15:P:122:THR:OG1	15:P:124:ASP:OD1	2.20	0.58
17:R:15:ARG:HB3	17:R:27:LEU:HD23	1.85	0.58
30:WA:1468:C:H5''	33:AA:31:SER:HB3	1.84	0.58
53:ZA:406:U:H2'	53:ZA:408:A:H8	1.68	0.58
53:ZA:687:C:O3'	58:HB:121:THR:OG1	2.20	0.58
61:KB:65:ARG:O	61:KB:66:HIS:ND1	2.36	0.58
5:E:195:LYS:O	37:EA:108:SER:OG	2.21	0.58
15:P:14:ARG:NH2	30:WA:2088:C:OP2	2.37	0.58
16:Q:64:ARG:NH2	30:WA:2638:U:OP1	2.36	0.58
27:AB:63:ARG:NH1	72:VB:37:ALA:O	2.35	0.58
30:WA:1204:G:H2'	30:WA:1205:G:C8	2.38	0.58
30:WA:4124:C:O2'	30:WA:4125:U:O2	2.15	0.58
30:WA:4589:A:H2'	30:WA:4590:U:O4'	2.03	0.58
48:PA:91:SER:O	48:PA:95:HIS:ND1	2.36	0.58
53:ZA:982:G:H2'	53:ZA:983:A:C8	2.38	0.58
53:ZA:1528:G:O2'	53:ZA:1666:C:OP1	2.21	0.58
53:ZA:1781:A:H2'	53:ZA:1782:G:C8	2.38	0.58
53:ZA:1798:C:H2'	53:ZA:1799:G:O4'	2.03	0.58
84:b:247:TYR:HB3	84:b:302:LEU:HB3	1.85	0.58
4:D:17:GLN:NE2	18:S:22:HIS:O	2.35	0.58
11:L:12:VAL:HG22	11:L:60:PHE:HB2	1.84	0.58
20:U:18:LEU:HD23	20:U:54:ALA:HB3	1.86	0.58
26:K:39:ARG:NH2	30:WA:1368:G:OP1	2.35	0.58
30:WA:2526:G:H2'	30:WA:2527:7MG:H82	1.86	0.58
53:ZA:857:U:H2'	53:ZA:858:A:C8	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SB:59:LEU:HD13	69:SB:64:VAL:HG11	1.83	0.58
71:UB:80:PHE:HB3	80:DC:52:PHE:HB3	1.85	0.58
79:CC:40:ARG:NH2	79:CC:61:SER:O	2.36	0.58
3:C:195:LYS:NZ	30:WA:2339:C:OP2	2.34	0.58
12:M:67:ARG:NH1	30:WA:2463:C:OP1	2.36	0.58
23:X:74:TYR:OH	32:YA:75:G:OP2	2.21	0.58
30:WA:4640:A:H2	30:WA:4668:G:H21	1.50	0.58
53:ZA:1600:G:H4'	76:ZB:43:LYS:HE3	1.86	0.58
55:EB:49:ARG:NH1	55:EB:49:ARG:O	2.36	0.58
8:H:64:ARG:NH2	30:WA:4698:C:OP1	2.37	0.58
13:N:89:PRO:HD3	30:WA:1919:C:H4'	1.86	0.58
30:WA:1650:C:H2'	30:WA:1651:A:H8	1.69	0.58
30:WA:1911:U:H2'	30:WA:1912:A:H8	1.68	0.58
53:ZA:1797:U:H2'	53:ZA:1798:C:C6	2.39	0.58
54:DB:15:GLY:HA2	54:DB:18:LYS:HE2	1.86	0.58
12:M:15:GLN:O	12:M:20:ARG:NH1	2.37	0.58
27:AB:85:ARG:NH1	27:AB:203:PHE:O	2.34	0.58
32:YA:102:G:OP2	32:YA:104:A:O2'	2.19	0.58
33:AA:56:LYS:O	33:AA:60:ASN:ND2	2.33	0.58
51:v:592:LEU:HD11	51:v:601:ARG:HB3	1.86	0.58
53:ZA:681:U:H4'	74:XB:9:THR:HG22	1.85	0.58
53:ZA:925:G:H21	64:NB:48:SER:HB2	1.69	0.58
55:EB:112:HIS:NE2	55:EB:237:SER:O	2.37	0.58
1:A:124:GLY:O	1:A:128:ARG:NH1	2.36	0.58
13:N:65:ASN:ND2	30:WA:4570:C:OP1	2.30	0.58
15:P:181:ARG:HH22	30:WA:1397:A:H5'	1.68	0.58
24:Y:103:ASP:HB2	24:Y:106:LEU:HB2	1.85	0.58
32:YA:96:C:H5''	39:GA:66:LYS:HG2	1.86	0.58
48:PA:26:SER:OG	48:PA:28:GLU:OE1	2.17	0.58
53:ZA:365:C:O2'	53:ZA:402:C:O2'	2.22	0.58
56:FB:50:PRO:HG2	56:FB:90:VAL:HG12	1.84	0.58
69:SB:34:LYS:NZ	69:SB:104:ASP:OD1	2.35	0.58
14:O:127:ARG:NH2	30:WA:2427:OMC:OP1	2.36	0.58
30:WA:1335:G:O2'	30:WA:1336:A:OP1	2.20	0.58
30:WA:4953:C:H3'	30:WA:4954:G:C5'	2.34	0.58
53:ZA:311:C:H5''	53:ZA:312:G:H5''	1.85	0.58
53:ZA:369:C:H5	53:ZA:1730:U:H5''	1.69	0.58
53:ZA:1036:A:N3	53:ZA:1844:U:O2'	2.37	0.58
53:ZA:1036:A:H4'	53:ZA:1855:G:H21	1.68	0.58
53:ZA:1679:A:OP1	79:CC:20:ARG:NH2	2.37	0.58
2:B:168:MET:HE1	2:B:173:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:192:TRP:CD1	30:WA:48:G:H5'	2.39	0.58
30:WA:1396:G:N2	30:WA:1399:G:OP2	2.32	0.58
30:WA:1404:A:H62	30:WA:1425:G:N2	1.99	0.58
49:QA:128:THR:HG22	49:QA:130:LEU:H	1.68	0.58
51:v:507:VAL:HA	51:v:575:PRO:HD3	1.85	0.58
53:ZA:59:U:O5'	53:ZA:503:C:N4	2.36	0.58
53:ZA:925:G:OP1	64:NB:121:ARG:NH1	2.37	0.58
53:ZA:930:C:O2'	53:ZA:1104:G:OP1	2.21	0.58
65:OB:29:GLY:O	65:OB:94:HIS:N	2.30	0.58
6:F:93:ARG:NH1	6:F:95:ARG:O	2.37	0.57
8:H:114:ILE:HB	8:H:124:ARG:HG3	1.83	0.57
27:AB:70:ASN:HD21	27:AB:72:ALA:HB3	1.69	0.57
53:ZA:1020:A:N7	64:NB:70:LYS:NZ	2.52	0.57
62:LB:84:ARG:O	62:LB:112:HIS:ND1	2.37	0.57
84:b:159:PRO:HG3	84:b:325:LEU:HD11	1.85	0.57
3:C:186:SER:O	3:C:188:ARG:NH1	2.36	0.57
3:C:290:SER:OG	48:PA:4:HIS:NE2	2.32	0.57
53:ZA:979:C:H2'	53:ZA:980:A:H8	1.69	0.57
58:HB:134:VAL:HG13	58:HB:166:VAL:HG11	1.85	0.57
59:IB:63:GLY:N	59:IB:76:THR:O	2.37	0.57
76:ZB:53:ALA:O	76:ZB:57:LYS:NZ	2.36	0.57
25:Z:64:LYS:NZ	30:WA:70:A:OP2	2.33	0.57
30:WA:1947:A:H2'	30:WA:1948:A:H8	1.69	0.57
30:WA:4704:U:H1'	30:WA:4705:A:H5''	1.87	0.57
46:NA:2:VAL:N	46:NA:90:HIS:O	2.38	0.57
50:RA:32:ILE:HD12	50:RA:39:PRO:HB3	1.85	0.57
66:PB:98:ASN:ND2	66:PB:121:ILE:O	2.37	0.57
80:DC:22:ARG:NH1	80:DC:36:LEU:O	2.31	0.57
12:M:193:ARG:O	12:M:197:THR:OG1	2.20	0.57
51:v:594:LYS:O	51:v:727:ARG:NH2	2.37	0.57
74:XB:46:HIS:HB3	74:XB:101:LEU:HD11	1.86	0.57
12:M:5:LYS:HG3	40:HA:40:VAL:HG11	1.87	0.57
13:N:68:ARG:NH2	30:WA:4569:M7A:OP1	2.36	0.57
28:BB:89:GLU:OE2	28:BB:99:ASN:ND2	2.33	0.57
30:WA:1938:G:H2'	30:WA:1939:A:C8	2.40	0.57
30:WA:3893:G:O2'	30:WA:3894:G:OP1	2.22	0.57
30:WA:4542:C:H2'	30:WA:4543:G:C8	2.39	0.57
42:JA:24:LYS:HG3	42:JA:35:LYS:HB2	1.86	0.57
51:v:191:THR:HG22	51:v:779:THR:HG22	1.87	0.57
52:w:195:ARG:NH2	53:ZA:1699:A:OP2	2.33	0.57
53:ZA:77:A:H62	57:GB:179:LEU:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:671:A:H4'	53:ZA:672:A:H5''	1.86	0.57
53:ZA:1593:C:OP1	76:ZB:103:HIS:NE2	2.27	0.57
63:MB:24:THR:O	63:MB:28:HIS:ND1	2.37	0.57
33:AA:36:ASP:HB3	33:AA:39:PHE:HB3	1.87	0.57
53:ZA:165:G:O2'	57:GB:53:SER:OG	2.21	0.57
60:JB:42:GLU:HA	60:JB:45:ARG:HG2	1.87	0.57
6:F:222:LYS:HE3	30:WA:1912:A:H4'	1.86	0.57
12:M:73:ARG:NH1	30:WA:32:G:OP1	2.37	0.57
30:WA:178:C:H2'	30:WA:179:G:C8	2.39	0.57
30:WA:1499:U:H2'	30:WA:1500:G:H8	1.70	0.57
30:WA:2002:U:OP2	50:RA:123:ARG:NH2	2.37	0.57
30:WA:4397:G:N2	30:WA:4400:U:O2	2.35	0.57
35:CA:64:ILE:HA	35:CA:106:VAL:HG22	1.86	0.57
37:EA:59:THR:OG1	37:EA:65:ASN:OD1	2.23	0.57
60:JB:162:ARG:HE	75:YB:31:GLY:HA2	1.68	0.57
2:B:217:ILE:HD11	2:B:333:LEU:HD21	1.86	0.57
3:C:146:GLU:OE2	3:C:178:ASN:ND2	2.38	0.57
23:X:34:LEU:HD23	23:X:38:LEU:HB3	1.85	0.57
30:WA:418:A:C2	32:YA:17:A:H1'	2.39	0.57
30:WA:1213:C:H2'	30:WA:1214:G:H8	1.70	0.57
30:WA:2013:U:O2'	30:WA:2016:C:N4	2.38	0.57
37:EA:40:GLU:O	37:EA:109:ARG:NH2	2.38	0.57
53:ZA:1367:U:HO2'	53:ZA:1466:G:HO2'	1.41	0.57
53:ZA:1464:C:OP2	68:RB:63:ARG:NH2	2.38	0.57
53:ZA:1620:A:H5''	66:PB:40:ARG:HH21	1.70	0.57
55:EB:126:VAL:HG12	55:EB:139:LEU:HD21	1.86	0.57
57:GB:74:ARG:HA	57:GB:96:SER:HA	1.87	0.57
12:M:181:HIS:O	12:M:195:ARG:NH2	2.36	0.57
18:S:87:LYS:NZ	30:WA:4310:G:N7	2.53	0.57
28:BB:144:LYS:HD3	28:BB:208:HIS:HB3	1.87	0.57
30:WA:1210:C:H2'	30:WA:1211:G:H8	1.70	0.57
41:IA:2:THR:O	41:IA:7:SER:OG	2.23	0.57
53:ZA:658:U:O2	74:XB:17:ARG:NH1	2.38	0.57
56:FB:97:PHE:HD1	56:FB:100:ILE:HD11	1.68	0.57
69:SB:13:LEU:HB2	69:SB:20:ILE:HB	1.85	0.57
70:TB:22:LEU:HD13	70:TB:28:LEU:HD21	1.87	0.57
83:GC:17:TRP:O	83:GC:36:ARG:N	2.34	0.57
29:CB:187:ARG:NH1	53:ZA:1142:G:OP2	2.37	0.57
30:WA:3705:C:O2'	30:WA:3779:A:N3	2.35	0.57
30:WA:4351:U:O2'	46:NA:80:LYS:O	2.22	0.57
30:WA:4609:G:N2	30:WA:4612:A:OP2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QA:47:LEU:HB3	49:QA:51:ALA:HB3	1.87	0.57
50:RA:108:GLU:O	50:RA:111:ASN:ND2	2.38	0.57
53:ZA:16:G:H21	53:ZA:1195:A:H62	1.53	0.57
70:TB:38:LYS:NZ	70:TB:40:ALA:O	2.36	0.57
18:S:20:ARG:HH12	31:XA:67:C:H4'	1.70	0.56
30:WA:703:U:H3'	30:WA:704:G:H5''	1.87	0.56
30:WA:1551:C:N4	30:WA:1617:G:H22	2.00	0.56
30:WA:4912:G:N1	30:WA:4918:G:O2'	2.37	0.56
32:YA:111:U:O4	41:IA:20:ARG:NH2	2.37	0.56
48:PA:28:GLU:OE2	48:PA:31:ASN:ND2	2.37	0.56
53:ZA:1144:A:H2'	53:ZA:1145:A:C8	2.40	0.56
23:X:50:ARG:NH2	32:YA:85:U:O4	2.38	0.56
24:Y:22:LYS:NZ	24:Y:129:TRP:O	2.37	0.56
24:Y:50:PRO:HD3	24:Y:68:ILE:HG12	1.86	0.56
30:WA:1932:U:OP1	30:WA:1954:U:O2'	2.13	0.56
30:WA:2313:A:N6	30:WA:2335:G:H1'	2.21	0.56
30:WA:3873:G:H22	30:WA:3905:G:H1'	1.69	0.56
53:ZA:26:U:H2'	53:ZA:27:A:H8	1.70	0.56
53:ZA:640:A:H2'	53:ZA:641:A:C8	2.41	0.56
71:UB:26:SER:HB3	71:UB:32:LEU:HB2	1.86	0.56
1:A:198:ARG:NH2	30:WA:3692:A:OP2	2.38	0.56
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.88	0.56
13:N:176:ARG:NH2	30:WA:4774:G:OP1	2.37	0.56
15:P:67:ILE:HD12	15:P:96:PRO:HD2	1.86	0.56
21:V:81:ALA:HB2	21:V:87:LEU:HD13	1.86	0.56
25:Z:10:LYS:NZ	30:WA:2292:G:O6	2.37	0.56
30:WA:2587:A:HO2'	30:WA:2658:C:HO2'	1.52	0.56
30:WA:2709:C:H2'	30:WA:2710:G:C8	2.40	0.56
30:WA:4752:C:H42	30:WA:4958:G:H1	1.52	0.56
51:v:649:ILE:HG22	51:v:663:THR:HB	1.87	0.56
52:w:219:GLY:HA3	54:DB:114:ALA:HB1	1.87	0.56
53:ZA:142:C:N4	53:ZA:329:G:OP2	2.38	0.56
53:ZA:146:G:HO2'	53:ZA:147:A:H8	1.53	0.56
53:ZA:527:C:O3'	60:JB:121:LYS:NZ	2.38	0.56
53:ZA:655:A:H4'	53:ZA:656:G:H3'	1.87	0.56
53:ZA:830:A:OP2	53:ZA:846:G:N2	2.38	0.56
53:ZA:1457:U:H2'	53:ZA:1458:G:H8	1.69	0.56
57:GB:159:ARG:HG2	57:GB:173:ALA:HB2	1.88	0.56
70:TB:104:LEU:HD22	70:TB:121:ARG:HG3	1.87	0.56
9:I:46:PHE:HB3	9:I:139:ARG:HG2	1.87	0.56
28:BB:89:GLU:HB3	28:BB:223:PHE:HE1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:290:CYS:O	51:v:295:ASP:N	2.34	0.56
53:ZA:532:C:O2'	53:ZA:533:A:OP1	2.23	0.56
65:OB:101:GLY:HA3	65:OB:134:PRO:HG2	1.87	0.56
75:YB:63:HIS:ND1	75:YB:68:LYS:O	2.37	0.56
83:GC:70:VAL:HG23	83:GC:79:LEU:HB3	1.87	0.56
83:GC:137:VAL:HB	83:GC:139:LYS:HZ2	1.70	0.56
9:I:30:LYS:HG2	9:I:63:GLU:HG3	1.87	0.56
23:X:11:ARG:HG3	30:WA:229:G:H5''	1.87	0.56
26:K:163:LYS:NZ	30:WA:512:C:OP2	2.39	0.56
27:AB:10:MET:HE1	27:AB:52:LYS:HA	1.88	0.56
30:WA:1183:U:H2'	30:WA:1184:G:C8	2.40	0.56
51:v:839:ARG:HG3	51:v:844:LEU:HB2	1.86	0.56
53:ZA:520:A:O2'	53:ZA:825:A:N3	2.35	0.56
53:ZA:916:A:O2'	64:NB:73:ARG:NH1	2.38	0.56
53:ZA:1754:G:H2'	53:ZA:1755:C:C6	2.41	0.56
55:EB:141:THR:OG1	55:EB:143:ASP:OD1	2.17	0.56
64:NB:84:LEU:HD23	64:NB:84:LEU:H	1.71	0.56
68:RB:37:GLU:OE1	83:GC:150:TRP:NE1	2.29	0.56
82:FC:100:LEU:HD23	82:FC:103:LEU:HD11	1.88	0.56
30:WA:2100:A:H2	30:WA:2102:A:H61	1.53	0.56
30:WA:2584:G:N2	30:WA:2587:A:OP2	2.29	0.56
53:ZA:171:A:OP1	57:GB:137:ARG:NH1	2.36	0.56
53:ZA:1486:A:H2'	53:ZA:1487:A:C8	2.40	0.56
53:ZA:1542:C:H5''	70:TB:62:ARG:HH22	1.70	0.56
53:ZA:1864:U:O2'	53:ZA:1866:A:N7	2.35	0.56
84:b:53:ASP:OD2	84:b:281:ARG:NH2	2.35	0.56
1:A:207:VAL:HG13	1:A:208:GLU:HG3	1.86	0.56
3:C:321:ASN:HB3	3:C:324:ILE:HB	1.87	0.56
7:G:126:ARG:NE	30:WA:4081:G:OP1	2.30	0.56
9:I:31:ILE:HB	9:I:66:GLU:HB2	1.87	0.56
10:J:150:CYS:SG	10:J:151:ILE:N	2.77	0.56
12:M:178:HIS:ND1	30:WA:68:U:OP1	2.25	0.56
29:CB:252:THR:HG22	29:CB:254:ASP:H	1.70	0.56
30:WA:2750:A:H2'	30:WA:2751:A:C8	2.40	0.56
53:ZA:530:U:H2'	53:ZA:531:A:H8	1.68	0.56
60:JB:63:LEU:O	60:JB:70:ARG:NH1	2.39	0.56
69:SB:70:ILE:HG12	69:SB:77:TYR:CZ	2.40	0.56
69:SB:132:ARG:HB2	69:SB:134:GLN:HE22	1.71	0.56
77:AC:12:LYS:HD3	77:AC:16:GLY:H	1.70	0.56
30:WA:2379:A:H2'	30:WA:2380:A:H8	1.71	0.56
40:HA:63:VAL:HG23	40:HA:65:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:RA:87:GLU:HB3	50:RA:90:ARG:HH21	1.71	0.56
53:ZA:28:U:H2'	53:ZA:29:G:C8	2.41	0.56
53:ZA:81:U:H3'	53:ZA:82:G:H8	1.69	0.56
53:ZA:373:G:H2'	53:ZA:374:G:H8	1.71	0.56
53:ZA:1288:U:H3	53:ZA:1311:C:H42	0.70	0.56
53:ZA:1533:A:OP2	56:FB:164:ARG:NH1	2.39	0.56
54:DB:106:ARG:NH1	54:DB:174:HIS:O	2.38	0.56
75:YB:76:TYR:OH	75:YB:86:GLU:OE1	2.19	0.56
79:CC:20:ARG:NH1	79:CC:28:THR:OG1	2.39	0.56
2:B:276:HIS:ND1	30:WA:4721:C:OP1	2.31	0.56
3:C:150:LEU:HB2	3:C:151:PRO:HD3	1.88	0.56
7:G:242:ARG:HH22	32:YA:154:G:H5'	1.71	0.56
26:K:27:ASN:HB3	32:YA:29:G:H5''	1.88	0.56
26:K:116:ARG:HH12	26:K:157:ILE:HD11	1.69	0.56
30:WA:3737:A:H2'	30:WA:3738:A:C8	2.40	0.56
53:ZA:582:U:H1'	75:YB:33:ALA:HB2	1.88	0.56
53:ZA:804:U:OP1	73:WB:82:GLN:NE2	2.33	0.56
53:ZA:1777:G:O2'	53:ZA:1778:C:OP1	2.22	0.56
54:DB:55:THR:HA	54:DB:58:VAL:HG12	1.88	0.56
1:A:93:LYS:NZ	30:WA:4120:G:OP1	2.38	0.56
5:E:126:ARG:NH2	30:WA:977:G:O2'	2.38	0.56
30:WA:1304:C:H2'	30:WA:1305:G:H8	1.71	0.56
30:WA:1829:G:H2'	30:WA:1830:A:C8	2.40	0.56
30:WA:4424:U:OP1	30:WA:4426:C:N4	2.39	0.56
51:v:114:GLU:OE2	51:v:400:LYS:NZ	2.37	0.56
53:ZA:466:G:H1'	57:GB:59:GLN:HE21	1.71	0.56
53:ZA:1488:C:O2'	53:ZA:1490:G:O5'	2.24	0.56
7:G:216:PRO:O	12:M:26:ARG:NH2	2.39	0.55
30:WA:2508:G:N2	30:WA:4089:G:N3	2.52	0.55
30:WA:4168:U:H5'	30:WA:4169:C:H5''	1.88	0.55
53:ZA:1131:G:H2'	53:ZA:1132:C:C6	2.42	0.55
53:ZA:1193:U:O2'	53:ZA:1194:A:OP1	2.22	0.55
53:ZA:1298:G:H21	53:ZA:1298:G:P	2.29	0.55
53:ZA:1395:C:H2'	53:ZA:1396:A:C8	2.41	0.55
75:YB:108:LYS:O	75:YB:112:ASN:ND2	2.36	0.55
83:GC:154:VAL:O	83:GC:155:ARG:NH1	2.37	0.55
5:E:64:MET:HG3	5:E:68:LYS:HE3	1.88	0.55
6:F:33:ARG:NH1	30:WA:1445:U:OP2	2.40	0.55
29:CB:191:VAL:HG11	29:CB:236:PHE:HA	1.88	0.55
30:WA:2764:G:O2'	30:WA:2767:G:N2	2.39	0.55
53:ZA:197:U:O2	53:ZA:202:G:O6	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:666:U:H2'	53:ZA:667:U:C6	2.42	0.55
53:ZA:1536:G:H2'	53:ZA:1537:A:H8	1.71	0.55
53:ZA:1568:C:H2'	53:ZA:1569:A:C8	2.42	0.55
53:ZA:1704:C:O2'	53:ZA:1831:A:N1	2.33	0.55
63:MB:33:ARG:HD3	63:MB:89:VAL:HG21	1.88	0.55
72:VB:21:ASN:HD22	73:WB:67:GLY:H	1.53	0.55
2:B:283:LYS:HD3	2:B:363:ILE:HD11	1.89	0.55
10:J:19:LYS:NZ	10:J:21:CYS:SG	2.71	0.55
11:L:101:LYS:NZ	30:WA:4882:G:OP1	2.29	0.55
16:Q:83:GLY:N	30:WA:2817:A:OP1	2.38	0.55
20:U:106:VAL:HG12	20:U:112:MET:HA	1.87	0.55
25:Z:117:LEU:HD12	25:Z:118:PRO:HD2	1.87	0.55
30:WA:1900:G:O2'	30:WA:1912:A:N3	2.37	0.55
30:WA:4647:U:H2'	30:WA:4648:G:C8	2.40	0.55
30:WA:4683:G:N2	30:WA:4718:G:H1'	2.21	0.55
34:BA:45:LEU:HD23	34:BA:96:ILE:HD12	1.88	0.55
51:v:109:VAL:HB	51:v:138:GLN:HE22	1.70	0.55
53:ZA:1252:C:OP1	71:UB:75:LYS:NZ	2.35	0.55
53:ZA:1491:G:H2'	53:ZA:1492:U:C6	2.42	0.55
73:WB:40:VAL:O	73:WB:44:HIS:ND1	2.36	0.55
1:A:3:ARG:HH11	30:WA:1633:C:H42	1.53	0.55
2:B:261:ARG:HB2	13:N:64:THR:HG21	1.88	0.55
4:D:23:ARG:NH1	30:WA:4285:A:OP2	2.40	0.55
7:G:282:ARG:HG2	7:G:285:GLU:HB2	1.88	0.55
27:AB:36:GLN:O	27:AB:53:ARG:NH1	2.40	0.55
27:AB:157:VAL:O	72:VB:65:SER:OG	2.19	0.55
28:BB:136:ARG:HE	28:BB:218:LEU:HD21	1.71	0.55
30:WA:321:U:H2'	30:WA:322:C:C6	2.41	0.55
48:PA:28:GLU:HG2	48:PA:31:ASN:HB2	1.88	0.55
56:FB:25:THR:OG1	56:FB:41:VAL:O	2.24	0.55
66:PB:118:GLU:O	69:SB:120:HIS:N	2.40	0.55
80:DC:20:SER:HB3	80:DC:27:ARG:HE	1.71	0.55
13:N:193:THR:HG23	13:N:202:LEU:HD23	1.89	0.55
30:WA:382:G:N1	30:WA:385:A:OP2	2.36	0.55
30:WA:4244:A:H2'	30:WA:4245:G:C8	2.41	0.55
30:WA:5062:C:H2'	30:WA:5063:A:C8	2.42	0.55
32:YA:57:C:OP2	41:IA:68:LYS:NZ	2.39	0.55
50:RA:72:GLU:HG2	50:RA:73:VAL:H	1.71	0.55
53:ZA:1568:C:OP1	70:TB:96:SER:OG	2.14	0.55
53:ZA:1744:G:O4'	53:ZA:1790:A:N6	2.40	0.55
67:QB:132:PHE:O	67:QB:140:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:RB:76:GLU:HB2	68:RB:80:ARG:HH21	1.72	0.55
1:A:156:LYS:NZ	30:WA:3667:A:OP2	2.34	0.55
2:B:217:ILE:HD13	2:B:284:ILE:HD11	1.88	0.55
3:C:110:ARG:NH1	30:WA:1513:A:OP1	2.35	0.55
15:P:144:LYS:HG2	30:WA:1465:C:H5''	1.89	0.55
30:WA:208:A:N3	30:WA:232:G:O2'	2.39	0.55
30:WA:4877:2MG:HM22	30:WA:4879:A:H62	1.72	0.55
53:ZA:438:G:H8	53:ZA:1800:A:H4'	1.72	0.55
59:IB:67:TRP:NE1	59:IB:191:GLU:OE2	2.32	0.55
70:TB:59:SER:O	70:TB:63:HIS:ND1	2.37	0.55
2:B:224:LYS:NZ	30:WA:4631:A:OP2	2.29	0.55
3:C:303:ARG:O	15:P:38:ARG:NH1	2.39	0.55
6:F:121:PHE:O	6:F:204:ASN:ND2	2.33	0.55
14:O:82:ARG:NH2	30:WA:2367:U:OP1	2.40	0.55
15:P:82:VAL:HG12	15:P:84:GLY:H	1.72	0.55
23:X:67:ILE:O	23:X:84:ARG:NH1	2.39	0.55
30:WA:1339:A:H2'	30:WA:1340:A:C8	2.42	0.55
30:WA:4512:A:H2'	30:WA:4513:C:C6	2.42	0.55
45:MA:15:ARG:NH2	53:ZA:1183:A:OP1	2.40	0.55
51:v:158:ASN:OD1	51:v:217:GLY:N	2.32	0.55
53:ZA:1164:G:H2'	53:ZA:1165:G:N3	2.22	0.55
53:ZA:1226:G:N1	53:ZA:1639:G:OP2	2.31	0.55
3:C:74:ALA:H	3:C:78:ARG:HH21	1.55	0.55
5:E:96:THR:HG22	5:E:109:VAL:HG22	1.89	0.55
5:E:224:LYS:O	30:WA:4945:C:N4	2.39	0.55
27:AB:50:ASN:HB3	27:AB:53:ARG:HD2	1.89	0.55
30:WA:7:C:H2'	30:WA:8:U:C6	2.42	0.55
53:ZA:624:C:N4	74:XB:63:ASN:OD1	2.34	0.55
71:UB:94:PRO:HD2	71:UB:97:ILE:HD12	1.89	0.55
2:B:47:LEU:HD22	2:B:166:THR:HG21	1.87	0.55
6:F:216:ARG:NH1	30:WA:719:C:OP1	2.40	0.55
18:S:63:ARG:NH2	33:AA:30:GLU:OE1	2.39	0.55
21:V:98:PRO:HA	21:V:101:ARG:HE	1.71	0.55
30:WA:1582:G:OP1	47:OA:17:ARG:NH2	2.33	0.55
30:WA:2003:A:O2'	30:WA:2004:A:OP1	2.24	0.55
51:v:610:PRO:HG2	51:v:613:LEU:HB2	1.88	0.55
53:ZA:3:C:O2	60:JB:18:ARG:NH1	2.40	0.55
53:ZA:926:A:OP1	64:NB:94:LYS:NZ	2.36	0.55
69:SB:80:PRO:HB2	69:SB:82:TRP:CD1	2.42	0.55
24:Y:133:LYS:NZ	30:WA:2758:G:OP1	2.32	0.55
30:WA:447:C:H2'	30:WA:448:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2367:U:H2'	30:WA:2368:A2M:H8	1.89	0.55
30:WA:3694:G:O2'	30:WA:3823:U:OP2	2.24	0.55
30:WA:4243:G:H2'	30:WA:4244:A:C8	2.42	0.55
46:NA:24:THR:HG23	46:NA:69:ARG:HB3	1.89	0.55
1:A:24:LYS:HG3	1:A:49:ILE:HD12	1.89	0.54
24:Y:95:VAL:HG13	24:Y:96:VAL:HG23	1.89	0.54
30:WA:66:A:O2'	30:WA:326:C:O2	2.22	0.54
30:WA:1080:G:H2'	30:WA:1081:G:C8	2.42	0.54
30:WA:1622:G:H1'	30:WA:2518:A:N6	2.22	0.54
30:WA:2880:C:H2'	47:OA:7:LYS:HE2	1.89	0.54
39:GA:103:LYS:O	39:GA:108:GLN:NE2	2.39	0.54
53:ZA:1858:G:OP2	65:OB:146:ARG:NH2	2.35	0.54
56:FB:127:ARG:HB2	56:FB:136:ARG:HH22	1.73	0.54
69:SB:121:ARG:O	69:SB:125:HIS:ND1	2.35	0.54
74:XB:60:LYS:HE2	74:XB:116:PRO:HB3	1.90	0.54
84:b:155:ARG:HG2	84:b:357:LEU:HA	1.90	0.54
1:A:200:ARG:NH2	1:A:217:GLN:OE1	2.40	0.54
2:B:55:HIS:NE2	21:V:16:GLY:HA3	2.22	0.54
4:D:5:LYS:HE3	30:WA:1783:C:H5''	1.89	0.54
15:P:79:THR:HB	15:P:136:THR:HG22	1.89	0.54
15:P:181:ARG:NH1	30:WA:1397:A:OP1	2.40	0.54
19:T:60:VAL:HG23	19:T:61:VAL:HG23	1.90	0.54
30:WA:1551:C:H42	30:WA:1617:G:N2	2.02	0.54
30:WA:2829:C:H2'	30:WA:2830:A:C8	2.42	0.54
30:WA:4964:U:H2'	30:WA:4965:G:N7	2.22	0.54
43:KA:20:ASN:O	43:KA:41:ARG:NH1	2.40	0.54
54:DB:106:ARG:HH21	54:DB:173:ARG:HD2	1.72	0.54
68:RB:37:GLU:OE2	83:GC:127:LYS:NZ	2.37	0.54
73:WB:103:VAL:HG12	73:WB:126:LEU:HD12	1.88	0.54
29:CB:102:LEU:HD13	29:CB:130:ILE:HD11	1.89	0.54
30:WA:1312:C:H2'	30:WA:1313:A:C8	2.39	0.54
30:WA:1764:G:H2'	30:WA:1765:G:H8	1.72	0.54
30:WA:1966:G:OP2	49:QA:59:THR:OG1	2.24	0.54
30:WA:5009:C:H2'	30:WA:5010:G:O4'	2.07	0.54
33:AA:43:MET:HG2	33:AA:47:LYS:HE3	1.90	0.54
49:QA:134:LYS:HE3	49:QA:177:MET:HE3	1.90	0.54
53:ZA:12:U:H2'	53:ZA:13:C:C6	2.43	0.54
53:ZA:552:G:H4'	81:EC:112:ASN:HB3	1.90	0.54
53:ZA:924:G:H21	64:NB:87:ASP:HB3	1.72	0.54
1:A:200:ARG:NH2	30:WA:3655:C:OP1	2.41	0.54
2:B:357:ARG:HD2	30:WA:4620:C:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:220:LYS:NZ	6:F:230:GLY:O	2.40	0.54
30:WA:1332:A2M:H5''	30:WA:1332:A2M:H8	1.90	0.54
30:WA:1668:C:O2'	30:WA:2325:G:N2	2.41	0.54
30:WA:1816:G:H21	33:AA:57:MET:HE2	1.72	0.54
53:ZA:561:A:O2'	60:JB:134:HIS:NE2	2.30	0.54
53:ZA:822:U:O4	53:ZA:826:A:N7	2.40	0.54
54:DB:47:GLU:HG2	54:DB:85:GLU:HB2	1.87	0.54
58:HB:53:VAL:HG21	58:HB:172:THR:HA	1.88	0.54
59:IB:83:TYR:HB3	59:IB:101:ILE:HD12	1.89	0.54
63:MB:89:VAL:HG13	63:MB:91:LEU:HG	1.90	0.54
83:GC:30:MET:HE2	83:GC:92:LEU:HD13	1.89	0.54
10:J:68:ILE:HD11	30:WA:4263:C:H5'	1.89	0.54
18:S:112:ASN:HB2	18:S:128:LEU:HD22	1.88	0.54
24:Y:36:ARG:NH1	24:Y:38:TYR:OH	2.29	0.54
30:WA:1852:C:H2'	30:WA:1853:C:C6	2.43	0.54
30:WA:2381:A:H2'	30:WA:2382:C:C6	2.42	0.54
30:WA:4741:C:H2'	30:WA:4742:G:C8	2.43	0.54
53:ZA:186:C:N4	53:ZA:187:G:O6	2.41	0.54
53:ZA:419:G:N2	53:ZA:661:U:O2	2.40	0.54
53:ZA:1290:G:N1	53:ZA:1310:U:O2	2.40	0.54
55:EB:57:THR:OG1	55:EB:60:GLU:OE1	2.24	0.54
59:IB:43:ILE:HG12	59:IB:57:ALA:HA	1.88	0.54
12:M:177:GLY:HA2	30:WA:67:C:O3'	2.08	0.54
30:WA:1314:C:H2'	30:WA:1315:C:C6	2.42	0.54
53:ZA:979:C:H2'	53:ZA:980:A:C8	2.43	0.54
53:ZA:981:A:H2'	53:ZA:982:G:H8	1.72	0.54
53:ZA:1129:G:H2'	53:ZA:1130:G:C4	2.43	0.54
57:GB:85:ARG:O	57:GB:87:ARG:NH1	2.40	0.54
67:QB:16:LYS:HB3	67:QB:19:ALA:HB3	1.88	0.54
75:YB:74:MET:N	75:YB:74:MET:SD	2.81	0.54
25:Z:136:LYS:NZ	30:WA:1404:A:OP1	2.35	0.54
30:WA:462:G:H2'	30:WA:463:A:H8	1.72	0.54
30:WA:2333:G:H2'	30:WA:2334:U:C6	2.43	0.54
30:WA:3875:C:H2'	30:WA:3876:A:H8	1.72	0.54
53:ZA:1670:C:H2'	53:ZA:1671:G:H8	1.73	0.54
53:ZA:1780:G:H2'	53:ZA:1781:A:C8	2.43	0.54
54:DB:175:VAL:HB	54:DB:182:LEU:HB2	1.89	0.54
57:GB:51:ARG:O	57:GB:112:VAL:N	2.34	0.54
58:HB:105:THR:HG23	58:HB:108:SER:H	1.72	0.54
59:IB:175:ILE:HD13	59:IB:185:ALA:HB1	1.90	0.54
60:JB:87:LEU:HD13	60:JB:100:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:BC:67:THR:OG1	78:BC:70:LYS:O	2.25	0.54
4:D:83:LEU:HB3	4:D:88:VAL:HB	1.90	0.54
12:M:104:GLU:HA	12:M:160:GLU:HG3	1.89	0.54
17:R:34:ALA:HB1	17:R:39:VAL:HG13	1.90	0.54
28:BB:136:ARG:HH12	53:ZA:941:C:H5''	1.72	0.54
30:WA:518:C:H2'	30:WA:519:G:H8	1.72	0.54
30:WA:1217:G:H2'	30:WA:1218:G:H8	1.73	0.54
30:WA:1332:A2M:H2'	30:WA:1333:C:C6	2.42	0.54
30:WA:1764:G:H2'	30:WA:1765:G:C8	2.43	0.54
30:WA:2594:C:H2'	30:WA:2595:G:O4'	2.08	0.54
30:WA:2668:G:N2	30:WA:2681:A:O2'	2.37	0.54
30:WA:4244:A:H2'	30:WA:4245:G:H8	1.73	0.54
30:WA:5060:G:H2'	30:WA:5061:A:H8	1.72	0.54
31:XA:82:G:H2'	31:XA:83:A:C8	2.43	0.54
51:v:115:VAL:HG11	51:v:142:VAL:HG23	1.90	0.54
51:v:507:VAL:HG22	51:v:554:LEU:HD11	1.90	0.54
53:ZA:373:G:H2'	53:ZA:374:G:C8	2.43	0.54
53:ZA:433:A:H5''	59:IB:22:HIS:HB3	1.89	0.54
53:ZA:1544:C:O2'	67:QB:80:GLN:OE1	2.24	0.54
58:HB:146:VAL:HG22	58:HB:152:ARG:HG2	1.90	0.54
13:N:116:LYS:HE3	17:R:169:THR:HB	1.90	0.54
20:U:82:ILE:HG23	20:U:121:VAL:HG13	1.90	0.54
23:X:26:ARG:NH1	23:X:75:ARG:O	2.41	0.54
30:WA:450:G:O6	30:WA:1304:C:N4	2.41	0.54
30:WA:2334:U:O2'	30:WA:2335:G:OP1	2.25	0.54
30:WA:3916:C:H2'	30:WA:3917:U:H6	1.72	0.54
50:RA:130:LYS:HD2	50:RA:133:LEU:HD12	1.88	0.54
51:v:24:VAL:O	51:v:32:LYS:NZ	2.40	0.54
53:ZA:1007:C:H2'	53:ZA:1008:A:C8	2.42	0.54
53:ZA:1810:U:H2'	53:ZA:1811:C:C6	2.43	0.54
58:HB:51:ILE:HD13	58:HB:179:LYS:HG2	1.90	0.54
63:MB:51:VAL:HB	63:MB:109:VAL:HB	1.89	0.54
14:O:69:ARG:NH1	30:WA:4985:C:N3	2.57	0.54
30:WA:1240:G:HO2'	30:WA:1241:G:H8	1.56	0.54
30:WA:2713:U:N3	84:b:255:TYR:O	2.39	0.54
30:WA:3714:U:HO2'	53:ZA:970:G:H1	1.56	0.54
30:WA:4709:C:H2'	30:WA:4710:A:H8	1.73	0.54
34:BA:44:LYS:NZ	34:BA:97:ILE:O	2.24	0.54
49:QA:132:PRO:HB3	49:QA:147:ILE:HD12	1.89	0.54
51:v:607:ARG:HD2	51:v:701:ARG:HD3	1.90	0.54
53:ZA:26:U:H2'	53:ZA:27:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:531:A:H3'	53:ZA:532:C:H5''	1.90	0.54
53:ZA:1338:G:O3'	71:UB:74:SER:OG	2.26	0.54
56:FB:125:SER:HB2	56:FB:136:ARG:HB3	1.88	0.54
60:JB:138:ARG:HH22	60:JB:153:SER:HA	1.73	0.54
2:B:19:ARG:NH2	30:WA:4628:OMG:OP1	2.41	0.53
16:Q:12:SER:OG	16:Q:17:CYS:O	2.22	0.53
30:WA:1277:G:H1'	33:AA:110:ALA:HA	1.89	0.53
30:WA:1508:A:H1'	30:WA:1509:G:C8	2.43	0.53
30:WA:2046:A:N7	30:WA:4439:C:O2'	2.40	0.53
53:ZA:1712:A:H2'	53:ZA:1713:C:C6	2.43	0.53
56:FB:19:LEU:HD23	56:FB:23:TRP:HE3	1.74	0.53
64:NB:54:LEU:O	64:NB:59:GLY:N	2.39	0.53
13:N:9:LEU:HD23	13:N:118:MET:HB2	1.89	0.53
16:Q:38:ARG:NH1	30:WA:2532:A:OP1	2.41	0.53
20:U:48:ARG:HB3	20:U:51:ARG:HE	1.73	0.53
21:V:8:PHE:HZ	21:V:49:ILE:HD12	1.72	0.53
24:Y:54:THR:H	24:Y:57:MET:HE2	1.72	0.53
30:WA:1630:OMG:N1	30:WA:3923:G:OP1	2.39	0.53
30:WA:2323:G:O6	36:DA:19:LYS:NZ	2.41	0.53
30:WA:4265:U:H2'	30:WA:4266:C:C6	2.43	0.53
51:v:261:TRP:CG	51:v:262:GLY:H	2.26	0.53
53:ZA:522:A:H5''	60:JB:145:PRO:HD2	1.90	0.53
53:ZA:1258:A:N1	53:ZA:1663:A:H1'	2.23	0.53
53:ZA:1486:A:H2'	53:ZA:1487:A:H8	1.73	0.53
53:ZA:1821:U:H2'	53:ZA:1822:A:C8	2.44	0.53
62:LB:89:ARG:NH1	62:LB:91:ASP:OD1	2.41	0.53
83:GC:7:LEU:HD21	83:GC:308:ARG:HD2	1.90	0.53
3:C:116:ASN:HB2	3:C:119:GLN:HG2	1.89	0.53
5:E:153:LEU:HD13	5:E:197:VAL:HG11	1.91	0.53
12:M:47:LYS:HD2	12:M:50:ARG:HD2	1.90	0.53
30:WA:2404:G:HO2'	30:WA:2827:G:HO2'	1.53	0.53
30:WA:2464:G:N2	30:WA:2467:C:OP2	2.38	0.53
30:WA:3921:G:H2'	30:WA:3922:A:C8	2.43	0.53
34:BA:61:GLU:OE2	34:BA:73:HIS:NE2	2.33	0.53
51:v:669:VAL:HG11	51:v:707:VAL:HG23	1.90	0.53
53:ZA:442:C:N4	53:ZA:449:A:H62	2.06	0.53
53:ZA:920:A:N7	53:ZA:1021:U:O4	2.41	0.53
53:ZA:1372:U:OP2	53:ZA:1385:G:N1	2.38	0.53
54:DB:172:VAL:HG22	54:DB:185:LYS:HG2	1.90	0.53
74:XB:54:LYS:HB3	74:XB:91:LEU:HD11	1.90	0.53
3:C:195:LYS:HE2	30:WA:2338:G:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:THR:HG23	10:J:63:ARG:HA	1.89	0.53
11:L:44:ARG:HB3	30:WA:939:A:H1'	1.90	0.53
12:M:176:LYS:NZ	30:WA:76:A:O3'	2.42	0.53
25:Z:26:ARG:NH1	30:WA:1660:C:OP2	2.41	0.53
26:K:49:ARG:NH2	39:GA:117:ARG:O	2.35	0.53
30:WA:67:C:OP2	30:WA:312:G:N2	2.41	0.53
30:WA:163:A:H2'	30:WA:164:G:H8	1.74	0.53
30:WA:426:A:H2'	30:WA:427:A:H8	1.72	0.53
30:WA:913:U:H2'	30:WA:914:G:O4'	2.08	0.53
30:WA:4528:A2M:H5'	30:WA:4529:G:H5'	1.90	0.53
48:PA:90:LEU:HG	48:PA:111:ILE:HG23	1.91	0.53
53:ZA:483:C:OP1	74:XB:76:LYS:NZ	2.42	0.53
53:ZA:621:C:H5'	74:XB:107:ARG:HH12	1.74	0.53
53:ZA:1615:U:O4	66:PB:40:ARG:NH1	2.42	0.53
61:KB:27:VAL:HG13	61:KB:43:LEU:HD13	1.90	0.53
71:UB:20:ILE:HG12	71:UB:98:VAL:HG21	1.89	0.53
74:XB:90:CYS:HA	74:XB:93:PHE:HD2	1.73	0.53
1:A:233:ARG:HB2	30:WA:4189:G:H5'	1.91	0.53
3:C:334:THR:HG22	3:C:337:ARG:HH12	1.73	0.53
23:X:103:LYS:NZ	30:WA:200:U:O4	2.34	0.53
30:WA:257:C:H2'	30:WA:258:G:H8	1.74	0.53
30:WA:743:C:N4	30:WA:744:G:O6	2.42	0.53
30:WA:911:G:H2'	30:WA:912:G:H8	1.74	0.53
30:WA:1807:A:H5''	30:WA:1808:G:H5'	1.89	0.53
30:WA:3702:U:H5''	30:WA:3703:G:H5'	1.90	0.53
30:WA:4996:U:H2'	30:WA:4997:G:C8	2.43	0.53
53:ZA:106:C:H2'	53:ZA:107:A:H8	1.74	0.53
53:ZA:934:G:N2	64:NB:110:ASP:OD2	2.42	0.53
53:ZA:1588:A:H2'	53:ZA:1589:A:H8	1.72	0.53
2:B:222:VAL:O	2:B:343:ARG:NH1	2.42	0.53
7:G:194:ASN:ND2	30:WA:151:G:N7	2.56	0.53
23:X:47:MET:HE3	23:X:48:PRO:HD2	1.89	0.53
24:Y:76:ASN:OD1	24:Y:77:TYR:N	2.41	0.53
30:WA:1210:C:H2'	30:WA:1211:G:C8	2.43	0.53
30:WA:5060:G:H2'	30:WA:5061:A:C8	2.44	0.53
51:v:664:ASP:HA	51:v:704:VAL:HG22	1.90	0.53
53:ZA:643:A:H4'	53:ZA:644:G:H5'	1.91	0.53
53:ZA:1373:C:O2'	68:RB:10:LYS:NZ	2.36	0.53
83:GC:238:ALA:H	83:GC:251:ALA:HB3	1.74	0.53
4:D:43:LYS:HE2	30:WA:1822:U:H4'	1.91	0.53
4:D:50:ARG:NH2	31:XA:6:C:O2'	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:103:ASP:HB2	22:W:40:ILE:HD11	1.91	0.53
30:WA:205:C:H42	30:WA:209:U:H5	1.55	0.53
30:WA:441:G:H2'	30:WA:442:G:H8	1.74	0.53
30:WA:961:A:N6	30:WA:1289:G:H1'	2.24	0.53
30:WA:1865:B8H:C5	30:WA:1865:B8H:C2	2.85	0.53
32:YA:12:G:C2	32:YA:13:G:C8	2.97	0.53
45:MA:12:ARG:HG2	45:MA:15:ARG:HH12	1.73	0.53
53:ZA:925:G:N2	53:ZA:1017:U:O2	2.27	0.53
53:ZA:1705:C:H2'	53:ZA:1706:G:C8	2.43	0.53
3:C:28:PHE:HA	3:C:129:ALA:HA	1.91	0.53
13:N:8:VAL:HG12	13:N:117:ARG:HG3	1.91	0.53
30:WA:1345:U:H2'	30:WA:1346:C:C6	2.43	0.53
30:WA:1674:A:H4'	30:WA:1690:G:H21	1.74	0.53
30:WA:4959:G:H2'	30:WA:4960:A:C8	2.43	0.53
51:v:425:LEU:HB3	51:v:447:ILE:HD11	1.91	0.53
53:ZA:107:A:H2'	53:ZA:108:G:H8	1.73	0.53
53:ZA:1220:A:N3	53:ZA:1677:U:O2'	2.33	0.53
77:AC:94:ASP:OD1	77:AC:94:ASP:N	2.40	0.53
84:b:260:LYS:HG3	84:b:263:ARG:HH21	1.74	0.53
30:WA:968:G:HO2'	30:WA:969:A:H8	1.57	0.53
30:WA:1999:C:H2'	30:WA:2000:G:C8	2.44	0.53
53:ZA:91:A:OP1	53:ZA:446:G:N2	2.42	0.53
53:ZA:581:U:H4'	75:YB:66:GLY:HA3	1.91	0.53
54:DB:193:ASP:OD2	54:DB:196:GLY:N	2.33	0.53
73:WB:49:GLU:O	73:WB:64:ASN:ND2	2.42	0.53
76:ZB:57:LYS:HD3	76:ZB:77:LEU:HD22	1.91	0.53
2:B:373:LYS:HD2	30:WA:4632:U:H4'	1.90	0.53
15:P:41:SER:OG	15:P:44:ASN:OD1	2.26	0.53
21:V:80:ARG:NH2	53:ZA:167:G:O2'	2.43	0.53
30:WA:22:G:OP1	41:IA:44:LYS:N	2.38	0.53
30:WA:1877:G:O2'	30:WA:4224:A:N3	2.37	0.53
30:WA:4139:C:H2'	30:WA:4140:G:H8	1.74	0.53
30:WA:4497:U:H5''	30:WA:4498:U:H5'	1.90	0.53
30:WA:4588:C:O2'	30:WA:4723:G:N2	2.41	0.53
31:XA:110:G:H2'	31:XA:111:C:C6	2.43	0.53
51:v:653:GLY:O	51:v:684:GLN:NE2	2.42	0.53
53:ZA:381:C:H5''	59:IB:54:LYS:HE3	1.90	0.53
53:ZA:434:G:H2'	53:ZA:435:A:C8	2.44	0.53
53:ZA:1101:U:H2'	53:ZA:1102:G:C8	2.43	0.53
53:ZA:1263:U:H3'	53:ZA:1264:C:H2'	1.90	0.53
53:ZA:1310:U:H4'	82:FC:143:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:OB:105:THR:HG22	65:OB:107:THR:H	1.73	0.53
76:ZB:96:LEU:O	76:ZB:112:ASN:ND2	2.40	0.53
3:C:69:THR:OG1	30:WA:4395:A:OP1	2.27	0.52
6:F:201:LYS:NZ	30:WA:1845:G:OP2	2.42	0.52
28:BB:28:LYS:HB3	28:BB:48:LEU:HD22	1.91	0.52
28:BB:134:LEU:HD12	28:BB:219:LYS:HB2	1.91	0.52
30:WA:930:G:H2'	30:WA:931:G:H8	1.74	0.52
30:WA:3853:U:H2'	30:WA:3854:A:C8	2.45	0.52
49:QA:114:GLY:HA2	49:QA:166:LYS:HG3	1.91	0.52
52:w:194:ASP:O	53:ZA:1331:C:N4	2.39	0.52
53:ZA:455:A:O2'	53:ZA:1735:A:N3	2.40	0.52
53:ZA:532:C:H2'	53:ZA:533:A:C8	2.43	0.52
53:ZA:1864:U:H3'	77:AC:5:ARG:HH21	1.73	0.52
84:b:202:ILE:HD12	84:b:205:PRO:HB3	1.90	0.52
5:E:181:PRO:HG2	5:E:184:LEU:HD12	1.90	0.52
10:J:95:ARG:HG2	10:J:175:LEU:HD11	1.90	0.52
16:Q:10:LEU:HB3	16:Q:41:ILE:HD13	1.91	0.52
30:WA:1471:G:OP2	33:AA:44:ARG:NH2	2.41	0.52
30:WA:2748:A:H2'	30:WA:2749:A:C8	2.44	0.52
30:WA:3624:G:H22	30:WA:3629:A:H1'	1.75	0.52
30:WA:3658:A:N1	30:WA:3697:A:H4'	2.24	0.52
30:WA:3816:G:O2'	30:WA:3819:U:OP2	2.26	0.52
68:RB:114:LEU:HB2	68:RB:117:LEU:HG	1.91	0.52
27:AB:136:GLU:OE1	53:ZA:1378:A:N6	2.42	0.52
30:WA:258:G:H2'	30:WA:259:C:C6	2.45	0.52
30:WA:760:G:H2'	30:WA:761:G:O4'	2.10	0.52
30:WA:1978:G:OP2	30:WA:1979:U:H3'	2.09	0.52
30:WA:2519:G:O2'	30:WA:2748:A:N6	2.41	0.52
30:WA:4476:U:H2'	30:WA:4477:B8W:C8	2.39	0.52
51:v:820:LEU:HD22	51:v:831:PRO:HG3	1.91	0.52
53:ZA:399:C:N3	62:LB:104:LYS:NZ	2.57	0.52
53:ZA:453:C:O2'	57:GB:92:ARG:O	2.24	0.52
53:ZA:1616:U:O2'	53:ZA:1661:A:N3	2.34	0.52
55:EB:31:PRO:HG3	55:EB:43:PRO:HG3	1.92	0.52
70:TB:132:ASP:OD1	70:TB:133:ARG:N	2.42	0.52
84:b:322:THR:HB	84:b:333:ILE:HB	1.91	0.52
2:B:11:HIS:NE2	30:WA:4463:C:OP1	2.42	0.52
7:G:104:LEU:HD21	30:WA:4091:G:C4	2.44	0.52
7:G:139:VAL:HG23	7:G:236:ILE:HG22	1.90	0.52
30:WA:2418:U:H2'	30:WA:2419:G:H8	1.75	0.52
30:WA:3646:U:H5	30:WA:3651:A:C2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4666:G:N2	30:WA:5009:C:O3'	2.41	0.52
32:YA:47:C:H1'	32:YA:61:A:H2'	1.91	0.52
51:v:851:LEU:H	51:v:851:LEU:HD23	1.75	0.52
53:ZA:5:U:H2'	53:ZA:6:G:H8	1.75	0.52
53:ZA:85:A:O3'	75:YB:118:ARG:NH2	2.42	0.52
53:ZA:1424:G:H2'	53:ZA:1425:G:H8	1.74	0.52
84:b:181:PRO:HG2	84:b:204:ASN:HB2	1.91	0.52
10:J:63:ARG:HH21	46:NA:103:VAL:HG21	1.74	0.52
27:AB:66:VAL:HG21	27:AB:185:MET:HB2	1.91	0.52
30:WA:1543:U:H2'	30:WA:1544:G:H8	1.74	0.52
30:WA:3767:B8H:C5	30:WA:3767:B8H:C2	2.86	0.52
30:WA:3915:C:H2'	30:WA:3916:C:H6	1.74	0.52
37:EA:16:ARG:HA	37:EA:21:GLN:HA	1.91	0.52
50:RA:117:ARG:HH12	50:RA:125:LEU:HA	1.74	0.52
51:v:159:LYS:HG2	89:v:900:GDP:C6	2.43	0.52
53:ZA:588:G:OP2	53:ZA:588:G:N2	2.37	0.52
64:NB:56:ASP:OD2	78:BC:52:THR:OG1	2.28	0.52
70:TB:65:TYR:HB2	70:TB:123:LEU:HD22	1.90	0.52
82:FC:133:ALA:N	82:FC:140:TYR:O	2.42	0.52
3:C:159:GLU:HA	3:C:217:ILE:HB	1.92	0.52
4:D:41:LYS:HD2	18:S:93:ILE:HG21	1.91	0.52
17:R:46:TYR:OH	31:XA:94:C:OP1	2.27	0.52
28:BB:189:ILE:HB	28:BB:190:PRO:HD3	1.92	0.52
30:WA:1809:A:H4'	30:WA:1810:A:O5'	2.10	0.52
30:WA:4953:C:H2'	30:WA:4954:G:N2	2.24	0.52
53:ZA:91:A:H5''	53:ZA:92:A:H5''	1.91	0.52
53:ZA:1217:A:H2'	53:ZA:1218:C:C6	2.44	0.52
53:ZA:1253:A:OP2	53:ZA:1526:G:N2	2.42	0.52
53:ZA:1662:U:O4	53:ZA:1663:A:N6	2.38	0.52
57:GB:102:VAL:HG13	57:GB:106:LEU:HD12	1.92	0.52
59:IB:31:ARG:HD2	59:IB:56:ARG:HH21	1.74	0.52
67:QB:102:GLU:O	67:QB:106:LYS:N	2.40	0.52
73:WB:8:ALA:HA	73:WB:74:VAL:HG11	1.92	0.52
75:YB:78:SER:OG	75:YB:80:ASP:OD1	2.24	0.52
84:b:79:SER:OG	84:b:89:PHE:N	2.41	0.52
9:I:7:ARG:NH2	30:WA:4410:G:OP2	2.43	0.52
9:I:118:ALA:O	30:WA:1869:G:O2'	2.26	0.52
17:R:170:LYS:NZ	30:WA:4879:A:O2'	2.31	0.52
23:X:59:ARG:HD2	30:WA:209:U:H5'	1.91	0.52
28:BB:228:LEU:HD12	28:BB:231:LEU:HD11	1.92	0.52
30:WA:406:C:O2'	30:WA:407:A:OP1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:418:A:H2'	30:WA:419:A:C8	2.45	0.52
30:WA:1829:G:H2'	30:WA:1830:A:H8	1.75	0.52
30:WA:1974:G:OP2	49:QA:112:ARG:NH1	2.42	0.52
30:WA:2366:G:O2'	30:WA:3864:G:O6	2.18	0.52
30:WA:4182:C:H2'	30:WA:4183:A:H8	1.74	0.52
52:w:286:TRP:HB2	61:KB:89:ILE:HG21	1.91	0.52
53:ZA:1036:A:H4'	53:ZA:1855:G:N2	2.24	0.52
63:MB:66:GLU:O	63:MB:70:ALA:N	2.42	0.52
12:M:125:SER:HB2	30:WA:3942:C:H1'	1.92	0.52
15:P:85:THR:HG23	15:P:104:ARG:HG3	1.91	0.52
20:U:92:ASP:OD1	20:U:92:ASP:N	2.41	0.52
28:BB:137:LEU:HD22	28:BB:215:VAL:HG22	1.92	0.52
30:WA:286:U:H2'	30:WA:287:U:C6	2.45	0.52
30:WA:491:C:H2'	30:WA:492:G:C8	2.45	0.52
30:WA:1388:G:H2'	30:WA:1389:G:H8	1.74	0.52
30:WA:2300:C:H2'	30:WA:2301:G:C8	2.45	0.52
30:WA:4459:G:H1	30:WA:4531:U:H3	1.56	0.52
51:v:7:ASP:HA	51:v:10:ARG:HE	1.74	0.52
53:ZA:535:G:O6	53:ZA:536:A:N6	2.43	0.52
53:ZA:1625:U:H2'	53:ZA:1626:C:H6	1.75	0.52
53:ZA:1828:C:H2'	53:ZA:1829:G:C8	2.45	0.52
54:DB:167:TYR:O	54:DB:190:LEU:N	2.34	0.52
61:KB:15:LEU:HD13	61:KB:21:MET:HB2	1.91	0.52
74:XB:71:ARG:HA	74:XB:82:THR:HA	1.91	0.52
76:ZB:51:ASP:H	76:ZB:54:THR:HB	1.74	0.52
83:GC:194:TYR:CE1	83:GC:212:LYS:HB2	2.45	0.52
4:D:45:ASN:O	4:D:45:ASN:ND2	2.42	0.52
13:N:18:ARG:NH2	30:WA:2058:C:O3'	2.40	0.52
25:Z:132:ARG:NH2	30:WA:1473:C:OP1	2.41	0.52
30:WA:49:U:H2'	30:WA:50:C:C6	2.44	0.52
30:WA:491:C:H2'	30:WA:492:G:H8	1.75	0.52
30:WA:1433:A:H4'	30:WA:1699:C:H5'	1.91	0.52
30:WA:2405:G:H21	38:FA:6:THR:HG22	1.75	0.52
30:WA:2814:G:O2'	30:WA:4649:G:OP1	2.25	0.52
30:WA:3689:G:H2'	30:WA:3690:C:C6	2.45	0.52
30:WA:4728:A:H2'	30:WA:4729:A:C8	2.44	0.52
35:CA:19:GLU:HG3	35:CA:102:LEU:HD21	1.91	0.52
37:EA:17:GLY:N	37:EA:20:ASN:O	2.36	0.52
53:ZA:44:U:O2	53:ZA:481:C:O2'	2.23	0.52
53:ZA:350:C:O2'	53:ZA:383:G:N1	2.43	0.52
1:A:53:GLY:O	1:A:192:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4292:G:H2'	30:WA:4293:C:C6	2.45	0.52
31:XA:75:G:N2	31:XA:100:A:OP2	2.35	0.52
32:YA:108:A:N6	32:YA:112:G:O6	2.43	0.52
36:DA:79:VAL:HG13	36:DA:84:GLU:HB2	1.91	0.52
50:RA:109:ILE:HD11	50:RA:143:VAL:HG21	1.93	0.52
53:ZA:1239:U:N3	53:ZA:1242:U:OP2	2.40	0.52
53:ZA:1310:U:C2	53:ZA:1311:C:H5	2.28	0.52
53:ZA:1396:A:H2	53:ZA:1449:G:H1	1.58	0.52
53:ZA:1593:C:O2	70:TB:12:GLN:NE2	2.43	0.52
55:EB:46:ILE:HG22	55:EB:51:ARG:HH12	1.74	0.52
61:KB:35:LEU:HD21	61:KB:40:VAL:HG21	1.92	0.52
78:BC:42:LYS:HD3	78:BC:42:LYS:H	1.75	0.52
1:A:178:PRO:HD2	47:OA:26:VAL:HG22	1.91	0.51
5:E:142:LYS:NZ	30:WA:713:C:OP1	2.42	0.51
6:F:105:ARG:NH2	15:P:4:ASP:OD1	2.43	0.51
12:M:116:LEU:HD22	12:M:135:ILE:HD11	1.91	0.51
30:WA:153:G:H2'	30:WA:154:G:H8	1.74	0.51
30:WA:711:G:H2'	30:WA:712:A:C8	2.44	0.51
30:WA:1610:7MG:H2'	30:WA:1611:U:O4'	2.11	0.51
30:WA:2003:A:H2'	30:WA:2004:A:C4	2.45	0.51
30:WA:3860:C:H2'	30:WA:3861:A:H8	1.75	0.51
32:YA:67:U:H2'	32:YA:68:G:C8	2.45	0.51
50:RA:15:LEU:N	50:RA:60:VAL:O	2.38	0.51
50:RA:117:ARG:NH2	50:RA:128:THR:OG1	2.43	0.51
53:ZA:1280:G:H2'	53:ZA:1281:G:H8	1.75	0.51
53:ZA:1481:G:O2'	53:ZA:1482:C:OP1	2.25	0.51
70:TB:126:GLN:HG2	70:TB:129:ARG:HE	1.76	0.51
1:A:208:GLU:HG2	30:WA:1634:G:H1	1.75	0.51
11:L:108:ASP:HB3	13:N:199:HIS:CD2	2.46	0.51
28:BB:176:VAL:HG23	28:BB:184:VAL:HG11	1.91	0.51
30:WA:1081:G:H22	30:WA:1241:G:N2	2.08	0.51
30:WA:4237:U:C2	46:NA:5:PRO:HD3	2.45	0.51
30:WA:4383:A:O2'	30:WA:4384:A:H2'	2.10	0.51
30:WA:4607:A:OP1	51:v:162:ARG:NH2	2.44	0.51
30:WA:4928:U:H2'	30:WA:4929:C:C6	2.44	0.51
53:ZA:864:A:H2'	53:ZA:865:A:H8	1.75	0.51
53:ZA:948:C:H2'	53:ZA:949:G:C8	2.43	0.51
78:BC:36:LYS:HB3	78:BC:43:ILE:HG12	1.91	0.51
4:D:193:GLU:OE2	4:D:197:LYS:NZ	2.43	0.51
12:M:44:ARG:NH1	30:WA:280:G:OP2	2.39	0.51
13:N:168:TYR:CE2	13:N:172:LYS:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:5:LYS:HD2	30:WA:4307:U:H4'	1.93	0.51
30:WA:1323:U:H2'	30:WA:1324:C:C6	2.46	0.51
30:WA:2103:G:H2'	30:WA:2104:C:C6	2.46	0.51
30:WA:2314:G:O2'	32:YA:18:U:O2	2.28	0.51
30:WA:2335:G:H2'	30:WA:2336:G:C4	2.44	0.51
30:WA:2420:U:H2'	30:WA:2421:G:C8	2.45	0.51
30:WA:2740:G:H2'	30:WA:2741:G:H8	1.74	0.51
30:WA:2816:G:N1	30:WA:2819:C:OP2	2.39	0.51
30:WA:3827:U:H3'	30:WA:3828:G:C8	2.46	0.51
30:WA:4179:U:H2'	30:WA:4180:G:H8	1.74	0.51
30:WA:4359:U:H5'	30:WA:4360:E6G:OP1	2.10	0.51
30:WA:4508:A:H2'	30:WA:4509:C:C6	2.44	0.51
53:ZA:433:A:H2'	53:ZA:434:G:C8	2.46	0.51
53:ZA:448:A:H62	59:IB:29:LEU:HD13	1.75	0.51
53:ZA:449:A:O2'	53:ZA:450:C:H4'	2.09	0.51
53:ZA:1098:C:H2'	53:ZA:1099:G:C8	2.46	0.51
53:ZA:1415:C:O2'	70:TB:132:ASP:OD2	2.23	0.51
78:BC:80:ARG:NH1	78:BC:81:ARG:O	2.43	0.51
83:GC:107:ASP:N	83:GC:107:ASP:OD1	2.42	0.51
84:b:57:MET:HA	84:b:60:THR:HG22	1.92	0.51
2:B:36:ASP:HB2	2:B:39:LYS:HE2	1.92	0.51
16:Q:78:ILE:HG22	16:Q:81:ARG:HH21	1.75	0.51
30:WA:178:C:H2'	30:WA:179:G:H8	1.74	0.51
30:WA:257:C:H2'	30:WA:258:G:C8	2.45	0.51
30:WA:275:C:H2'	30:WA:276:C:C6	2.45	0.51
30:WA:1081:G:H22	30:WA:1241:G:H22	1.59	0.51
30:WA:4490:C:O2'	44:LA:88:LYS:NZ	2.40	0.51
53:ZA:17:C:H2'	53:ZA:18:C:H6	1.75	0.51
53:ZA:319:C:H2'	53:ZA:320:G:H8	1.74	0.51
53:ZA:1018:U:H5'	64:NB:71:ILE:HD12	1.93	0.51
53:ZA:1839:U:H2'	53:ZA:1840:U:H6	1.75	0.51
55:EB:44:LEU:HD13	55:EB:72:ILE:HD11	1.92	0.51
56:FB:40:ALA:HB1	56:FB:45:TYR:CD1	2.45	0.51
57:GB:4:ASN:O	57:GB:111:LEU:N	2.37	0.51
75:YB:57:VAL:HG23	75:YB:73:GLY:HA3	1.93	0.51
7:G:207:LEU:HB3	7:G:257:PHE:HB2	1.92	0.51
8:H:90:TYR:HE2	8:H:155:SER:HB3	1.75	0.51
14:O:10:ASN:N	14:O:10:ASN:OD1	2.43	0.51
16:Q:101:ILE:HD13	30:WA:2902:G:H4'	1.92	0.51
17:R:63:TYR:OH	30:WA:730:2MG:OP1	2.22	0.51
26:K:74:ARG:NH2	30:WA:109:G:OP2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BB:40:ASN:OD1	28:BB:75:GLN:NE2	2.43	0.51
30:WA:1674:A:N3	30:WA:1857:U:O2'	2.35	0.51
30:WA:2764:G:H2'	30:WA:2765:G:C4	2.46	0.51
30:WA:3722:A:H2'	30:WA:3723:A2M:C8	2.37	0.51
53:ZA:1236:G:H21	53:ZA:1522:A:H62	1.57	0.51
83:GC:218:LEU:HB3	83:GC:227:LEU:HD12	1.92	0.51
8:H:111:LEU:HD11	8:H:125:ARG:HB2	1.93	0.51
16:Q:96:MET:HG2	16:Q:100:ARG:HE	1.75	0.51
24:Y:25:ILE:HA	24:Y:43:VAL:HG12	1.93	0.51
25:Z:34:ASN:HB2	30:WA:94:A:H5''	1.91	0.51
30:WA:2085:U:H2'	30:WA:2086:C:C6	2.46	0.51
30:WA:2263:C:H5''	30:WA:2264:G:H8	1.75	0.51
30:WA:4667:C:O2'	30:WA:5009:C:OP1	2.29	0.51
31:XA:38:U:N3	31:XA:41:G:OP2	2.33	0.51
37:EA:88:PHE:CD1	37:EA:92:LEU:HD11	2.45	0.51
53:ZA:77:A:H2	57:GB:175:LYS:HG3	1.76	0.51
53:ZA:107:A:H2'	53:ZA:108:G:C8	2.45	0.51
53:ZA:1515:G:H2'	53:ZA:1516:G:H8	1.76	0.51
58:HB:50:GLU:HB3	58:HB:60:ILE:HG22	1.93	0.51
76:ZB:58:LEU:HD12	76:ZB:62:VAL:HG21	1.93	0.51
30:WA:1505:A:H5''	30:WA:1506:C:H5'	1.92	0.51
30:WA:1983:C:H2'	30:WA:1984:A:C8	2.45	0.51
30:WA:3878:G:H2'	30:WA:3879:G:C8	2.46	0.51
30:WA:4397:G:H2'	30:WA:4452:5MC:HM51	1.93	0.51
33:AA:102:PRO:HA	33:AA:109:ARG:HH12	1.75	0.51
49:QA:77:LYS:HD2	49:QA:198:ILE:HG12	1.93	0.51
53:ZA:925:G:H2'	53:ZA:926:A:H8	1.76	0.51
53:ZA:1653:U:H2'	53:ZA:1654:G:C8	2.46	0.51
70:TB:6:VAL:O	70:TB:11:GLN:NE2	2.42	0.51
72:VB:36:VAL:N	72:VB:51:LYS:O	2.35	0.51
84:b:33:ARG:HG2	84:b:337:PRO:HG3	1.92	0.51
10:J:27:GLY:HA2	10:J:68:ILE:HB	1.91	0.51
12:M:138:PHE:HA	12:M:143:ARG:HH21	1.75	0.51
12:M:145:ASN:HB3	12:M:148:THR:HG22	1.93	0.51
13:N:12:ARG:HB2	13:N:37:ARG:HD2	1.92	0.51
15:P:172:ARG:HD2	25:Z:57:GLY:HA3	1.93	0.51
22:W:135:LYS:NZ	30:WA:2441:U:OP2	2.44	0.51
27:AB:33:GLN:HB3	27:AB:154:LEU:HD12	1.91	0.51
28:BB:150:ILE:HG13	53:ZA:1124:C:H5''	1.93	0.51
30:WA:139:G:H2'	30:WA:140:G:H8	1.76	0.51
30:WA:158:A:N1	30:WA:276:C:O2'	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:674:C:H2'	30:WA:675:G:H8	1.75	0.51
30:WA:2700:A:OP2	42:JA:28:ASN:ND2	2.44	0.51
30:WA:4323:C:O2'	46:NA:18:HIS:ND1	2.30	0.51
30:WA:4583:G:H2'	30:WA:4584:U:H6	1.75	0.51
51:v:766:LYS:HB3	51:v:792:GLU:HB3	1.93	0.51
53:ZA:17:C:H4'	53:ZA:1166:G:C8	2.46	0.51
53:ZA:1474:A:H2'	53:ZA:1475:G:N3	2.26	0.51
53:ZA:1583:C:OP2	53:ZA:1584:G:O2'	2.28	0.51
83:GC:8:ARG:HE	83:GC:311:GLN:HB2	1.76	0.51
83:GC:197:THR:HG21	83:GC:238:ALA:HA	1.93	0.51
4:D:152:ARG:O	4:D:157:ASN:ND2	2.44	0.51
12:M:96:ARG:NH1	12:M:104:GLU:OE2	2.44	0.51
18:S:109:VAL:HA	18:S:112:ASN:HD21	1.75	0.51
26:K:32:LYS:NZ	30:WA:1367:G:OP2	2.42	0.51
27:AB:94:THR:OG1	27:AB:186:ARG:NH2	2.44	0.51
30:WA:268:G:H2'	30:WA:269:G:H8	1.76	0.51
30:WA:1499:U:H2'	30:WA:1500:G:C8	2.45	0.51
53:ZA:75:G:O6	57:GB:171:THR:OG1	2.26	0.51
53:ZA:84:A:H4'	75:YB:120:THR:HA	1.93	0.51
53:ZA:92:A:O4'	55:EB:3:ARG:NH1	2.44	0.51
53:ZA:1189:A:H2'	53:ZA:1190:A:H8	1.76	0.51
53:ZA:1610:G:OP1	69:SB:121:ARG:NH2	2.34	0.51
64:NB:4:MET:HE3	64:NB:121:ARG:HG2	1.93	0.51
30:WA:1217:G:O2'	30:WA:1218:G:OP1	2.28	0.51
30:WA:3915:C:H2'	30:WA:3916:C:C6	2.45	0.51
30:WA:4734:A:OP2	30:WA:5073:G:N1	2.35	0.51
42:JA:37:ARG:HH21	42:JA:42:LEU:HB2	1.76	0.51
51:v:373:TYR:CZ	51:v:492:HIS:HB2	2.46	0.51
53:ZA:14:C:H2'	53:ZA:15:U:C6	2.46	0.51
53:ZA:1588:A:H2'	53:ZA:1589:A:C8	2.46	0.51
54:DB:192:TRP:NE1	54:DB:201:LYS:O	2.43	0.51
59:IB:8:TRP:HA	59:IB:18:ARG:HD2	1.92	0.51
66:PB:121:ILE:HG22	69:SB:120:HIS:HD2	1.75	0.51
72:VB:20:SER:OG	72:VB:22:ARG:NE	2.41	0.51
1:A:243:THR:HG23	30:WA:3751:A:H5'	1.92	0.50
30:WA:423:G:H2'	30:WA:424:U:C6	2.46	0.50
30:WA:1203:C:H2'	30:WA:1204:G:C8	2.46	0.50
30:WA:2409:A:H1'	41:IA:12:ARG:HH11	1.75	0.50
30:WA:4385:A:OP1	46:NA:58:LYS:NZ	2.43	0.50
35:CA:36:VAL:HG11	35:CA:44:ARG:HD2	1.92	0.50
46:NA:75:PRO:HA	46:NA:78:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PA:49:VAL:HG11	48:PA:97:ILE:HD11	1.92	0.50
53:ZA:1017:U:OP1	64:NB:62:GLN:NE2	2.38	0.50
53:ZA:1309:C:H2'	53:ZA:1310:U:O4'	2.10	0.50
53:ZA:1563:G:OP1	70:TB:121:ARG:NH1	2.43	0.50
53:ZA:1613:G:OP1	69:SB:88:LYS:NZ	2.40	0.50
53:ZA:1856:C:H2'	53:ZA:1857:G:C8	2.47	0.50
69:SB:15:VAL:O	69:SB:18:THR:OG1	2.27	0.50
6:F:72:ARG:NH2	30:WA:728:C:OP1	2.41	0.50
25:Z:21:ARG:NH2	30:WA:1323:U:OP1	2.44	0.50
30:WA:975:G:H2'	30:WA:976:C:O4'	2.12	0.50
30:WA:4591:G:O6	30:WA:4722:A:N6	2.44	0.50
30:WA:4902:G:H1'	30:WA:4932:G:H1	1.76	0.50
51:v:300:VAL:HG11	51:v:340:MET:HE3	1.93	0.50
53:ZA:928:G:H2'	53:ZA:929:G:C8	2.47	0.50
79:CC:18:LEU:HB2	79:CC:29:GLN:HG3	1.93	0.50
1:A:28:ARG:HB3	1:A:123:ARG:HB3	1.93	0.50
1:A:177:LYS:O	30:WA:2744:C:N4	2.36	0.50
3:C:37:VAL:HG13	3:C:237:ILE:HD11	1.93	0.50
5:E:156:LEU:HD11	5:E:198:ILE:HG13	1.92	0.50
5:E:188:PRO:HG3	30:WA:4943:A:H1'	1.93	0.50
17:R:113:MET:HG3	17:R:119:ALA:HB3	1.94	0.50
25:Z:105:ARG:HD2	26:K:161:PHE:HB3	1.93	0.50
29:CB:125:LYS:NZ	53:ZA:1356:G:O3'	2.44	0.50
30:WA:126:C:H2'	30:WA:127:G:H8	1.76	0.50
30:WA:260:C:H2'	30:WA:261:G:H8	1.76	0.50
30:WA:712:A:H2'	30:WA:713:C:C6	2.46	0.50
30:WA:2064:C:H2'	30:WA:2065:G:H8	1.77	0.50
30:WA:4158:C:H2'	30:WA:4159:G:H8	1.76	0.50
30:WA:4583:G:H2'	30:WA:4584:U:C6	2.46	0.50
30:WA:4641:PSU:O2	35:CA:79:ASN:ND2	2.38	0.50
30:WA:4766:G:H2'	30:WA:4767:A:C8	2.43	0.50
30:WA:4953:C:H3'	30:WA:4954:G:H5''	1.93	0.50
53:ZA:1115:U:O2	53:ZA:1117:C:N4	2.44	0.50
53:ZA:1858:G:N7	65:OB:146:ARG:NH1	2.59	0.50
77:AC:22:ARG:NH2	77:AC:27:ALA:O	2.40	0.50
2:B:15:GLY:O	30:WA:4592:G:N2	2.37	0.50
3:C:170:LEU:HD23	3:C:221:PHE:HZ	1.75	0.50
6:F:189:LEU:HD21	6:F:207:LEU:HD21	1.92	0.50
22:W:63:LYS:NZ	32:YA:135:C:OP1	2.40	0.50
30:WA:260:C:H2'	30:WA:261:G:C8	2.46	0.50
30:WA:498:G:O2'	30:WA:499:C:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2290:A:H2'	30:WA:2291:G:H8	1.76	0.50
30:WA:3814:G:OP2	30:WA:3814:G:N2	2.30	0.50
30:WA:4306:U:OP2	30:WA:4308:C:N4	2.44	0.50
30:WA:4464:U:H2'	30:WA:4465:U:C6	2.46	0.50
53:ZA:145:G:OP2	57:GB:178:ARG:NH2	2.44	0.50
53:ZA:1481:G:HO2'	53:ZA:1482:C:P	2.35	0.50
53:ZA:1779:G:H2'	53:ZA:1780:G:C5	2.47	0.50
59:IB:25:ARG:HB2	59:IB:28:GLU:HG2	1.93	0.50
63:MB:17:ALA:HB1	63:MB:120:ALA:HB1	1.92	0.50
68:RB:69:ILE:HG22	68:RB:71:ILE:HG13	1.93	0.50
7:G:156:ARG:NH2	7:G:245:ARG:O	2.45	0.50
9:I:99:ILE:HG22	9:I:123:GLN:HB2	1.93	0.50
30:WA:927:C:H5'	30:WA:928:C:H5''	1.93	0.50
30:WA:1947:A:N3	30:WA:4437:C:O2'	2.38	0.50
30:WA:4301:B8H:C5	30:WA:4301:B8H:C2	2.85	0.50
30:WA:4509:C:H2'	30:WA:4510:C:C6	2.47	0.50
30:WA:4653:A:H2'	30:WA:4654:G:H8	1.77	0.50
48:PA:10:VAL:HG13	48:PA:14:SER:HB3	1.92	0.50
50:RA:117:ARG:HH12	50:RA:125:LEU:HD23	1.76	0.50
51:v:18:ASN:ND2	51:v:94:ASP:O	2.45	0.50
53:ZA:526:A:H5'	81:EC:104:ARG:HH22	1.77	0.50
53:ZA:1025:U:H2'	53:ZA:1026:C:O4'	2.12	0.50
53:ZA:1275:G:N2	53:ZA:1506:A:OP2	2.42	0.50
54:DB:70:THR:HG22	54:DB:86:LEU:HD13	1.92	0.50
59:IB:6:ASP:O	59:IB:9:HIS:ND1	2.44	0.50
68:RB:28:PHE:HA	68:RB:55:THR:HG21	1.94	0.50
84:b:189:GLN:HG3	84:b:224:TYR:HE1	1.75	0.50
84:b:268:GLU:HG2	84:b:271:ARG:HH22	1.76	0.50
1:A:72:ARG:HH12	30:WA:2509:C:H42	1.60	0.50
15:P:12:LYS:HG2	30:WA:2087:G:H5''	1.93	0.50
22:W:110:LYS:NZ	22:W:121:VAL:O	2.44	0.50
30:WA:275:C:OP1	40:HA:35:LYS:NZ	2.45	0.50
30:WA:2084:G:H2'	30:WA:2085:U:H6	1.74	0.50
30:WA:3695:U:H2'	30:WA:3696:G:O4'	2.11	0.50
30:WA:3758:G:O6	30:WA:3781:G:N2	2.45	0.50
42:JA:17:ARG:NH2	42:JA:38:CYS:SG	2.85	0.50
49:QA:142:GLY:HA2	51:v:180:ARG:HH21	1.77	0.50
51:v:11:ALA:O	51:v:15:LYS:NZ	2.34	0.50
53:ZA:563:G:OP1	60:JB:133:ARG:NH2	2.40	0.50
55:EB:68:ARG:HD2	55:EB:76:VAL:HG11	1.92	0.50
17:R:161:ARG:HH11	17:R:164:LYS:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:85:GLN:HA	25:Z:88:VAL:HG22	1.93	0.50
29:CB:131:GLY:HA3	29:CB:137:VAL:HA	1.93	0.50
30:WA:2050:G:O6	30:WA:3875:C:O2'	2.29	0.50
51:v:749:ILE:HG22	51:v:810:PRO:HA	1.93	0.50
53:ZA:295:C:H2'	53:ZA:296:U:C6	2.47	0.50
53:ZA:561:A:HO2'	60:JB:134:HIS:HE2	1.52	0.50
53:ZA:561:A:H5''	60:JB:164:PRO:HG3	1.93	0.50
54:DB:107:TYR:HA	54:DB:110:LEU:HG	1.94	0.50
64:NB:3:ARG:HB2	64:NB:6:ALA:HB3	1.93	0.50
83:GC:152:SER:OG	83:GC:168:CYS:SG	2.57	0.50
6:F:45:ARG:NH1	30:WA:2107:G:H5''	2.26	0.50
12:M:49:ARG:HH12	30:WA:152:U:P	2.34	0.50
12:M:75:VAL:HG21	12:M:80:THR:HG22	1.93	0.50
17:R:154:LEU:HB3	17:R:157:ARG:HD3	1.94	0.50
30:WA:1510:C:H2'	30:WA:1511:G:H8	1.75	0.50
30:WA:2313:A:H61	30:WA:2335:G:H1'	1.76	0.50
30:WA:2525:C:H2'	30:WA:2526:G:C8	2.45	0.50
30:WA:4257:C:OP2	30:WA:4258:A:O2'	2.28	0.50
32:YA:92:U:H2'	32:YA:93:C:O4'	2.11	0.50
49:QA:51:ALA:HA	49:QA:91:THR:HB	1.94	0.50
53:ZA:94:G:O2'	53:ZA:508:A:O2'	2.24	0.50
53:ZA:122:G:OP1	55:EB:75:LYS:NZ	2.32	0.50
53:ZA:1109:C:H2'	53:ZA:1110:G:O4'	2.12	0.50
53:ZA:1113:A:H2'	53:ZA:1114:U:C6	2.47	0.50
53:ZA:1712:A:H2'	53:ZA:1713:C:H6	1.76	0.50
72:VB:73:ALA:HB1	72:VB:78:ILE:HB	1.93	0.50
4:D:40:ASP:HB2	4:D:43:LYS:HG2	1.94	0.50
30:WA:478:G:H2'	30:WA:479:G:H8	1.77	0.50
30:WA:1437:C:H2'	30:WA:1438:G:O4'	2.12	0.50
30:WA:4164:C:H2'	30:WA:4165:C:C6	2.46	0.50
51:v:602:LEU:HG	51:v:707:VAL:HG12	1.94	0.50
53:ZA:220:U:H2'	53:ZA:221:A:H8	1.76	0.50
2:B:57:VAL:HG22	2:B:73:VAL:HG12	1.94	0.49
5:E:144:ARG:NE	37:EA:110:ILE:OXT	2.44	0.49
27:AB:17:LYS:HB3	27:AB:173:LEU:HD11	1.95	0.49
30:WA:928:C:OP1	30:WA:930:G:O2'	2.28	0.49
30:WA:1744:G:H2'	30:WA:1745:C:C6	2.46	0.49
30:WA:2544:C:H2'	30:WA:2545:C:C6	2.47	0.49
30:WA:2613:G:H2'	30:WA:2614:G:H8	1.76	0.49
41:IA:46:LYS:HZ2	41:IA:54:LYS:HD2	1.77	0.49
50:RA:46:ILE:HG12	50:RA:71:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1756:C:H2'	53:ZA:1757:G:H5''	1.93	0.49
53:ZA:1822:A:H2'	53:ZA:1823:A:N3	2.28	0.49
3:C:189:MET:HG2	3:C:195:LYS:HE3	1.94	0.49
8:H:7:ASN:HB3	8:H:58:ASP:HB3	1.93	0.49
8:H:120:GLU:HB2	30:WA:4617:C:C2	2.47	0.49
14:O:116:HIS:HB3	14:O:149:ILE:HB	1.94	0.49
30:WA:275:C:O2'	30:WA:276:C:OP1	2.30	0.49
30:WA:4997:G:H2'	30:WA:4998:G:C8	2.47	0.49
51:v:32:LYS:HE2	51:v:105:SER:H	1.76	0.49
53:ZA:1713:C:H2'	53:ZA:1714:U:C6	2.48	0.49
56:FB:101:HIS:HB2	56:FB:108:PRO:HG3	1.94	0.49
57:GB:77:LEU:HD13	57:GB:84:TYR:HB2	1.94	0.49
3:C:207:PRO:HB3	3:C:249:PHE:CD2	2.47	0.49
4:D:65:ALA:HB2	4:D:74:ILE:HD13	1.94	0.49
27:AB:30:LEU:HD13	27:AB:38:ILE:HD12	1.94	0.49
30:WA:49:U:H2'	30:WA:50:C:H6	1.77	0.49
30:WA:441:G:H2'	30:WA:442:G:C8	2.48	0.49
30:WA:2098:G:H5''	30:WA:2100:A:C8	2.47	0.49
30:WA:4581:U:H2'	30:WA:4582:U:C6	2.47	0.49
53:ZA:158:A:N6	53:ZA:466:G:N7	2.60	0.49
53:ZA:987:A:OP1	77:AC:32:LYS:NZ	2.44	0.49
53:ZA:1094:C:H2'	53:ZA:1095:U:C6	2.47	0.49
53:ZA:1217:A:H2'	53:ZA:1218:C:H6	1.77	0.49
53:ZA:1515:G:H2'	53:ZA:1516:G:C8	2.47	0.49
62:LB:77:VAL:HG22	62:LB:88:ILE:HG22	1.95	0.49
69:SB:26:ILE:HD11	69:SB:52:LEU:HA	1.94	0.49
2:B:60:VAL:HG12	2:B:62:ARG:HG2	1.94	0.49
9:I:22:PHE:CZ	30:WA:1793:A:H2'	2.48	0.49
29:CB:138:GLY:HA2	29:CB:241:PHE:HE1	1.77	0.49
30:WA:248:C:H2'	30:WA:249:C:H6	1.76	0.49
30:WA:1960:G:H2'	30:WA:1961:A:H8	1.78	0.49
30:WA:2014:A:C3'	30:WA:2015:A:H5'	2.43	0.49
30:WA:2563:C:N4	30:WA:2564:G:O6	2.45	0.49
30:WA:3604:A:H2'	30:WA:3605:G:H8	1.77	0.49
30:WA:3938:G:H2'	30:WA:3939:G:H8	1.77	0.49
32:YA:38:U:H5'	39:GA:81:LEU:HD13	1.94	0.49
53:ZA:57:U:O2'	53:ZA:499:G:N2	2.38	0.49
53:ZA:573:U:N3	53:ZA:576:A:OP2	2.35	0.49
53:ZA:792:C:H2'	53:ZA:793:G:C8	2.47	0.49
53:ZA:1201:U:H2'	53:ZA:1202:U:C6	2.48	0.49
53:ZA:1208:A:O2'	53:ZA:1835:A:N6	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1268:C:N4	53:ZA:1269:G:O6	2.45	0.49
53:ZA:1304:U:OP1	82:FC:93:HIS:N	2.46	0.49
56:FB:176:GLU:OE2	56:FB:187:SER:OG	2.31	0.49
59:IB:119:LEU:HD12	59:IB:120:PRO:HD2	1.94	0.49
8:H:89:ARG:HE	8:H:187:VAL:HA	1.78	0.49
20:U:42:VAL:HG13	20:U:61:VAL:HG12	1.95	0.49
26:K:16:LYS:HE2	30:WA:46:U:OP1	2.13	0.49
28:BB:122:GLU:O	28:BB:165:ARG:NH1	2.35	0.49
30:WA:438:G:OP1	36:DA:16:ARG:NH2	2.46	0.49
30:WA:1805:U:H2'	30:WA:1806:A:C8	2.48	0.49
30:WA:2379:A:H2'	30:WA:2380:A:C8	2.46	0.49
30:WA:3921:G:H2'	30:WA:3922:A:H8	1.77	0.49
32:YA:94:G:OP2	41:IA:72:ARG:NH1	2.44	0.49
50:RA:35:LEU:HD22	50:RA:37:LEU:HB2	1.95	0.49
53:ZA:17:C:H2'	53:ZA:18:C:C6	2.47	0.49
53:ZA:1290:G:H2'	53:ZA:1291:A:C8	2.48	0.49
53:ZA:1376:A:N6	53:ZA:1377:U:O2	2.45	0.49
53:ZA:1536:G:H2'	53:ZA:1537:A:C8	2.47	0.49
53:ZA:1613:G:OP2	66:PB:39:ALA:N	2.43	0.49
53:ZA:1808:U:H2'	53:ZA:1809:A:C8	2.47	0.49
55:EB:222:LEU:HA	55:EB:225:ILE:HD12	1.95	0.49
57:GB:85:ARG:HD2	75:YB:118:ARG:NH1	2.28	0.49
59:IB:172:LEU:HB3	59:IB:190:LEU:HD12	1.95	0.49
63:MB:116:LYS:HA	63:MB:121:LYS:HG2	1.95	0.49
67:QB:37:ARG:HD2	67:QB:42:ILE:HB	1.94	0.49
2:B:228:TYR:O	30:WA:2840:A:O2'	2.29	0.49
6:F:97:ILE:HD12	15:P:4:ASP:HB2	1.94	0.49
14:O:40:HIS:NE2	14:O:110:ASP:O	2.38	0.49
30:WA:652:C:H2'	30:WA:653:G:C8	2.47	0.49
30:WA:1217:G:H2'	30:WA:1218:G:C8	2.47	0.49
30:WA:2453:G:H2'	30:WA:2454:A:C8	2.47	0.49
30:WA:2786:G:O2'	43:KA:3:SER:O	2.30	0.49
30:WA:2849:A:O2'	30:WA:4636:G:H4'	2.11	0.49
30:WA:3741:A:H2'	30:WA:3742:A:C8	2.48	0.49
30:WA:3770:G:H21	30:WA:3771:A:N6	2.10	0.49
48:PA:47:LYS:HB2	48:PA:102:TYR:CZ	2.48	0.49
48:PA:107:ARG:HG3	48:PA:108:MET:N	2.28	0.49
51:v:513:ASN:ND2	51:v:516:ASP:OD1	2.34	0.49
53:ZA:1106:C:H2'	53:ZA:1107:G:H8	1.78	0.49
1:A:37:ARG:NH2	30:WA:4092:G:OP2	2.45	0.49
10:J:143:ASP:N	10:J:143:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:267:G:H2'	30:WA:268:G:H8	1.77	0.49
30:WA:429:A:H2'	30:WA:430:G:C8	2.47	0.49
30:WA:429:A:H2'	30:WA:430:G:H8	1.78	0.49
30:WA:1913:A:H2'	30:WA:1914:P7G:O4'	2.12	0.49
30:WA:2562:G:N2	30:WA:2575:U:O2	2.36	0.49
30:WA:3902:B8K:O2'	30:WA:3903:G:OP2	2.30	0.49
30:WA:4709:C:H2'	30:WA:4710:A:C8	2.47	0.49
37:EA:106:TYR:CD2	37:EA:107:PRO:HD3	2.48	0.49
53:ZA:23:G:H2'	53:ZA:24:C:O4'	2.13	0.49
53:ZA:87:U:H2'	53:ZA:88:G:H8	1.78	0.49
53:ZA:114:G:OP1	62:LB:69:ARG:NH2	2.30	0.49
53:ZA:1408:U:H5''	67:QB:24:HIS:CD2	2.47	0.49
53:ZA:1462:U:H2'	53:ZA:1464:C:C4	2.46	0.49
53:ZA:1617:G:N2	53:ZA:1620:A:OP2	2.41	0.49
57:GB:59:GLN:OE1	57:GB:59:GLN:N	2.46	0.49
58:HB:143:ARG:HB2	58:HB:155:LYS:HB2	1.94	0.49
66:PB:18:ARG:NH2	69:SB:88:LYS:O	2.43	0.49
7:G:242:ARG:NH2	32:YA:154:G:H5'	2.27	0.49
14:O:60:PHE:HD2	14:O:67:VAL:HG21	1.76	0.49
20:U:82:ILE:HG22	20:U:83:ARG:HG3	1.95	0.49
30:WA:715:G:H2'	30:WA:716:G:H8	1.77	0.49
30:WA:1514:C:H2'	30:WA:1515:G:H8	1.78	0.49
30:WA:1622:G:O3'	41:IA:12:ARG:NH2	2.46	0.49
30:WA:3866:A:H2'	30:WA:3867:A:H8	1.77	0.49
30:WA:4278:A:H2'	30:WA:4279:A:C8	2.47	0.49
30:WA:4368:A:H5''	46:NA:36:GLN:HB2	1.93	0.49
32:YA:30:U:H2'	32:YA:31:G:C8	2.48	0.49
32:YA:69:U:H2'	32:YA:70:G:O4'	2.12	0.49
51:v:134:GLY:HA2	51:v:181:ILE:HD11	1.94	0.49
53:ZA:1012:A:OP1	64:NB:3:ARG:NH1	2.46	0.49
62:LB:111:VAL:HG11	62:LB:128:VAL:HG11	1.94	0.49
3:C:293:LEU:O	3:C:299:GLN:NE2	2.45	0.49
5:E:189:LEU:HD21	5:E:256:VAL:HG11	1.95	0.49
20:U:13:LYS:HD2	20:U:128:LEU:HD11	1.93	0.49
27:AB:145:ILE:HG13	27:AB:159:ILE:HB	1.95	0.49
30:WA:744:G:N1	30:WA:925:G:O6	2.46	0.49
30:WA:2418:U:H2'	30:WA:2419:G:C8	2.47	0.49
30:WA:2448:G:OP2	30:WA:2521:G:N2	2.36	0.49
30:WA:3939:G:H2'	30:WA:3940:C:C6	2.48	0.49
30:WA:4213:U:OP1	30:WA:4339:U:O2'	2.24	0.49
30:WA:4864:C:H2'	30:WA:4865:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4902:G:H2'	30:WA:4903:G:C8	2.48	0.49
43:KA:20:ASN:ND2	43:KA:42:ARG:O	2.41	0.49
53:ZA:223:C:H2'	53:ZA:224:A:C8	2.48	0.49
53:ZA:1100:A:H4'	68:RB:132:ARG:HH12	1.78	0.49
60:JB:60:LEU:O	60:JB:70:ARG:NH1	2.46	0.49
69:SB:98:VAL:HG11	69:SB:106:LYS:HG3	1.94	0.49
4:D:208:MET:HG3	4:D:219:TYR:HE1	1.77	0.49
12:M:38:ARG:NH2	32:YA:142:U:OP1	2.33	0.49
12:M:145:ASN:ND2	12:M:147:ASP:OD1	2.46	0.49
26:K:8:MET:HE2	26:K:10:LEU:HD21	1.95	0.49
26:K:36:ARG:NH1	30:WA:1370:U:OP2	2.43	0.49
26:K:162:LYS:NZ	30:WA:645:G:OP2	2.41	0.49
30:WA:243:A:H2'	30:WA:244:G:C8	2.47	0.49
30:WA:426:A:H2'	30:WA:427:A:C8	2.48	0.49
30:WA:734:A:N6	30:WA:937:G:O6	2.41	0.49
30:WA:987:U:H2'	30:WA:988:C:C6	2.47	0.49
30:WA:1334:G:O2'	30:WA:2354:A:OP1	2.30	0.49
30:WA:1367:G:H2'	30:WA:1368:G:H8	1.78	0.49
30:WA:3758:G:H2'	30:WA:3759:G:O4'	2.13	0.49
49:QA:26:LYS:HA	49:QA:194:ASP:HA	1.93	0.49
53:ZA:497:C:H2'	53:ZA:498:C:C6	2.48	0.49
53:ZA:1269:G:H2'	53:ZA:1270:G:C8	2.48	0.49
53:ZA:1457:U:H2'	53:ZA:1458:G:C8	2.48	0.49
53:ZA:1482:C:H2'	53:ZA:1483:A:O4'	2.12	0.49
53:ZA:1566:G:N7	70:TB:101:ARG:NH2	2.60	0.49
4:D:29:ASP:HB2	4:D:150:LEU:HD21	1.95	0.48
5:E:95:VAL:HG13	5:E:112:LEU:HD11	1.94	0.48
28:BB:157:GLN:HB2	28:BB:160:GLN:HG2	1.95	0.48
30:WA:1823:G:O2'	30:WA:1824:G:OP1	2.26	0.48
32:YA:7:U:H2'	32:YA:8:U:C6	2.47	0.48
49:QA:192:VAL:O	49:QA:199:TYR:N	2.40	0.48
53:ZA:811:A:H2'	53:ZA:812:A:H8	1.78	0.48
53:ZA:958:G:H3'	53:ZA:959:G:C8	2.46	0.48
66:PB:83:MET:HB3	66:PB:116:LEU:HG	1.95	0.48
3:C:100:ARG:NH2	30:WA:1526:C:OP1	2.44	0.48
15:P:99:LYS:HE3	15:P:119:LYS:HE3	1.94	0.48
16:Q:134:ASN:HB2	16:Q:137:ILE:HG13	1.94	0.48
17:R:68:PHE:H	30:WA:730:2MG:HN1	1.61	0.48
17:R:118:ARG:O	17:R:120:ARG:NH1	2.45	0.48
22:W:94:ASN:OD1	22:W:146:ALA:N	2.39	0.48
30:WA:318:A:H2'	30:WA:319:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:658:C:H2'	30:WA:659:C:C6	2.48	0.48
30:WA:1516:U:H2'	30:WA:1517:G:H8	1.76	0.48
30:WA:1559:A:N6	30:WA:1578:G:H1'	2.29	0.48
30:WA:2107:G:H2'	30:WA:2108:A:O4'	2.13	0.48
35:CA:68:LEU:HD11	35:CA:84:ILE:HD12	1.96	0.48
37:EA:45:LYS:NZ	37:EA:108:SER:HA	2.27	0.48
51:v:120:ARG:NH1	51:v:495:ARG:O	2.47	0.48
51:v:395:MET:HE2	51:v:494:MET:HE1	1.96	0.48
51:v:420:LEU:HB3	51:v:465:PRO:HD3	1.94	0.48
51:v:710:HIS:CD2	51:v:715:DDE:HD2	2.48	0.48
53:ZA:812:A:H5'	55:EB:16:LYS:HD2	1.95	0.48
53:ZA:1047:C:H2'	53:ZA:1048:G:O4'	2.13	0.48
53:ZA:1484:A:H4'	54:DB:159:HIS:NE2	2.28	0.48
57:GB:85:ARG:HD2	75:YB:118:ARG:HH11	1.78	0.48
58:HB:17:ASP:HB3	58:HB:20:GLU:HG2	1.95	0.48
62:LB:35:ARG:HE	62:LB:63:THR:HG21	1.77	0.48
63:MB:33:ARG:HD2	63:MB:91:LEU:HD11	1.95	0.48
64:NB:130:LYS:NZ	64:NB:139:TRP:O	2.37	0.48
83:GC:235:ILE:O	83:GC:253:GLY:N	2.46	0.48
4:D:222:GLN:HE22	31:XA:47:G:H21	1.62	0.48
5:E:50:PRO:HG2	5:E:58:ARG:HB3	1.95	0.48
6:F:226:PHE:CG	6:F:235:ARG:HG2	2.49	0.48
14:O:5:SER:O	32:YA:11:C:O2'	2.21	0.48
26:K:31:ARG:HD2	26:K:35:ARG:HH21	1.78	0.48
30:WA:447:C:H2'	30:WA:448:G:H8	1.76	0.48
30:WA:1484:G:H2'	30:WA:1485:C:C6	2.48	0.48
30:WA:1871:UR3:H3U2	30:WA:4410:G:H8	1.79	0.48
30:WA:2524:U:O2'	30:WA:2535:U:O2	2.24	0.48
51:v:290:CYS:HA	51:v:294:LEU:HB2	1.95	0.48
51:v:325:SER:HA	51:v:328:LYS:HE3	1.96	0.48
53:ZA:452:G:O4'	57:GB:88:ARG:NH1	2.47	0.48
53:ZA:1670:C:H2'	53:ZA:1671:G:C8	2.48	0.48
54:DB:148:LYS:HE2	54:DB:150:MET:HE2	1.95	0.48
57:GB:149:LYS:H	57:GB:149:LYS:HD2	1.78	0.48
2:B:77:THR:HG21	2:B:337:VAL:HG22	1.94	0.48
10:J:120:ASP:HB2	10:J:123:ILE:HG12	1.95	0.48
30:WA:500:G:H2'	30:WA:500:G:N3	2.27	0.48
30:WA:1667:C:H2'	30:WA:1668:C:C6	2.48	0.48
39:GA:97:LYS:HA	39:GA:100:GLU:HG2	1.95	0.48
41:IA:22:CYS:SG	41:IA:24:SER:OG	2.66	0.48
48:PA:119:ARG:O	48:PA:122:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QA:48:ARG:NH1	50:RA:123:ARG:O	2.46	0.48
53:ZA:962:A:N1	53:ZA:1055:A:O2'	2.46	0.48
55:EB:130:PHE:O	55:EB:138:HIS:N	2.37	0.48
60:JB:136:ARG:NH1	60:JB:159:PHE:O	2.46	0.48
1:A:117:GLU:HG2	1:A:124:GLY:N	2.29	0.48
24:Y:79:HIS:ND1	30:WA:2585:U:O2'	2.36	0.48
26:K:46:ILE:O	26:K:149:GLN:NE2	2.46	0.48
30:WA:476:G:H2'	30:WA:477:C:C6	2.49	0.48
30:WA:1448:A:H2'	30:WA:1449:G:O4'	2.14	0.48
30:WA:2508:G:H2'	30:WA:2509:C:O4'	2.13	0.48
30:WA:2762:A:H2'	30:WA:2763:G:C5	2.49	0.48
30:WA:5007:U:H2'	30:WA:5008:U:C6	2.48	0.48
39:GA:4:ILE:HD11	39:GA:9:LEU:HD11	1.95	0.48
51:v:579:TYR:O	51:v:580:ARG:NH1	2.39	0.48
53:ZA:24:C:N4	53:ZA:25:A:H62	2.11	0.48
53:ZA:923:G:OP1	64:NB:3:ARG:NH2	2.46	0.48
53:ZA:927:C:H2'	53:ZA:928:G:C8	2.48	0.48
53:ZA:1286:G:N2	53:ZA:1313:A:H62	2.11	0.48
53:ZA:1692:U:H2'	53:ZA:1693:G:C8	2.49	0.48
53:ZA:1781:A:H2'	53:ZA:1782:G:H8	1.77	0.48
2:B:120:LYS:N	30:WA:4973:A:OP1	2.45	0.48
3:C:42:THR:HG23	30:WA:2345:C:H4'	1.95	0.48
3:C:306:ARG:HG2	30:WA:2104:C:H3'	1.95	0.48
21:V:93:LYS:O	21:V:96:GLN:NE2	2.46	0.48
28:BB:91:VAL:HG12	28:BB:93:GLY:H	1.78	0.48
28:BB:113:MET:HE3	28:BB:209:ASP:HB3	1.96	0.48
30:WA:1550:G:H2'	30:WA:1551:C:C6	2.49	0.48
30:WA:3925:U:H2'	30:WA:3926:U:C6	2.49	0.48
30:WA:4582:U:H2'	30:WA:4583:G:C8	2.48	0.48
51:v:110:ASP:HB3	51:v:553:HIS:HB2	1.95	0.48
53:ZA:94:G:OP1	55:EB:6:LYS:NZ	2.47	0.48
53:ZA:130:G:N2	53:ZA:180:G:OP1	2.46	0.48
53:ZA:730:C:H2'	53:ZA:731:G:H8	1.77	0.48
59:IB:78:ILE:HA	59:IB:104:ILE:HG22	1.95	0.48
79:CC:13:ARG:C	79:CC:32:VAL:HG23	2.37	0.48
4:D:56:THR:OG1	4:D:59:ASP:OD1	2.28	0.48
5:E:205:ASP:N	5:E:205:ASP:OD1	2.46	0.48
7:G:211:ALA:HB2	7:G:243:LEU:HD22	1.96	0.48
27:AB:141:ASN:OD1	27:AB:141:ASN:N	2.45	0.48
30:WA:443:G:H5''	37:EA:54:LYS:HB3	1.95	0.48
30:WA:447:C:C2	30:WA:1306:G:N2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2674:C:H2'	30:WA:2675:C:O4'	2.14	0.48
30:WA:3789:A:O2'	30:WA:3790:A2M:H3'	2.13	0.48
32:YA:66:A:H2'	32:YA:67:U:C6	2.48	0.48
32:YA:141:C:H2'	32:YA:142:U:C6	2.48	0.48
51:v:200:MET:HE3	51:v:203:ILE:HD13	1.96	0.48
51:v:374:GLU:HB2	51:v:495:ARG:HG2	1.94	0.48
53:ZA:61:A:N1	53:ZA:335:G:O2'	2.36	0.48
53:ZA:857:U:H4'	55:EB:201:HIS:CE1	2.49	0.48
53:ZA:969:U:OP1	53:ZA:970:G:O2'	2.19	0.48
53:ZA:1032:C:H2'	53:ZA:1033:G:O4'	2.13	0.48
53:ZA:1189:A:H2'	53:ZA:1190:A:C8	2.48	0.48
74:XB:22:TRP:HE3	74:XB:28:LYS:HG3	1.79	0.48
2:B:348:ARG:HH12	2:B:351:LEU:HG	1.79	0.48
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.96	0.48
4:D:225:GLN:HB2	31:XA:49:A:OP1	2.14	0.48
5:E:122:GLU:OE2	36:DA:94:SER:OG	2.30	0.48
17:R:112:ASP:OD1	17:R:116:ARG:NH1	2.42	0.48
23:X:22:PRO:O	23:X:26:ARG:HG2	2.13	0.48
24:Y:4:PHE:O	24:Y:9:LYS:NZ	2.33	0.48
25:Z:32:ARG:NH1	30:WA:1521:G:OP1	2.47	0.48
30:WA:325:U:H2'	30:WA:326:C:C6	2.49	0.48
48:PA:17:LEU:HD21	48:PA:19:LYS:HE3	1.96	0.48
49:QA:160:LEU:HG	49:QA:161:ILE:HG12	1.95	0.48
53:ZA:164:A:H2'	53:ZA:165:G:N3	2.29	0.48
53:ZA:220:U:H2'	53:ZA:221:A:C8	2.49	0.48
53:ZA:430:C:H2'	53:ZA:431:G:H8	1.77	0.48
53:ZA:1269:G:H2'	53:ZA:1270:G:H8	1.78	0.48
53:ZA:1424:G:H2'	53:ZA:1425:G:C8	2.48	0.48
53:ZA:1471:C:H2'	53:ZA:1472:C:C6	2.48	0.48
59:IB:37:LYS:HB2	59:IB:59:ARG:HG3	1.96	0.48
65:OB:117:ARG:HB2	77:AC:49:ALA:HB2	1.95	0.48
75:YB:92:ALA:HB2	75:YB:97:TYR:HD2	1.79	0.48
4:D:184:ASP:HB2	4:D:187:SER:HB3	1.96	0.48
9:I:54:SER:HB2	9:I:135:ILE:HD11	1.96	0.48
25:Z:12:ARG:NH1	30:WA:2350:G:OP2	2.46	0.48
25:Z:77:LYS:NZ	30:WA:1507:G:H1	2.12	0.48
26:K:116:ARG:NH2	26:K:155:MET:O	2.47	0.48
30:WA:112:C:C2	30:WA:113:A:C8	3.01	0.48
30:WA:163:A:H2'	30:WA:164:G:C8	2.48	0.48
30:WA:1556:C:H2'	30:WA:1557:G:O4'	2.14	0.48
30:WA:2796:C:OP1	43:KA:48:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2816:G:H22	30:WA:2818:A:H3'	1.78	0.48
30:WA:2835:G:H2'	30:WA:2836:G:H8	1.78	0.48
30:WA:3875:C:H2'	30:WA:3876:A:C8	2.49	0.48
37:EA:92:LEU:H	37:EA:92:LEU:HD12	1.78	0.48
51:v:651:CYS:SG	51:v:652:PHE:N	2.87	0.48
53:ZA:56:G:OP1	75:YB:111:LYS:NZ	2.36	0.48
53:ZA:152:U:H2'	53:ZA:153:G:C8	2.48	0.48
53:ZA:1474:A:H4'	67:QB:121:VAL:HG23	1.95	0.48
58:HB:146:VAL:O	73:WB:49:GLU:HG3	2.14	0.48
64:NB:19:ARG:HD2	78:BC:84:HIS:CE1	2.49	0.48
73:WB:53:ILE:HD11	78:BC:8:LEU:HD23	1.95	0.48
4:D:265:ARG:HH12	4:D:269:PRO:HD3	1.79	0.48
6:F:181:TYR:CZ	6:F:202:GLU:HG2	2.49	0.48
6:F:221:LYS:HB3	6:F:230:GLY:HA2	1.96	0.48
6:F:237:ASP:OD1	6:F:237:ASP:N	2.46	0.48
8:H:37:ASP:OD2	8:H:39:ASN:ND2	2.46	0.48
12:M:60:VAL:HG11	32:YA:141:C:H5''	1.95	0.48
14:O:64:ASN:ND2	14:O:80:GLN:OE1	2.44	0.48
17:R:87:ARG:NH2	30:WA:2039:G:H5'	2.28	0.48
27:AB:42:LYS:HE3	27:AB:48:ILE:HD11	1.95	0.48
30:WA:48:G:H8	30:WA:49:U:H5	1.61	0.48
30:WA:401:G:C2	30:WA:402:A:H1'	2.49	0.48
30:WA:1194:C:H2'	30:WA:1195:G:H8	1.79	0.48
30:WA:3793:C:O2'	30:WA:3794:C:OP1	2.30	0.48
30:WA:4693:C:H2'	30:WA:4694:U:C6	2.48	0.48
52:w:286:TRP:HE1	61:KB:85:LEU:HD22	1.79	0.48
53:ZA:676:C:H2'	53:ZA:677:G:O4'	2.14	0.48
53:ZA:1413:G:H2'	53:ZA:1414:A:C8	2.48	0.48
53:ZA:1711:U:H2'	53:ZA:1712:A:C8	2.49	0.48
71:UB:26:SER:HB2	71:UB:110:VAL:HG13	1.95	0.48
80:DC:53:ILE:HG13	80:DC:55:LEU:HG	1.96	0.48
3:C:304:ALA:HB1	30:WA:2104:C:C6	2.49	0.47
5:E:68:LYS:HB2	5:E:70:LEU:HG	1.96	0.47
14:O:108:ASP:N	14:O:152:GLU:OE2	2.40	0.47
16:Q:105:LEU:HD23	16:Q:138:LEU:HD23	1.95	0.47
19:T:42:PHE:CE1	19:T:46:ARG:HD2	2.49	0.47
21:V:52:THR:HG23	21:V:55:TYR:H	1.78	0.47
26:K:147:ALA:HB1	39:GA:120:ALA:HB3	1.96	0.47
27:AB:30:LEU:HB2	27:AB:47:TYR:CZ	2.49	0.47
27:AB:59:LEU:O	27:AB:63:ARG:HG2	2.14	0.47
30:WA:1480:G:H2'	30:WA:1481:C:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2782:G:H5''	30:WA:2783:G:H5'	1.96	0.47
30:WA:5051:U:OP2	35:CA:83:ARG:NH2	2.44	0.47
53:ZA:12:U:H2'	53:ZA:13:C:H6	1.78	0.47
53:ZA:406:U:H2'	53:ZA:408:A:C8	2.46	0.47
53:ZA:996:A:H2'	53:ZA:997:A:C8	2.49	0.47
53:ZA:1253:A:H4'	53:ZA:1254:C:O5'	2.13	0.47
63:MB:61:TYR:OH	63:MB:108:CYS:SG	2.60	0.47
64:NB:4:MET:SD	64:NB:124:ARG:NH1	2.86	0.47
65:OB:34:PHE:HB3	65:OB:41:PHE:HB2	1.94	0.47
77:AC:46:GLU:HG2	77:AC:47:ALA:H	1.78	0.47
2:B:298:LEU:HD23	2:B:298:LEU:H	1.78	0.47
4:D:106:ALA:HB2	4:D:166:ALA:HA	1.95	0.47
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.95	0.47
5:E:122:GLU:HG3	36:DA:7:LEU:HD22	1.95	0.47
6:F:94:ILE:HD13	6:F:140:ALA:HB2	1.95	0.47
8:H:51:LYS:HB2	8:H:53:LYS:HG3	1.95	0.47
30:WA:168:C:H2'	30:WA:169:A:H8	1.80	0.47
30:WA:287:U:H2'	30:WA:288:G:C8	2.49	0.47
30:WA:1473:C:H2'	30:WA:1474:C:H6	1.79	0.47
30:WA:1970:G:H2'	30:WA:1971:C:C6	2.48	0.47
30:WA:2494:C:O2'	30:WA:2496:C:N4	2.47	0.47
30:WA:3626:A:C8	30:WA:4647:U:H1'	2.49	0.47
30:WA:4950:G:N1	37:EA:3:GLY:O	2.38	0.47
32:YA:94:G:C5	41:IA:84:PRO:HD3	2.49	0.47
51:v:369:CYS:SG	51:v:370:GLU:HG3	2.55	0.47
53:ZA:426:A:H2'	53:ZA:426:A:N3	2.29	0.47
53:ZA:468:A:H2'	53:ZA:469:A:C8	2.49	0.47
53:ZA:587:A:O4'	53:ZA:592:C:N4	2.47	0.47
53:ZA:921:G:C2	78:BC:22:LYS:HG2	2.49	0.47
53:ZA:1162:C:H2'	53:ZA:1163:C:O4'	2.13	0.47
53:ZA:1617:G:N2	53:ZA:1619:A:H3'	2.29	0.47
54:DB:18:LYS:HG2	54:DB:39:VAL:HG11	1.95	0.47
58:HB:101:LEU:O	58:HB:116:ARG:NH1	2.47	0.47
59:IB:107:THR:HG22	59:IB:110:ARG:HH21	1.78	0.47
62:LB:103:GLU:HG3	74:XB:10:ALA:HB3	1.96	0.47
83:GC:164:ILE:HG23	83:GC:176:VAL:HG13	1.95	0.47
1:A:196:TRP:O	1:A:198:ARG:N	2.48	0.47
6:F:126:LYS:HB2	18:S:133:ALA:HB3	1.95	0.47
11:L:81:ASP:OD2	11:L:84:THR:OG1	2.21	0.47
26:K:124:LEU:HD11	39:GA:119:TYR:HB2	1.96	0.47
28:BB:168:MET:HG2	28:BB:197:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:35:U:O2'	30:WA:1530:A:N1	2.45	0.47
30:WA:1350:C:H2'	30:WA:1351:A:C8	2.49	0.47
30:WA:1990:G:O2'	30:WA:2008:G:OP2	2.28	0.47
30:WA:3732:A:H2'	30:WA:3733:A:C8	2.50	0.47
30:WA:4158:C:H2'	30:WA:4159:G:C8	2.49	0.47
32:YA:148:A:H2'	32:YA:149:G:C8	2.50	0.47
53:ZA:55:U:OP1	53:ZA:451:G:N1	2.28	0.47
53:ZA:114:G:O2'	53:ZA:115:U:H5''	2.14	0.47
53:ZA:652:U:H2'	53:ZA:653:A:C8	2.50	0.47
53:ZA:917:U:H2'	53:ZA:918:U:O4'	2.14	0.47
53:ZA:1716:C:H2'	53:ZA:1717:C:H6	1.78	0.47
53:ZA:1859:A:P	77:AC:10:ARG:HH12	2.38	0.47
54:DB:170:THR:HG22	54:DB:187:LYS:HG2	1.96	0.47
1:A:5:ILE:HG12	1:A:8:GLN:HG3	1.96	0.47
1:A:24:LYS:N	1:A:51:ASP:OD1	2.40	0.47
3:C:245:HIS:NE2	30:WA:2343:C:O2	2.44	0.47
5:E:76:ALA:HA	33:AA:117:ARG:HD3	1.97	0.47
6:F:125:ASN:H	6:F:128:SER:HB3	1.78	0.47
10:J:50:PHE:HD1	10:J:70:VAL:HG22	1.79	0.47
13:N:61:ARG:HA	13:N:70:PRO:HD2	1.96	0.47
16:Q:170:ARG:HA	16:Q:173:ARG:HE	1.80	0.47
29:CB:94:ILE:HD11	29:CB:159:LYS:HD3	1.96	0.47
30:WA:115:C:O2'	30:WA:276:C:OP1	2.32	0.47
30:WA:314:G:O2'	30:WA:4360:E6G:OP2	2.22	0.47
30:WA:1559:A:H61	30:WA:1578:G:H1'	1.78	0.47
30:WA:1667:C:H2'	30:WA:1668:C:H6	1.78	0.47
30:WA:2332:G:H2'	30:WA:2333:G:H8	1.79	0.47
30:WA:2522:A:N3	30:WA:2544:C:O2'	2.46	0.47
30:WA:2629:G:H2'	30:WA:2630:U:H6	1.79	0.47
51:v:159:LYS:HG2	89:v:900:GDP:C5	2.50	0.47
53:ZA:1015:U:O2'	64:NB:55:ARG:NH1	2.47	0.47
53:ZA:1049:A:OP2	53:ZA:1068:G:N1	2.30	0.47
53:ZA:1112:U:H2'	53:ZA:1113:A:H8	1.79	0.47
53:ZA:1288:U:O2	53:ZA:1311:C:N3	2.48	0.47
55:EB:11:ARG:HA	55:EB:28:ALA:HB2	1.96	0.47
57:GB:218:LYS:HA	57:GB:221:LYS:HE3	1.97	0.47
63:MB:26:LEU:HB3	63:MB:31:LEU:HD21	1.97	0.47
83:GC:289:LEU:HA	83:GC:300:ALA:HA	1.96	0.47
2:B:268:ARG:HH21	30:WA:3901:C:H1'	1.79	0.47
4:D:209:ARG:HE	4:D:233:PRO:HB2	1.79	0.47
14:O:4:TYR:CE2	14:O:16:LYS:HB3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:97:LYS:HB2	21:V:100:VAL:HG23	1.96	0.47
26:K:91:ALA:HB1	26:K:96:ILE:HB	1.96	0.47
28:BB:131:ASP:OD1	28:BB:131:ASP:N	2.25	0.47
30:WA:281:U:H2'	30:WA:282:C:H6	1.78	0.47
30:WA:300:A:H2'	30:WA:301:G:H8	1.80	0.47
30:WA:659:C:H2'	30:WA:660:G:H8	1.78	0.47
30:WA:1460:G:O2'	30:WA:1461:JMH:OP1	2.30	0.47
30:WA:1651:A:O2'	41:IA:49:TRP:O	2.26	0.47
30:WA:2410:G:HO2'	30:WA:2796:C:HO2'	1.62	0.47
30:WA:2452:U:H2'	30:WA:2453:G:H8	1.80	0.47
30:WA:2658:C:OP2	38:FA:54:ARG:NH1	2.48	0.47
30:WA:3612:U:H2'	30:WA:3613:A:C8	2.50	0.47
30:WA:4242:C:OP1	30:WA:4332:C:O2'	2.30	0.47
34:BA:101:ASP:N	34:BA:101:ASP:OD1	2.47	0.47
47:OA:46:LYS:HE3	47:OA:58:GLY:HA3	1.96	0.47
53:ZA:1558:C:H2'	53:ZA:1559:C:C6	2.50	0.47
53:ZA:1678:A2M:O2'	53:ZA:1679:A:H5''	2.15	0.47
56:FB:127:ARG:HB2	56:FB:136:ARG:NH2	2.29	0.47
60:JB:18:ARG:HB3	60:JB:21:GLU:HB2	1.97	0.47
65:OB:95:ILE:HG21	65:OB:116:LEU:HD21	1.96	0.47
83:GC:163:PRO:HB2	83:GC:179:LEU:HB2	1.96	0.47
7:G:237:LEU:HD21	7:G:242:ARG:HD2	1.97	0.47
18:S:43:LYS:HD2	30:WA:1737:C:H5''	1.97	0.47
20:U:89:ARG:HB2	20:U:95:PHE:CE2	2.50	0.47
30:WA:2272:U:OP1	48:PA:37:SER:OG	2.19	0.47
30:WA:2498:G:O2'	32:YA:127:U:OP1	2.25	0.47
30:WA:2649:G:H2'	30:WA:2650:G:H8	1.79	0.47
30:WA:4417:C:H2'	30:WA:4418:C:O2	2.14	0.47
30:WA:4864:C:H2'	30:WA:4865:G:C8	2.50	0.47
51:v:674:GLU:HG2	51:v:716:ARG:HH21	1.80	0.47
53:ZA:25:A:O2'	53:ZA:26:U:H6	1.97	0.47
53:ZA:96:C:H2'	53:ZA:97:U:C6	2.49	0.47
53:ZA:1693:G:N2	53:ZA:1834:A:H8	2.12	0.47
53:ZA:1714:U:H2'	53:ZA:1715:A:C8	2.49	0.47
57:GB:48:TYR:CZ	57:GB:117:GLY:HA3	2.50	0.47
73:WB:24:GLN:NE2	78:BC:7:LEU:H	2.11	0.47
1:A:40:TYR:OH	30:WA:4123:U:O2	2.26	0.47
9:I:3:ARG:NH2	30:WA:4436:U:OP2	2.44	0.47
11:L:6:PHE:O	11:L:11:ARG:NE	2.48	0.47
11:L:120:ASN:ND2	30:WA:4885:C:OP2	2.47	0.47
17:R:87:ARG:HD3	31:XA:87:G:H4'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:135:ARG:NH1	30:WA:2758:G:H5'	2.30	0.47
28:BB:78:GLU:HG3	28:BB:79:VAL:H	1.80	0.47
30:WA:661:G:H2'	30:WA:662:C:C6	2.49	0.47
30:WA:1083:C:OP1	30:WA:1221:C:O2'	2.32	0.47
30:WA:1192:U:H2'	30:WA:1193:G:N3	2.29	0.47
30:WA:1306:G:H2'	30:WA:1307:C:C2	2.50	0.47
30:WA:2312:A:H2'	30:WA:2313:A:C8	2.50	0.47
30:WA:2707:C:H2'	30:WA:2708:G:O4'	2.14	0.47
30:WA:4093:C:H2'	30:WA:4094:G:C8	2.49	0.47
30:WA:4093:C:H2'	30:WA:4094:G:H8	1.79	0.47
30:WA:4327:G:N2	30:WA:4330:A:OP2	2.42	0.47
30:WA:4781:G:H2'	30:WA:4782:C:H5''	1.97	0.47
30:WA:5011:U:H4'	30:WA:5012:A:H5'	1.97	0.47
51:v:144:ARG:HG3	51:v:188:ILE:HD11	1.95	0.47
51:v:605:LYS:HE2	51:v:705:HIS:CE1	2.50	0.47
53:ZA:427:U:H5''	53:ZA:428:U:OP2	2.15	0.47
53:ZA:1203:G:H2'	53:ZA:1204:A:C8	2.50	0.47
53:ZA:1683:C:H2'	53:ZA:1684:C:H6	1.80	0.47
54:DB:32:ASP:OD1	54:DB:57:ASN:ND2	2.48	0.47
55:EB:20:LEU:HD11	55:EB:46:ILE:HD12	1.96	0.47
70:TB:10:ASN:ND2	70:TB:13:GLU:OE1	2.48	0.47
77:AC:46:GLU:CD	77:AC:46:GLU:H	2.23	0.47
82:FC:143:LYS:N	82:FC:143:LYS:HE3	2.30	0.47
2:B:229:LYS:HG3	2:B:272:LYS:HD3	1.97	0.47
8:H:163:GLN:HE22	30:WA:4691:G:H21	1.63	0.47
9:I:21:ARG:HG3	9:I:24:ARG:HH21	1.79	0.47
28:BB:27:LYS:HA	28:BB:51:ARG:NH1	2.30	0.47
30:WA:1081:G:N2	30:WA:1241:G:H22	2.13	0.47
30:WA:2527:7MG:OP1	38:FA:29:ARG:NH1	2.45	0.47
30:WA:2653:G:H2'	30:WA:2654:G:C8	2.49	0.47
30:WA:2714:C:OP1	84:b:263:ARG:HB3	2.14	0.47
30:WA:3916:C:H2'	30:WA:3917:U:C6	2.49	0.47
30:WA:3928:A:H2'	30:WA:3929:C:C6	2.50	0.47
30:WA:4463:C:H2'	30:WA:4464:U:C6	2.50	0.47
30:WA:4939:A:H2'	30:WA:4940:C:C6	2.50	0.47
49:QA:99:ARG:HG3	49:QA:189:ILE:HD12	1.97	0.47
53:ZA:502:C:H3'	53:ZA:503:C:C6	2.49	0.47
53:ZA:1094:C:H2'	53:ZA:1095:U:H6	1.78	0.47
53:ZA:1213:C:H2'	53:ZA:1214:A:H8	1.80	0.47
53:ZA:1823:A:H3'	53:ZA:1824:A:C8	2.50	0.47
56:FB:72:LEU:HB2	56:FB:151:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:HB:144:ILE:O	73:WB:52:ILE:N	2.45	0.47
8:H:20:LEU:HB3	8:H:25:VAL:HG12	1.97	0.47
9:I:28:ASP:OD2	9:I:32:ARG:NH2	2.47	0.47
12:M:85:VAL:HG23	30:WA:43:U:OP1	2.15	0.47
14:O:69:ARG:HH11	30:WA:4986:G:H1'	1.79	0.47
18:S:39:ILE:HG22	18:S:99:SER:HB3	1.96	0.47
18:S:130:ARG:NH2	30:WA:1807:A:N3	2.54	0.47
25:Z:32:ARG:HG3	30:WA:37:U:H4'	1.97	0.47
25:Z:134:GLU:OE2	26:K:178:ALA:N	2.46	0.47
30:WA:668:A:H4'	48:PA:46:ARG:HH22	1.80	0.47
30:WA:1252:G:H2'	30:WA:1253:U:C6	2.50	0.47
30:WA:2737:G:H2'	30:WA:2738:C:C6	2.50	0.47
30:WA:2837:A:H2'	30:WA:2838:A:C8	2.48	0.47
30:WA:3646:U:H5	30:WA:3651:A:H2	1.63	0.47
30:WA:3714:U:H2'	30:WA:3715:G:C8	2.50	0.47
30:WA:4599:U:H2'	30:WA:4600:G:C8	2.46	0.47
41:IA:75:ARG:HG3	41:IA:76:HIS:ND1	2.29	0.47
53:ZA:30:C:O2'	53:ZA:596:U:OP1	2.33	0.47
53:ZA:375:U:H2'	53:ZA:376:A:C8	2.50	0.47
53:ZA:734:C:H2'	53:ZA:735:C:C6	2.50	0.47
53:ZA:1454:A:O5'	68:RB:3:ARG:NH2	2.48	0.47
57:GB:48:TYR:CE1	57:GB:117:GLY:HA3	2.50	0.47
58:HB:15:LYS:HD3	58:HB:16:PRO:HD2	1.97	0.47
67:QB:16:LYS:HG3	67:QB:17:LYS:H	1.80	0.47
68:RB:110:ASP:N	68:RB:110:ASP:OD1	2.47	0.47
83:GC:35:SER:OG	83:GC:36:ARG:N	2.48	0.47
2:B:74:GLU:OE1	2:B:285:TYR:OH	2.30	0.47
10:J:19:LYS:HB2	10:J:75:ARG:CZ	2.45	0.47
10:J:151:ILE:HG13	10:J:155:HIS:HB3	1.97	0.47
26:K:19:GLN:OE1	30:WA:1523:A:N6	2.48	0.47
30:WA:4238:A:H4'	46:NA:98:LYS:HE3	1.97	0.47
32:YA:109:C:O2	32:YA:111:U:N3	2.48	0.47
49:QA:20:LEU:HD22	49:QA:54:LEU:HD12	1.97	0.47
51:v:839:ARG:HD3	51:v:845:LYS:O	2.14	0.47
53:ZA:106:C:OP1	53:ZA:431:G:O2'	2.30	0.47
53:ZA:179:C:H2'	53:ZA:180:G:C8	2.50	0.47
53:ZA:334:C:H41	57:GB:190:ARG:NE	2.13	0.47
53:ZA:1093:A:H2'	53:ZA:1094:C:H6	1.80	0.47
53:ZA:1135:C:H2'	53:ZA:1136:U:C6	2.50	0.47
53:ZA:1567:G:OP1	53:ZA:1567:G:N2	2.37	0.47
55:EB:153:LEU:HD23	55:EB:172:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:b:64:PHE:O	84:b:65:LYS:HG2	2.14	0.47
84:b:122:ALA:HB3	84:b:320:LYS:H	1.80	0.47
84:b:123:HIS:HE1	84:b:125:PHE:HB3	1.80	0.47
2:B:249:ARG:NH2	30:WA:3850:A:OP2	2.48	0.46
5:E:45:HIS:ND1	5:E:46:CYS:O	2.40	0.46
23:X:50:ARG:HG2	23:X:51:LYS:H	1.80	0.46
30:WA:19:G:H2'	30:WA:20:U:C6	2.50	0.46
30:WA:509:G:O2'	30:WA:511:U:OP2	2.29	0.46
30:WA:746:G:O2'	30:WA:747:G:H5'	2.15	0.46
30:WA:1681:C:H41	30:WA:4383:A:H5''	1.80	0.46
30:WA:2548:A:H4'	32:YA:127:U:H1'	1.97	0.46
30:WA:2694:C:H2'	30:WA:2695:C:C6	2.50	0.46
30:WA:4178:G:H2'	30:WA:4179:U:C6	2.50	0.46
32:YA:19:C:H2'	32:YA:20:A:C8	2.49	0.46
40:HA:33:LEU:HG	40:HA:38:LYS:HB2	1.97	0.46
51:v:476:ASP:OD1	51:v:476:ASP:N	2.48	0.46
53:ZA:1093:A:H2'	53:ZA:1094:C:C6	2.50	0.46
53:ZA:1542:C:OP1	70:TB:62:ARG:NH2	2.47	0.46
53:ZA:1661:A:OP1	80:DC:19:ARG:NH2	2.47	0.46
59:IB:64:ASN:C	59:IB:64:ASN:HD22	2.23	0.46
69:SB:76:GLN:N	69:SB:76:GLN:OE1	2.48	0.46
78:BC:56:CYS:SG	78:BC:57:VAL:N	2.88	0.46
82:FC:106:TYR:HA	82:FC:117:LEU:H	1.80	0.46
11:L:96:GLU:OE2	11:L:100:ARG:NE	2.47	0.46
13:N:58:LEU:HD11	13:N:145:VAL:HG13	1.98	0.46
17:R:127:MET:HA	18:S:153:PRO:HD2	1.96	0.46
23:X:11:ARG:NH1	30:WA:229:G:OP1	2.42	0.46
29:CB:82:TYR:CE2	29:CB:164:PRO:HD3	2.50	0.46
30:WA:14:C:N3	32:YA:143:G:N1	2.37	0.46
30:WA:684:C:H2'	30:WA:685:G:O4'	2.15	0.46
30:WA:1460:G:H2'	30:WA:1461:JMH:C6	2.45	0.46
30:WA:2416:C:H2'	30:WA:2417:A:C8	2.51	0.46
30:WA:2499:U:H2'	30:WA:2500:U:C6	2.50	0.46
30:WA:4912:G:H3'	30:WA:4918:G:H21	1.80	0.46
48:PA:27:THR:O	48:PA:27:THR:OG1	2.33	0.46
51:v:746:LEU:HB2	51:v:815:ASP:HB2	1.98	0.46
53:ZA:1112:U:H2'	53:ZA:1113:A:C8	2.50	0.46
53:ZA:1407:U:H2'	53:ZA:1408:U:C6	2.50	0.46
58:HB:192:PHE:HB2	78:BC:12:PRO:HB3	1.97	0.46
63:MB:100:PRO:HB2	63:MB:103:VAL:HG22	1.97	0.46
67:QB:102:GLU:CD	83:GC:55:PRO:HG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SB:20:ILE:HD11	69:SB:33:ILE:HD11	1.97	0.46
70:TB:107:LEU:HB3	70:TB:113:VAL:HG22	1.97	0.46
71:UB:32:LEU:HD21	71:UB:87:ARG:HD3	1.97	0.46
75:YB:35:VAL:HG13	75:YB:40:ILE:HD11	1.97	0.46
5:E:277:VAL:HG21	37:EA:2:SER:HB2	1.98	0.46
7:G:155:TYR:OH	7:G:264:ASP:OD2	2.22	0.46
12:M:140:LYS:HD3	12:M:144:ARG:HH21	1.80	0.46
17:R:156:HIS:CE1	17:R:174:THR:HG21	2.50	0.46
17:R:161:ARG:HH21	30:WA:1926:C:H41	1.64	0.46
27:AB:176:TRP:CD2	27:AB:199:PRO:HB3	2.50	0.46
30:WA:1822:U:H2'	30:WA:1823:G:O4'	2.15	0.46
30:WA:2524:U:H1'	30:WA:2525:C:C6	2.50	0.46
30:WA:4961:A:H2'	30:WA:4962:C:O4'	2.15	0.46
53:ZA:77:A:N3	53:ZA:77:A:H2'	2.29	0.46
53:ZA:536:A:N6	53:ZA:547:G:O6	2.48	0.46
53:ZA:1126:G:H2'	53:ZA:1127:C:C6	2.50	0.46
53:ZA:1171:G:O2'	53:ZA:1187:G:O6	2.30	0.46
53:ZA:1361:G:OP2	53:ZA:1362:U:O2'	2.24	0.46
53:ZA:1569:A:O2'	53:ZA:1626:C:O2	2.31	0.46
53:ZA:1745:A:N3	57:GB:66:GLY:HA3	2.30	0.46
55:EB:246:LEU:HD23	55:EB:246:LEU:H	1.78	0.46
57:GB:181:THR:HG23	57:GB:184:VAL:H	1.81	0.46
60:JB:59:GLU:O	60:JB:62:THR:OG1	2.25	0.46
70:TB:42:HIS:HB2	70:TB:83:GLN:HA	1.97	0.46
73:WB:24:GLN:NE2	78:BC:5:LYS:O	2.48	0.46
1:A:54:ARG:HG2	1:A:56:ALA:H	1.80	0.46
3:C:221:PHE:HB3	3:C:227:ILE:HG21	1.97	0.46
3:C:298:ILE:O	3:C:302:LEU:HG	2.16	0.46
9:I:177:ASN:HB2	9:I:180:GLU:HG2	1.97	0.46
11:L:86:TRP:O	11:L:89:THR:HG22	2.15	0.46
12:M:172:ARG:HG2	30:WA:29:G:H5''	1.97	0.46
13:N:14:HIS:HD2	13:N:19:LEU:HD13	1.81	0.46
25:Z:28:HIS:CD2	25:Z:32:ARG:HD3	2.50	0.46
27:AB:185:MET:O	72:VB:46:PHE:N	2.48	0.46
30:WA:20:U:H3'	30:WA:21:G:C8	2.50	0.46
30:WA:221:C:H2'	30:WA:222:C:C6	2.51	0.46
30:WA:1574:U:O4	47:OA:2:ALA:N	2.48	0.46
30:WA:1582:G:C2	30:WA:3642:U:H1'	2.51	0.46
30:WA:2290:A:H2'	30:WA:2291:G:C8	2.50	0.46
30:WA:2386:A:H1'	30:WA:2388:C:P	2.55	0.46
30:WA:2687:G:H2'	30:WA:2688:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:3638:C:H2'	30:WA:3639:G:C8	2.50	0.46
30:WA:4556:U:H2'	30:WA:4557:U:C6	2.50	0.46
30:WA:4696:A:H2'	30:WA:4697:A:O4'	2.16	0.46
53:ZA:1172:U:H2'	53:ZA:1173:A:H8	1.80	0.46
64:NB:30:SER:HB3	64:NB:67:THR:HG22	1.98	0.46
7:G:215:ASP:HB2	7:G:216:PRO:HD3	1.97	0.46
14:O:94:MET:HE1	14:O:146:ILE:HB	1.96	0.46
19:T:21:PHE:CE1	19:T:80:LYS:HB2	2.51	0.46
30:WA:2557:G:H1'	30:WA:2771:A:H61	1.80	0.46
30:WA:2763:G:H2'	30:WA:2764:G:C8	2.50	0.46
30:WA:4598:C:H2'	30:WA:4599:U:H6	1.80	0.46
30:WA:4601:C:H2'	30:WA:4602:UR3:H6	1.97	0.46
44:LA:92:THR:OG1	44:LA:94:ASN:OD1	2.21	0.46
50:RA:37:LEU:HG	50:RA:38:SER:H	1.81	0.46
53:ZA:56:G:H2'	53:ZA:57:U:C6	2.50	0.46
53:ZA:393:U:O2'	53:ZA:394:G:N3	2.48	0.46
53:ZA:459:C:H2'	53:ZA:460:A:C8	2.50	0.46
53:ZA:794:A:H2'	53:ZA:795:A:C8	2.51	0.46
53:ZA:896:U:H2'	53:ZA:897:U:C6	2.51	0.46
53:ZA:1010:G:H2'	53:ZA:1011:A:C8	2.51	0.46
53:ZA:1500:G:H2'	53:ZA:1501:C:C6	2.50	0.46
53:ZA:1606:G:H1'	53:ZA:1632:G:N2	2.29	0.46
59:IB:12:ARG:HE	59:IB:18:ARG:NH1	2.13	0.46
65:OB:146:ARG:HG3	77:AC:29:CYS:SG	2.56	0.46
67:QB:40:GLU:O	67:QB:48:GLN:NE2	2.49	0.46
67:QB:50:LYS:HE3	67:QB:85:ARG:NH1	2.30	0.46
69:SB:48:ALA:HB2	69:SB:70:ILE:HD12	1.97	0.46
6:F:180:LYS:HE3	6:F:181:TYR:CZ	2.50	0.46
7:G:99:GLN:HG3	7:G:100:PRO:HD2	1.97	0.46
12:M:113:LEU:HD11	32:YA:141:C:H5'	1.97	0.46
21:V:80:ARG:NH1	57:GB:11:GLY:HA3	2.31	0.46
23:X:1:MET:HE2	30:WA:227:A:H4'	1.98	0.46
26:K:62:PRO:HG3	30:WA:74:G:H1'	1.96	0.46
27:AB:102:ARG:NH2	27:AB:103:PHE:O	2.49	0.46
29:CB:176:LYS:O	29:CB:200:ARG:NH2	2.34	0.46
29:CB:256:TRP:CD1	73:WB:68:ARG:HG2	2.51	0.46
30:WA:259:C:H2'	30:WA:260:C:C6	2.51	0.46
30:WA:1333:C:H2'	30:WA:1334:G:H8	1.80	0.46
30:WA:1660:C:O2	30:WA:4395:A:O2'	2.34	0.46
30:WA:4480:G:H5''	30:WA:4481:C:H5'	1.97	0.46
46:NA:4:VAL:O	46:NA:94:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:607:U:O4	54:DB:114:ALA:N	2.48	0.46
53:ZA:905:C:H2'	53:ZA:906:U:C6	2.51	0.46
53:ZA:956:G:H2'	53:ZA:957:A:H8	1.80	0.46
53:ZA:1017:U:H2'	53:ZA:1018:U:C6	2.51	0.46
53:ZA:1213:C:H2'	53:ZA:1214:A:C8	2.51	0.46
53:ZA:1287:A:N6	53:ZA:1312:G:H1'	2.31	0.46
53:ZA:1474:A:H2'	53:ZA:1475:G:C4	2.51	0.46
55:EB:127:ARG:HE	55:EB:142:HIS:HA	1.80	0.46
77:AC:46:GLU:OE1	77:AC:46:GLU:N	2.47	0.46
2:B:47:LEU:HD21	2:B:344:VAL:HG23	1.96	0.46
9:I:57:TYR:HD1	9:I:130:HIS:HA	1.81	0.46
9:I:171:TRP:O	9:I:174:THR:OG1	2.24	0.46
27:AB:34:MET:HG2	27:AB:154:LEU:HD11	1.97	0.46
28:BB:103:MET:HE3	28:BB:215:VAL:HG23	1.96	0.46
30:WA:714:C:H2'	30:WA:715:G:H8	1.81	0.46
30:WA:1182:C:H2'	30:WA:1183:U:H6	1.81	0.46
30:WA:1361:G:H2'	30:WA:1362:U:C6	2.50	0.46
30:WA:4347:C:O3'	46:NA:37:GLY:HA3	2.15	0.46
30:WA:4513:C:N3	30:WA:4517:U:H5	2.14	0.46
51:v:766:LYS:HE3	51:v:796:PHE:HA	1.98	0.46
53:ZA:65:C:C6	57:GB:174:PRO:HB3	2.51	0.46
53:ZA:387:C:H2'	53:ZA:388:U:C6	2.51	0.46
53:ZA:565:G:H2'	53:ZA:566:U:C6	2.51	0.46
53:ZA:1733:U:H2'	53:ZA:1734:G:O4'	2.15	0.46
8:H:120:GLU:HB2	30:WA:4617:C:O2	2.16	0.46
9:I:42:LYS:N	9:I:45:GLU:OE2	2.42	0.46
12:M:65:ARG:HD2	12:M:127:TYR:CG	2.51	0.46
13:N:54:TYR:CE1	13:N:145:VAL:HG11	2.51	0.46
18:S:70:HIS:N	30:WA:4319:C:OP1	2.47	0.46
21:V:101:ARG:HA	21:V:104:GLN:HG2	1.98	0.46
26:K:186:ARG:HE	40:HA:9:VAL:HG11	1.81	0.46
29:CB:142:LYS:HB2	29:CB:157:LEU:HD12	1.98	0.46
29:CB:191:VAL:HG13	29:CB:230:THR:HG22	1.98	0.46
29:CB:204:ILE:HD11	29:CB:220:ASP:HA	1.97	0.46
30:WA:146:G:H2'	30:WA:147:A:H8	1.81	0.46
30:WA:1516:U:H2'	30:WA:1517:G:C8	2.50	0.46
30:WA:1895:G:N2	30:WA:1944:A:H61	2.14	0.46
30:WA:2073:C:O2'	30:WA:2074:A:H5'	2.15	0.46
30:WA:2083:C:H2'	30:WA:2084:G:C8	2.51	0.46
45:MA:21:ARG:NH2	53:ZA:1175:G:OP1	2.48	0.46
51:v:430:MET:HB2	51:v:484:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1305:C:H2'	53:ZA:1306:U:C5	2.51	0.46
53:ZA:1312:G:OP2	53:ZA:1312:G:H8	1.99	0.46
53:ZA:1473:G:H2'	53:ZA:1475:G:H22	1.80	0.46
53:ZA:1652:G:H1	53:ZA:1672:U:H3	1.62	0.46
57:GB:137:ARG:HD2	57:GB:140:ARG:HG3	1.97	0.46
61:KB:3:MET:HG2	61:KB:44:HIS:CG	2.51	0.46
66:PB:98:ASN:HB3	66:PB:122:THR:HA	1.96	0.46
70:TB:72:VAL:HG22	70:TB:104:LEU:HD12	1.98	0.46
75:YB:62:THR:HA	75:YB:69:THR:HG22	1.98	0.46
83:GC:121:VAL:HG21	83:GC:165:ILE:HD13	1.98	0.46
7:G:85:PHE:HE1	24:Y:53:VAL:HG12	1.79	0.46
7:G:198:THR:O	7:G:202:ASN:ND2	2.49	0.46
15:P:53:MET:HB3	15:P:57:ASN:HB2	1.98	0.46
30:WA:113:A:C4	30:WA:114:G:C8	3.03	0.46
30:WA:680:C:H2'	30:WA:681:G:C8	2.43	0.46
30:WA:2639:C:H2'	30:WA:2640:U:C6	2.51	0.46
30:WA:2653:G:H2'	30:WA:2654:G:H8	1.80	0.46
30:WA:2683:A:H2'	30:WA:2684:G:H8	1.80	0.46
30:WA:3625:G:OP1	30:WA:3627:C:N4	2.49	0.46
30:WA:5007:U:H2'	30:WA:5008:U:H6	1.81	0.46
32:YA:87:G:OP1	39:GA:5:LYS:NZ	2.37	0.46
50:RA:26:SER:HB3	50:RA:32:ILE:HD11	1.98	0.46
51:v:539:GLU:HG3	51:v:540:GLU:H	1.80	0.46
53:ZA:457:C:C2	53:ZA:458:A:C8	3.04	0.46
53:ZA:519:A:H5''	60:JB:11:LYS:HG2	1.97	0.46
55:EB:151:ASP:HB3	55:EB:154:ILE:HG13	1.98	0.46
56:FB:142:SER:OG	79:CC:49:PRO:O	2.29	0.46
58:HB:145:ARG:HB2	73:WB:51:GLU:HG2	1.98	0.46
60:JB:131:ARG:NH1	60:JB:143:ASN:O	2.49	0.46
83:GC:8:ARG:HB2	83:GC:309:VAL:HG23	1.97	0.46
1:A:244:GLY:HA3	30:WA:3751:A:H5''	1.97	0.46
3:C:190:ARG:HB2	3:C:202:ILE:HG23	1.98	0.46
16:Q:97:ARG:HH21	30:WA:2730:A:H5''	1.81	0.46
17:R:95:ARG:NH2	17:R:112:ASP:OD2	2.44	0.46
26:K:66:TYR:OH	30:WA:1388:G:OP1	2.29	0.46
30:WA:168:C:H2'	30:WA:169:A:C8	2.51	0.46
30:WA:268:G:H2'	30:WA:269:G:C8	2.50	0.46
30:WA:1090:C:H2'	30:WA:1091:C:H6	1.81	0.46
30:WA:1433:A:H1'	30:WA:1699:C:OP1	2.16	0.46
30:WA:1509:G:H2'	30:WA:1510:C:H6	1.81	0.46
30:WA:1830:A:H2'	30:WA:1831:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:1983:C:O2'	50:RA:97:ASN:OD1	2.28	0.46
30:WA:4596:U:H2'	30:WA:4597:C:C6	2.51	0.46
30:WA:4710:A:H2'	30:WA:4711:G:O4'	2.16	0.46
53:ZA:27:A:H2'	53:ZA:28:U:C6	2.51	0.46
53:ZA:1293:A:H1'	82:FC:138:ARG:CZ	2.45	0.46
55:EB:71:LYS:NZ	55:EB:74:GLY:HA2	2.31	0.46
71:UB:22:ILE:HG22	71:UB:114:VAL:HG13	1.98	0.46
80:DC:6:LEU:HA	80:DC:9:SER:HB3	1.98	0.46
80:DC:21:CYS:HB3	80:DC:26:ASN:H	1.81	0.46
3:C:60:HIS:NE2	3:C:100:ARG:HD3	2.31	0.45
4:D:33:ARG:NE	31:XA:7:G:OP1	2.25	0.45
5:E:264:ILE:HG23	5:E:270:LEU:HD23	1.97	0.45
7:G:155:TYR:HB3	7:G:188:VAL:HA	1.97	0.45
30:WA:521:U:H3	30:WA:642:G:H1	1.64	0.45
30:WA:1792:A:N3	30:WA:4215:U:O2'	2.47	0.45
30:WA:2085:U:H2'	30:WA:2086:C:H6	1.81	0.45
30:WA:2629:G:H2'	30:WA:2630:U:C6	2.51	0.45
30:WA:2758:G:H2'	30:WA:2759:B9B:C4	2.46	0.45
30:WA:4764:C:H2'	30:WA:4765:G:C8	2.52	0.45
36:DA:85:LEU:HD11	36:DA:111:ILE:HG23	1.99	0.45
53:ZA:986:G:H22	65:OB:135:ILE:HD13	1.81	0.45
83:GC:298:LEU:HD22	83:GC:310:TRP:HD1	1.81	0.45
2:B:389:MET:O	30:WA:5046:G:N1	2.42	0.45
4:D:232:THR:OG1	4:D:234:ASP:OD1	2.24	0.45
9:I:150:GLU:OE2	9:I:153:ARG:NH2	2.48	0.45
11:L:24:LEU:O	11:L:43:THR:OG1	2.30	0.45
13:N:14:HIS:HE1	13:N:119:VAL:HG23	1.82	0.45
15:P:97:LYS:HG3	15:P:118:GLY:HA2	1.97	0.45
19:T:105:ASN:OD1	19:T:109:SER:OG	2.25	0.45
23:X:22:PRO:HB2	32:YA:90:C:O2'	2.16	0.45
24:Y:12:LEU:HB2	24:Y:81:MET:HB3	1.99	0.45
27:AB:91:ALA:HB1	27:AB:96:ALA:O	2.16	0.45
30:WA:1081:G:H1	30:WA:1241:G:H22	1.63	0.45
30:WA:1332:A2M:HM'3	30:WA:1332:A2M:H1'	1.74	0.45
30:WA:1805:U:H2'	30:WA:1806:A:H8	1.78	0.45
30:WA:3604:A:H2'	30:WA:3605:G:C8	2.51	0.45
32:YA:64:U:C2	32:YA:65:A:C8	3.05	0.45
36:DA:75:ARG:HB2	36:DA:95:TYR:CD2	2.51	0.45
53:ZA:568:C:H2'	53:ZA:569:A:O4'	2.16	0.45
53:ZA:1280:G:H2'	53:ZA:1281:G:C8	2.52	0.45
53:ZA:1471:C:H2'	53:ZA:1472:C:H6	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:FB:31:ASN:ND2	56:FB:114:ASN:OD1	2.49	0.45
62:LB:68:ILE:HD13	62:LB:131:CYS:HB3	1.99	0.45
1:A:21:LYS:HD2	30:WA:1546:C:H5''	1.98	0.45
13:N:85:ARG:HG3	13:N:99:LEU:HD11	1.98	0.45
28:BB:62:LEU:HD23	28:BB:91:VAL:HG11	1.96	0.45
30:WA:2417:A:H2'	30:WA:2418:U:C6	2.51	0.45
30:WA:4268:C:H2'	30:WA:4269:G:O4'	2.16	0.45
30:WA:4904:G:O2'	30:WA:4907:C:O4'	2.32	0.45
51:v:30:HIS:O	51:v:158:ASN:ND2	2.44	0.45
53:ZA:884:C:H2'	53:ZA:885:U:O4'	2.16	0.45
53:ZA:1129:G:O2'	53:ZA:1130:G:O4'	2.24	0.45
53:ZA:1456:G:H2'	53:ZA:1457:U:C6	2.51	0.45
53:ZA:1456:G:H2'	53:ZA:1457:U:H6	1.81	0.45
53:ZA:1541:G:H4'	70:TB:15:VAL:HG21	1.97	0.45
55:EB:9:LEU:HB2	55:EB:30:ARG:HD3	1.99	0.45
77:AC:46:GLU:HG2	77:AC:47:ALA:N	2.31	0.45
3:C:180:ILE:HD11	3:C:227:ILE:HD11	1.98	0.45
3:C:274:LYS:NZ	30:WA:1381:C:OP1	2.49	0.45
9:I:115:MET:HE3	30:WA:1873:A:H61	1.82	0.45
11:L:117:LYS:NZ	30:WA:4934:C:OP1	2.49	0.45
24:Y:136:PHE:OXT	30:WA:4127:G:O2'	2.34	0.45
30:WA:318:A:H2'	30:WA:319:A:C8	2.51	0.45
30:WA:381:U:H2'	30:WA:382:G:O4'	2.16	0.45
30:WA:1333:C:N4	30:WA:1334:G:O6	2.49	0.45
43:KA:25:GLN:O	43:KA:28:TRP:NE1	2.49	0.45
51:v:127:VAL:HG21	51:v:143:LEU:HD13	1.98	0.45
53:ZA:110:U:O2'	53:ZA:111:A:OP1	2.27	0.45
53:ZA:470:G:H2'	53:ZA:471:G:C8	2.52	0.45
53:ZA:1365:G:H2'	53:ZA:1366:G:H8	1.80	0.45
53:ZA:1689:C:H2'	53:ZA:1690:U:C6	2.51	0.45
71:UB:54:VAL:O	71:UB:87:ARG:HG3	2.15	0.45
76:ZB:94:LYS:HB3	76:ZB:96:LEU:HD13	1.97	0.45
83:GC:285:GLN:N	83:GC:303:THR:OG1	2.50	0.45
1:A:243:THR:OG1	30:WA:3753:A:H5''	2.16	0.45
2:B:161:ARG:HB3	2:B:184:GLN:HA	1.98	0.45
10:J:20:LEU:HD13	10:J:132:VAL:HG22	1.99	0.45
19:T:84:LYS:HB2	19:T:110:TYR:CZ	2.52	0.45
27:AB:55:TRP:CZ2	27:AB:59:LEU:HD21	2.51	0.45
30:WA:162:A:H2'	30:WA:163:A:H8	1.81	0.45
30:WA:442:G:OP1	37:EA:51:TYR:OH	2.35	0.45
30:WA:2379:A:H5'	35:CA:64:ILE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2649:G:H2'	30:WA:2650:G:C8	2.52	0.45
30:WA:2789:C:H2'	30:WA:2790:C:H6	1.81	0.45
30:WA:4459:G:HO2'	30:WA:4505:PSU:HO2'	1.64	0.45
30:WA:4969:C:H5''	30:WA:4970:U:H5	1.81	0.45
34:BA:47:ILE:HD12	34:BA:94:LEU:HD11	1.98	0.45
47:OA:11:VAL:HG21	47:OA:23:ARG:O	2.16	0.45
50:RA:56:LEU:HD13	50:RA:82:ILE:HG23	1.98	0.45
53:ZA:824:C:C2	60:JB:144:ILE:HG12	2.51	0.45
53:ZA:986:G:C5	65:OB:137:SER:HA	2.52	0.45
53:ZA:1221:G:H2'	53:ZA:1222:G:H8	1.81	0.45
57:GB:51:ARG:N	57:GB:112:VAL:O	2.40	0.45
74:XB:39:ASN:ND2	74:XB:43:GLY:H	2.15	0.45
78:BC:50:ALA:O	78:BC:51:GLN:HG2	2.16	0.45
84:b:257:LEU:HD13	84:b:262:SER:HB3	1.98	0.45
4:D:197:LYS:HB3	4:D:202:GLN:HB2	1.99	0.45
7:G:308:LYS:HE3	7:G:308:LYS:HB3	1.73	0.45
21:V:35:LYS:HE2	21:V:51:TRP:CZ2	2.51	0.45
30:WA:221:C:H2'	30:WA:222:C:H6	1.81	0.45
30:WA:3630:G:O2'	30:WA:3631:G:OP1	2.31	0.45
30:WA:3872:A2M:H2'	30:WA:3873:G:C8	2.51	0.45
30:WA:5035:U:H2'	30:WA:5036:G:H8	1.82	0.45
37:EA:36:ARG:O	37:EA:39:THR:HG22	2.16	0.45
51:v:352:GLN:O	51:v:356:ILE:HG12	2.16	0.45
51:v:774:SER:HB2	51:v:783:VAL:HG13	1.98	0.45
53:ZA:381:C:H5'	59:IB:48:VAL:HG13	1.99	0.45
53:ZA:928:G:H2'	53:ZA:929:G:H8	1.81	0.45
53:ZA:1277:C:H2'	53:ZA:1278:A:H8	1.80	0.45
53:ZA:1752:C:H3'	53:ZA:1753:C:H5''	1.97	0.45
53:ZA:1788:A:H2'	53:ZA:1789:G:O4'	2.16	0.45
57:GB:67:VAL:HG11	57:GB:99:GLY:HA2	1.99	0.45
61:KB:91:PRO:HD2	61:KB:94:LEU:HD22	1.98	0.45
62:LB:113:LEU:HD23	62:LB:142:VAL:HG21	1.98	0.45
69:SB:34:LYS:HE2	69:SB:103:LEU:HD23	1.99	0.45
77:AC:60:ASP:OD1	77:AC:60:ASP:N	2.49	0.45
81:EC:95:GLN:HB2	81:EC:97:LYS:HE2	1.98	0.45
1:A:182:ALA:HB2	30:WA:3657:A:O2'	2.17	0.45
11:L:29:ASP:OD1	11:L:30:VAL:N	2.48	0.45
30:WA:1398:A:H2'	30:WA:1399:G:C8	2.51	0.45
30:WA:1510:C:H2'	30:WA:1511:G:C8	2.51	0.45
30:WA:2269:C:H2'	30:WA:2270:G:O4'	2.16	0.45
30:WA:2545:C:H2'	30:WA:2546:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:2700:A:H1'	30:WA:2702:A:N7	2.32	0.45
30:WA:4716:C:H2'	30:WA:4717:C:C6	2.51	0.45
35:CA:85:ARG:NH2	35:CA:118:GLN:O	2.42	0.45
53:ZA:151:C:H2'	53:ZA:152:U:H6	1.80	0.45
53:ZA:602:G:OP2	53:ZA:603:C:O2'	2.32	0.45
53:ZA:851:C:H4'	53:ZA:852:G:H8	1.81	0.45
53:ZA:1430:C:H2'	53:ZA:1431:G:H8	1.82	0.45
53:ZA:1538:C:H2'	53:ZA:1539:U:C6	2.52	0.45
53:ZA:1673:U:H2'	53:ZA:1674:G:O4'	2.17	0.45
53:ZA:1860:A:N7	77:AC:34:LYS:NZ	2.64	0.45
69:SB:62:ASP:OD1	69:SB:63:GLU:N	2.49	0.45
77:AC:25:ASN:OD1	77:AC:26:CYS:N	2.49	0.45
79:CC:13:ARG:N	79:CC:33:GLU:O	2.44	0.45
83:GC:17:TRP:HE1	83:GC:36:ARG:NH1	2.15	0.45
1:A:152:SER:OG	30:WA:3666:G:N7	2.49	0.45
6:F:226:PHE:N	6:F:232:ALA:O	2.49	0.45
7:G:126:ARG:NH2	30:WA:4167:C:O2	2.39	0.45
10:J:37:ALA:HB2	10:J:50:PHE:HE1	1.82	0.45
15:P:54:SER:O	15:P:58:ARG:HG2	2.16	0.45
24:Y:59:LYS:O	24:Y:62:ILE:HG13	2.17	0.45
30:WA:307:A:O5'	30:WA:307:A:H8	1.99	0.45
30:WA:1313:A:H2'	30:WA:1314:C:H6	1.82	0.45
30:WA:1482:C:H2'	30:WA:1483:C:H6	1.82	0.45
30:WA:1738:G:N3	30:WA:4219:A:H2'	2.32	0.45
30:WA:2263:C:H5''	30:WA:2264:G:C8	2.52	0.45
32:YA:93:C:H3'	41:IA:72:ARG:HH12	1.82	0.45
51:v:453:MET:N	51:v:453:MET:SD	2.89	0.45
53:ZA:537:C:O2'	53:ZA:538:U:O5'	2.35	0.45
53:ZA:821:G:H5''	60:JB:150:ARG:HH22	1.80	0.45
53:ZA:1480:A:O5'	67:QB:131:LYS:HE2	2.17	0.45
53:ZA:1643:U:H2'	53:ZA:1644:C:C6	2.51	0.45
59:IB:66:SER:HA	59:IB:73:THR:HG22	1.98	0.45
69:SB:39:ARG:HG3	69:SB:83:PHE:HZ	1.82	0.45
70:TB:104:LEU:HB3	70:TB:121:ARG:HE	1.81	0.45
73:WB:87:GLU:HA	73:WB:90:GLN:HG2	1.99	0.45
74:XB:85:VAL:HB	74:XB:90:CYS:HB2	1.99	0.45
84:b:162:GLN:HG3	84:b:164:THR:H	1.82	0.45
1:A:221:LYS:HD3	1:A:233:ARG:NH2	2.32	0.45
3:C:60:HIS:HA	3:C:92:PHE:HE1	1.82	0.45
5:E:261:LEU:HG	5:E:265:LYS:HE3	1.99	0.45
6:F:102:PRO:HA	6:F:105:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:217:ILE:HD12	7:G:217:ILE:HA	1.82	0.45
8:H:104:VAL:HG23	8:H:113:GLU:HB2	1.99	0.45
14:O:94:MET:HG2	14:O:148:MET:HE2	1.98	0.45
26:K:61:CYS:SG	30:WA:102:G:H5''	2.57	0.45
28:BB:97:LEU:HD12	28:BB:232:HIS:CE1	2.52	0.45
29:CB:81:ILE:HG23	29:CB:86:LEU:HB2	1.99	0.45
30:WA:1317:G:H2'	30:WA:1318:A:O4'	2.17	0.45
30:WA:2116:U:N3	30:WA:2117:G:N7	2.65	0.45
30:WA:2687:G:H2'	30:WA:2688:C:H6	1.81	0.45
36:DA:99:ILE:HB	36:DA:124:ASN:HD21	1.82	0.45
38:FA:60:ARG:HB2	38:FA:63:VAL:HG23	1.97	0.45
49:QA:198:ILE:H	49:QA:198:ILE:HG13	1.54	0.45
53:ZA:164:A:H2'	53:ZA:165:G:C4	2.52	0.45
53:ZA:1267:C:N3	53:ZA:1516:G:N1	2.64	0.45
53:ZA:1370:A:H2'	53:ZA:1372:U:H5'	1.99	0.45
53:ZA:1518:C:OP1	53:ZA:1519:U:O2'	2.26	0.45
53:ZA:1706:G:H2'	53:ZA:1707:U:H6	1.81	0.45
55:EB:11:ARG:N	55:EB:26:VAL:O	2.39	0.45
56:FB:124:ASP:OD1	56:FB:125:SER:N	2.50	0.45
60:JB:49:THR:HA	60:JB:52:LYS:HZ3	1.82	0.45
64:NB:4:MET:HG2	64:NB:5:HIS:CE1	2.52	0.45
65:OB:28:PHE:HB3	65:OB:47:LEU:HD11	1.97	0.45
66:PB:85:ILE:HG22	66:PB:112:ILE:HD13	1.99	0.45
69:SB:28:PHE:O	69:SB:31:THR:OG1	2.28	0.45
76:ZB:46:ASN:HB3	76:ZB:79:ILE:C	2.42	0.45
2:B:25:HIS:CG	30:WA:4989:C:H4'	2.52	0.45
6:F:30:LYS:HG3	30:WA:1444:U:H6	1.80	0.45
14:O:16:LYS:HG2	14:O:149:ILE:HG12	1.99	0.45
14:O:83:TRP:O	30:WA:3861:A:H5''	2.16	0.45
15:P:67:ILE:HD11	15:P:98:LEU:HD11	1.99	0.45
15:P:178:ARG:N	25:Z:51:GLY:HA2	2.32	0.45
24:Y:135:ARG:HH12	30:WA:2758:G:H5'	1.82	0.45
28:BB:129:THR:HG22	28:BB:176:VAL:HG22	1.99	0.45
29:CB:132:ASP:HB3	29:CB:136:HIS:HB2	1.99	0.45
30:WA:44:A:N3	30:WA:94:A:H2	2.15	0.45
30:WA:48:G:H2'	30:WA:48:G:N3	2.32	0.45
30:WA:416:U:H2'	30:WA:417:G:O4'	2.17	0.45
30:WA:989:U:H2'	30:WA:990:C:C6	2.52	0.45
30:WA:1215:U:O2'	30:WA:1217:G:H5'	2.17	0.45
30:WA:1477:C:H2'	30:WA:1478:U:C6	2.52	0.45
30:WA:2607:G:H2'	30:WA:2608:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4403:C:C2'	30:WA:4404:U:H5'	2.47	0.45
30:WA:4464:U:H2'	30:WA:4465:U:H6	1.82	0.45
37:EA:33:VAL:HG12	37:EA:38:GLU:HB3	1.99	0.45
40:HA:77:VAL:HG21	40:HA:86:LYS:HD2	1.98	0.45
51:v:219:HIS:HA	51:v:337:LYS:HE3	1.99	0.45
51:v:692:LEU:O	51:v:839:ARG:NH2	2.50	0.45
51:v:804:THR:HG22	51:v:807:GLN:HB2	1.99	0.45
53:ZA:101:U:H5''	59:IB:19:LYS:HE3	1.99	0.45
53:ZA:115:U:H2'	53:ZA:116:U:C6	2.52	0.45
53:ZA:128:U:H3'	53:ZA:129:C:H6	1.82	0.45
53:ZA:128:U:H3'	53:ZA:129:C:C6	2.53	0.45
53:ZA:455:A:P	57:GB:94:ARG:HG3	2.57	0.45
53:ZA:508:A:H3'	53:ZA:509:G:H8	1.81	0.45
53:ZA:1100:A:H4'	68:RB:132:ARG:NH1	2.31	0.45
53:ZA:1584:G:C4	53:ZA:1586:U:H1'	2.51	0.45
53:ZA:1692:U:H2'	53:ZA:1693:G:H8	1.82	0.45
56:FB:89:THR:HA	56:FB:92:ILE:HG22	1.99	0.45
57:GB:162:LEU:N	57:GB:170:ARG:O	2.45	0.45
62:LB:84:ARG:HB3	62:LB:112:HIS:CE1	2.52	0.45
79:CC:29:GLN:HA	79:CC:45:ASN:HA	1.98	0.45
83:GC:17:TRP:HE1	83:GC:36:ARG:HH11	1.64	0.45
8:H:94:SER:HB3	8:H:142:ASP:HB3	1.98	0.44
13:N:156:LEU:HD23	30:WA:4915:A:C4	2.52	0.44
14:O:64:ASN:ND2	30:WA:3897:U:H4'	2.32	0.44
30:WA:2416:C:H2'	30:WA:2417:A:H8	1.81	0.44
30:WA:2544:C:H2'	30:WA:2545:C:H6	1.81	0.44
32:YA:28:C:H2'	32:YA:29:G:H8	1.82	0.44
32:YA:102:G:H5''	41:IA:39:TYR:HE1	1.82	0.44
39:GA:89:ARG:HA	39:GA:92:ARG:HH21	1.82	0.44
51:v:231:MET:HE1	51:v:343:TRP:HE1	1.82	0.44
51:v:609:PHE:CE1	51:v:701:ARG:HB2	2.53	0.44
51:v:609:PHE:HE1	51:v:701:ARG:HB2	1.81	0.44
53:ZA:156:G:N2	57:GB:60:GLY:O	2.38	0.44
53:ZA:944:A:O2'	65:OB:136:PRO:HB3	2.17	0.44
53:ZA:1566:G:N1	53:ZA:1568:C:OP2	2.51	0.44
53:ZA:1706:G:O2'	53:ZA:1850:A:O3'	2.35	0.44
53:ZA:1805:G:H2'	53:ZA:1806:A:C8	2.53	0.44
66:PB:49:LEU:HB2	66:PB:54:HIS:CE1	2.51	0.44
70:TB:51:ASN:OD1	70:TB:51:ASN:N	2.48	0.44
4:D:178:LYS:HE2	4:D:179:ARG:HH12	1.81	0.44
5:E:175:LEU:HD21	30:WA:4946:G:C5	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:ARG:NH2	30:WA:1900:G:OP1	2.50	0.44
13:N:6:VAL:HG22	13:N:32:LYS:HB2	2.00	0.44
23:X:52:ASP:HB2	23:X:110:LYS:HG3	1.98	0.44
30:WA:36:U:H5''	30:WA:1657:U:O4'	2.17	0.44
30:WA:161:G:H2'	30:WA:162:A:H8	1.81	0.44
30:WA:665:G:H2'	30:WA:666:C:C6	2.53	0.44
30:WA:934:G:O2'	30:WA:935:C:O4'	2.35	0.44
30:WA:1762:U:H2'	30:WA:1763:G:H8	1.82	0.44
30:WA:2055:OMG:HM23	30:WA:2055:OMG:H1'	1.71	0.44
30:WA:2700:A:H4'	30:WA:2701:A:H5'	2.00	0.44
30:WA:4197:A:H2'	30:WA:4198:C:H6	1.82	0.44
30:WA:4329:A:H2'	30:WA:4330:A:C8	2.52	0.44
30:WA:4877:2MG:HM22	30:WA:4879:A:N6	2.31	0.44
50:RA:124:GLU:HG2	50:RA:125:LEU:H	1.82	0.44
51:v:254:GLU:HA	51:v:257:MET:HE2	1.98	0.44
51:v:672:LEU:HD13	51:v:707:VAL:HG21	2.00	0.44
53:ZA:929:G:N2	53:ZA:1104:G:H4'	2.32	0.44
53:ZA:1055:A:H61	53:ZA:1064:C:N4	2.15	0.44
61:KB:48:ALA:O	61:KB:51:SER:OG	2.25	0.44
84:b:159:PRO:HG3	84:b:325:LEU:HD21	1.99	0.44
2:B:52:GLY:HA2	2:B:341:LYS:HE3	1.98	0.44
15:P:124:ASP:OD1	15:P:125:GLN:N	2.51	0.44
24:Y:89:ILE:HG12	24:Y:91:LEU:HG	1.99	0.44
28:BB:32:ASP:O	28:BB:96:CYS:N	2.43	0.44
30:WA:490:C:H2'	30:WA:491:C:C6	2.53	0.44
30:WA:1333:C:H2'	30:WA:1334:G:C8	2.52	0.44
30:WA:2297:C:H2'	30:WA:2298:U:C6	2.52	0.44
30:WA:4074:U:H2'	30:WA:4075:U:C6	2.52	0.44
30:WA:4774:G:H2'	30:WA:4775:U:O4'	2.17	0.44
37:EA:36:ARG:HG3	37:EA:80:ASN:HA	1.99	0.44
51:v:390:PRO:HB3	51:v:465:PRO:HG3	2.00	0.44
53:ZA:85:A:H2'	53:ZA:86:C:H6	1.82	0.44
53:ZA:1221:G:H2'	53:ZA:1222:G:C8	2.52	0.44
55:EB:212:ASP:OD1	55:EB:216:ASN:N	2.50	0.44
59:IB:57:ALA:HB2	59:IB:183:GLY:HA2	2.00	0.44
61:KB:14:LEU:HD21	61:KB:34:GLU:HG2	1.99	0.44
2:B:20:LYS:HD3	30:WA:4722:A:H4'	1.99	0.44
3:C:284:MET:HE3	15:P:124:ASP:HB3	1.98	0.44
5:E:108:ARG:HH21	30:WA:469:C:H42	1.66	0.44
17:R:71:SER:O	17:R:76:LYS:NZ	2.51	0.44
30:WA:1509:G:H2'	30:WA:1510:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:3828:G:H5'	30:WA:3829:A:OP1	2.17	0.44
30:WA:4465:U:H2'	30:WA:4466:C:C6	2.53	0.44
30:WA:4605:G:O2'	30:WA:4614:G:O6	2.29	0.44
30:WA:4728:A:H2'	30:WA:4729:A:H8	1.82	0.44
30:WA:4892:C:H2'	30:WA:4893:C:C6	2.52	0.44
31:XA:3:C:H2'	31:XA:4:U:H6	1.81	0.44
51:v:19:ILE:HA	51:v:99:LEU:O	2.18	0.44
51:v:668:GLY:HA2	53:ZA:1503:C:O2'	2.18	0.44
53:ZA:639:C:H2'	53:ZA:640:A:C8	2.53	0.44
53:ZA:944:A:H1'	65:OB:136:PRO:HB3	2.00	0.44
53:ZA:1260:A:H2	53:ZA:1619:A:H2'	1.83	0.44
53:ZA:1401:A:H2'	53:ZA:1402:A:C8	2.53	0.44
53:ZA:1427:C:H2'	53:ZA:1429:G:H8	1.82	0.44
53:ZA:1517:G:H2'	53:ZA:1518:C:C2	2.53	0.44
53:ZA:1780:G:O2'	53:ZA:1781:A:O4'	2.23	0.44
53:ZA:1839:U:H1'	53:ZA:1863:A:N1	2.33	0.44
54:DB:29:LEU:HD22	54:DB:58:VAL:HG23	1.98	0.44
59:IB:38:ILE:HA	59:IB:60:LEU:O	2.17	0.44
59:IB:107:THR:OG1	59:IB:108:PRO:HD3	2.18	0.44
63:MB:59:PRO:O	63:MB:63:LYS:HD3	2.17	0.44
65:OB:116:LEU:HD23	65:OB:119:LEU:HD21	1.99	0.44
75:YB:98:GLU:OE2	75:YB:101:LYS:NZ	2.47	0.44
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.82	0.44
2:B:93:VAL:HG23	2:B:102:PHE:HB2	2.00	0.44
3:C:95:MET:HE3	3:C:95:MET:HB2	1.88	0.44
29:CB:172:ASN:OD1	29:CB:173:LYS:N	2.50	0.44
30:WA:436:C:H2'	30:WA:437:G:H8	1.83	0.44
30:WA:2100:A:H2'	30:WA:2101:G:C8	2.52	0.44
30:WA:2389:U:H2'	30:WA:2390:U:C6	2.52	0.44
30:WA:2506:C:H2'	30:WA:2507:A:O4'	2.17	0.44
30:WA:2815:U:H2'	30:WA:2816:G:O4'	2.18	0.44
30:WA:3782:G:O2'	30:WA:3820:G:O6	2.31	0.44
30:WA:4160:C:H2'	30:WA:4161:G:O4'	2.18	0.44
31:XA:110:G:H2'	31:XA:111:C:H6	1.83	0.44
32:YA:15:G:H2'	32:YA:16:G:C8	2.52	0.44
32:YA:66:A:H2'	32:YA:67:U:H6	1.81	0.44
51:v:79:TYR:HE2	51:v:81:LEU:HD23	1.82	0.44
53:ZA:1512:C:O2'	80:DC:7:TYR:O	2.30	0.44
53:ZA:1552:G:O4'	54:DB:9:ARG:NH1	2.50	0.44
53:ZA:1720:U:H5''	53:ZA:1721:U:H5''	2.00	0.44
73:WB:112:ASP:OD1	73:WB:112:ASP:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:TYR:O	33:AA:117:ARG:NE	2.51	0.44
12:M:41:ARG:NH1	30:WA:8:U:OP1	2.51	0.44
15:P:179:GLY:H	25:Z:51:GLY:H	1.64	0.44
16:Q:44:LEU:HD22	16:Q:49:LEU:HD12	1.99	0.44
28:BB:155:TYR:OH	53:ZA:989:C:OP2	2.23	0.44
30:WA:129:C:H2'	30:WA:130:C:C6	2.53	0.44
30:WA:518:C:H2'	30:WA:519:G:C8	2.53	0.44
30:WA:728:C:H2'	30:WA:729:U:C6	2.52	0.44
30:WA:1524:C:H2'	30:WA:1525:C:C6	2.52	0.44
30:WA:1782:C:H2'	30:WA:1783:C:H6	1.83	0.44
30:WA:4634:U:H2'	30:WA:4635:G:H8	1.82	0.44
51:v:86:LEU:HD11	51:v:96:ALA:HB2	1.99	0.44
53:ZA:161:U:O4	75:YB:115:LYS:NZ	2.33	0.44
53:ZA:220:U:O4	53:ZA:302:A:N6	2.38	0.44
53:ZA:432:G:H2'	53:ZA:433:A:H8	1.82	0.44
53:ZA:566:U:H2'	53:ZA:567:C:O4'	2.18	0.44
53:ZA:993:G:OP1	53:ZA:1131:G:N2	2.48	0.44
53:ZA:1218:C:H2'	53:ZA:1219:JMH:C6	2.47	0.44
53:ZA:1521:C:O2'	69:SB:136:THR:O	2.28	0.44
53:ZA:1594:A:H62	76:ZB:104:ARG:NH1	2.16	0.44
60:JB:37:LEU:HD11	60:JB:106:LEU:HD21	2.00	0.44
64:NB:16:LEU:HB2	73:WB:57:ARG:NH2	2.33	0.44
3:C:77:PRO:O	3:C:90:GLY:HA2	2.18	0.44
3:C:209:VAL:HB	3:C:229:LEU:HD13	1.99	0.44
4:D:205:ALA:HB1	4:D:233:PRO:HB3	1.99	0.44
14:O:121:LYS:O	32:YA:13:G:O2'	2.34	0.44
16:Q:68:LEU:HA	16:Q:71:ARG:HD3	1.99	0.44
19:T:80:LYS:HZ1	19:T:109:SER:H	1.65	0.44
30:WA:2272:U:C2	48:PA:24:THR:HG21	2.52	0.44
30:WA:2637:U:H2'	30:WA:2638:U:C6	2.53	0.44
30:WA:2645:G:H2'	30:WA:2646:A:C8	2.53	0.44
30:WA:4139:C:H2'	30:WA:4140:G:C8	2.53	0.44
30:WA:4573:A:O2'	30:WA:4986:G:N7	2.50	0.44
31:XA:38:U:H1'	31:XA:42:A:H61	1.82	0.44
37:EA:63:LYS:HD2	37:EA:64:PRO:HD2	1.99	0.44
50:RA:117:ARG:HH22	50:RA:125:LEU:HA	1.83	0.44
53:ZA:31:U:H2'	53:ZA:32:U:C6	2.53	0.44
53:ZA:177:G:O2'	53:ZA:313:A:N6	2.51	0.44
53:ZA:382:C:H2'	53:ZA:383:G:C8	2.52	0.44
53:ZA:683:G:N1	53:ZA:1022:U:OP2	2.33	0.44
53:ZA:688:U:H1'	53:ZA:689:U:OP2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1427:C:H2'	53:ZA:1429:G:C8	2.52	0.44
53:ZA:1589:A:N3	53:ZA:1653:U:O2'	2.45	0.44
53:ZA:1809:A:H2'	53:ZA:1810:U:C6	2.52	0.44
59:IB:36:THR:HG21	59:IB:179:PRO:HB2	2.00	0.44
66:PB:31:GLU:H	66:PB:31:GLU:CD	2.25	0.44
67:QB:9:SER:HB2	67:QB:24:HIS:HE1	1.83	0.44
1:A:109:GLU:OE2	1:A:139:HIS:ND1	2.50	0.44
4:D:286:SER:OG	30:WA:1186:C:OP2	2.25	0.44
8:H:43:VAL:O	30:WA:4769:A:O2'	2.21	0.44
12:M:178:HIS:HA	12:M:181:HIS:NE2	2.33	0.44
21:V:104:GLN:HA	21:V:107:GLN:HG2	1.99	0.44
23:X:126:ARG:HB3	30:WA:196:C:H4'	2.00	0.44
25:Z:4:ARG:NH2	30:WA:2346:A:OP2	2.37	0.44
26:K:103:ARG:NH2	30:WA:325:U:H5''	2.33	0.44
30:WA:379:G:O2'	30:WA:380:U:H5'	2.18	0.44
30:WA:1206:G:H2'	30:WA:1207:U:C6	2.53	0.44
30:WA:1674:A:H4'	30:WA:1690:G:N2	2.32	0.44
30:WA:1830:A:H2'	30:WA:1831:G:H8	1.83	0.44
30:WA:1871:UR3:O5'	30:WA:1871:UR3:H6	2.17	0.44
30:WA:2056:C:H2'	30:WA:2057:G:O4'	2.18	0.44
30:WA:2449:U:O2'	32:YA:112:G:O2'	2.35	0.44
30:WA:2470:C:H1'	30:WA:3677:G:H22	1.83	0.44
30:WA:2470:C:H2'	30:WA:2471:G:O4'	2.17	0.44
50:RA:130:LYS:NZ	50:RA:151:ILE:HA	2.32	0.44
51:v:259:LYS:HB3	51:v:264:ARG:NH1	2.32	0.44
51:v:829:SER:O	51:v:832:SER:OG	2.30	0.44
52:w:191:ARG:HD3	52:w:191:ARG:HA	1.85	0.44
53:ZA:141:A:N1	53:ZA:178:C:N4	2.66	0.44
53:ZA:150:A:H61	57:GB:133:LEU:HD13	1.82	0.44
53:ZA:479:C:H2'	53:ZA:480:G:C8	2.53	0.44
53:ZA:916:A:C5	64:NB:73:ARG:HD3	2.52	0.44
53:ZA:957:A:C5	53:ZA:958:G:C2	3.06	0.44
53:ZA:1703:C:H2'	53:ZA:1704:C:O4'	2.17	0.44
55:EB:103:TYR:CG	55:EB:189:LEU:HD11	2.52	0.44
56:FB:92:ILE:HD11	56:FB:169:ILE:HG23	1.98	0.44
59:IB:46:VAL:HG21	59:IB:56:ARG:HE	1.83	0.44
67:QB:34:VAL:O	67:QB:37:ARG:HG2	2.17	0.44
83:GC:21:ILE:HD11	83:GC:31:ILE:HD11	2.00	0.44
1:A:6:ARG:HH12	1:A:199:VAL:H	1.65	0.44
7:G:96:GLN:HE22	30:WA:4121:C:H3'	1.82	0.44
7:G:216:PRO:C	7:G:218:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:143:HIS:HA	13:N:147:TRP:HB3	2.00	0.44
24:Y:51:ARG:HB3	24:Y:65:ARG:HH21	1.83	0.44
30:WA:747:G:H2'	30:WA:748:A:C8	2.53	0.44
30:WA:1213:C:H2'	30:WA:1214:G:C8	2.52	0.44
30:WA:1539:A2M:H8	30:WA:1642:A:H61	1.83	0.44
30:WA:4602:UR3:H6	30:WA:4602:UR3:O5'	2.17	0.44
30:WA:4959:G:H2'	30:WA:4960:A:H8	1.82	0.44
32:YA:40:A:H2'	32:YA:41:A:C8	2.52	0.44
32:YA:132:G:H2'	32:YA:133:G:H8	1.83	0.44
36:DA:79:VAL:N	36:DA:98:GLU:O	2.45	0.44
51:v:15:LYS:O	51:v:16:LYS:HG2	2.17	0.44
53:ZA:531:A:H2'	53:ZA:532:C:O4'	2.18	0.44
53:ZA:1062:A:H2'	53:ZA:1063:C:C6	2.53	0.44
53:ZA:1343:U:H2'	53:ZA:1344:A:O4'	2.18	0.44
53:ZA:1628:C:H2'	53:ZA:1629:C:C6	2.53	0.44
54:DB:113:LEU:HD21	54:DB:118:ALA:HB2	1.99	0.44
57:GB:137:ARG:HD3	57:GB:178:ARG:NH2	2.33	0.44
1:A:23:ARG:HA	1:A:52:PRO:HD2	1.99	0.43
1:A:104:VAL:HG23	1:A:162:ASN:O	2.18	0.43
2:B:234:ARG:NH2	2:B:268:ARG:O	2.31	0.43
2:B:286:LYS:HB3	2:B:332:MET:HE2	1.99	0.43
10:J:19:LYS:HB2	10:J:75:ARG:NH1	2.33	0.43
13:N:54:TYR:OH	13:N:73:PHE:O	2.36	0.43
17:R:160:ARG:HB3	30:WA:1926:C:H1'	1.99	0.43
30:WA:478:G:H2'	30:WA:479:G:C8	2.52	0.43
30:WA:748:A:O2'	30:WA:749:A:H5'	2.18	0.43
30:WA:1319:C:O2	30:WA:3886:G:O2'	2.31	0.43
30:WA:1598:A:H5''	30:WA:2844:U:H5''	2.00	0.43
30:WA:1969:A:H3'	30:WA:1970:G:H8	1.83	0.43
30:WA:2522:A:O2'	38:FA:66:ARG:NH2	2.51	0.43
30:WA:2542:A:OP2	42:JA:37:ARG:NH2	2.51	0.43
30:WA:4440:U:H2'	30:WA:4441:U:C6	2.53	0.43
53:ZA:349:A:H2'	53:ZA:350:C:C6	2.53	0.43
53:ZA:396:U:H4'	59:IB:14:THR:HG22	2.00	0.43
53:ZA:1006:C:H2'	53:ZA:1007:C:C6	2.53	0.43
53:ZA:1689:C:H2'	53:ZA:1690:U:H6	1.83	0.43
54:DB:135:GLU:N	54:DB:187:LYS:O	2.47	0.43
58:HB:60:ILE:HG23	58:HB:90:LYS:HD2	1.99	0.43
77:AC:10:ARG:HB2	77:AC:33:ASP:OD2	2.17	0.43
9:I:30:LYS:HG3	9:I:66:GLU:OE1	2.19	0.43
30:WA:300:A:H2'	30:WA:301:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:311:G:H2'	30:WA:312:G:H8	1.84	0.43
30:WA:463:A:H61	30:WA:693:A:H61	1.66	0.43
30:WA:652:C:H2'	30:WA:653:G:H8	1.82	0.43
30:WA:1669:U:H5''	36:DA:58:ILE:HB	1.99	0.43
30:WA:2500:U:O2'	30:WA:2501:G:H5'	2.17	0.43
30:WA:2748:A:H2'	30:WA:2749:A:H8	1.83	0.43
30:WA:2816:G:N2	30:WA:2818:A:H3'	2.33	0.43
30:WA:3872:A2M:HM'3	30:WA:3872:A2M:H1'	1.81	0.43
30:WA:4499:OMG:HM23	30:WA:4499:OMG:H1'	1.79	0.43
51:v:209:LEU:O	51:v:357:HIS:NE2	2.50	0.43
53:ZA:164:A:O2'	53:ZA:165:G:O4'	2.23	0.43
53:ZA:509:G:H2'	53:ZA:510:G:H8	1.83	0.43
53:ZA:815:U:C2	53:ZA:816:A:C8	3.06	0.43
53:ZA:931:C:H2'	53:ZA:932:G:C8	2.52	0.43
53:ZA:1096:G:H1	53:ZA:1136:U:H3	1.64	0.43
53:ZA:1483:A:H4'	54:DB:159:HIS:O	2.17	0.43
53:ZA:1678:A2M:N3	53:ZA:1678:A2M:HM'2	2.34	0.43
55:EB:103:TYR:HA	55:EB:109:PHE:HA	2.01	0.43
73:WB:55:ASP:HB3	78:BC:25:VAL:HG13	1.99	0.43
83:GC:260:ASP:OD2	83:GC:263:GLY:N	2.51	0.43
5:E:186:ARG:HD3	30:WA:4941:G:C5	2.53	0.43
17:R:35:PRO:HD2	17:R:39:VAL:HG11	2.00	0.43
30:WA:420:A:H62	32:YA:14:OMU:HN3	1.66	0.43
30:WA:985:G:H2'	30:WA:986:C:H6	1.83	0.43
30:WA:2500:U:H2'	30:WA:2501:G:C8	2.49	0.43
30:WA:2781:G:H2'	30:WA:2782:G:C8	2.53	0.43
30:WA:4085:C:H2'	30:WA:4086:G:H8	1.83	0.43
30:WA:4704:U:H4'	30:WA:4705:A:OP1	2.17	0.43
34:BA:17:ARG:NH1	34:BA:107:SER:OG	2.51	0.43
51:v:79:TYR:OH	51:v:348:ASP:OD1	2.30	0.43
51:v:215:GLY:HA3	51:v:222:ALA:HA	1.99	0.43
51:v:261:TRP:CD1	51:v:262:GLY:H	2.36	0.43
52:w:213:SER:OG	53:ZA:630:U:O4	2.26	0.43
53:ZA:386:C:H1'	59:IB:5:ARG:HA	1.99	0.43
53:ZA:687:C:H3'	53:ZA:688:U:H5''	2.00	0.43
53:ZA:1102:G:N1	53:ZA:1131:G:C6	2.86	0.43
53:ZA:1584:G:O4'	53:ZA:1586:U:O2'	2.36	0.43
56:FB:61:PHE:CZ	79:CC:49:PRO:HB2	2.53	0.43
59:IB:190:LEU:HB2	59:IB:195:LEU:HD13	2.00	0.43
59:IB:193:LYS:HA	59:IB:196:GLU:HG2	2.01	0.43
69:SB:38:ARG:O	69:SB:42:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SB:120:HIS:O	69:SB:124:ARG:HG2	2.18	0.43
75:YB:29:HIS:O	75:YB:29:HIS:ND1	2.48	0.43
83:GC:172:LYS:HB3	83:GC:191:HIS:O	2.18	0.43
1:A:72:ARG:NH1	30:WA:4089:G:O6	2.51	0.43
1:A:117:GLU:OE2	1:A:163:ARG:NE	2.40	0.43
1:A:245:ARG:HD2	30:WA:3752:A:N7	2.33	0.43
3:C:48:ASN:HB2	30:WA:1376:G:OP2	2.19	0.43
7:G:196:VAL:HG22	7:G:256:ALA:HB2	1.99	0.43
15:P:15:ARG:HG3	30:WA:1696:G:H5'	2.01	0.43
25:Z:121:PRO:HA	25:Z:141:GLY:O	2.19	0.43
29:CB:137:VAL:HG11	29:CB:244:ILE:HD12	2.00	0.43
29:CB:229:CYS:HB2	53:ZA:15:U:OP2	2.18	0.43
30:WA:319:A:H1'	30:WA:3731:A:N3	2.34	0.43
30:WA:956:G:H5'	37:EA:109:ARG:HD3	1.99	0.43
30:WA:1309:A:O5'	36:DA:33:ARG:NH1	2.50	0.43
30:WA:2681:A:C5	30:WA:2682:G:C8	3.07	0.43
30:WA:2838:A:OP1	35:CA:44:ARG:NH1	2.51	0.43
30:WA:4658:C:H4'	35:CA:75:LYS:O	2.19	0.43
30:WA:4672:C:H2'	30:WA:4673:U:O4'	2.18	0.43
30:WA:5008:U:H2'	30:WA:5009:C:C6	2.53	0.43
35:CA:88:LEU:HD12	35:CA:106:VAL:HG12	2.00	0.43
51:v:121:VAL:HG13	51:v:415:ARG:HB3	2.00	0.43
53:ZA:602:G:N2	53:ZA:621:C:N3	2.66	0.43
53:ZA:815:U:OP1	60:JB:10:ARG:NH2	2.42	0.43
53:ZA:929:G:H21	53:ZA:1104:G:H4'	1.83	0.43
53:ZA:1259:A:H1'	53:ZA:1264:C:H42	1.83	0.43
53:ZA:1495:G:H2'	53:ZA:1496:U:C6	2.53	0.43
61:KB:89:ILE:H	61:KB:89:ILE:HG13	1.46	0.43
75:YB:103:SER:HB2	75:YB:106:GLN:HG2	1.99	0.43
2:B:86:VAL:HG12	2:B:201:LEU:HD12	2.00	0.43
3:C:315:LYS:HD2	6:F:167:ALA:HB1	2.01	0.43
26:K:101:ARG:NH2	30:WA:76:A:H5'	2.33	0.43
27:AB:21:ALA:HB1	27:AB:170:SER:HA	1.99	0.43
27:AB:85:ARG:HE	27:AB:85:ARG:HB2	1.69	0.43
28:BB:118:GLN:O	53:ZA:988:C:O2'	2.35	0.43
30:WA:32:G:H21	30:WA:50:C:H5	1.65	0.43
30:WA:1296:G:H2'	30:WA:1297:G:H8	1.83	0.43
30:WA:2380:A:H2'	30:WA:2381:A:H8	1.83	0.43
30:WA:2409:A:O2'	41:IA:12:ARG:O	2.32	0.43
30:WA:2809:OMC:HM23	30:WA:2809:OMC:H1'	1.77	0.43
30:WA:3723:A2M:H2'	30:WA:3724:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:4191:A:H2'	30:WA:4192:G:C8	2.53	0.43
30:WA:4224:A:H2'	30:WA:4225:6MZ:C8	2.49	0.43
30:WA:4598:C:H2'	30:WA:4599:U:C6	2.53	0.43
32:YA:154:G:C6	32:YA:155:C:N4	2.86	0.43
41:IA:46:LYS:NZ	41:IA:54:LYS:HD2	2.34	0.43
41:IA:70:VAL:HG22	41:IA:73:ARG:HH21	1.84	0.43
44:LA:68:MET:HG2	44:LA:79:PRO:HA	2.00	0.43
52:w:201:ARG:HG3	53:ZA:626:G:C5	2.54	0.43
53:ZA:922:A:H2'	53:ZA:923:G:O4'	2.18	0.43
53:ZA:1038:U:H2'	53:ZA:1039:C:C6	2.54	0.43
53:ZA:1646:C:H2'	53:ZA:1678:A2M:N1	2.34	0.43
53:ZA:1792:G:H2'	53:ZA:1793:A:H8	1.83	0.43
53:ZA:1810:U:H2'	53:ZA:1811:C:H6	1.82	0.43
53:ZA:1836:G:OP1	53:ZA:1839:U:H4'	2.19	0.43
59:IB:138:ASN:HB2	59:IB:139:LYS:HD2	2.00	0.43
60:JB:176:LYS:O	60:JB:180:LYS:HG2	2.18	0.43
63:MB:21:VAL:HG21	63:MB:121:LYS:HD3	1.99	0.43
75:YB:58:PHE:HE1	75:YB:74:MET:HE1	1.83	0.43
83:GC:18:VAL:HA	83:GC:35:SER:HA	1.99	0.43
2:B:117:ARG:NH2	2:B:178:ALA:O	2.51	0.43
4:D:230:ASN:O	4:D:230:ASN:ND2	2.52	0.43
7:G:105:THR:O	32:YA:150:C:N4	2.49	0.43
10:J:19:LYS:HD3	10:J:75:ARG:NH2	2.34	0.43
10:J:64:ARG:NE	10:J:65:ASN:OD1	2.42	0.43
17:R:161:ARG:HG2	17:R:164:LYS:HB3	2.00	0.43
23:X:30:MET:HB3	23:X:101:PRO:HG2	2.00	0.43
23:X:59:ARG:HB2	23:X:103:LYS:HG3	1.99	0.43
27:AB:5:LEU:O	27:AB:9:GLN:HG2	2.18	0.43
27:AB:44:ASP:OD1	27:AB:44:ASP:N	2.48	0.43
30:WA:58:G:H4'	30:WA:59:A:H4'	2.00	0.43
30:WA:66:A:H61	30:WA:282:C:HO2'	1.67	0.43
30:WA:252:C:H2'	30:WA:253:G:C8	2.53	0.43
30:WA:398:A2M:H8	30:WA:398:A2M:O5'	2.18	0.43
30:WA:1889:C:H2'	30:WA:1890:G:H8	1.84	0.43
30:WA:2013:U:H3'	30:WA:2014:A:C5'	2.48	0.43
30:WA:2086:C:H2'	30:WA:2087:G:C8	2.53	0.43
30:WA:2575:U:H2'	30:WA:2576:C:C6	2.53	0.43
31:XA:3:C:H2'	31:XA:4:U:C6	2.53	0.43
45:MA:1:MET:HG3	45:MA:6:ARG:HB3	2.01	0.43
53:ZA:1050:A:H4'	53:ZA:1846:G:O2'	2.19	0.43
53:ZA:1455:A:OP1	68:RB:5:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:FB:103:LEU:HD11	76:ZB:67:LEU:HD22	2.00	0.43
64:NB:70:LYS:HE2	64:NB:70:LYS:HB3	1.87	0.43
67:QB:117:ARG:O	67:QB:121:VAL:HG12	2.19	0.43
71:UB:22:ILE:HG22	71:UB:114:VAL:HG22	2.01	0.43
3:C:32:ILE:HD12	3:C:130:ALA:HB2	2.01	0.43
9:I:66:GLU:HG3	9:I:69:ARG:HH21	1.84	0.43
10:J:72:CYS:SG	10:J:73:THR:N	2.92	0.43
25:Z:77:LYS:CE	30:WA:1507:G:H22	2.31	0.43
30:WA:424:U:H2'	30:WA:425:U:C6	2.53	0.43
30:WA:434:A:H2'	30:WA:435:A:O4'	2.18	0.43
30:WA:451:C:O2'	30:WA:1299:G:H2'	2.19	0.43
30:WA:968:G:O2'	30:WA:969:A:H8	2.00	0.43
30:WA:1198:C:H2'	30:WA:1199:C:C6	2.53	0.43
30:WA:1215:U:O2'	30:WA:1217:G:H8	2.01	0.43
30:WA:1732:U:H2'	30:WA:1733:U:C6	2.54	0.43
30:WA:1782:C:H2'	30:WA:1783:C:C6	2.53	0.43
30:WA:2003:A:C2	30:WA:2025:U:H4'	2.53	0.43
30:WA:2310:U:O2'	36:DA:104:SER:OG	2.32	0.43
30:WA:2426:G:OP2	30:WA:2833:U:H1'	2.19	0.43
30:WA:4191:A:H2'	30:WA:4192:G:H8	1.83	0.43
30:WA:4263:C:H2'	30:WA:4264:C:C6	2.54	0.43
30:WA:4431:C:H2'	30:WA:4432:G:O4'	2.18	0.43
30:WA:4694:U:H2'	30:WA:4695:B8K:O4'	2.19	0.43
49:QA:85:ASN:OD1	49:QA:85:ASN:N	2.51	0.43
51:v:747:VAL:HG12	51:v:812:CYS:HB3	2.00	0.43
53:ZA:112:U:H2'	53:ZA:115:U:H5	1.84	0.43
53:ZA:291:G:N2	62:LB:40:ILE:O	2.36	0.43
53:ZA:1298:G:H5'	66:PB:77:LYS:HB2	1.99	0.43
53:ZA:1480:A:H2'	53:ZA:1481:G:H8	1.84	0.43
53:ZA:1561:A:H4'	53:ZA:1583:C:H4'	1.99	0.43
57:GB:20:ASP:OD1	57:GB:21:GLU:N	2.51	0.43
62:LB:93:LEU:HB3	62:LB:102:PHE:HB3	2.01	0.43
75:YB:85:ASN:O	75:YB:85:ASN:ND2	2.51	0.43
80:DC:23:VAL:HB	80:DC:42:CYS:SG	2.58	0.43
1:A:83:HIS:CE1	1:A:86:GLN:HB2	2.53	0.43
4:D:22:ARG:NH1	31:XA:7:G:H8	2.17	0.43
4:D:116:ASP:OD1	4:D:116:ASP:N	2.50	0.43
4:D:217:ASP:OD1	4:D:217:ASP:N	2.51	0.43
11:L:90:ARG:O	11:L:94:LYS:HG2	2.19	0.43
22:W:77:ILE:HG22	22:W:100:VAL:HG12	2.01	0.43
22:W:80:PRO:HG2	22:W:155:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:36:GLY:HA3	25:Z:40:HIS:CD2	2.54	0.43
26:K:29:PRO:HB2	30:WA:1377:A:H4'	2.01	0.43
26:K:129:ARG:NH1	30:WA:173:C:H5''	2.33	0.43
29:CB:130:ILE:O	29:CB:138:GLY:N	2.51	0.43
30:WA:86:U:H2'	30:WA:87:A:C8	2.54	0.43
30:WA:480:C:OP1	48:PA:67:ARG:NH1	2.51	0.43
30:WA:964:G:O2'	30:WA:2268:A:N6	2.51	0.43
30:WA:2451:C:HO2'	30:WA:2750:A:HO2'	1.63	0.43
30:WA:3856:U:H2'	30:WA:3857:A:O4'	2.18	0.43
30:WA:4193:U:H2'	30:WA:4194:U:H6	1.81	0.43
32:YA:78:G:H2'	32:YA:79:G:C8	2.53	0.43
53:ZA:380:G:P	59:IB:56:ARG:HH22	2.42	0.43
53:ZA:616:A:H8	53:ZA:616:A:OP2	2.01	0.43
53:ZA:616:A:N3	81:EC:85:VAL:HG21	2.33	0.43
53:ZA:1056:U:H2'	53:ZA:1057:C:C6	2.54	0.43
53:ZA:1102:G:H2'	53:ZA:1103:C:C6	2.54	0.43
53:ZA:1706:G:H2'	53:ZA:1707:U:C6	2.54	0.43
54:DB:74:GLN:NE2	54:DB:81:GLU:OE2	2.51	0.43
66:PB:13:ARG:HD2	66:PB:13:ARG:HA	1.81	0.43
82:FC:107:LYS:N	82:FC:115:SER:O	2.45	0.43
13:N:128:ARG:NH2	30:WA:2062:A:OP1	2.52	0.43
17:R:164:LYS:HB3	17:R:165:PRO:HD3	2.01	0.43
20:U:97:TYR:CZ	21:V:21:TYR:HD1	2.36	0.43
30:WA:155:C:H3'	30:WA:156:G:H8	1.84	0.43
30:WA:288:G:H2'	30:WA:289:C:C6	2.54	0.43
30:WA:759:G:O2'	30:WA:760:G:H5'	2.18	0.43
30:WA:1198:C:H2'	30:WA:1199:C:H6	1.84	0.43
30:WA:1473:C:H2'	30:WA:1474:C:C6	2.53	0.43
30:WA:2369:OMG:H1'	30:WA:2369:OMG:HM23	1.76	0.43
30:WA:2492:G:O6	30:WA:2494:C:O2'	2.22	0.43
30:WA:2627:G:H2'	30:WA:2628:A:C8	2.54	0.43
30:WA:4471:C:H2'	30:WA:4472:A:H8	1.84	0.43
30:WA:4643:U:H2'	30:WA:4644:G:N3	2.34	0.43
30:WA:4904:G:O2'	30:WA:4907:C:O5'	2.34	0.43
30:WA:4945:C:H5'	30:WA:4946:G:H5''	2.00	0.43
34:BA:22:MET:HE1	34:BA:85:CYS:HB3	1.99	0.43
51:v:19:ILE:HG12	51:v:99:LEU:HB3	2.00	0.43
53:ZA:307:G:H1'	59:IB:45:THR:HG22	2.01	0.43
53:ZA:1545:A:H2'	53:ZA:1546:G:C8	2.53	0.43
53:ZA:1709:G:H2'	53:ZA:1710:C:C6	2.54	0.43
56:FB:179:ASN:HB2	56:FB:187:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:GB:93:LYS:HG2	57:GB:95:LYS:HE2	2.01	0.43
61:KB:23:ALA:HB2	61:KB:32:HIS:HE2	1.84	0.43
69:SB:53:THR:O	69:SB:55:ARG:NH2	2.52	0.43
80:DC:21:CYS:SG	80:DC:24:CYS:N	2.77	0.43
83:GC:178:ASN:HB3	83:GC:181:ASN:OD1	2.19	0.43
83:GC:241:PHE:HE1	83:GC:261:LEU:HD21	1.84	0.43
2:B:222:VAL:HG23	2:B:343:ARG:NH1	2.34	0.43
6:F:186:MET:HE3	6:F:186:MET:HB2	1.94	0.43
17:R:127:MET:HE1	18:S:155:PRO:HA	2.00	0.43
22:W:145:ASP:OD1	22:W:145:ASP:N	2.49	0.43
27:AB:122:LEU:HB2	27:AB:142:LEU:HD11	2.00	0.43
28:BB:143:THR:HA	28:BB:207:LEU:HG	2.00	0.43
30:WA:176:G:H2'	30:WA:177:G:H8	1.84	0.43
30:WA:272:U:H2'	30:WA:273:U:C6	2.54	0.43
30:WA:993:C:H2'	30:WA:994:C:H6	1.84	0.43
30:WA:1179:G:H2'	30:WA:1180:G:C8	2.53	0.43
30:WA:1515:G:H2'	30:WA:1516:U:C6	2.54	0.43
30:WA:1582:G:H3'	30:WA:1582:G:N3	2.34	0.43
30:WA:1599:C:O2'	30:WA:1602:G:H1'	2.19	0.43
30:WA:4271:G:N3	30:WA:4271:G:H2'	2.34	0.43
30:WA:4655:G:H4'	30:WA:5013:C:H4'	2.01	0.43
30:WA:4868:G:H2'	30:WA:4869:U:C6	2.54	0.43
30:WA:5019:A:H2'	30:WA:5020:G:O4'	2.19	0.43
46:NA:61:LYS:HE2	46:NA:61:LYS:HB3	1.84	0.43
48:PA:108:MET:O	48:PA:112:ARG:HG2	2.19	0.43
53:ZA:63:U:O2'	53:ZA:170:A:N3	2.39	0.43
53:ZA:170:A:H2'	53:ZA:171:A:C8	2.54	0.43
53:ZA:1390:U:H2'	53:ZA:1391:C:H6	1.83	0.43
55:EB:66:MET:HA	55:EB:66:MET:HE2	2.01	0.43
56:FB:125:SER:HB2	56:FB:136:ARG:HD3	2.01	0.43
65:OB:67:ASP:N	65:OB:67:ASP:OD1	2.52	0.43
66:PB:98:ASN:HD21	66:PB:120:SER:HB2	1.84	0.43
71:UB:20:ILE:HD12	71:UB:116:ILE:HA	2.00	0.43
84:b:31:VAL:HG21	84:b:56:ILE:HD13	2.00	0.43
2:B:135:LYS:HA	2:B:138:GLN:NE2	2.33	0.42
2:B:357:ARG:HH11	30:WA:4620:C:H5''	1.83	0.42
17:R:169:THR:HG21	30:WA:4880:G:C5	2.54	0.42
22:W:95:THR:HG22	22:W:139:ARG:HA	2.01	0.42
25:Z:35:ALA:HB2	30:WA:38:A:H5''	2.01	0.42
28:BB:120:MET:HG3	28:BB:142:PHE:CE1	2.50	0.42
29:CB:205:VAL:HG12	53:ZA:3:C:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:86:U:H2'	30:WA:87:A:H8	1.84	0.42
30:WA:307:A:H2'	30:WA:308:G:N3	2.34	0.42
30:WA:347:A:H2'	30:WA:348:G:C8	2.54	0.42
30:WA:704:G:H4'	30:WA:705:C:C5	2.54	0.42
30:WA:2083:C:H2'	30:WA:2084:G:H8	1.83	0.42
30:WA:2540:G:H2'	30:WA:2541:A:C8	2.54	0.42
30:WA:3928:A:H2'	30:WA:3929:C:H6	1.84	0.42
30:WA:4259:G:H2'	30:WA:4259:G:N3	2.33	0.42
31:XA:94:C:H2'	31:XA:95:C:H6	1.84	0.42
36:DA:69:MET:HA	36:DA:75:ARG:HD3	1.99	0.42
37:EA:46:ARG:H	37:EA:107:PRO:HG2	1.84	0.42
37:EA:57:THR:HG21	37:EA:68:ARG:HG2	2.00	0.42
50:RA:53:TRP:HB3	50:RA:56:LEU:HB2	2.01	0.42
53:ZA:1146:C:H2'	53:ZA:1147:C:C6	2.53	0.42
53:ZA:1237:C:H2'	53:ZA:1238:U:C6	2.54	0.42
53:ZA:1588:A:N3	53:ZA:1654:G:O2'	2.44	0.42
53:ZA:1599:U:H2'	56:FB:166:ILE:HD11	2.00	0.42
62:LB:17:PHE:CZ	62:LB:19:ASN:HB2	2.54	0.42
64:NB:110:ASP:O	64:NB:114:ARG:HG2	2.18	0.42
71:UB:23:THR:HB	71:UB:113:GLU:HB3	2.01	0.42
74:XB:39:ASN:HD22	74:XB:43:GLY:H	1.66	0.42
83:GC:168:CYS:HB3	83:GC:198:VAL:HB	2.00	0.42
6:F:164:LYS:HE2	30:WA:2087:G:H21	1.83	0.42
13:N:175:MET:SD	13:N:179:LYS:NZ	2.92	0.42
18:S:2:THR:N	30:WA:4225:6MZ:OP1	2.52	0.42
30:WA:113:A:H61	30:WA:158:A:H62	1.67	0.42
30:WA:251:C:H2'	30:WA:252:C:C6	2.53	0.42
30:WA:1242:C:O2'	30:WA:1243:C:OP1	2.28	0.42
30:WA:1979:U:H4'	30:WA:1980:G:H3'	2.00	0.42
30:WA:2086:C:H2'	30:WA:2087:G:H8	1.84	0.42
30:WA:2640:U:H2'	30:WA:2641:U:C6	2.54	0.42
30:WA:2697:U:H2'	30:WA:2698:G:O4'	2.19	0.42
30:WA:2713:U:OP2	30:WA:2713:U:H4'	2.18	0.42
30:WA:2754:C:H2'	30:WA:2755:G:C8	2.55	0.42
30:WA:2866:OMC:HM23	30:WA:2866:OMC:H1'	1.85	0.42
30:WA:3876:A:H2'	30:WA:3877:A:C8	2.53	0.42
30:WA:4745:G:H2'	30:WA:4748:G:P	2.60	0.42
30:WA:4965:G:H2'	30:WA:4966:G:C8	2.54	0.42
32:YA:32:C:H2'	32:YA:33:G:O4'	2.19	0.42
32:YA:94:G:H1'	41:IA:82:THR:O	2.20	0.42
34:BA:31:TYR:OH	34:BA:59:GLU:OE2	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:472:C:O2	53:ZA:475:C:N4	2.46	0.42
53:ZA:526:A:H5'	81:EC:104:ARG:NH2	2.34	0.42
53:ZA:934:G:H1	53:ZA:1008:A:H2	1.65	0.42
66:PB:18:ARG:NH1	66:PB:37:TYR:HA	2.34	0.42
67:QB:116:ASP:HB3	67:QB:119:LEU:HD23	2.01	0.42
83:GC:87:LEU:HD21	83:GC:108:VAL:HG11	2.01	0.42
1:A:13:GLY:O	1:A:17:ARG:NH1	2.49	0.42
9:I:53:VAL:HG11	18:S:158:PHE:HZ	1.84	0.42
16:Q:70:ARG:HG3	16:Q:76:MET:HE2	2.00	0.42
17:R:27:LEU:HD21	18:S:141:VAL:HG11	2.01	0.42
28:BB:33:VAL:HB	28:BB:44:ILE:HB	2.01	0.42
28:BB:121:ILE:HG12	28:BB:164:ILE:HD11	2.01	0.42
29:CB:194:ARG:HB3	29:CB:225:SER:HB2	2.00	0.42
30:WA:1090:C:H2'	30:WA:1091:C:C6	2.53	0.42
30:WA:2616:A:O5'	30:WA:2693:G:H4'	2.18	0.42
30:WA:2798:G:H5'	30:WA:2799:C:H5''	2.00	0.42
30:WA:3657:A:H2'	30:WA:3658:A:C8	2.54	0.42
30:WA:3888:U:H2'	30:WA:3889:U:C6	2.53	0.42
30:WA:4883:C:H2'	30:WA:4884:C:H6	1.84	0.42
30:WA:4922:C:H2'	30:WA:4923:C:C6	2.54	0.42
30:WA:4971:A:H2'	30:WA:4972:A:C8	2.54	0.42
32:YA:28:C:H2'	32:YA:29:G:C8	2.54	0.42
36:DA:70:LEU:HD11	36:DA:76:LYS:HG3	2.02	0.42
46:NA:26:TYR:HB3	46:NA:67:VAL:HB	2.01	0.42
47:OA:22:LEU:O	47:OA:26:VAL:HG23	2.18	0.42
49:QA:45:MET:SD	49:QA:48:ARG:NE	2.84	0.42
49:QA:130:LEU:HD13	49:QA:177:MET:HE2	2.00	0.42
51:v:541:SER:HB3	51:v:841:ARG:HH21	1.83	0.42
51:v:710:HIS:O	51:v:716:ARG:NH1	2.53	0.42
53:ZA:81:U:H3'	53:ZA:82:G:C8	2.53	0.42
53:ZA:84:A:H5''	75:YB:122:LYS:HD2	2.01	0.42
53:ZA:96:C:H2'	53:ZA:97:U:H6	1.84	0.42
53:ZA:430:C:H2'	53:ZA:431:G:C8	2.53	0.42
53:ZA:507:G:P	75:YB:104:ARG:HH22	2.41	0.42
53:ZA:604:A:N3	53:ZA:639:C:O2'	2.45	0.42
53:ZA:1285:G:H1'	82:FC:100:LEU:HD11	2.01	0.42
53:ZA:1546:G:H2'	53:ZA:1547:C:C6	2.54	0.42
61:KB:29:MET:HB2	61:KB:42:ASN:HB3	2.00	0.42
64:NB:134:VAL:HG13	64:NB:135:LEU:HG	2.00	0.42
73:WB:6:VAL:HG12	73:WB:34:ILE:HD11	2.01	0.42
1:A:65:ASP:OD2	1:A:68:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:O	30:WA:3663:C:H5''	2.20	0.42
3:C:336:ARG:HA	3:C:339:THR:HG22	2.00	0.42
8:H:63:ASN:O	8:H:67:LEU:HG	2.20	0.42
10:J:169:LYS:HD2	10:J:170:TYR:CE2	2.54	0.42
12:M:181:HIS:CD2	30:WA:99:A:H4'	2.54	0.42
13:N:121:PRO:HA	13:N:124:LEU:HB2	2.02	0.42
30:WA:93:G:H2'	30:WA:94:A:C8	2.55	0.42
30:WA:269:G:H2'	30:WA:270:U:C6	2.55	0.42
30:WA:505:G:H2'	30:WA:506:G:C8	2.55	0.42
30:WA:1214:G:O2'	30:WA:1215:U:H5'	2.19	0.42
30:WA:1504:C:H2'	30:WA:1505:A:O4'	2.19	0.42
30:WA:1527:OMG:HN1	30:WA:1660:C:H42	1.66	0.42
30:WA:1570:A:H2	53:ZA:1030:A:H5'	1.84	0.42
30:WA:1871:UR3:H3U2	30:WA:4410:G:C8	2.54	0.42
30:WA:1888:OMG:OP1	36:DA:47:ARG:NH2	2.48	0.42
30:WA:2627:G:H2'	30:WA:2628:A:H8	1.84	0.42
30:WA:2881:G:C8	47:OA:16:THR:HG22	2.54	0.42
30:WA:3870:A:H61	30:WA:3886:G:H1	1.66	0.42
30:WA:4508:A:H2'	30:WA:4509:C:H6	1.84	0.42
41:IA:64:MET:HE3	41:IA:67:LEU:HD23	2.01	0.42
43:KA:24:PRO:HG2	43:KA:27:ILE:HG13	2.02	0.42
51:v:20:ARG:HB2	51:v:100:ILE:HD12	2.01	0.42
51:v:524:LEU:HD22	51:v:546:ILE:HD11	2.01	0.42
53:ZA:877:C:O2'	53:ZA:878:G:O4'	2.35	0.42
53:ZA:912:C:H2'	53:ZA:914:U:O4'	2.20	0.42
53:ZA:945:U:H2'	53:ZA:946:U:C6	2.54	0.42
53:ZA:959:G:H1'	53:ZA:964:A:N6	2.35	0.42
53:ZA:1711:U:H2'	53:ZA:1712:A:H8	1.84	0.42
53:ZA:1847:G:H2'	53:ZA:1848:U:C6	2.54	0.42
73:WB:3:ARG:HH21	73:WB:28:ARG:HH12	1.68	0.42
75:YB:100:LYS:HG3	75:YB:107:ARG:HH21	1.84	0.42
83:GC:57:ARG:NH2	83:GC:95:GLY:H	2.17	0.42
8:H:117:PHE:O	8:H:120:GLU:HG2	2.19	0.42
11:L:11:ARG:NH2	11:L:61:ILE:HD11	2.34	0.42
13:N:18:ARG:HH21	30:WA:2059:U:P	2.42	0.42
20:U:13:LYS:HB2	20:U:128:LEU:HD21	2.00	0.42
30:WA:250:C:H2'	30:WA:251:C:C6	2.53	0.42
30:WA:272:U:H2'	30:WA:273:U:H6	1.85	0.42
30:WA:655:C:H2'	30:WA:656:C:H6	1.84	0.42
30:WA:675:G:H2'	30:WA:676:C:H6	1.85	0.42
30:WA:1401:U:H2'	30:WA:1402:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:1916:C:H1'	30:WA:1922:A:H2'	2.01	0.42
30:WA:1962:U:O2'	30:WA:1963:A:H5'	2.19	0.42
30:WA:2064:C:H2'	30:WA:2065:G:C8	2.54	0.42
30:WA:2297:C:H2'	30:WA:2298:U:H6	1.85	0.42
30:WA:2352:A:OP1	36:DA:22:ARG:NH2	2.42	0.42
30:WA:2638:U:H2'	30:WA:2639:C:C6	2.55	0.42
30:WA:3638:C:H2'	30:WA:3639:G:H8	1.85	0.42
30:WA:3830:A2M:H2'	30:WA:3831:C:O4'	2.19	0.42
30:WA:3832:G:O2'	30:WA:3834:G:OP2	2.31	0.42
30:WA:4679:C:H2'	30:WA:4680:U:C6	2.55	0.42
32:YA:13:G:H2'	32:YA:14:OMU:H6	2.02	0.42
47:OA:57:CYS:SG	47:OA:60:CYS:HB2	2.59	0.42
49:QA:76:GLU:OE1	49:QA:76:GLU:N	2.46	0.42
51:v:200:MET:HE3	51:v:203:ILE:HG21	2.01	0.42
51:v:406:ASP:OD2	53:ZA:478:G:O2'	2.34	0.42
51:v:629:LYS:NZ	53:ZA:1319:U:O2'	2.34	0.42
51:v:693:CYS:SG	51:v:835:VAL:HG12	2.59	0.42
51:v:827:ASN:OD1	51:v:828:SER:N	2.52	0.42
53:ZA:77:A:C2	57:GB:175:LYS:HG3	2.55	0.42
53:ZA:558:G:H2'	53:ZA:559:G:C8	2.54	0.42
53:ZA:1337:4AC:H2'	53:ZA:1338:G:H8	1.83	0.42
53:ZA:1754:G:C4	53:ZA:1779:G:N2	2.86	0.42
53:ZA:1810:U:H4'	53:ZA:1811:C:OP1	2.20	0.42
59:IB:139:LYS:HD2	59:IB:139:LYS:N	2.35	0.42
66:PB:30:TYR:O	66:PB:34:MET:HG3	2.20	0.42
66:PB:68:PRO:HA	66:PB:69:PRO:HD3	1.97	0.42
67:QB:112:LEU:HD22	67:QB:119:LEU:HG	2.01	0.42
83:GC:107:ASP:HB2	83:GC:125:ARG:HD3	2.00	0.42
4:D:223:PHE:HB3	4:D:226:TYR:HB2	2.01	0.42
16:Q:105:LEU:HD22	16:Q:135:LYS:HG3	2.02	0.42
17:R:161:ARG:HH21	30:WA:1926:C:N4	2.18	0.42
30:WA:99:A:H2'	30:WA:100:C:O2	2.19	0.42
30:WA:691:C:H2'	30:WA:692:C:C6	2.55	0.42
30:WA:1444:U:O2'	30:WA:1445:U:OP2	2.26	0.42
30:WA:2026:G:H4'	49:QA:84:GLY:C	2.45	0.42
30:WA:2639:C:H2'	30:WA:2640:U:H6	1.84	0.42
30:WA:3705:C:H2'	30:WA:3751:A:H61	1.84	0.42
30:WA:4486:U:H2'	30:WA:4487:U:H6	1.83	0.42
30:WA:5035:U:H2'	30:WA:5036:G:C8	2.55	0.42
32:YA:52:A:H62	43:KA:27:ILE:HD13	1.85	0.42
51:v:653:GLY:N	51:v:660:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:93:U:O2'	55:EB:8:HIS:ND1	2.39	0.42
53:ZA:418:A:N3	53:ZA:418:A:H2'	2.35	0.42
53:ZA:419:G:H4'	73:WB:88:LYS:HE2	2.02	0.42
53:ZA:816:A:H2'	53:ZA:817:G:O4'	2.19	0.42
54:DB:127:MET:HE3	54:DB:154:ASP:HB3	2.01	0.42
58:HB:20:GLU:HB3	58:HB:48:ALA:O	2.19	0.42
60:JB:38:ARG:HG2	60:JB:42:GLU:OE2	2.19	0.42
61:KB:58:VAL:HA	61:KB:72:THR:HG23	2.00	0.42
64:NB:23:PRO:HB3	78:BC:84:HIS:HD2	1.84	0.42
83:GC:304:ASP:O	83:GC:306:LEU:HG	2.20	0.42
2:B:30:LYS:HG3	30:WA:4721:C:OP2	2.19	0.42
3:C:83:GLY:H	30:WA:368:C:H1'	1.85	0.42
3:C:204:ARG:HD2	30:WA:2304:G:OP2	2.20	0.42
6:F:57:HIS:O	6:F:61:ARG:HG3	2.19	0.42
7:G:212:HIS:ND1	7:G:238:LYS:HA	2.34	0.42
19:T:105:ASN:OD1	19:T:106:THR:N	2.52	0.42
23:X:100:HIS:CD2	30:WA:231:U:H4'	2.55	0.42
27:AB:24:HIS:HB3	27:AB:51:LEU:HD21	2.01	0.42
30:WA:125:C:H2'	30:WA:126:C:H6	1.85	0.42
30:WA:1313:A:H2'	30:WA:1314:C:C6	2.55	0.42
30:WA:1353:G:H2'	30:WA:1354:P4U:C6	2.50	0.42
30:WA:1860:G:OP1	33:AA:4:SER:HB2	2.18	0.42
30:WA:2644:U:O2	38:FA:26:PRO:HB3	2.20	0.42
30:WA:4238:A:OP1	46:NA:97:LYS:HG3	2.20	0.42
30:WA:4418:C:H2'	30:WA:4419:A:O4'	2.20	0.42
30:WA:4903:G:H22	30:WA:4928:U:H1'	1.84	0.42
32:YA:14:OMU:H1'	32:YA:14:OMU:HM23	1.49	0.42
48:PA:51:VAL:HB	48:PA:113:ARG:HD3	2.01	0.42
53:ZA:376:A:N1	53:ZA:389:A:N6	2.68	0.42
53:ZA:1338:G:H2'	53:ZA:1339:U:C6	2.55	0.42
58:HB:156:VAL:O	58:HB:188:GLU:N	2.53	0.42
69:SB:39:ARG:HG3	69:SB:83:PHE:CZ	2.54	0.42
70:TB:104:LEU:HB3	70:TB:121:ARG:NE	2.34	0.42
74:XB:60:LYS:HD3	74:XB:60:LYS:HA	1.90	0.42
75:YB:23:MET:SD	75:YB:23:MET:N	2.92	0.42
1:A:3:ARG:HD3	30:WA:1633:C:N4	2.32	0.42
6:F:156:ARG:NH1	6:F:211:LYS:O	2.53	0.42
10:J:108:GLY:HA3	30:WA:4256:A:H5''	2.00	0.42
16:Q:163:ARG:NH2	53:ZA:871:U:H3	2.18	0.42
18:S:112:ASN:HA	18:S:115:LYS:HG2	2.02	0.42
30:WA:115:C:H2'	30:WA:116:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:162:A:H2'	30:WA:163:A:C8	2.55	0.42
30:WA:519:G:H2'	30:WA:520:C:C6	2.55	0.42
30:WA:1277:G:N2	30:WA:1444:U:O2	2.53	0.42
30:WA:2453:G:OP2	30:WA:2515:G:N1	2.30	0.42
30:WA:4952:U:O2'	30:WA:4953:C:P	2.78	0.42
31:XA:28:C:O2'	31:XA:54:A:N1	2.52	0.42
37:EA:50:VAL:HG22	37:EA:69:VAL:HG12	2.02	0.42
47:OA:21:SER:HA	47:OA:24:LYS:HG2	2.02	0.42
51:v:429:ILE:HG12	51:v:485:ILE:HD12	2.02	0.42
53:ZA:561:A:N7	60:JB:173:VAL:HG21	2.35	0.42
53:ZA:1399:C:H5''	83:GC:100:ARG:CZ	2.49	0.42
53:ZA:1462:U:H2'	53:ZA:1464:C:N4	2.35	0.42
53:ZA:1627:C:OP1	70:TB:83:GLN:NE2	2.53	0.42
53:ZA:1808:U:H2'	53:ZA:1809:A:H8	1.84	0.42
63:MB:25:ALA:O	63:MB:29:ASP:N	2.53	0.42
1:A:5:ILE:HD13	1:A:232:GLY:HA2	2.02	0.42
1:A:213:GLY:HA3	30:WA:4549:A:H5''	2.01	0.42
2:B:106:PHE:HB2	2:B:133:TYR:CE1	2.54	0.42
2:B:340:THR:OG1	2:B:341:LYS:N	2.53	0.42
7:G:283:TYR:OH	40:HA:46:GLU:OE2	2.34	0.42
11:L:31:ILE:H	11:L:36:ALA:HA	1.85	0.42
13:N:126:VAL:HG11	30:WA:4768:U:C5	2.55	0.42
14:O:69:ARG:NH2	30:WA:4573:A:N3	2.68	0.42
22:W:119:ILE:HD13	22:W:149:VAL:HG11	2.00	0.42
24:Y:89:ILE:HD11	24:Y:117:LYS:HB3	2.01	0.42
25:Z:36:GLY:HA3	25:Z:40:HIS:NE2	2.35	0.42
30:WA:7:C:H2'	30:WA:8:U:H6	1.82	0.42
30:WA:254:G:H2'	30:WA:255:C:O4'	2.20	0.42
30:WA:271:C:H2'	30:WA:272:U:H6	1.85	0.42
30:WA:910:G:H2'	30:WA:911:G:H8	1.84	0.42
30:WA:1321:C:H2'	30:WA:1322:OMG:H8	1.84	0.42
30:WA:1879:A:OP1	33:AA:9:THR:HG22	2.20	0.42
30:WA:2599:C:H2'	30:WA:2600:C:C6	2.55	0.42
30:WA:2646:A:H2'	30:WA:2647:A:O4'	2.20	0.42
30:WA:2726:G:C2'	30:WA:2727:G:H5'	2.50	0.42
30:WA:2769:A:H2'	30:WA:2770:A:H8	1.83	0.42
30:WA:4625:OMU:HM23	30:WA:4625:OMU:H1'	1.59	0.42
32:YA:109:C:O2'	41:IA:20:ARG:NH2	2.53	0.42
33:AA:47:LYS:HA	33:AA:50:ASN:ND2	2.34	0.42
36:DA:44:ARG:HG3	36:DA:49:PHE:CD2	2.45	0.42
47:OA:50:ARG:HH21	47:OA:56:HIS:CG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QA:41:GLN:O	49:QA:45:MET:HG2	2.20	0.42
53:ZA:441:C:H2'	53:ZA:442:C:C6	2.54	0.42
53:ZA:506:G:P	75:YB:104:ARG:HH21	2.43	0.42
53:ZA:940:U:H2'	53:ZA:941:C:C6	2.55	0.42
53:ZA:1003:U:H2'	53:ZA:1004:U:C6	2.55	0.42
53:ZA:1016:U:H6	64:NB:61:ALA:HB1	1.84	0.42
53:ZA:1405:A:H2'	53:ZA:1406:G:O4'	2.19	0.42
54:DB:67:ARG:O	54:DB:70:THR:OG1	2.33	0.42
54:DB:154:ASP:OD1	54:DB:155:GLY:N	2.53	0.42
56:FB:144:LEU:HD23	79:CC:49:PRO:HG2	2.02	0.42
69:SB:89:ASP:OD1	69:SB:90:VAL:N	2.53	0.42
72:VB:38:GLU:OE1	72:VB:38:GLU:N	2.53	0.42
76:ZB:50:PHE:CZ	76:ZB:58:LEU:HD22	2.54	0.42
77:AC:23:CYS:SG	77:AC:24:THR:N	2.93	0.42
84:b:116:GLY:O	84:b:192:GLN:HA	2.19	0.42
2:B:161:ARG:HD3	2:B:182:GLU:HB3	2.02	0.42
7:G:163:LYS:HG2	7:G:166:ARG:HH22	1.85	0.42
8:H:113:GLU:HG2	8:H:125:ARG:HB3	2.02	0.42
12:M:24:ARG:NH1	30:WA:3943:G:OP2	2.42	0.42
13:N:49:ARG:HD2	30:WA:1935:U:OP2	2.20	0.42
13:N:121:PRO:HD2	17:R:166:ARG:O	2.20	0.42
14:O:30:ARG:NH2	30:WA:424:U:OP1	2.44	0.42
16:Q:13:SER:OG	16:Q:38:ARG:NH2	2.50	0.42
16:Q:24:LEU:HD22	16:Q:50:ILE:HD12	2.00	0.42
17:R:154:LEU:HD13	17:R:157:ARG:NH1	2.35	0.42
26:K:58:ILE:HG23	26:K:70:VAL:HG11	2.01	0.42
29:CB:259:THR:HB	72:VB:15:ARG:HH21	1.84	0.42
30:WA:6:C:H2'	30:WA:7:C:H6	1.84	0.42
30:WA:1674:A:C2	30:WA:1857:U:H4'	2.54	0.42
48:PA:46:ARG:NH1	48:PA:70:GLN:HG3	2.35	0.42
50:RA:153:ASP:OD1	50:RA:154:ASP:N	2.53	0.42
53:ZA:421:G:OP1	62:LB:97:ARG:HG2	2.19	0.42
53:ZA:616:A:H4'	81:EC:81:ARG:O	2.19	0.42
53:ZA:1413:G:H2'	53:ZA:1414:A:H8	1.85	0.42
53:ZA:1856:C:H2'	53:ZA:1857:G:H8	1.84	0.42
57:GB:56:ASN:HA	57:GB:62:PRO:HA	2.02	0.42
58:HB:43:LEU:HD22	58:HB:72:PHE:HD2	1.85	0.42
59:IB:21:TYR:CZ	59:IB:22:HIS:HD2	2.38	0.42
59:IB:139:LYS:O	59:IB:140:LYS:HG2	2.20	0.42
67:QB:89:SER:HB3	67:QB:119:LEU:HD12	2.02	0.42
83:GC:206:LEU:HD13	83:GC:218:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:GC:258:ILE:HB	83:GC:267:VAL:HB	2.01	0.42
84:b:107:LYS:HE2	84:b:107:LYS:HB2	1.90	0.42
2:B:62:ARG:HG3	2:B:65:SER:OG	2.20	0.41
4:D:208:MET:HE3	4:D:208:MET:HB2	1.95	0.41
24:Y:15:ALA:HB2	38:FA:88:ARG:HH21	1.85	0.41
25:Z:103:VAL:HB	25:Z:108:TYR:HB2	2.01	0.41
27:AB:102:ARG:HH21	27:AB:105:PRO:HD3	1.84	0.41
29:CB:60:TRP:CE2	29:CB:92:GLU:HB2	2.55	0.41
29:CB:94:ILE:HD12	29:CB:95:ASP:N	2.35	0.41
29:CB:169:TYR:O	73:WB:98:GLN:NE2	2.53	0.41
30:WA:270:U:H2'	30:WA:271:C:C6	2.55	0.41
30:WA:301:G:H2'	30:WA:302:C:C6	2.54	0.41
30:WA:1515:G:H2'	30:WA:1516:U:H6	1.85	0.41
30:WA:1961:A:H2'	30:WA:1962:U:H5'	2.02	0.41
30:WA:2593:C:H4'	30:WA:2594:C:H5''	2.01	0.41
30:WA:3793:C:N4	30:WA:3817:C:O4'	2.53	0.41
30:WA:3818:A:N3	30:WA:4543:G:O2'	2.46	0.41
30:WA:4454:A:H1'	86:WA:5199:ANM:O3	2.20	0.41
30:WA:4472:A:H61	30:WA:4495:C:H42	1.68	0.41
30:WA:5057:C:H2'	30:WA:5058:U:O4'	2.20	0.41
31:XA:64:G:H2'	31:XA:65:G:H8	1.84	0.41
49:QA:57:LYS:HB3	49:QA:60:MET:HB3	2.02	0.41
53:ZA:224:A:H2'	53:ZA:225:G:C8	2.55	0.41
53:ZA:1282:A:H3'	53:ZA:1282:A:OP2	2.20	0.41
53:ZA:1332:A:O2'	54:DB:141:LYS:NZ	2.39	0.41
53:ZA:1503:C:H2'	53:ZA:1504:U:C6	2.55	0.41
53:ZA:1614:A:H2'	53:ZA:1615:U:C6	2.55	0.41
54:DB:134:CYS:SG	54:DB:135:GLU:N	2.92	0.41
56:FB:119:SER:O	56:FB:193:LYS:HG3	2.20	0.41
66:PB:75:VAL:HA	66:PB:93:MET:HB2	2.01	0.41
67:QB:105:LYS:HE2	67:QB:105:LYS:HB3	1.81	0.41
79:CC:11:LEU:HB2	79:CC:35:MET:SD	2.60	0.41
5:E:163:LYS:HG2	5:E:277:VAL:HG12	2.02	0.41
12:M:28:TRP:HA	12:M:31:ARG:NH1	2.35	0.41
23:X:87:ARG:NH2	30:WA:404:U:O3'	2.53	0.41
30:WA:268:G:C2	30:WA:269:G:C5	3.09	0.41
30:WA:446:C:H2'	30:WA:447:C:C6	2.55	0.41
30:WA:2436:A:H2'	30:WA:2437:U:C6	2.55	0.41
30:WA:2862:A:H2'	30:WA:2863:A:O4'	2.19	0.41
30:WA:2902:G:H2'	30:WA:2903:G:H8	1.84	0.41
30:WA:3701:C:O2'	30:WA:3821:A:N1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:3731:A:H2'	30:WA:3732:A:C8	2.55	0.41
30:WA:4267:C:H2'	30:WA:4268:C:H6	1.85	0.41
31:XA:111:C:H2'	31:XA:112:U:O4'	2.20	0.41
34:BA:53:PRO:HG2	34:BA:56:ARG:HH11	1.85	0.41
53:ZA:15:U:H2'	53:ZA:16:G:O4'	2.20	0.41
53:ZA:432:G:H2'	53:ZA:433:A:C8	2.55	0.41
53:ZA:643:A:OP2	60:JB:38:ARG:NH1	2.44	0.41
53:ZA:1129:G:H2'	53:ZA:1130:G:N3	2.34	0.41
53:ZA:1238:U:H2'	53:ZA:1239:U:O4'	2.20	0.41
53:ZA:1571:G:H2'	53:ZA:1572:C:C6	2.56	0.41
54:DB:34:TYR:HE1	54:DB:37:VAL:HG13	1.85	0.41
61:KB:15:LEU:HD22	61:KB:49:MET:HE1	2.03	0.41
63:MB:106:CYS:SG	63:MB:107:SER:N	2.93	0.41
69:SB:17:ASN:O	69:SB:17:ASN:ND2	2.53	0.41
72:VB:3:ASN:OD1	72:VB:7:GLU:N	2.52	0.41
75:YB:120:THR:HG22	75:YB:121:ALA:H	1.85	0.41
84:b:79:SER:HG	84:b:89:PHE:H	1.63	0.41
84:b:113:HIS:NE2	84:b:276:MET:HE2	2.35	0.41
1:A:198:ARG:NH1	30:WA:3693:U:OP2	2.53	0.41
1:A:210:PRO:HG2	1:A:235:VAL:HG21	2.02	0.41
3:C:71:ARG:HB2	3:C:73:VAL:HG22	2.02	0.41
4:D:128:ASP:OD1	4:D:129:GLU:N	2.49	0.41
10:J:112:HIS:HE1	10:J:125:ILE:HA	1.86	0.41
29:CB:108:LYS:HB3	29:CB:233:LEU:HD11	2.03	0.41
30:WA:119:G:H3'	30:WA:120:A:H5''	2.02	0.41
30:WA:217:C:H3'	30:WA:218:A:H2'	2.02	0.41
30:WA:1917:G:H2'	30:WA:1918:C:C6	2.55	0.41
30:WA:1937:A:H2'	30:WA:1938:G:C8	2.55	0.41
30:WA:2776:G:H2'	30:WA:2777:C:O4'	2.20	0.41
30:WA:3727:G:H2'	30:WA:3728:A2M:H8	2.03	0.41
30:WA:4159:G:H2'	30:WA:4160:C:C6	2.55	0.41
30:WA:4183:A:H2'	30:WA:4184:G:C8	2.55	0.41
30:WA:4765:G:H2'	30:WA:4766:G:O4'	2.19	0.41
34:BA:64:ALA:O	34:BA:68:LYS:N	2.54	0.41
46:NA:38:LYS:NZ	46:NA:42:ASP:OD1	2.53	0.41
53:ZA:97:U:H2'	53:ZA:98:C:C6	2.55	0.41
53:ZA:344:U:H2'	53:ZA:345:U:C6	2.55	0.41
53:ZA:443:U:H2'	53:ZA:444:G:O4'	2.20	0.41
53:ZA:649:U:H2'	53:ZA:650:A:C8	2.52	0.41
53:ZA:684:G:C6	53:ZA:685:A:C5	3.08	0.41
53:ZA:964:A:H2'	53:ZA:965:U:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:996:A:H2'	53:ZA:997:A:H8	1.84	0.41
53:ZA:1092:G:C2	53:ZA:1093:A:N7	2.88	0.41
53:ZA:1406:G:H2'	53:ZA:1407:U:C6	2.56	0.41
53:ZA:1540:G:C6	53:ZA:1594:A:C6	3.08	0.41
53:ZA:1667:U:H2'	53:ZA:1668:U:C6	2.55	0.41
55:EB:31:PRO:HD2	55:EB:38:LEU:HD11	2.02	0.41
55:EB:105:THR:HG22	55:EB:245:ARG:H	1.85	0.41
58:HB:58:LYS:HB2	58:HB:90:LYS:HG2	2.01	0.41
64:NB:88:LEU:HD11	64:NB:122:ILE:HG23	2.03	0.41
65:OB:126:ILE:HG13	77:AC:53:ILE:HG23	2.01	0.41
65:OB:148:GLY:O	65:OB:150:ARG:NH1	2.53	0.41
70:TB:18:LEU:HD13	70:TB:134:ILE:HG21	2.01	0.41
79:CC:23:SER:OG	79:CC:24:GLN:OE1	2.32	0.41
3:C:190:ARG:O	3:C:195:LYS:NZ	2.44	0.41
4:D:234:ASP:OD1	4:D:235:MET:N	2.54	0.41
16:Q:21:LYS:NZ	30:WA:2826:U:OP1	2.42	0.41
25:Z:72:THR:HG22	25:Z:110:LYS:HB3	2.03	0.41
26:K:48:PRO:HB2	39:GA:120:ALA:HB2	2.02	0.41
30:WA:1350:C:H2'	30:WA:1351:A:H8	1.84	0.41
30:WA:1746:G:O6	31:XA:103:A:O2'	2.22	0.41
30:WA:1791:A:H2'	30:WA:1794:C:C5	2.55	0.41
30:WA:1852:C:H2'	30:WA:1853:C:H6	1.86	0.41
30:WA:3792:G:H1'	30:WA:3794:C:N4	2.35	0.41
30:WA:3812:A:H2'	30:WA:3813:C:H6	1.86	0.41
30:WA:4225:6MZ:O5'	30:WA:4225:6MZ:H8	2.19	0.41
40:HA:55:ARG:O	40:HA:59:GLU:HG2	2.20	0.41
53:ZA:1384:C:C2	53:ZA:1385:G:C8	3.09	0.41
57:GB:2:LYS:HB3	57:GB:15:LEU:HD21	2.03	0.41
57:GB:71:GLY:O	57:GB:99:GLY:N	2.53	0.41
59:IB:98:LYS:HB2	59:IB:178:ARG:HG2	2.02	0.41
60:JB:49:THR:HA	60:JB:52:LYS:NZ	2.36	0.41
62:LB:16:ILE:H	62:LB:16:ILE:HG13	1.58	0.41
69:SB:84:LEU:HD12	69:SB:95:TYR:HB3	2.01	0.41
73:WB:90:GLN:HB2	73:WB:94:LEU:HD12	2.03	0.41
74:XB:77:ASN:HB3	74:XB:79:LYS:HE3	2.02	0.41
83:GC:172:LYS:HG2	83:GC:193:GLY:O	2.20	0.41
84:b:207:ASP:OD1	84:b:207:ASP:N	2.53	0.41
2:B:291:TYR:OH	2:B:315:ASN:ND2	2.53	0.41
4:D:220:LYS:HE2	4:D:220:LYS:HB2	1.87	0.41
25:Z:42:ARG:NH2	30:WA:4381:A:O2'	2.53	0.41
28:BB:65:ARG:NH1	65:OB:50:LYS:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:129:C:H2'	30:WA:130:C:H6	1.86	0.41
30:WA:139:G:H2'	30:WA:140:G:C8	2.56	0.41
30:WA:288:G:H2'	30:WA:289:C:H6	1.86	0.41
30:WA:694:C:H2'	30:WA:695:C:C6	2.55	0.41
30:WA:1367:G:H2'	30:WA:1368:G:C8	2.54	0.41
30:WA:1743:A:H2'	30:WA:1744:G:H8	1.86	0.41
30:WA:1834:G:H2'	30:WA:1835:G:O4'	2.21	0.41
30:WA:1862:C:H2'	30:WA:1863:A:C8	2.56	0.41
30:WA:4721:C:H2'	30:WA:4722:A:H8	1.84	0.41
32:YA:93:C:H3'	41:IA:72:ARG:NH1	2.36	0.41
36:DA:67:LYS:HG2	36:DA:68:HIS:ND1	2.35	0.41
47:OA:47:MET:HE2	47:OA:71:TYR:CE1	2.56	0.41
53:ZA:1054:G:H2'	53:ZA:1055:A:H8	1.85	0.41
53:ZA:1119:A:O5'	53:ZA:1119:A:H8	2.04	0.41
55:EB:36:HIS:CG	55:EB:85:GLY:HA3	2.55	0.41
68:RB:103:LYS:O	68:RB:107:LYS:HG2	2.20	0.41
75:YB:14:THR:HG22	75:YB:21:LYS:HE3	2.02	0.41
82:FC:106:TYR:HB3	82:FC:116:ARG:HA	2.01	0.41
83:GC:249:CYS:HB2	83:GC:289:LEU:HD11	2.02	0.41
2:B:334:LYS:NZ	30:WA:4679:C:O3'	2.54	0.41
14:O:15:CYS:SG	14:O:150:LEU:HB2	2.60	0.41
15:P:181:ARG:NH2	30:WA:1397:A:OP2	2.54	0.41
30:WA:164:G:H2'	30:WA:165:A:H8	1.85	0.41
30:WA:490:C:H2'	30:WA:491:C:H6	1.86	0.41
30:WA:505:G:H2'	30:WA:506:G:H8	1.85	0.41
30:WA:1860:G:H2'	30:WA:1861:C:C6	2.56	0.41
30:WA:2557:G:H1'	30:WA:2771:A:N6	2.35	0.41
30:WA:3850:A:H2'	30:WA:3851:C:C6	2.55	0.41
34:BA:52:CYS:SG	34:BA:57:LYS:HB2	2.61	0.41
35:CA:37:GLY:O	35:CA:41:ARG:HG3	2.20	0.41
47:OA:26:VAL:HG12	47:OA:30:GLU:HG3	2.01	0.41
48:PA:65:LYS:O	48:PA:102:TYR:OH	2.29	0.41
50:RA:85:LEU:HD13	50:RA:100:HIS:HB3	2.02	0.41
50:RA:104:ILE:HD12	50:RA:104:ILE:HA	1.93	0.41
51:v:396:MET:HE1	51:v:472:LEU:HD11	2.02	0.41
51:v:592:LEU:HD13	51:v:603:TYR:CZ	2.56	0.41
53:ZA:175:A:H2'	53:ZA:176:U:C6	2.56	0.41
53:ZA:866:U:H2'	53:ZA:867:G:C8	2.55	0.41
53:ZA:1120:U:H5''	78:BC:72:ARG:HH22	1.85	0.41
53:ZA:1298:G:OP1	53:ZA:1298:G:N2	2.44	0.41
53:ZA:1455:A:C2	53:ZA:1456:G:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1805:G:H2'	53:ZA:1806:A:H8	1.84	0.41
58:HB:144:ILE:HB	73:WB:52:ILE:HB	2.01	0.41
66:PB:49:LEU:HB2	66:PB:54:HIS:NE2	2.36	0.41
70:TB:74:SER:O	70:TB:78:ILE:HG13	2.21	0.41
7:G:113:TYR:CE1	7:G:114:ILE:HG13	2.56	0.41
9:I:76:MET:O	9:I:80:CYS:N	2.54	0.41
9:I:187:GLU:OE1	9:I:189:ARG:HB2	2.20	0.41
28:BB:149:GLN:HE22	28:BB:154:SER:HB2	1.85	0.41
30:WA:65:A:C2	30:WA:76:A:H5''	2.56	0.41
30:WA:2043:U:H2'	30:WA:2044:G:O4'	2.21	0.41
30:WA:2553:C:H2'	30:WA:2554:G:H8	1.85	0.41
30:WA:2683:A:H2'	30:WA:2684:G:C8	2.54	0.41
30:WA:2732:C:H2'	30:WA:2733:U:C6	2.56	0.41
30:WA:2895:C:H42	30:WA:3616:A:H61	1.68	0.41
30:WA:3615:A:H2'	30:WA:3616:A:H8	1.86	0.41
30:WA:3827:U:H3'	30:WA:3828:G:H8	1.83	0.41
30:WA:4460:G:H2'	30:WA:4461:C:H6	1.86	0.41
30:WA:4780:C:H2'	30:WA:4781:G:C8	2.56	0.41
30:WA:4999:G:H2'	30:WA:5000:U:C6	2.55	0.41
30:WA:5041:C:H2'	30:WA:5042:U:C6	2.56	0.41
36:DA:77:PHE:CD2	36:DA:88:LEU:HD11	2.56	0.41
51:v:609:PHE:CD2	51:v:699:GLY:HA2	2.55	0.41
53:ZA:112:U:H2'	53:ZA:115:U:C5	2.55	0.41
53:ZA:675:U:H2'	53:ZA:676:C:H6	1.86	0.41
53:ZA:991:G:C6	53:ZA:1134:G:H4'	2.56	0.41
53:ZA:1214:A:H2'	53:ZA:1217:A:N7	2.36	0.41
53:ZA:1279:C:H2'	53:ZA:1280:G:H8	1.85	0.41
53:ZA:1390:U:H2'	53:ZA:1391:C:C6	2.55	0.41
53:ZA:1777:G:O2'	53:ZA:1778:C:P	2.78	0.41
55:EB:139:LEU:O	55:EB:146:THR:HA	2.20	0.41
68:RB:20:TYR:HD1	68:RB:23:ARG:HD2	1.86	0.41
81:EC:90:LEU:H	81:EC:90:LEU:HD22	1.86	0.41
84:b:23:MET:O	84:b:27:ILE:HG12	2.20	0.41
1:A:241:ARG:NH1	30:WA:3664:G:OP1	2.47	0.41
2:B:254:ILE:HG21	2:B:262:VAL:HG22	2.03	0.41
3:C:152:LEU:HD21	3:C:174:LEU:HD13	2.03	0.41
10:J:26:VAL:HG23	10:J:28:GLU:H	1.84	0.41
12:M:137:PRO:O	12:M:143:ARG:NH2	2.53	0.41
14:O:85:LYS:HE3	14:O:85:LYS:HB2	1.81	0.41
18:S:68:THR:OG1	18:S:71:ALA:O	2.32	0.41
19:T:19:LEU:HD22	19:T:78:PHE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:82:ILE:HG22	23:X:83:GLU:H	1.86	0.41
25:Z:74:ASN:HA	25:Z:112:LEU:O	2.21	0.41
25:Z:100:ILE:HG12	25:Z:123:ILE:HB	2.03	0.41
26:K:129:ARG:HH12	30:WA:173:C:H5''	1.86	0.41
27:AB:90:PHE:CD2	27:AB:179:ALA:HB2	2.56	0.41
28:BB:87:ILE:HG22	28:BB:101:HIS:HB2	2.01	0.41
30:WA:704:G:H4'	30:WA:705:C:H5	1.85	0.41
30:WA:1394:A:H2'	30:WA:1395:U:C6	2.56	0.41
30:WA:1464:A:H2'	30:WA:1465:C:O4'	2.20	0.41
30:WA:1817:C:H2'	30:WA:1818:U:C6	2.56	0.41
30:WA:2014:A:H3'	30:WA:2015:A:H5'	2.01	0.41
30:WA:2286:U:C2	30:WA:2287:A:C8	3.09	0.41
30:WA:2555:G:O2'	30:WA:2592:A:N1	2.44	0.41
30:WA:3712:U:H2'	30:WA:3713:C:H6	1.85	0.41
30:WA:4350:C:H2'	30:WA:4351:U:H6	1.85	0.41
30:WA:4952:U:HO2'	30:WA:4953:C:P	2.43	0.41
37:EA:83:MET:HE2	37:EA:83:MET:HB2	1.93	0.41
39:GA:98:HIS:O	39:GA:101:SER:OG	2.36	0.41
40:HA:86:LYS:O	40:HA:89:GLU:HG2	2.21	0.41
50:RA:82:ILE:HD12	50:RA:82:ILE:HA	1.91	0.41
53:ZA:363:A:N1	53:ZA:401:A:N6	2.68	0.41
53:ZA:788:G:H2'	53:ZA:789:G:O4'	2.20	0.41
53:ZA:1149:A:O2'	53:ZA:1150:A:H3'	2.20	0.41
53:ZA:1284:A:N7	63:MB:91:LEU:HD13	2.36	0.41
55:EB:69:PHE:CE1	55:EB:94:LYS:HD2	2.56	0.41
55:EB:136:ILE:HG23	55:EB:149:TYR:CE1	2.56	0.41
74:XB:94:ILE:HG22	74:XB:125:VAL:HG21	2.03	0.41
83:GC:109:LEU:HD21	83:GC:125:ARG:NH1	2.36	0.41
84:b:73:GLY:N	84:b:113:HIS:O	2.33	0.41
84:b:253:LYS:NZ	84:b:299:HIS:O	2.53	0.41
1:A:40:TYR:HA	1:A:91:GLY:HA3	2.02	0.41
5:E:48:ARG:HD3	30:WA:986:C:OP1	2.21	0.41
10:J:35:ARG:HG2	10:J:123:ILE:HG22	2.02	0.41
11:L:14:TYR:CZ	11:L:22:GLY:HA2	2.56	0.41
12:M:49:ARG:NE	30:WA:114:G:OP1	2.47	0.41
25:Z:125:LYS:HE3	25:Z:125:LYS:HB2	1.89	0.41
28:BB:109:LYS:HE3	28:BB:113:MET:SD	2.60	0.41
29:CB:113:GLN:OE1	29:CB:120:GLN:HG3	2.21	0.41
30:WA:19:G:C6	32:YA:139:G:N1	2.89	0.41
30:WA:25:A:C8	30:WA:341:G:C8	3.09	0.41
30:WA:138:G:H2'	30:WA:139:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:222:C:H2'	30:WA:223:G:O4'	2.21	0.41
30:WA:710:C:H2'	30:WA:711:G:H8	1.85	0.41
30:WA:732:G:C6	30:WA:936:A:C4	3.09	0.41
30:WA:1252:G:O6	33:AA:111:ARG:NH2	2.54	0.41
30:WA:1256:C:H2'	30:WA:1257:C:C6	2.56	0.41
30:WA:1638:G:H5'	30:WA:1639:A:OP1	2.21	0.41
30:WA:1881:U:H2'	30:WA:1882:G:C8	2.56	0.41
30:WA:1998:C:H2'	30:WA:1999:C:C6	2.56	0.41
30:WA:2548:A:N6	30:WA:2551:G:H22	2.19	0.41
30:WA:2701:A:H5''	42:JA:70:LYS:HD2	2.03	0.41
30:WA:2853:G:O2'	30:WA:3843:U:O4	2.23	0.41
30:WA:3728:A2M:OP2	40:HA:68:ARG:NH2	2.54	0.41
30:WA:3739:U:H2'	30:WA:3740:G:O4'	2.20	0.41
30:WA:4418:C:H5	30:WA:4434:C:H42	1.68	0.41
30:WA:4463:C:H2'	30:WA:4464:U:H6	1.85	0.41
30:WA:4478:A:P	44:LA:76:ARG:HH21	2.44	0.41
30:WA:4479:A:H2'	30:WA:4481:C:H5''	2.02	0.41
30:WA:4999:G:H2'	30:WA:5000:U:H6	1.85	0.41
30:WA:5063:A:H2'	30:WA:5064:C:H6	1.86	0.41
34:BA:61:GLU:HG2	34:BA:71:VAL:HG11	2.02	0.41
35:CA:42:ALA:HB3	35:CA:43:PRO:HD3	2.02	0.41
35:CA:54:MET:HE2	35:CA:60:PRO:HA	2.02	0.41
51:v:21:ASN:HB3	51:v:122:THR:HA	2.02	0.41
51:v:116:THR:HB	51:v:497:MET:HE2	2.03	0.41
51:v:160:MET:HE2	51:v:178:PHE:HZ	1.86	0.41
51:v:162:ARG:O	51:v:166:GLU:HG2	2.20	0.41
51:v:488:PHE:CE1	51:v:490:HIS:HB2	2.56	0.41
52:w:217:ALA:HB2	54:DB:143:ARG:CZ	2.51	0.41
53:ZA:57:U:H5''	53:ZA:504:G:H1'	2.03	0.41
53:ZA:319:C:H2'	53:ZA:320:G:C8	2.54	0.41
53:ZA:360:A:H4'	53:ZA:361:U:H3'	2.02	0.41
53:ZA:429:C:H2'	53:ZA:430:C:C6	2.56	0.41
53:ZA:559:G:O2'	53:ZA:560:A:H8	2.03	0.41
53:ZA:941:C:H2'	53:ZA:942:G:C8	2.56	0.41
53:ZA:1039:C:H2'	53:ZA:1040:G:H8	1.85	0.41
53:ZA:1199:A:H2'	53:ZA:1200:A:C8	2.55	0.41
53:ZA:1336:C:H2'	53:ZA:1337:4AC:H6	2.02	0.41
53:ZA:1337:4AC:H2'	53:ZA:1338:G:C8	2.55	0.41
53:ZA:1502:C:H2'	53:ZA:1503:C:H6	1.86	0.41
53:ZA:1545:A:N6	53:ZA:1588:A:C4	2.89	0.41
54:DB:42:THR:OG1	54:DB:45:ARG:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DB:67:ARG:NH1	61:KB:95:ARG:O	2.54	0.41
56:FB:59:LYS:NZ	56:FB:62:ARG:HH21	2.18	0.41
57:GB:58:LYS:HE2	57:GB:58:LYS:HB3	1.86	0.41
66:PB:84:ILE:HD13	66:PB:84:ILE:HA	1.94	0.41
69:SB:5:ILE:N	69:SB:6:PRO:HD2	2.35	0.41
69:SB:55:ARG:HE	69:SB:55:ARG:N	2.13	0.41
69:SB:66:ARG:O	69:SB:70:ILE:HG13	2.21	0.41
69:SB:102:GLY:O	69:SB:106:LYS:HG2	2.21	0.41
73:WB:55:ASP:OD1	73:WB:55:ASP:N	2.51	0.41
74:XB:17:ARG:HA	74:XB:17:ARG:NE	2.36	0.41
76:ZB:50:PHE:HE2	76:ZB:87:ALA:HB2	1.85	0.41
77:AC:15:ARG:N	77:AC:15:ARG:HD2	2.36	0.41
83:GC:57:ARG:HH21	83:GC:95:GLY:H	1.69	0.41
84:b:174:ALA:HB1	84:b:180:THR:HA	2.03	0.41
2:B:254:ILE:HD13	2:B:268:ARG:HH12	1.85	0.41
10:J:12:MET:HE3	10:J:137:PRO:HB2	2.03	0.41
13:N:109:PRO:HB2	13:N:111:PRO:HD2	2.02	0.41
19:T:106:THR:OG1	19:T:107:LYS:N	2.54	0.41
26:K:59:VAL:O	26:K:71:ARG:N	2.44	0.41
29:CB:168:GLY:N	29:CB:179:THR:O	2.52	0.41
30:WA:6:C:H2'	30:WA:7:C:C6	2.56	0.41
30:WA:1199:C:H2'	30:WA:1200:G:C8	2.55	0.41
30:WA:1241:G:O2'	30:WA:1242:C:H5'	2.21	0.41
30:WA:1279:G:H2'	30:WA:1280:A:C8	2.56	0.41
30:WA:1476:U:H2'	30:WA:1477:C:C6	2.57	0.41
30:WA:1495:G:H2'	30:WA:1496:A:H8	1.86	0.41
30:WA:1563:A:H2'	30:WA:1564:G:H8	1.86	0.41
30:WA:1629:G:C5	30:WA:1648:A:C8	3.09	0.41
30:WA:1778:U:H2'	30:WA:1779:C:C6	2.56	0.41
30:WA:2756:G:C2	30:WA:2757:G:N7	2.89	0.41
30:WA:3642:U:O4	30:WA:3656:A:H2	2.04	0.41
30:WA:4237:U:O4	46:NA:8:ARG:NH2	2.54	0.41
35:CA:57:MET:O	35:CA:59:THR:N	2.54	0.41
49:QA:171:GLU:OE1	49:QA:171:GLU:N	2.47	0.41
51:v:218:LEU:HD23	51:v:218:LEU:HA	1.96	0.41
51:v:219:HIS:HB2	51:v:221:TRP:HD1	1.85	0.41
51:v:759:ILE:HG13	51:v:800:LEU:HD11	2.03	0.41
53:ZA:5:U:H2'	53:ZA:6:G:C8	2.53	0.41
57:GB:50:VAL:HG21	57:GB:111:LEU:HB3	2.02	0.41
59:IB:48:VAL:HB	59:IB:52:ASN:C	2.46	0.41
61:KB:58:VAL:HG23	61:KB:70:TYR:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:KB:80:ARG:NE	61:KB:87:PRO:HA	2.36	0.41
63:MB:58:GLU:HB2	63:MB:61:TYR:HB3	2.03	0.41
66:PB:21:ASP:OD1	66:PB:22:LEU:N	2.54	0.41
66:PB:115:TYR:H	66:PB:118:GLU:CD	2.28	0.41
71:UB:21:ARG:HG3	71:UB:90:ASP:OD1	2.21	0.41
83:GC:120:ILE:HG12	83:GC:132:TRP:O	2.21	0.41
83:GC:298:LEU:HB3	83:GC:310:TRP:HB2	2.02	0.41
2:B:65:SER:HA	30:WA:4621:A:H4'	2.02	0.40
3:C:199:ARG:NE	30:WA:2300:C:OP1	2.41	0.40
7:G:140:LEU:HD21	7:G:144:THR:HG22	2.03	0.40
19:T:44:GLN:HA	19:T:63:LEU:HD21	2.03	0.40
19:T:84:LYS:HB2	19:T:110:TYR:CE2	2.56	0.40
22:W:143:ASP:N	22:W:143:ASP:OD1	2.54	0.40
25:Z:22:ILE:H	25:Z:22:ILE:HD12	1.86	0.40
26:K:186:ARG:HH21	40:HA:9:VAL:HG11	1.86	0.40
29:CB:254:ASP:HB3	72:VB:1:MET:N	2.36	0.40
30:WA:363:A:N1	30:WA:376:A:H5''	2.36	0.40
30:WA:985:G:H2'	30:WA:986:C:C6	2.56	0.40
30:WA:1966:G:N2	30:WA:2029:G:O2'	2.54	0.40
30:WA:2034:A:H2'	30:WA:2035:A:C8	2.56	0.40
30:WA:4081:G:OP2	30:WA:4168:U:N3	2.30	0.40
30:WA:4718:G:C5	30:WA:4719:C:C5	3.09	0.40
44:LA:57:ARG:O	44:LA:61:GLN:HG3	2.20	0.40
45:MA:2:ARG:HB3	45:MA:5:TRP:CD1	2.55	0.40
53:ZA:56:G:C6	53:ZA:90:G:N1	2.89	0.40
53:ZA:106:C:H2'	53:ZA:107:A:C8	2.54	0.40
53:ZA:1004:U:H2'	53:ZA:1005:G:C8	2.50	0.40
53:ZA:1008:A:H2'	53:ZA:1009:A:O4'	2.21	0.40
53:ZA:1089:G:N7	74:XB:3:LYS:NZ	2.69	0.40
53:ZA:1129:G:H5'	78:BC:19:HIS:CD2	2.56	0.40
53:ZA:1254:C:O2'	71:UB:71:GLY:O	2.28	0.40
53:ZA:1337:4AC:OP1	80:DC:44:ARG:NH2	2.54	0.40
53:ZA:1446:A:H5''	71:UB:58:THR:HG23	2.03	0.40
53:ZA:1643:U:O2'	67:QB:142:GLN:HA	2.21	0.40
53:ZA:1668:U:H5''	67:QB:132:PHE:HB3	2.03	0.40
53:ZA:1867:U:O2'	77:AC:38:LYS:HG2	2.21	0.40
57:GB:48:TYR:OH	57:GB:119:LYS:O	2.34	0.40
61:KB:6:LYS:HE2	61:KB:6:LYS:HB3	1.87	0.40
65:OB:116:LEU:HD23	65:OB:116:LEU:HA	1.94	0.40
73:WB:42:MET:HE2	73:WB:49:GLU:HA	2.02	0.40
79:CC:37:ASP:OD2	79:CC:39:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HD12	1:A:225:ILE:HA	1.95	0.40
3:C:323:ARG:HH22	30:WA:1285:A:H2	1.69	0.40
5:E:160:HIS:HB3	5:E:163:LYS:HE2	2.03	0.40
5:E:211:ILE:HG23	5:E:215:LEU:HD12	2.03	0.40
16:Q:19:LYS:HG2	30:WA:2828:G:OP1	2.21	0.40
16:Q:38:ARG:HG3	30:WA:2531:C:H5''	2.02	0.40
16:Q:90:PRO:HG2	16:Q:93:VAL:HB	2.03	0.40
22:W:100:VAL:HG21	22:W:109:ILE:HD11	2.04	0.40
30:WA:1550:G:H2'	30:WA:1551:C:H6	1.84	0.40
30:WA:1906:C:H2'	30:WA:1907:G:H8	1.86	0.40
30:WA:2055:OMG:H2'	30:WA:2056:C:C6	2.57	0.40
30:WA:2408:A:OP1	38:FA:10:ARG:HD2	2.21	0.40
30:WA:2409:A:H2'	30:WA:2410:G:O4'	2.20	0.40
30:WA:2571:G:H2'	30:WA:2572:G:C8	2.55	0.40
30:WA:3789:A:H61	30:WA:3819:U:H1'	1.85	0.40
30:WA:5060:G:N2	35:CA:118:GLN:OE1	2.49	0.40
34:BA:26:LYS:HG3	34:BA:97:ILE:HB	2.03	0.40
51:v:653:GLY:HA2	51:v:660:ASN:HB2	2.03	0.40
52:w:209:LYS:HD3	54:DB:143:ARG:HH11	1.86	0.40
53:ZA:498:C:N4	53:ZA:499:G:O6	2.55	0.40
53:ZA:618:C:OP1	74:XB:87:ASN:HA	2.21	0.40
53:ZA:946:U:H2'	53:ZA:947:G:C8	2.56	0.40
53:ZA:1367:U:H2'	53:ZA:1368:U:C6	2.56	0.40
53:ZA:1688:C:H2'	53:ZA:1689:C:H6	1.86	0.40
55:EB:184:THR:HA	55:EB:189:LEU:HD13	2.03	0.40
56:FB:51:HIS:ND1	67:QB:82:TYR:OH	2.49	0.40
69:SB:23:ARG:HH12	76:ZB:45:ASN:HB3	1.87	0.40
1:A:46:LYS:HE3	1:A:46:LYS:HB3	1.92	0.40
4:D:33:ARG:NH2	4:D:72:ASP:OD2	2.54	0.40
4:D:42:ASN:HD22	18:S:69:GLN:HA	1.87	0.40
9:I:95:HIS:HB3	9:I:126:VAL:O	2.21	0.40
12:M:101:VAL:O	12:M:105:ARG:HG2	2.21	0.40
15:P:167:VAL:HG12	15:P:169:SER:H	1.86	0.40
15:P:179:GLY:H	25:Z:51:GLY:N	2.19	0.40
17:R:43:ARG:NH1	31:XA:95:C:OP1	2.54	0.40
17:R:95:ARG:NE	17:R:97:TYR:OH	2.47	0.40
19:T:101:ARG:HB2	19:T:115:PHE:CZ	2.57	0.40
22:W:80:PRO:HA	22:W:98:PHE:HA	2.03	0.40
28:BB:150:ILE:HG22	68:RB:131:PRO:HG3	2.03	0.40
30:WA:509:G:HO2'	30:WA:511:U:P	2.43	0.40
30:WA:993:C:H2'	30:WA:994:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:WA:1181:A:H2'	30:WA:1182:C:C6	2.57	0.40
30:WA:1196:C:H2'	30:WA:1197:C:C6	2.57	0.40
30:WA:1880:C:H2'	30:WA:1881:U:C6	2.56	0.40
30:WA:1943:C:H4'	30:WA:1944:A:O4'	2.20	0.40
30:WA:2659:C:H2'	30:WA:2660:C:H6	1.86	0.40
30:WA:3925:U:H2'	30:WA:3926:U:H6	1.85	0.40
30:WA:4628:OMG:HM23	30:WA:4628:OMG:H1'	1.87	0.40
32:YA:11:C:H2'	32:YA:12:G:C8	2.52	0.40
39:GA:21:LEU:O	39:GA:25:LYS:HG2	2.22	0.40
53:ZA:151:C:H2'	53:ZA:152:U:C6	2.56	0.40
53:ZA:381:C:H5'	59:IB:48:VAL:CG1	2.51	0.40
53:ZA:386:C:H5''	59:IB:10:LYS:HD2	2.01	0.40
53:ZA:529:A:H2'	53:ZA:530:U:C6	2.57	0.40
53:ZA:651:U:H2'	53:ZA:652:U:C6	2.56	0.40
53:ZA:1120:U:P	78:BC:72:ARG:HH12	2.44	0.40
53:ZA:1233:G:C6	53:ZA:1526:G:C6	3.09	0.40
53:ZA:1538:C:H2'	53:ZA:1539:U:H6	1.87	0.40
53:ZA:1713:C:H2'	53:ZA:1714:U:H6	1.85	0.40
55:EB:75:LYS:HE3	55:EB:75:LYS:HB2	1.95	0.40
61:KB:64:TRP:CD2	80:DC:23:VAL:HG22	2.56	0.40
65:OB:113:GLN:NE2	77:AC:42:ARG:HH12	2.19	0.40
71:UB:30:LYS:HA	71:UB:30:LYS:HD3	1.93	0.40
2:B:312:LYS:HD2	2:B:370:THR:HG21	2.02	0.40
6:F:45:ARG:HH12	30:WA:2107:G:H5''	1.87	0.40
18:S:13:TYR:OH	30:WA:1795:U:OP2	2.19	0.40
19:T:97:ARG:NH2	30:WA:2629:G:OP2	2.55	0.40
22:W:131:ASP:O	43:KA:14:ALA:HB1	2.21	0.40
30:WA:30:C:H2'	30:WA:31:U:H6	1.86	0.40
30:WA:316:U:OP1	30:WA:316:U:H3'	2.22	0.40
30:WA:505:G:O2'	30:WA:506:G:P	2.80	0.40
30:WA:714:C:H2'	30:WA:715:G:C8	2.56	0.40
30:WA:1419:C:H2'	30:WA:1420:C:C6	2.56	0.40
30:WA:1900:G:H2'	30:WA:1901:A:O4'	2.21	0.40
30:WA:2523:G:H1'	30:WA:2544:C:H1'	2.04	0.40
30:WA:3669:G:H2'	30:WA:3670:G:H8	1.86	0.40
30:WA:3699:U:H2'	30:WA:3700:U:C6	2.57	0.40
30:WA:3701:C:H2'	30:WA:3702:U:O4'	2.21	0.40
35:CA:23:ARG:HG3	35:CA:121:ASN:HA	2.04	0.40
49:QA:18:ILE:HG13	49:QA:68:HIS:CD2	2.56	0.40
51:v:13:MET:HB3	51:v:464:VAL:HG21	2.03	0.40
51:v:749:ILE:HD11	51:v:784:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ZA:1174:U:C2	53:ZA:1175:G:C8	3.10	0.40
53:ZA:1177:U:H2'	53:ZA:1178:U:C6	2.57	0.40
53:ZA:1389:C:OP2	68:RB:45:LYS:HD2	2.21	0.40
53:ZA:1479:G:H4'	67:QB:128:GLU:OE2	2.22	0.40
53:ZA:1606:G:N2	53:ZA:1632:G:O2'	2.45	0.40
53:ZA:1754:G:H2'	53:ZA:1755:C:H6	1.84	0.40
56:FB:121:PRO:HA	56:FB:193:LYS:HD3	2.02	0.40
61:KB:32:HIS:CD2	61:KB:45:VAL:HG21	2.56	0.40
64:NB:20:ARG:HH11	73:WB:56:HIS:CG	2.39	0.40
67:QB:93:VAL:HG13	67:QB:105:LYS:HG2	2.02	0.40
76:ZB:73:VAL:HG12	76:ZB:79:ILE:HD11	2.04	0.40
77:AC:7:ASN:O	77:AC:9:GLY:N	2.54	0.40
83:GC:294:ASP:OD1	83:GC:295:GLY:N	2.54	0.40
1:A:83:HIS:HB3	47:OA:64:VAL:HG22	2.03	0.40
2:B:200:ARG:O	2:B:203:GLN:HG2	2.21	0.40
3:C:303:ARG:HG2	15:P:38:ARG:O	2.21	0.40
7:G:119:GLN:HG3	12:M:28:TRP:CH2	2.56	0.40
9:I:52:MET:HE1	9:I:155:ALA:HB3	2.03	0.40
15:P:65:ARG:NH1	30:WA:1507:G:OP1	2.42	0.40
16:Q:23:TRP:CD1	30:WA:2392:G:H5''	2.57	0.40
22:W:64:SER:HB2	39:GA:69:LEU:HD13	2.03	0.40
24:Y:100:VAL:HG23	24:Y:106:LEU:HB3	2.03	0.40
27:AB:149:ASN:OD1	27:AB:150:THR:N	2.48	0.40
30:WA:25:A:H2'	30:WA:26:C:H6	1.86	0.40
30:WA:754:G:O6	30:WA:913:U:O4	2.40	0.40
30:WA:1376:G:H5'	30:WA:1378:A:H1'	2.02	0.40
30:WA:4422:C:H2'	30:WA:4423:G:O4'	2.20	0.40
30:WA:5063:A:H2'	30:WA:5064:C:C6	2.56	0.40
33:AA:8:THR:HG22	33:AA:10:HIS:H	1.86	0.40
33:AA:40:LEU:O	33:AA:44:ARG:HG3	2.21	0.40
36:DA:85:LEU:HD23	36:DA:85:LEU:HA	1.96	0.40
49:QA:47:LEU:O	49:QA:51:ALA:N	2.50	0.40
51:v:631:ARG:NE	51:v:649:ILE:HD11	2.37	0.40
53:ZA:102:A:H4'	53:ZA:104:A:C8	2.56	0.40
53:ZA:126:G:H5''	57:GB:195:LYS:HD3	2.04	0.40
53:ZA:200:G:H2'	53:ZA:201:C:C6	2.56	0.40
53:ZA:1296:U:H2'	53:ZA:1297:U:O4'	2.22	0.40
53:ZA:1320:G:H3'	53:ZA:1321:G:H8	1.87	0.40
53:ZA:1687:C:H2'	53:ZA:1688:C:H6	1.86	0.40
57:GB:7:PHE:CZ	57:GB:116:LYS:HG2	2.57	0.40
58:HB:129:ILE:O	58:HB:133:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:KB:72:THR:O	61:KB:76:ILE:N	2.54	0.40
68:RB:29:HIS:HB2	83:GC:36:ARG:NH2	2.37	0.40
68:RB:32:LYS:HE3	68:RB:33:ARG:NH1	2.37	0.40
75:YB:20:ARG:NH2	75:YB:76:TYR:OH	2.53	0.40
76:ZB:72:VAL:HG13	76:ZB:76:ARG:HH21	1.87	0.40
83:GC:298:LEU:HD22	83:GC:310:TRP:CD1	2.56	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	246/257 (96%)	236 (96%)	10 (4%)	0	100	100
2	B	392/403 (97%)	377 (96%)	15 (4%)	0	100	100
3	C	359/425 (84%)	353 (98%)	6 (2%)	0	100	100
4	D	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
5	E	207/291 (71%)	200 (97%)	7 (3%)	0	100	100
6	F	223/247 (90%)	216 (97%)	7 (3%)	0	100	100
7	G	229/319 (72%)	224 (98%)	4 (2%)	1 (0%)	30	59
8	H	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
9	I	201/214 (94%)	199 (99%)	2 (1%)	0	100	100
10	J	168/178 (94%)	164 (98%)	3 (2%)	1 (1%)	21	51
11	L	136/218 (62%)	131 (96%)	5 (4%)	0	100	100
12	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
13	N	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
14	O	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
15	P	185/188 (98%)	182 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	178/196 (91%)	174 (98%)	4 (2%)	0	100	100
17	R	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
18	S	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
19	T	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
20	U	129/140 (92%)	129 (100%)	0	0	100	100
21	V	94/157 (60%)	89 (95%)	5 (5%)	0	100	100
22	W	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
23	X	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
24	Y	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
25	Z	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
26	K	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
27	AB	215/295 (73%)	210 (98%)	5 (2%)	0	100	100
28	BB	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
29	CB	219/293 (75%)	218 (100%)	1 (0%)	0	100	100
33	AA	100/245 (41%)	96 (96%)	4 (4%)	0	100	100
34	BA	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
35	CA	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
36	DA	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
37	EA	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
38	FA	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
39	GA	120/123 (98%)	120 (100%)	0	0	100	100
40	HA	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
41	IA	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
42	JA	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
43	KA	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
44	LA	49/102 (48%)	47 (96%)	2 (4%)	0	100	100
45	MA	23/25 (92%)	23 (100%)	0	0	100	100
46	NA	101/106 (95%)	97 (96%)	4 (4%)	0	100	100
47	OA	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
48	PA	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
49	QA	194/318 (61%)	190 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	RA	151/165 (92%)	147 (97%)	4 (3%)	0	100	100
51	v	827/839 (99%)	802 (97%)	25 (3%)	0	100	100
52	w	42/46 (91%)	38 (90%)	4 (10%)	0	100	100
54	DB	226/243 (93%)	222 (98%)	4 (2%)	0	100	100
55	EB	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
56	FB	181/204 (89%)	174 (96%)	7 (4%)	0	100	100
57	GB	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
58	HB	181/194 (93%)	180 (99%)	1 (1%)	0	100	100
59	IB	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
60	JB	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
61	KB	94/165 (57%)	90 (96%)	4 (4%)	0	100	100
62	LB	134/158 (85%)	128 (96%)	6 (4%)	0	100	100
63	MB	115/132 (87%)	112 (97%)	2 (2%)	1 (1%)	14	41
64	NB	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
65	OB	134/168 (80%)	132 (98%)	2 (2%)	0	100	100
66	PB	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
67	QB	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
68	RB	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
69	SB	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
70	TB	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
71	UB	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
72	VB	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
73	WB	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	XB	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
75	YB	122/130 (94%)	118 (97%)	4 (3%)	0	100	100
76	ZB	73/125 (58%)	72 (99%)	1 (1%)	0	100	100
77	AC	95/115 (83%)	91 (96%)	4 (4%)	0	100	100
78	BC	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
79	CC	60/69 (87%)	60 (100%)	0	0	100	100
80	DC	53/56 (95%)	53 (100%)	0	0	100	100
81	EC	53/133 (40%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	FC	66/156 (42%)	63 (96%)	3 (4%)	0	100	100
83	GC	311/317 (98%)	293 (94%)	18 (6%)	0	100	100
84	b	313/394 (79%)	302 (96%)	11 (4%)	0	100	100
All	All	12680/14654 (86%)	12346 (97%)	331 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	217	ILE
63	MB	74	ILE
10	J	10	ASN

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	190/199 (96%)	186 (98%)	4 (2%)	47	77
2	B	342/348 (98%)	341 (100%)	1 (0%)	86	96
3	C	301/346 (87%)	300 (100%)	1 (0%)	86	96
4	D	247/250 (99%)	246 (100%)	1 (0%)	84	94
5	E	189/251 (75%)	184 (97%)	5 (3%)	40	73
6	F	196/215 (91%)	196 (100%)	0	100	100
7	G	200/272 (74%)	198 (99%)	2 (1%)	68	89
8	H	169/171 (99%)	167 (99%)	2 (1%)	63	86
9	I	175/181 (97%)	174 (99%)	1 (1%)	78	93
10	J	143/149 (96%)	142 (99%)	1 (1%)	76	92
11	L	117/161 (73%)	115 (98%)	2 (2%)	53	82
12	M	171/172 (99%)	170 (99%)	1 (1%)	78	93
13	N	171/173 (99%)	171 (100%)	0	100	100
14	O	134/163 (82%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	164/165 (99%)	163 (99%)	1 (1%)	78	93
16	Q	159/175 (91%)	158 (99%)	1 (1%)	78	93
17	R	157/157 (100%)	157 (100%)	0	100	100
18	S	139/140 (99%)	137 (99%)	2 (1%)	59	85
19	T	89/114 (78%)	89 (100%)	0	100	100
20	U	101/107 (94%)	100 (99%)	1 (1%)	68	89
21	V	81/126 (64%)	81 (100%)	0	100	100
22	W	106/134 (79%)	105 (99%)	1 (1%)	70	90
23	X	124/135 (92%)	123 (99%)	1 (1%)	73	90
24	Y	117/118 (99%)	117 (100%)	0	100	100
25	Z	119/120 (99%)	119 (100%)	0	100	100
26	K	175/176 (99%)	172 (98%)	3 (2%)	53	82
27	AB	181/245 (74%)	178 (98%)	3 (2%)	53	82
28	BB	194/231 (84%)	192 (99%)	2 (1%)	68	89
29	CB	187/225 (83%)	184 (98%)	3 (2%)	55	83
33	AA	84/184 (46%)	82 (98%)	2 (2%)	43	75
34	BA	84/98 (86%)	82 (98%)	2 (2%)	43	75
35	CA	98/110 (89%)	97 (99%)	1 (1%)	68	89
36	DA	114/121 (94%)	110 (96%)	4 (4%)	32	66
37	EA	88/89 (99%)	88 (100%)	0	100	100
38	FA	98/100 (98%)	97 (99%)	1 (1%)	68	89
39	GA	109/110 (99%)	108 (99%)	1 (1%)	70	90
40	HA	86/89 (97%)	85 (99%)	1 (1%)	63	86
41	IA	73/80 (91%)	71 (97%)	2 (3%)	39	73
42	JA	64/65 (98%)	62 (97%)	2 (3%)	35	69
43	KA	47/48 (98%)	47 (100%)	0	100	100
44	LA	47/89 (53%)	47 (100%)	0	100	100
45	MA	24/24 (100%)	24 (100%)	0	100	100
46	NA	91/94 (97%)	90 (99%)	1 (1%)	65	88
47	OA	74/75 (99%)	73 (99%)	1 (1%)	59	85
48	PA	108/121 (89%)	107 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	QA	164/258 (64%)	159 (97%)	5 (3%)	36	70
50	RA	126/137 (92%)	121 (96%)	5 (4%)	28	62
51	v	706/713 (99%)	687 (97%)	19 (3%)	39	73
52	w	37/37 (100%)	37 (100%)	0	100	100
54	DB	190/202 (94%)	183 (96%)	7 (4%)	30	64
55	EB	224/225 (100%)	218 (97%)	6 (3%)	39	73
56	FB	158/170 (93%)	153 (97%)	5 (3%)	34	68
57	GB	207/218 (95%)	202 (98%)	5 (2%)	43	75
58	HB	165/174 (95%)	164 (99%)	1 (1%)	78	93
59	IB	178/180 (99%)	176 (99%)	2 (1%)	65	88
60	JB	161/168 (96%)	158 (98%)	3 (2%)	50	79
61	KB	87/136 (64%)	85 (98%)	2 (2%)	44	76
62	LB	126/142 (89%)	124 (98%)	2 (2%)	55	83
63	MB	99/108 (92%)	95 (96%)	4 (4%)	28	62
64	NB	130/131 (99%)	128 (98%)	2 (2%)	57	84
65	OB	106/130 (82%)	105 (99%)	1 (1%)	70	90
66	PB	109/130 (84%)	107 (98%)	2 (2%)	51	80
67	QB	117/121 (97%)	114 (97%)	3 (3%)	40	73
68	RB	119/121 (98%)	113 (95%)	6 (5%)	22	53
69	SB	125/132 (95%)	121 (97%)	4 (3%)	34	68
70	TB	111/115 (96%)	106 (96%)	5 (4%)	24	58
71	UB	92/107 (86%)	89 (97%)	3 (3%)	33	67
72	VB	67/67 (100%)	62 (92%)	5 (8%)	12	37
73	WB	112/113 (99%)	110 (98%)	2 (2%)	51	80
74	XB	113/115 (98%)	110 (97%)	3 (3%)	39	73
75	YB	107/112 (96%)	103 (96%)	4 (4%)	30	64
76	ZB	66/103 (64%)	64 (97%)	2 (3%)	36	70
77	AC	84/98 (86%)	80 (95%)	4 (5%)	23	55
78	BC	75/76 (99%)	75 (100%)	0	100	100
79	CC	55/62 (89%)	51 (93%)	4 (7%)	13	38
80	DC	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	EC	46/106 (43%)	45 (98%)	1 (2%)	45	77
82	FC	61/140 (44%)	60 (98%)	1 (2%)	55	83
83	GC	272/275 (99%)	264 (97%)	8 (3%)	37	71
84	b	239/336 (71%)	231 (97%)	8 (3%)	33	67
All	All	11009/12423 (89%)	10817 (98%)	192 (2%)	52	82

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	101	VAL
1	A	142	GLU
1	A	218	HIS
2	B	344	VAL
3	C	313	VAL
4	D	153	THR
5	E	178	VAL
5	E	187	VAL
5	E	197	VAL
5	E	267	VAL
5	E	290	VAL
7	G	217	ILE
7	G	221	VAL
8	H	16	VAL
8	H	20	LEU
9	I	31	ILE
10	J	155	HIS
11	L	12	VAL
11	L	125	ASN
12	M	174	LEU
15	P	31	LEU
16	Q	167	LYS
18	S	74	ILE
18	S	80	VAL
20	U	92	ASP
22	W	50	LYS
23	X	111	LEU
26	K	59	VAL
26	K	67	HIS
26	K	154	VAL
27	AB	44	ASP

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Mol	Chain	Res	Type
27	AB	76	VAL
27	AB	197	VAL
28	BB	127	VAL
28	BB	131	ASP
29	CB	86	LEU
29	CB	102	LEU
29	CB	248	TYR
33	AA	32	LEU
33	AA	72	ILE
34	BA	28	VAL
34	BA	42	LYS
35	CA	113	THR
36	DA	13	VAL
36	DA	21	ILE
36	DA	58	ILE
36	DA	87	VAL
38	FA	32	TYR
39	GA	4	ILE
40	HA	29	ARG
41	IA	54	LYS
41	IA	58	THR
42	JA	37	ARG
42	JA	47	ILE
46	NA	23	VAL
47	OA	52	VAL
48	PA	106	LEU
49	QA	30	VAL
49	QA	53	VAL
49	QA	55	MET
49	QA	159	GLN
49	QA	198	ILE
50	RA	64	ILE
50	RA	91	ASP
50	RA	107	ASP
50	RA	111	ASN
50	RA	129	ILE
51	v	6	VAL
51	v	15	LYS
51	v	28	VAL
51	v	236	PHE
51	v	278	THR
51	v	344	LEU

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Mol	Chain	Res	Type
51	v	489	GLU
51	v	504	VAL
51	v	505	VAL
51	v	577	VAL
51	v	622	VAL
51	v	684	GLN
51	v	704	VAL
51	v	707	VAL
51	v	770	VAL
51	v	783	VAL
51	v	797	THR
51	v	804	THR
51	v	856	ASP
54	DB	39	VAL
54	DB	113	LEU
54	DB	136	VAL
54	DB	159	HIS
54	DB	168	VAL
54	DB	188	ILE
54	DB	218	LEU
55	EB	62	LYS
55	EB	67	GLN
55	EB	105	THR
55	EB	146	THR
55	EB	148	ARG
55	EB	230	LYS
56	FB	20	PHE
56	FB	63	LYS
56	FB	97	PHE
56	FB	100	ILE
56	FB	117	ILE
57	GB	32	MET
57	GB	98	ARG
57	GB	121	ILE
57	GB	158	VAL
57	GB	179	LEU
58	HB	92	VAL
59	IB	29	LEU
59	IB	75	LYS
60	JB	65	GLU
60	JB	92	MET
60	JB	102	ILE

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Mol	Chain	Res	Type
61	KB	66	HIS
61	KB	89	ILE
62	LB	16	ILE
62	LB	145	VAL
63	MB	74	ILE
63	MB	77	ILE
63	MB	83	LYS
63	MB	110	VAL
64	NB	36	GLN
64	NB	94	LYS
65	OB	135	ILE
66	PB	14	LYS
66	PB	44	ARG
67	QB	18	THR
67	QB	53	GLU
67	QB	118	THR
68	RB	24	LEU
68	RB	31	ASN
68	RB	71	ILE
68	RB	76	GLU
68	RB	102	THR
68	RB	108	LEU
69	SB	36	VAL
69	SB	52	LEU
69	SB	55	ARG
69	SB	59	LEU
70	TB	34	VAL
70	TB	37	VAL
70	TB	51	ASN
70	TB	75	MET
70	TB	118	ASP
71	UB	46	LYS
71	UB	50	VAL
71	UB	84	ILE
72	VB	1	MET
72	VB	11	LEU
72	VB	13	VAL
72	VB	52	THR
72	VB	59	ILE
73	WB	74	VAL
73	WB	80	ASP
74	XB	7	LEU

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Mol	Chain	Res	Type
74	XB	105	PHE
74	XB	129	SER
75	YB	35	VAL
75	YB	51	THR
75	YB	111	LYS
75	YB	120	THR
76	ZB	48	VAL
76	ZB	100	VAL
77	AC	40	VAL
77	AC	50	VAL
77	AC	63	VAL
77	AC	94	ASP
79	CC	10	LYS
79	CC	17	VAL
79	CC	32	VAL
79	CC	42	ILE
81	EC	82	VAL
82	FC	143	LYS
83	GC	47	ARG
83	GC	50	THR
83	GC	69	VAL
83	GC	91	ASP
83	GC	92	LEU
83	GC	99	ARG
83	GC	107	ASP
83	GC	266	ILE
84	b	58	GLU
84	b	59	GLU
84	b	147	HIS
84	b	156	LEU
84	b	157	VAL
84	b	253	LYS
84	b	276	MET
84	b	343	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
2	B	175	GLN
3	C	38	ASN
3	C	142	HIS

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Mol	Chain	Res	Type
6	F	118	ASN
8	H	39	ASN
8	H	63	ASN
9	I	59	GLN
9	I	144	ASN
9	I	166	HIS
9	I	177	ASN
9	I	202	ASN
10	J	23	ASN
10	J	98	ASN
11	L	70	GLN
12	M	109	HIS
15	P	188	ASN
16	Q	34	ASN
16	Q	40	GLN
17	R	66	GLN
18	S	112	ASN
20	U	27	ASN
22	W	107	HIS
25	Z	40	HIS
26	K	104	ASN
27	AB	113	GLN
28	BB	118	GLN
29	CB	136	HIS
33	AA	6	ASN
35	CA	34	HIS
36	DA	52	GLN
36	DA	124	ASN
37	EA	91	ASN
38	FA	100	GLN
40	HA	20	ASN
41	IA	66	HIS
49	QA	105	ASN
51	v	101	ASN
51	v	138	GLN
51	v	433	ASN
51	v	492	HIS
51	v	588	ASN
51	v	853	ASN
56	FB	31	ASN
56	FB	82	ASN
57	GB	65	GLN

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Mol	Chain	Res	Type
58	HB	44	ASN
60	JB	177	ASN
61	KB	42	ASN
61	KB	50	GLN
62	LB	94	HIS
67	QB	8	GLN
67	QB	24	HIS
68	RB	83	ASN
68	RB	116	ASN
69	SB	101	ASN
73	WB	24	GLN
73	WB	98	GLN
77	AC	8	ASN
78	BC	19	HIS
78	BC	84	HIS
79	CC	29	GLN
83	GC	237	ASN
83	GC	305	ASN
84	b	29	ASN
84	b	161	ASN
84	b	162	GLN
84	b	303	GLN
84	b	306	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	WA	3517/3635 (96%)	662 (18%)	34 (0%)
31	XA	119/120 (99%)	11 (9%)	0
32	YA	149/156 (95%)	27 (18%)	1 (0%)
53	ZA	1688/1869 (90%)	373 (22%)	15 (0%)
All	All	5473/5780 (94%)	1073 (19%)	50 (0%)

All (1073) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	WA	12	A
30	WA	13	U
30	WA	25	A
30	WA	39	A
30	WA	42	A

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Mol	Chain	Res	Type
30	WA	49	U
30	WA	59	A
30	WA	64	A
30	WA	65	A
30	WA	71	C
30	WA	73	A
30	WA	76	A
30	WA	91	G
30	WA	108	A
30	WA	109	G
30	WA	110	C
30	WA	116	G
30	WA	118	C
30	WA	119	G
30	WA	120	A
30	WA	122	U
30	WA	126	C
30	WA	132	G
30	WA	134	G
30	WA	135	G
30	WA	136	C
30	WA	149	A
30	WA	157	U
30	WA	159	C
30	WA	172	C
30	WA	200	U
30	WA	201	C
30	WA	209	U
30	WA	216	C
30	WA	219	G
30	WA	224	U
30	WA	233	U
30	WA	234	G
30	WA	237	B9B
30	WA	246	G
30	WA	264	C
30	WA	266	C
30	WA	274	C
30	WA	275	C
30	WA	276	C
30	WA	280	G
30	WA	297	U

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Mol	Chain	Res	Type
30	WA	306	A
30	WA	309	C
30	WA	310	G
30	WA	315	G
30	WA	316	U
30	WA	322	C
30	WA	326	C
30	WA	334	A
30	WA	340	C
30	WA	350	C
30	WA	386	A
30	WA	387	G
30	WA	391	U
30	WA	393	U
30	WA	396	A
30	WA	398	A2M
30	WA	399	G
30	WA	407	A
30	WA	408	A
30	WA	409	G
30	WA	410	A
30	WA	412	G
30	WA	413	G
30	WA	449	C
30	WA	450	G
30	WA	452	A
30	WA	453	G
30	WA	454	U
30	WA	457	G
30	WA	459	C
30	WA	466	A
30	WA	468	U
30	WA	469	C
30	WA	482	C
30	WA	483	G
30	WA	484	G
30	WA	485	U
30	WA	488	G
30	WA	489	G
30	WA	493	U
30	WA	494	G
30	WA	497	G

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Mol	Chain	Res	Type
30	WA	498	G
30	WA	499	C
30	WA	500	G
30	WA	501	G
30	WA	506	G
30	WA	511	U
30	WA	662	C
30	WA	667	G
30	WA	668	A
30	WA	686	C
30	WA	693	A
30	WA	698	G
30	WA	703	U
30	WA	704	G
30	WA	705	C
30	WA	732	G
30	WA	739	C
30	WA	741	G
30	WA	747	G
30	WA	749	A
30	WA	751	G
30	WA	760	G
30	WA	915	U
30	WA	916	U
30	WA	917	A
30	WA	919	A
30	WA	920	G
30	WA	925	G
30	WA	929	C
30	WA	930	G
30	WA	933	A
30	WA	934	G
30	WA	936	A
30	WA	937	G
30	WA	938	C
30	WA	940	G
30	WA	946	C
30	WA	949	A
30	WA	950	U
30	WA	961	A
30	WA	964	G
30	WA	965	A

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Mol	Chain	Res	Type
30	WA	966	G
30	WA	969	A
30	WA	971	A
30	WA	972	C
30	WA	973	C
30	WA	974	C
30	WA	978	C
30	WA	984	C
30	WA	989	U
30	WA	991	C
30	WA	1076	G
30	WA	1078	C
30	WA	1079	G
30	WA	1084	A
30	WA	1085	C
30	WA	1104	G
30	WA	1176	G
30	WA	1186	C
30	WA	1191	G
30	WA	1193	G
30	WA	1201	G
30	WA	1203	C
30	WA	1204	G
30	WA	1208	C
30	WA	1217	G
30	WA	1218	G
30	WA	1222	C
30	WA	1240	G
30	WA	1241	G
30	WA	1242	C
30	WA	1243	C
30	WA	1244	A
30	WA	1245	C
30	WA	1279	G
30	WA	1282	C
30	WA	1283	G
30	WA	1284	C
30	WA	1286	C
30	WA	1290	G
30	WA	1291	U
30	WA	1293	G
30	WA	1299	G

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Mol	Chain	Res	Type
30	WA	1300	A
30	WA	1301	U
30	WA	1302	G
30	WA	1303	U
30	WA	1307	C
30	WA	1309	A
30	WA	1320	C
30	WA	1332	A2M
30	WA	1336	A
30	WA	1354	P4U
30	WA	1360	A
30	WA	1361	G
30	WA	1364	G
30	WA	1365	G
30	WA	1377	A
30	WA	1378	A
30	WA	1383	G
30	WA	1393	A
30	WA	1400	G
30	WA	1403	A
30	WA	1404	A
30	WA	1411	C
30	WA	1427	G
30	WA	1441	G
30	WA	1444	U
30	WA	1445	U
30	WA	1461	JMH
30	WA	1463	C
30	WA	1487	G
30	WA	1488	C
30	WA	1489	G
30	WA	1490	C
30	WA	1502	A
30	WA	1503	G
30	WA	1506	C
30	WA	1507	G
30	WA	1523	A
30	WA	1528	A
30	WA	1530	A
30	WA	1539	A2M
30	WA	1552	A
30	WA	1573	C

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Mol	Chain	Res	Type
30	WA	1579	B9B
30	WA	1583	U
30	WA	1587	PSU
30	WA	1596	U
30	WA	1601	U
30	WA	1607	U
30	WA	1617	G
30	WA	1618	A
30	WA	1629	G
30	WA	1630	OMG
30	WA	1636	A
30	WA	1638	G
30	WA	1639	A
30	WA	1643	A
30	WA	1659	G
30	WA	1666	C
30	WA	1681	C
30	WA	1682	PSU
30	WA	1700	U
30	WA	1739	G
30	WA	1746	G
30	WA	1747	A
30	WA	1755	G
30	WA	1758	G
30	WA	1760	C
30	WA	1761	U
30	WA	1766	G
30	WA	1769	G
30	WA	1774	G
30	WA	1778	U
30	WA	1786	U
30	WA	1792	A
30	WA	1809	A
30	WA	1810	A
30	WA	1824	G
30	WA	1826	G
30	WA	1836	G
30	WA	1838	G
30	WA	1840	G
30	WA	1841	G
30	WA	1842	A
30	WA	1847	G

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Mol	Chain	Res	Type
30	WA	1860	G
30	WA	1865	B8H
30	WA	1871	UR3
30	WA	1874	G
30	WA	1887	U
30	WA	1902	A
30	WA	1923	U
30	WA	1925	C
30	WA	1926	C
30	WA	1927	G
30	WA	1935	U
30	WA	1936	C
30	WA	1937	A
30	WA	1938	G
30	WA	1941	C
30	WA	1953	G
30	WA	1962	U
30	WA	1963	A
30	WA	1966	G
30	WA	1969	A
30	WA	1979	U
30	WA	1980	G
30	WA	1981	G
30	WA	1989	A
30	WA	1995	A
30	WA	2002	U
30	WA	2003	A
30	WA	2004	A
30	WA	2006	G
30	WA	2008	G
30	WA	2009	U
30	WA	2013	U
30	WA	2014	A
30	WA	2015	A
30	WA	2026	G
30	WA	2028	C
30	WA	2030	A
30	WA	2031	A
30	WA	2052	A
30	WA	2053	U
30	WA	2060	G
30	WA	2061	G

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Mol	Chain	Res	Type
30	WA	2074	A
30	WA	2089	U
30	WA	2098	G
30	WA	2099	C
30	WA	2102	A
30	WA	2103	G
30	WA	2105	G
30	WA	2106	A
30	WA	2107	G
30	WA	2109	A
30	WA	2110	A
30	WA	2112	A
30	WA	2113	G
30	WA	2264	G
30	WA	2265	C
30	WA	2266	G
30	WA	2273	A
30	WA	2280	G
30	WA	2294	C
30	WA	2305	A
30	WA	2306	G
30	WA	2311	G
30	WA	2317	U
30	WA	2318	A
30	WA	2319	G
30	WA	2321	G
30	WA	2335	G
30	WA	2336	G
30	WA	2338	G
30	WA	2353	G
30	WA	2356	C
30	WA	2365	A
30	WA	2369	OMG
30	WA	2385	B8W
30	WA	2387	A
30	WA	2400	A
30	WA	2401	A
30	WA	2415	C
30	WA	2422	A
30	WA	2427	OMC
30	WA	2429	OMG
30	WA	2430	U

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Mol	Chain	Res	Type
30	WA	2474	C
30	WA	2476	G
30	WA	2480	G
30	WA	2488	G
30	WA	2492	G
30	WA	2493	C
30	WA	2494	C
30	WA	2495	U
30	WA	2496	C
30	WA	2501	G
30	WA	2508	G
30	WA	2509	C
30	WA	2510	C
30	WA	2511	G
30	WA	2525	C
30	WA	2534	A
30	WA	2535	U
30	WA	2542	A
30	WA	2549	G
30	WA	2551	G
30	WA	2552	G
30	WA	2557	G
30	WA	2558	A
30	WA	2564	G
30	WA	2567	G
30	WA	2568	C
30	WA	2571	G
30	WA	2574	G
30	WA	2576	C
30	WA	2588	C
30	WA	2591	G
30	WA	2594	C
30	WA	2632	C
30	WA	2643	G
30	WA	2645	G
30	WA	2654	G
30	WA	2658	C
30	WA	2667	G
30	WA	2674	C
30	WA	2679	A
30	WA	2686	G
30	WA	2691	G

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Mol	Chain	Res	Type
30	WA	2692	U
30	WA	2700	A
30	WA	2701	A
30	WA	2712	U
30	WA	2713	U
30	WA	2714	C
30	WA	2715	C
30	WA	2716	G
30	WA	2717	G
30	WA	2719	G
30	WA	2720	G
30	WA	2721	C
30	WA	2726	G
30	WA	2727	G
30	WA	2730	A
30	WA	2731	G
30	WA	2745	U
30	WA	2758	G
30	WA	2759	B9B
30	WA	2760	A
30	WA	2761	G
30	WA	2763	G
30	WA	2764	G
30	WA	2765	G
30	WA	2766	U
30	WA	2767	G
30	WA	2768	U
30	WA	2769	A
30	WA	2774	U
30	WA	2777	C
30	WA	2778	OMG
30	WA	2792	A
30	WA	2793	U
30	WA	2795	U
30	WA	2803	A
30	WA	2819	C
30	WA	2831	U
30	WA	2832	G
30	WA	2847	G
30	WA	2860	G
30	WA	2861	C
30	WA	2884	A

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Mol	Chain	Res	Type
30	WA	2903	G
30	WA	3610	C
30	WA	3620	G
30	WA	3623	C
30	WA	3630	G
30	WA	3631	G
30	WA	3640	A
30	WA	3667	A
30	WA	3678	C
30	WA	3697	A
30	WA	3716	A
30	WA	3717	A
30	WA	3728	A2M
30	WA	3729	A
30	WA	3734	PSU
30	WA	3741	A
30	WA	3764	A
30	WA	3766	C
30	WA	3777	U
30	WA	3778	U
30	WA	3779	A
30	WA	3781	G
30	WA	3782	G
30	WA	3783	U
30	WA	3789	A
30	WA	3791	U
30	WA	3794	C
30	WA	3797	OMG
30	WA	3816	G
30	WA	3818	A
30	WA	3819	U
30	WA	3822	A
30	WA	3824	G
30	WA	3828	G
30	WA	3829	A
30	WA	3844	G
30	WA	3845	U
30	WA	3872	A2M
30	WA	3873	G
30	WA	3882	A
30	WA	3883	C
30	WA	3884	G

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Mol	Chain	Res	Type
30	WA	3885	P7G
30	WA	3892	OMC
30	WA	3894	G
30	WA	3897	U
30	WA	3902	B8K
30	WA	3903	G
30	WA	3905	G
30	WA	3906	A
30	WA	3910	A
30	WA	3911	A
30	WA	3912	G
30	WA	3913	A
30	WA	3920	U
30	WA	3921	G
30	WA	3922	A
30	WA	3954	A
30	WA	3956	G
30	WA	4069	C
30	WA	4071	U
30	WA	4073	U
30	WA	4078	A
30	WA	4081	G
30	WA	4089	G
30	WA	4090	A
30	WA	4091	G
30	WA	4093	C
30	WA	4103	A
30	WA	4104	G
30	WA	4105	C
30	WA	4121	C
30	WA	4125	U
30	WA	4126	G
30	WA	4130	C
30	WA	4132	A
30	WA	4133	A
30	WA	4143	C
30	WA	4163	C
30	WA	4167	C
30	WA	4168	U
30	WA	4175	A
30	WA	4188	G
30	WA	4189	G

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Mol	Chain	Res	Type
30	WA	4196	G
30	WA	4208	A
30	WA	4234	U
30	WA	4238	A
30	WA	4239	A
30	WA	4256	A
30	WA	4259	G
30	WA	4260	A
30	WA	4263	C
30	WA	4271	G
30	WA	4273	A
30	WA	4276	A
30	WA	4278	A
30	WA	4286	A
30	WA	4295	U
30	WA	4296	G
30	WA	4298	PSU
30	WA	4309	A
30	WA	4310	G
30	WA	4311	OMU
30	WA	4319	C
30	WA	4323	C
30	WA	4324	C
30	WA	4334	G
30	WA	4335	G
30	WA	4337	C
30	WA	4354	C
30	WA	4355	C
30	WA	4360	E6G
30	WA	4378	G
30	WA	4382	G
30	WA	4383	A
30	WA	4385	A
30	WA	4392	C
30	WA	4398	G
30	WA	4399	A
30	WA	4400	U
30	WA	4401	A
30	WA	4404	U
30	WA	4420	1MA
30	WA	4424	U
30	WA	4427	A

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Mol	Chain	Res	Type
30	WA	4445	G
30	WA	4454	A
30	WA	4455	PSU
30	WA	4456	G
30	WA	4469	A
30	WA	4471	C
30	WA	4481	C
30	WA	4505	PSU
30	WA	4517	U
30	WA	4518	A
30	WA	4525	G
30	WA	4527	G
30	WA	4528	A2M
30	WA	4529	G
30	WA	4553	A
30	WA	4565	C
30	WA	4572	G
30	WA	4578	G
30	WA	4579	U
30	WA	4580	G
30	WA	4582	U
30	WA	4589	A
30	WA	4591	G
30	WA	4594	A
30	WA	4595	A
30	WA	4632	U
30	WA	4641	PSU
30	WA	4642	OMG
30	WA	4657	G
30	WA	4661	A
30	WA	4675	C
30	WA	4676	B8T
30	WA	4677	A
30	WA	4682	U
30	WA	4700	C
30	WA	4705	A
30	WA	4714	U
30	WA	4725	C
30	WA	4741	C
30	WA	4742	G
30	WA	4744	C
30	WA	4745	G

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Mol	Chain	Res	Type
30	WA	4750	G
30	WA	4754	C
30	WA	4755	G
30	WA	4756	G
30	WA	4759	G
30	WA	4762	C
30	WA	4764	C
30	WA	4770	G
30	WA	4776	C
30	WA	4782	C
30	WA	4873	G
30	WA	4875	OMG
30	WA	4876	C
30	WA	4880	G
30	WA	4887	U
30	WA	4888	C
30	WA	4890	U
30	WA	4900	C
30	WA	4903	G
30	WA	4904	G
30	WA	4907	C
30	WA	4908	G
30	WA	4911	C
30	WA	4915	A
30	WA	4917	G
30	WA	4919	G
30	WA	4920	G
30	WA	4924	G
30	WA	4925	C
30	WA	4926	C
30	WA	4927	C
30	WA	4930	U
30	WA	4942	C
30	WA	4948	A
30	WA	4949	C
30	WA	4952	U
30	WA	4953	C
30	WA	4954	G
30	WA	4955	U
30	WA	4956	G
30	WA	4958	G
30	WA	4961	A

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Mol	Chain	Res	Type
30	WA	4962	C
30	WA	4963	C
30	WA	4964	U
30	WA	4967	C
30	WA	4968	G
30	WA	4969	C
30	WA	4970	U
30	WA	4980	G
30	WA	4981	U
30	WA	4984	A
30	WA	4993	U
30	WA	4995	C
30	WA	4998	G
30	WA	5011	U
30	WA	5018	C
30	WA	5019	A
30	WA	5022	G
30	WA	5036	G
30	WA	5046	G
30	WA	5052	C
30	WA	5055	C
30	WA	5058	U
30	WA	5059	C
30	WA	5060	G
30	WA	5066	A
30	WA	5067	G
30	WA	5074	U
31	XA	7	G
31	XA	11	A
31	XA	22	A
31	XA	53	U
31	XA	54	A
31	XA	64	G
31	XA	89	G
31	XA	100	A
31	XA	102	U
31	XA	110	G
31	XA	120	U
32	YA	15	G
32	YA	23	C
32	YA	34	U
32	YA	35	C

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Mol	Chain	Res	Type
32	YA	38	U
32	YA	39	G
32	YA	59	A
32	YA	62	A
32	YA	63	U
32	YA	75	G
32	YA	87	G
32	YA	90	C
32	YA	94	G
32	YA	103	A
32	YA	105	C
32	YA	108	A
32	YA	110	U
32	YA	111	U
32	YA	114	G
32	YA	122	G
32	YA	125	C
32	YA	126	C
32	YA	127	U
32	YA	128	C
32	YA	129	C
32	YA	137	A
32	YA	147	G
53	ZA	2	A
53	ZA	3	C
53	ZA	25	A
53	ZA	26	U
53	ZA	33	G
53	ZA	41	G
53	ZA	42	A
53	ZA	44	U
53	ZA	46	A
53	ZA	56	G
53	ZA	65	C
53	ZA	67	C
53	ZA	68	A
53	ZA	72	C
53	ZA	74	G
53	ZA	75	G
53	ZA	76	U
53	ZA	77	A
53	ZA	78	C

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Mol	Chain	Res	Type
53	ZA	92	A
53	ZA	103	A
53	ZA	111	A
53	ZA	113	G
53	ZA	114	G
53	ZA	115	U
53	ZA	126	G
53	ZA	127	C
53	ZA	129	C
53	ZA	130	G
53	ZA	141	A
53	ZA	142	C
53	ZA	143	U
53	ZA	147	A
53	ZA	155	G
53	ZA	158	A
53	ZA	161	U
53	ZA	163	U
53	ZA	168	C
53	ZA	170	A
53	ZA	175	A
53	ZA	178	C
53	ZA	181	A
53	ZA	184	G
53	ZA	185	G
53	ZA	189	U
53	ZA	200	G
53	ZA	203	G
53	ZA	206	G
53	ZA	305	U
53	ZA	306	C
53	ZA	307	G
53	ZA	310	C
53	ZA	322	C
53	ZA	323	C
53	ZA	330	G
53	ZA	335	G
53	ZA	338	G
53	ZA	347	G
53	ZA	351	G
53	ZA	360	A
53	ZA	362	C

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Mol	Chain	Res	Type
53	ZA	364	A
53	ZA	368	U
53	ZA	369	C
53	ZA	370	G
53	ZA	372	U
53	ZA	385	G
53	ZA	386	C
53	ZA	391	C
53	ZA	393	U
53	ZA	394	G
53	ZA	398	A
53	ZA	400	C
53	ZA	407	G
53	ZA	408	A
53	ZA	409	C
53	ZA	417	C
53	ZA	418	A
53	ZA	426	A
53	ZA	428	U
53	ZA	429	C
53	ZA	435	A
53	ZA	438	G
53	ZA	448	A
53	ZA	450	C
53	ZA	452	G
53	ZA	455	A
53	ZA	465	A
53	ZA	466	G
53	ZA	472	C
53	ZA	473	A
53	ZA	474	G
53	ZA	482	G
53	ZA	485	A
53	ZA	487	U
53	ZA	492	C
53	ZA	496	C
53	ZA	502	C
53	ZA	532	C
53	ZA	533	A
53	ZA	537	C
53	ZA	542	U
53	ZA	546	G

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Mol	Chain	Res	Type
53	ZA	550	C
53	ZA	551	U
53	ZA	554	A
53	ZA	555	A
53	ZA	556	U
53	ZA	559	G
53	ZA	560	A
53	ZA	562	U
53	ZA	568	C
53	ZA	583	A
53	ZA	587	A
53	ZA	588	G
53	ZA	589	G
53	ZA	590	A
53	ZA	591	U
53	ZA	594	A
53	ZA	598	G
53	ZA	603	C
53	ZA	606	G
53	ZA	607	U
53	ZA	609	U
53	ZA	611	G
53	ZA	612	U
53	ZA	614	C
53	ZA	616	A
53	ZA	617	G
53	ZA	627	U
53	ZA	628	A
53	ZA	629	A
53	ZA	632	C
53	ZA	643	A
53	ZA	644	G
53	ZA	660	C
53	ZA	668	A
53	ZA	669	A
53	ZA	671	A
53	ZA	672	A
53	ZA	673	G
53	ZA	688	U
53	ZA	689	U
53	ZA	752	G
53	ZA	753	C

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Mol	Chain	Res	Type
53	ZA	754	G
53	ZA	799	U
53	ZA	801	U
53	ZA	811	A
53	ZA	815	U
53	ZA	821	G
53	ZA	822	U
53	ZA	823	U
53	ZA	830	A
53	ZA	844	U
53	ZA	847	A
53	ZA	869	A
53	ZA	870	A
53	ZA	871	U
53	ZA	872	A
53	ZA	873	G
53	ZA	875	A
53	ZA	879	C
53	ZA	888	U
53	ZA	890	U
53	ZA	894	G
53	ZA	908	A
53	ZA	910	G
53	ZA	911	C
53	ZA	912	C
53	ZA	913	A
53	ZA	914	U
53	ZA	919	A
53	ZA	920	A
53	ZA	922	A
53	ZA	930	C
53	ZA	933	G
53	ZA	934	G
53	ZA	954	U
53	ZA	955	A
53	ZA	968	U
53	ZA	970	G
53	ZA	971	G
53	ZA	990	A
53	ZA	992	A
53	ZA	999	G
53	ZA	1014	G

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Mol	Chain	Res	Type
53	ZA	1017	U
53	ZA	1019	C
53	ZA	1020	A
53	ZA	1021	U
53	ZA	1023	A
53	ZA	1034	A
53	ZA	1035	A
53	ZA	1040	G
53	ZA	1041	G
53	ZA	1045	U
53	ZA	1055	A
53	ZA	1056	U
53	ZA	1057	C
53	ZA	1058	A
53	ZA	1061	U
53	ZA	1062	A
53	ZA	1073	U
53	ZA	1078	C
53	ZA	1083	A
53	ZA	1085	C
53	ZA	1088	U
53	ZA	1089	G
53	ZA	1095	U
53	ZA	1096	G
53	ZA	1097	G
53	ZA	1100	A
53	ZA	1103	C
53	ZA	1108	G
53	ZA	1115	U
53	ZA	1116	C
53	ZA	1132	C
53	ZA	1136	U
53	ZA	1137	U
53	ZA	1149	A
53	ZA	1150	A
53	ZA	1153	C
53	ZA	1154	U
53	ZA	1155	U
53	ZA	1161	U
53	ZA	1164	G
53	ZA	1194	A
53	ZA	1195	A

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Mol	Chain	Res	Type
53	ZA	1207	G
53	ZA	1215	C
53	ZA	1216	C
53	ZA	1220	A
53	ZA	1224	G
53	ZA	1241	A
53	ZA	1242	U
53	ZA	1243	PSU
53	ZA	1248	B8N
53	ZA	1251	A
53	ZA	1253	A
53	ZA	1254	C
53	ZA	1256	G
53	ZA	1257	G
53	ZA	1258	A
53	ZA	1259	A
53	ZA	1264	C
53	ZA	1274	G
53	ZA	1275	G
53	ZA	1277	C
53	ZA	1281	G
53	ZA	1282	A
53	ZA	1283	C
53	ZA	1284	A
53	ZA	1285	G
53	ZA	1286	G
53	ZA	1288	U
53	ZA	1292	C
53	ZA	1293	A
53	ZA	1301	A
53	ZA	1302	G
53	ZA	1304	U
53	ZA	1308	U
53	ZA	1311	C
53	ZA	1313	A
53	ZA	1324	G
53	ZA	1327	G
53	ZA	1342	U
53	ZA	1345	G
53	ZA	1364	U
53	ZA	1371	U
53	ZA	1372	U

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Mol	Chain	Res	Type
53	ZA	1377	U
53	ZA	1378	A
53	ZA	1382	A
53	ZA	1393	G
53	ZA	1395	C
53	ZA	1397	U
53	ZA	1402	A
53	ZA	1414	A
53	ZA	1425	G
53	ZA	1428	G
53	ZA	1429	G
53	ZA	1438	A
53	ZA	1439	A
53	ZA	1442	U
53	ZA	1454	A
53	ZA	1462	U
53	ZA	1473	G
53	ZA	1477	U
53	ZA	1482	C
53	ZA	1484	A
53	ZA	1489	A
53	ZA	1490	G
53	ZA	1494	U
53	ZA	1495	G
53	ZA	1497	G
53	ZA	1498	A
53	ZA	1507	G
53	ZA	1508	A
53	ZA	1510	G
53	ZA	1517	G
53	ZA	1521	C
53	ZA	1522	A
53	ZA	1535	U
53	ZA	1536	G
53	ZA	1544	C
53	ZA	1551	U
53	ZA	1553	C
53	ZA	1560	U
53	ZA	1567	G
53	ZA	1568	C
53	ZA	1574	C
53	ZA	1575	G

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Mol	Chain	Res	Type
53	ZA	1576	G
53	ZA	1579	A
53	ZA	1580	A
53	ZA	1582	C
53	ZA	1585	U
53	ZA	1586	U
53	ZA	1587	G
53	ZA	1588	A
53	ZA	1601	A
53	ZA	1603	G
53	ZA	1604	G
53	ZA	1620	A
53	ZA	1621	U
53	ZA	1623	A
53	ZA	1624	U
53	ZA	1637	A
53	ZA	1638	G
53	ZA	1646	C
53	ZA	1648	G
53	ZA	1657	G
53	ZA	1658	G
53	ZA	1665	G
53	ZA	1678	A2M
53	ZA	1679	A
53	ZA	1680	G
53	ZA	1683	C
53	ZA	1695	A
53	ZA	1698	C
53	ZA	1715	A
53	ZA	1721	U
53	ZA	1722	G
53	ZA	1726	G
53	ZA	1729	U
53	ZA	1732	G
53	ZA	1748	G
53	ZA	1753	C
53	ZA	1756	C
53	ZA	1757	G
53	ZA	1774	C
53	ZA	1778	C
53	ZA	1779	G
53	ZA	1783	C

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Mol	Chain	Res	Type
53	ZA	1784	G
53	ZA	1787	G
53	ZA	1806	A
53	ZA	1811	C
53	ZA	1823	A
53	ZA	1824	A
53	ZA	1825	A
53	ZA	1826	G
53	ZA	1831	A
53	ZA	1836	G
53	ZA	1838	U
53	ZA	1849	G
53	ZA	1851	A
53	ZA	1861	G
53	ZA	1862	G
53	ZA	1863	A
53	ZA	1865	C
53	ZA	1866	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	WA	12	A
30	WA	48	G
30	WA	125	C
30	WA	275	C
30	WA	385	A
30	WA	406	C
30	WA	505	G
30	WA	1217	G
30	WA	1242	C
30	WA	1244	A
30	WA	1335	G
30	WA	1376	G
30	WA	1444	U
30	WA	1638	G
30	WA	1809	A
30	WA	1823	G
30	WA	2003	A
30	WA	2051	G
30	WA	2104	C
30	WA	2109	A

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Mol	Chain	Res	Type
30	WA	2334	U
30	WA	2644	U
30	WA	2712	U
30	WA	3630	G
30	WA	3765	A
30	WA	3793	C
30	WA	3893	G
30	WA	4124	C
30	WA	4237	U
30	WA	4453	G
30	WA	4704	U
30	WA	4889	G
30	WA	4907	C
30	WA	4952	U
32	YA	124	U
53	ZA	110	U
53	ZA	140	U
53	ZA	427	U
53	ZA	434	G
53	ZA	532	C
53	ZA	553	U
53	ZA	642	U
53	ZA	688	U
53	ZA	1088	U
53	ZA	1193	U
53	ZA	1253	A
53	ZA	1481	G
53	ZA	1664	A
53	ZA	1777	G
53	ZA	1810	U

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

110 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
30	PSU	WA	4298	30	18,21,22	4.48	7 (38%)	21,30,33	2.83	5 (23%)
30	B8H	WA	1865	30	19,22,23	6.88	8 (42%)	21,32,35	2.48	5 (23%)
30	OMG	WA	2778	30	23,26,27	2.48	9 (39%)	32,38,41	2.13	11 (34%)
30	OMC	WA	4541	30	19,22,23	3.03	8 (42%)	25,31,34	0.74	0
30	7MG	WA	4555	30	23,26,27	3.34	10 (43%)	27,39,42	2.20	9 (33%)
30	B8T	WA	4676	30	19,22,23	3.28	8 (42%)	25,31,34	0.86	1 (4%)
30	P4U	WA	1354	30	21,24,25	3.49	8 (38%)	28,33,36	1.53	2 (7%)
30	P7G	WA	3885	30	24,28,29	3.53	10 (41%)	25,41,44	1.30	2 (8%)
30	OMG	WA	4375	30	23,26,27	2.45	9 (39%)	32,38,41	2.07	11 (34%)
51	DDE	v	715	51	18,20,21	2.11	5 (27%)	17,28,30	1.21	1 (5%)
30	A2M	WA	1332	30	22,25,26	2.65	11 (50%)	30,36,39	2.28	9 (30%)
30	I4U	WA	1664	30,85	20,24,25	3.51	8 (40%)	27,34,37	1.77	2 (7%)
30	5MC	WA	4452	30	19,22,23	3.82	8 (42%)	26,32,35	1.05	1 (3%)
30	PSU	WA	3769	30	18,21,22	4.53	6 (33%)	21,30,33	2.99	5 (23%)
30	UR3	WA	4602	30	19,22,23	3.19	9 (47%)	26,32,35	1.54	4 (15%)
30	B8W	WA	4190	30	23,26,27	2.19	6 (26%)	33,38,41	3.36	17 (51%)
30	OMG	WA	4642	30	23,26,27	2.47	9 (39%)	32,38,41	2.13	11 (34%)
32	OMU	YA	14	30,32	19,22,23	3.08	8 (42%)	25,31,34	1.84	5 (20%)
30	PSU	WA	4408	30	18,21,22	4.47	7 (38%)	21,30,33	2.98	6 (28%)
30	B8W	WA	2385	30	23,26,27	2.17	6 (26%)	33,38,41	3.39	16 (48%)
30	E6G	WA	4360	30	24,27,28	1.80	5 (20%)	34,39,42	2.42	13 (38%)
30	OMG	WA	2369	30	23,26,27	2.46	9 (39%)	32,38,41	2.11	11 (34%)
30	OMG	WA	1527	30	23,26,27	2.45	9 (39%)	32,38,41	2.10	11 (34%)
53	B8N	ZA	1248	53	25,29,30	2.49	5 (20%)	28,42,45	2.02	6 (21%)
30	OMC	WA	3914	30	19,22,23	3.01	8 (42%)	25,31,34	0.77	0
30	OMG	WA	3797	30	23,26,27	2.47	9 (39%)	32,38,41	2.12	11 (34%)
30	A2M	WA	3872	30	22,25,26	2.64	11 (50%)	30,36,39	2.30	9 (30%)
53	JMH	ZA	1219	53	18,22,23	2.90	6 (33%)	23,32,35	1.41	5 (21%)
30	OMC	WA	2866	30	19,22,23	3.04	8 (42%)	25,31,34	0.86	1 (4%)
30	OMG	WA	4875	30	23,26,27	2.46	9 (39%)	32,38,41	2.08	11 (34%)
30	PSU	WA	2513	30	18,21,22	4.53	6 (33%)	21,30,33	3.02	6 (28%)
30	PSU	WA	4455	30,85	18,21,22	4.48	6 (33%)	21,30,33	3.06	6 (28%)
30	JMH	WA	1461	30	18,22,23	2.86	6 (33%)	23,32,35	1.41	3 (13%)
30	A2M	WA	2406	30	22,25,26	2.66	11 (50%)	30,36,39	2.38	10 (33%)
30	A2M	WA	3728	30	22,25,26	2.66	11 (50%)	30,36,39	2.31	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	5MC	WA	4340	30	19,22,23	3.89	8 (42%)	26,32,35	1.03	2 (7%)
30	A2M	WA	4528	30,85	22,25,26	2.65	11 (50%)	30,36,39	2.39	10 (33%)
30	A2M	WA	1876	30	22,25,26	2.65	11 (50%)	30,36,39	2.43	10 (33%)
53	5MC	ZA	1374	53	19,22,23	3.88	8 (42%)	26,32,35	1.01	2 (7%)
30	OMU	WA	4625	30	19,22,23	3.03	8 (42%)	25,31,34	1.79	5 (20%)
30	PSU	WA	4641	30	18,21,22	4.70	6 (33%)	21,30,33	3.25	6 (28%)
30	OMG	WA	2429	30	23,26,27	2.46	9 (39%)	32,38,41	2.06	11 (34%)
30	E7G	WA	2302	30	24,27,28	3.33	11 (45%)	28,40,43	2.40	9 (32%)
30	B9B	WA	1579	30	25,28,29	1.77	6 (24%)	35,40,43	2.35	14 (40%)
30	B8H	WA	3767	-	19,22,23	6.87	8 (42%)	21,32,35	2.46	5 (23%)
53	4AC	ZA	1337	53	21,24,25	3.68	9 (42%)	28,34,37	1.20	4 (14%)
30	OMG	WA	2055	30	23,26,27	2.45	9 (39%)	32,38,41	2.06	11 (34%)
30	1MA	WA	4420	30	21,25,26	2.47	5 (23%)	30,37,40	1.93	8 (26%)
30	B8K	WA	4695	30	24,28,29	3.34	12 (50%)	29,42,45	2.45	11 (37%)
30	A2M	WA	3723	30	22,25,26	2.65	11 (50%)	30,36,39	2.30	10 (33%)
30	P7G	WA	1914	30	24,28,29	3.61	10 (41%)	25,41,44	1.33	2 (8%)
30	OMC	WA	2370	30	19,22,23	3.01	8 (42%)	25,31,34	0.70	0
30	2MG	WA	4877	30	23,26,27	2.61	7 (30%)	33,38,41	2.31	12 (36%)
30	I4U	WA	4199	30	20,24,25	3.51	8 (40%)	27,34,37	1.57	2 (7%)
30	OMG	WA	1630	30	23,26,27	2.46	9 (39%)	32,38,41	2.13	11 (34%)
30	2MG	WA	730	30	23,26,27	2.69	7 (30%)	33,38,41	2.38	12 (36%)
30	6MZ	WA	4225	30	22,25,26	2.44	4 (18%)	29,36,39	2.24	10 (34%)
30	1MA	WA	1328	30,85	21,25,26	2.45	4 (19%)	30,37,40	1.91	8 (26%)
30	5MU	WA	4088	30	19,22,23	8.29	7 (36%)	27,32,35	3.55	10 (37%)
30	A2M	WA	2368	30,85	22,25,26	2.65	11 (50%)	30,36,39	2.33	10 (33%)
30	B8W	WA	4134	30	23,26,27	2.16	6 (26%)	33,38,41	3.38	16 (48%)
30	OMG	WA	1888	30	23,26,27	2.48	9 (39%)	32,38,41	2.14	11 (34%)
30	OMC	WA	2427	30	19,22,23	3.04	8 (42%)	25,31,34	0.75	0
30	OMG	WA	1322	30	23,26,27	2.46	9 (39%)	32,38,41	2.12	11 (34%)
30	B8W	WA	4477	30	23,26,27	2.20	6 (26%)	33,38,41	3.33	15 (45%)
53	A2M	ZA	1678	53	22,25,26	2.67	11 (50%)	30,36,39	2.31	8 (26%)
30	5MC	WA	3787	30	19,22,23	3.83	8 (42%)	26,32,35	1.03	2 (7%)
30	OMC	WA	3892	30	19,22,23	3.03	8 (42%)	25,31,34	0.73	0
30	A2M	WA	1529	30	22,25,26	2.66	11 (50%)	30,36,39	2.33	8 (26%)
30	B9B	WA	237	30	25,28,29	1.77	5 (20%)	35,40,43	2.34	13 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMG	WA	4499	30	23,26,27	2.47	9 (39%)	32,38,41	2.13	11 (34%)
30	MHG	WA	4376	30	29,32,33	3.56	10 (34%)	34,46,49	2.53	11 (32%)
30	B8K	WA	3902	30	24,28,29	3.26	12 (50%)	29,42,45	2.36	10 (34%)
53	PSU	ZA	1243	53	18,21,22	4.54	6 (33%)	21,30,33	2.99	6 (28%)
30	PSU	WA	3734	30	18,21,22	4.54	6 (33%)	21,30,33	2.94	5 (23%)
30	B9H	WA	2791	30	21,25,26	2.90	5 (23%)	22,35,38	1.57	5 (22%)
30	A2M	WA	3790	30	22,25,26	2.69	11 (50%)	30,36,39	2.45	11 (36%)
30	E7G	WA	1802	30	24,27,28	3.35	11 (45%)	28,40,43	2.38	9 (32%)
30	A2M	WA	398	30	22,25,26	2.65	11 (50%)	30,36,39	2.33	10 (33%)
30	B8T	WA	4488	30	19,22,23	3.28	8 (42%)	25,31,34	0.87	1 (4%)
30	OMG	WA	4628	30	23,26,27	2.46	9 (39%)	32,38,41	2.07	11 (34%)
30	A2M	WA	4576	30	22,25,26	2.68	11 (50%)	30,36,39	2.35	10 (33%)
30	UR3	WA	1871	30	19,22,23	3.21	8 (42%)	26,32,35	1.59	4 (15%)
30	UR3	WA	4535	30	19,22,23	3.23	8 (42%)	26,32,35	1.60	3 (11%)
30	PSU	WA	1682	30	18,21,22	4.53	7 (38%)	21,30,33	3.04	7 (33%)
30	2MG	WA	1522	30	23,26,27	2.62	8 (34%)	33,38,41	2.28	13 (39%)
30	A2M	WA	3830	30	22,25,26	2.63	11 (50%)	30,36,39	2.31	10 (33%)
30	A2M	WA	1539	30,85	22,25,26	2.63	11 (50%)	30,36,39	2.31	10 (33%)
44	MLZ	LA	72	44	8,9,10	0.72	0	4,9,11	0.86	0
30	PSU	WA	4447	30	18,21,22	4.49	6 (33%)	21,30,33	2.89	6 (28%)
30	OMG	WA	373	30	23,26,27	2.46	9 (39%)	32,38,41	2.05	11 (34%)
30	PSU	WA	1587	30	18,21,22	4.50	7 (38%)	21,30,33	2.85	5 (23%)
30	B9B	WA	2759	30	25,28,29	1.76	5 (20%)	35,40,43	2.38	14 (40%)
30	B8H	WA	4301	30	19,22,23	6.85	8 (42%)	21,32,35	2.48	5 (23%)
30	OMG	WA	4201	30	23,26,27	2.45	9 (39%)	32,38,41	2.09	11 (34%)
30	OMC	WA	3874	30	19,22,23	3.00	8 (42%)	25,31,34	0.70	0
30	OMC	WA	2809	30	19,22,23	3.00	8 (42%)	25,31,34	0.69	0
30	7MG	WA	2527	30	23,26,27	3.37	10 (43%)	27,39,42	2.21	9 (33%)
30	OMC	WA	3706	30,85	19,22,23	3.02	8 (42%)	25,31,34	0.71	0
3	MLZ	C	333	3	8,9,10	0.68	0	4,9,11	0.84	0
30	PSU	WA	4505	30	18,21,22	4.50	6 (33%)	21,30,33	3.04	5 (23%)
30	PSU	WA	4633	30	18,21,22	4.51	6 (33%)	21,30,33	3.07	6 (28%)
30	BGH	WA	3904	30	25,29,30	4.54	17 (68%)	30,43,46	2.37	11 (36%)
30	PSU	WA	4536	30	18,21,22	4.56	6 (33%)	21,30,33	2.97	5 (23%)
30	M7A	WA	4569	30	19,25,26	1.57	2 (10%)	25,37,40	4.33	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	WA	3720	30	18,21,22	4.52	6 (33%)	21,30,33	2.97	5 (23%)
30	7MG	WA	1610	30	23,26,27	3.35	10 (43%)	27,39,42	2.22	9 (33%)
30	OMU	WA	4311	30	19,22,23	3.03	8 (42%)	25,31,34	1.82	5 (20%)
30	B8W	WA	4534	30	23,26,27	2.16	6 (26%)	33,38,41	3.42	16 (48%)
30	PSU	WA	1688	30	18,21,22	4.51	6 (33%)	21,30,33	3.06	6 (28%)

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
30	PSU	WA	4298	30	-	2/7/25/26	0/2/2/2
30	B8H	WA	1865	30	-	2/7/25/26	0/2/2/2
30	OMG	WA	2778	30	-	2/9/27/28	0/3/3/3
30	OMC	WA	4541	30	-	0/9/27/28	0/2/2/2
30	7MG	WA	4555	30	-	2/7/37/38	0/3/3/3
30	B8T	WA	4676	30	-	5/7/27/28	0/2/2/2
30	P4U	WA	1354	30	-	4/10/29/30	0/2/2/2
30	P7G	WA	3885	30	-	2/10/40/41	0/3/3/3
30	OMG	WA	4375	30	-	0/9/27/28	0/3/3/3
51	DDE	v	715	51	-	4/20/21/23	0/1/1/1
30	A2M	WA	1332	30	-	1/9/27/28	0/3/3/3
30	I4U	WA	1664	30,85	-	0/9/29/30	0/2/2/2
30	5MC	WA	4452	30	-	4/7/25/26	0/2/2/2
30	PSU	WA	3769	30	-	0/7/25/26	0/2/2/2
30	UR3	WA	4602	30	-	0/7/25/26	0/2/2/2
30	B8W	WA	4190	30	-	2/9/27/28	0/3/3/3
30	OMG	WA	4642	30	-	3/9/27/28	0/3/3/3
32	OMU	YA	14	30,32	-	5/9/27/28	0/2/2/2
30	PSU	WA	4408	30	-	0/7/25/26	0/2/2/2
30	B8W	WA	2385	30	-	4/9/27/28	0/3/3/3
30	E6G	WA	4360	30	-	5/10/28/29	0/3/3/3
30	OMG	WA	2369	30	-	3/9/27/28	0/3/3/3
30	OMG	WA	1527	30	-	0/9/27/28	0/3/3/3
53	B8N	ZA	1248	53	-	3/16/34/35	0/2/2/2
30	OMC	WA	3914	30	-	0/9/27/28	0/2/2/2
30	OMG	WA	3797	30	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A2M	WA	3872	30	-	4/9/27/28	0/3/3/3
53	JMH	ZA	1219	53	-	0/7/25/26	0/2/2/2
30	OMC	WA	2866	30	-	1/9/27/28	0/2/2/2
30	OMG	WA	4875	30	-	3/9/27/28	0/3/3/3
30	PSU	WA	2513	30	-	0/7/25/26	0/2/2/2
30	PSU	WA	4455	30,85	-	3/7/25/26	0/2/2/2
30	JMH	WA	1461	30	-	0/7/25/26	0/2/2/2
30	A2M	WA	2406	30	-	0/9/27/28	0/3/3/3
30	A2M	WA	3728	30	-	3/9/27/28	0/3/3/3
30	5MC	WA	4340	30	-	2/7/25/26	0/2/2/2
30	A2M	WA	4528	30,85	-	1/9/27/28	0/3/3/3
30	A2M	WA	1876	30	-	0/9/27/28	0/3/3/3
53	5MC	ZA	1374	53	-	0/7/25/26	0/2/2/2
30	OMU	WA	4625	30	-	1/9/27/28	0/2/2/2
30	PSU	WA	4641	30	-	2/7/25/26	0/2/2/2
30	OMG	WA	2429	30	-	2/9/27/28	0/3/3/3
30	E7G	WA	2302	30	-	2/9/39/40	0/3/3/3
30	B9B	WA	1579	30	-	3/11/29/30	0/3/3/3
30	B8H	WA	3767	-	-	3/7/25/26	0/2/2/2
53	4AC	ZA	1337	53	-	0/11/29/30	0/2/2/2
30	OMG	WA	2055	30	-	1/9/27/28	0/3/3/3
30	1MA	WA	4420	30	-	2/7/25/26	0/3/3/3
30	B8K	WA	4695	30	-	0/11/41/42	0/3/3/3
30	A2M	WA	3723	30	-	0/9/27/28	0/3/3/3
30	P7G	WA	1914	30	-	1/10/40/41	0/3/3/3
30	OMC	WA	2370	30	-	0/9/27/28	0/2/2/2
30	2MG	WA	4877	30	-	1/9/27/28	0/3/3/3
30	I4U	WA	4199	30	-	4/9/29/30	0/2/2/2
30	OMG	WA	1630	30	-	1/9/27/28	0/3/3/3
30	2MG	WA	730	30	-	0/9/27/28	0/3/3/3
30	6MZ	WA	4225	30	-	0/9/27/28	0/3/3/3
30	1MA	WA	1328	30,85	-	2/7/25/26	0/3/3/3
30	5MU	WA	4088	30	-	0/7/25/26	0/2/2/2
30	A2M	WA	2368	30,85	-	0/9/27/28	0/3/3/3
30	B8W	WA	4134	30	-	2/9/27/28	0/3/3/3
30	OMG	WA	1888	30	-	1/9/27/28	0/3/3/3
30	OMC	WA	2427	30	-	0/9/27/28	0/2/2/2
30	OMG	WA	1322	30	-	1/9/27/28	0/3/3/3
30	B8W	WA	4477	30	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	A2M	ZA	1678	53	-	1/9/27/28	0/3/3/3
30	5MC	WA	3787	30	-	1/7/25/26	0/2/2/2
30	OMC	WA	3892	30	-	3/9/27/28	0/2/2/2
30	A2M	WA	1529	30	-	1/9/27/28	0/3/3/3
30	B9B	WA	237	30	-	4/11/29/30	0/3/3/3
30	OMG	WA	4499	30	-	0/9/27/28	0/3/3/3
30	MHG	WA	4376	30	-	6/16/46/47	0/3/3/3
30	B8K	WA	3902	30	-	3/11/41/42	0/3/3/3
53	PSU	ZA	1243	53	-	2/7/25/26	0/2/2/2
30	PSU	WA	3734	30	-	2/7/25/26	0/2/2/2
30	B9H	WA	2791	30	-	1/12/47/48	0/2/2/2
30	A2M	WA	3790	30	-	4/9/27/28	0/3/3/3
30	E7G	WA	1802	30	-	2/9/39/40	0/3/3/3
30	A2M	WA	398	30	-	3/9/27/28	0/3/3/3
30	B8T	WA	4488	30	-	0/7/27/28	0/2/2/2
30	OMG	WA	4628	30	-	0/9/27/28	0/3/3/3
30	A2M	WA	4576	30	-	1/9/27/28	0/3/3/3
30	UR3	WA	1871	30	-	2/7/25/26	0/2/2/2
30	UR3	WA	4535	30	-	0/7/25/26	0/2/2/2
30	PSU	WA	1682	30	-	0/7/25/26	0/2/2/2
30	2MG	WA	1522	30	-	1/9/27/28	0/3/3/3
30	A2M	WA	3830	30	-	2/9/27/28	0/3/3/3
30	A2M	WA	1539	30,85	-	2/9/27/28	0/3/3/3
44	MLZ	LA	72	44	-	1/7/8/10	-
30	PSU	WA	4447	30	-	0/7/25/26	0/2/2/2
30	OMG	WA	373	30	-	1/9/27/28	0/3/3/3
30	PSU	WA	1587	30	-	2/7/25/26	0/2/2/2
30	B9B	WA	2759	30	-	2/11/29/30	0/3/3/3
30	B8H	WA	4301	30	-	2/7/25/26	0/2/2/2
30	OMG	WA	4201	30	-	0/9/27/28	0/3/3/3
30	OMC	WA	3874	30	-	0/9/27/28	0/2/2/2
30	OMC	WA	2809	30	-	1/9/27/28	0/2/2/2
30	7MG	WA	2527	30	-	0/7/37/38	0/3/3/3
30	OMC	WA	3706	30,85	-	4/9/27/28	0/2/2/2
3	MLZ	C	333	3	-	4/7/8/10	-
30	PSU	WA	4505	30	-	3/7/25/26	0/2/2/2
30	PSU	WA	4633	30	-	0/7/25/26	0/2/2/2
30	BGH	WA	3904	30	-	0/13/43/44	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	WA	4536	30	-	0/7/25/26	0/2/2/2
30	M7A	WA	4569	30	-	0/7/37/38	0/3/3/3
30	PSU	WA	3720	30	-	0/7/25/26	0/2/2/2
30	7MG	WA	1610	30	-	0/7/37/38	0/3/3/3
30	OMU	WA	4311	30	-	0/9/27/28	0/2/2/2
30	B8W	WA	4534	30	-	0/9/27/28	0/3/3/3
30	PSU	WA	1688	30	-	0/7/25/26	0/2/2/2

All (880) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4088	5MU	C4-C5	23.43	1.82	1.44
30	WA	4088	5MU	C6-N1	17.74	1.68	1.38
30	WA	1865	B8H	C6-C5	-15.85	1.12	1.35
30	WA	4301	B8H	C6-C5	-15.75	1.12	1.35
30	WA	3767	B8H	C6-C5	-15.75	1.12	1.35
30	WA	4088	5MU	C4-N3	-14.71	1.11	1.38
30	WA	1865	B8H	C4-N3	-14.66	1.11	1.38
30	WA	4301	B8H	C4-N3	-14.63	1.11	1.38
30	WA	3767	B8H	C4-N3	-14.56	1.11	1.38
30	WA	3767	B8H	C4-C5	14.24	1.83	1.44
30	WA	1865	B8H	C4-C5	14.05	1.83	1.44
30	WA	4301	B8H	C4-C5	14.00	1.83	1.44
30	WA	4088	5MU	C6-C5	-13.65	1.12	1.34
30	WA	4641	PSU	C6-C5	13.25	1.50	1.35
30	WA	1865	B8H	C6-N1	13.13	1.68	1.36
30	WA	3767	B8H	C6-N1	13.09	1.68	1.36
30	WA	4301	B8H	C6-N1	13.06	1.68	1.36
30	WA	4536	PSU	C6-C5	12.59	1.49	1.35
53	ZA	1243	PSU	C6-C5	12.54	1.49	1.35
30	WA	3769	PSU	C6-C5	12.54	1.49	1.35
30	WA	3734	PSU	C6-C5	12.54	1.49	1.35
30	WA	2513	PSU	C6-C5	12.50	1.49	1.35
30	WA	3720	PSU	C6-C5	12.50	1.49	1.35
30	WA	4633	PSU	C6-C5	12.49	1.49	1.35
30	WA	1688	PSU	C6-C5	12.48	1.49	1.35
30	WA	1587	PSU	C6-C5	12.45	1.49	1.35
30	WA	4447	PSU	C6-C5	12.44	1.49	1.35
30	WA	1682	PSU	C6-C5	12.42	1.49	1.35
30	WA	4505	PSU	C6-C5	12.38	1.49	1.35
30	WA	4455	PSU	C6-C5	12.32	1.48	1.35
30	WA	4408	PSU	C6-C5	12.29	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4298	PSU	C6-C5	12.26	1.48	1.35
30	WA	4199	I4U	C4-N3	10.80	1.45	1.31
30	WA	1664	I4U	C4-N3	10.74	1.45	1.31
30	WA	1354	P4U	C4-N3	10.71	1.45	1.31
30	WA	4641	PSU	C2-N1	10.16	1.49	1.36
30	WA	4376	MHG	C8-N9	10.09	1.52	1.45
30	WA	4536	PSU	C2-N1	10.02	1.49	1.36
30	WA	1682	PSU	C2-N1	10.02	1.49	1.36
30	WA	2513	PSU	C2-N1	9.97	1.49	1.36
30	WA	3734	PSU	C2-N1	9.95	1.49	1.36
30	WA	3904	BGH	C3'-C4'	-9.95	1.27	1.53
53	ZA	1243	PSU	C2-N1	9.94	1.49	1.36
30	WA	4455	PSU	C2-N1	9.93	1.49	1.36
30	WA	4505	PSU	C2-N1	9.89	1.49	1.36
30	WA	1688	PSU	C2-N1	9.87	1.49	1.36
30	WA	3720	PSU	C2-N1	9.86	1.49	1.36
30	WA	4225	6MZ	C6-N6	9.86	1.45	1.34
30	WA	4633	PSU	C2-N1	9.85	1.49	1.36
30	WA	4408	PSU	C2-N1	9.82	1.49	1.36
30	WA	4298	PSU	C2-N1	9.81	1.49	1.36
30	WA	3769	PSU	C2-N1	9.80	1.49	1.36
30	WA	1587	PSU	C2-N1	9.79	1.49	1.36
30	WA	4447	PSU	C2-N1	9.73	1.49	1.36
30	WA	3904	BGH	O4'-C4'	9.65	1.66	1.45
30	WA	1914	P7G	C8-N9	9.62	1.52	1.45
30	WA	4535	UR3	C2-N1	9.31	1.51	1.38
30	WA	4452	5MC	C6-C5	9.30	1.49	1.34
53	ZA	1374	5MC	C6-C5	9.26	1.49	1.34
30	WA	1871	UR3	C2-N1	9.24	1.51	1.38
30	WA	4340	5MC	C6-C5	9.16	1.49	1.34
30	WA	3787	5MC	C6-C5	9.13	1.49	1.34
30	WA	4602	UR3	C2-N1	9.12	1.51	1.38
30	WA	4420	1MA	C2-N3	9.04	1.47	1.30
30	WA	1328	1MA	C2-N3	8.99	1.46	1.30
30	WA	3885	P7G	C8-N9	8.92	1.51	1.45
30	WA	2527	7MG	C8-N9	8.70	1.51	1.45
30	WA	4555	7MG	C8-N9	8.58	1.51	1.45
30	WA	1802	E7G	C8-N9	8.54	1.51	1.45
30	WA	1610	7MG	C8-N9	8.49	1.51	1.45
30	WA	4376	MHG	C2-N3	8.42	1.48	1.32
30	WA	2302	E7G	C8-N9	8.33	1.51	1.45
53	ZA	1337	4AC	C4-N3	8.30	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	2791	B9H	C2-N3	8.19	1.47	1.37
30	WA	3904	BGH	C8-N9	7.96	1.51	1.45
30	WA	4376	MHG	C5-N7	7.94	1.45	1.35
30	WA	730	2MG	C2-N3	7.94	1.47	1.32
30	WA	4536	PSU	C2-N3	7.61	1.50	1.37
30	WA	1914	P7G	C5-N7	7.61	1.45	1.35
30	WA	3769	PSU	C2-N3	7.56	1.49	1.37
53	ZA	1248	B8N	C4-N3	-7.53	1.27	1.40
30	WA	1682	PSU	C2-N3	7.52	1.49	1.37
30	WA	4877	2MG	C2-N3	7.52	1.46	1.32
30	WA	3734	PSU	C2-N3	7.49	1.49	1.37
30	WA	4505	PSU	C2-N3	7.49	1.49	1.37
30	WA	2513	PSU	C2-N3	7.49	1.49	1.37
30	WA	3720	PSU	C2-N3	7.47	1.49	1.37
30	WA	1522	2MG	C2-N3	7.47	1.46	1.32
53	ZA	1243	PSU	C2-N3	7.47	1.49	1.37
32	YA	14	OMU	C2-N1	7.45	1.50	1.38
30	WA	4633	PSU	C2-N3	7.45	1.49	1.37
30	WA	4455	PSU	C2-N3	7.45	1.49	1.37
30	WA	1688	PSU	C2-N3	7.44	1.49	1.37
30	WA	3885	P7G	C5-N7	7.42	1.44	1.35
30	WA	4447	PSU	C2-N3	7.40	1.49	1.37
53	ZA	1337	4AC	C2-N3	7.40	1.51	1.36
30	WA	4641	PSU	C2-N3	7.40	1.49	1.37
30	WA	4676	B8T	C4-N3	7.39	1.45	1.32
30	WA	4298	PSU	C2-N3	7.38	1.49	1.37
30	WA	2791	B9H	C6-C5	7.37	1.48	1.33
30	WA	4408	PSU	C2-N3	7.37	1.49	1.37
30	WA	4488	B8T	C4-N3	7.36	1.45	1.32
30	WA	1587	PSU	C2-N3	7.34	1.49	1.37
30	WA	1802	E7G	C5-N7	7.24	1.44	1.35
30	WA	4695	B8K	C8-N9	7.24	1.50	1.45
30	WA	2302	E7G	C5-N7	7.10	1.44	1.35
32	YA	14	OMU	C2-N3	7.07	1.50	1.38
30	WA	4625	OMU	C2-N3	7.00	1.50	1.38
30	WA	2527	7MG	C5-N7	6.98	1.44	1.35
30	WA	730	2MG	C4-N3	6.98	1.50	1.34
30	WA	4311	OMU	C2-N3	6.94	1.50	1.38
30	WA	4340	5MC	C5-C4	6.94	1.49	1.44
30	WA	4340	5MC	C4-N3	6.93	1.45	1.34
30	WA	4311	OMU	C2-N1	6.93	1.49	1.38
30	WA	4555	7MG	C5-N7	6.90	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4625	OMU	C2-N1	6.90	1.49	1.38
53	ZA	1374	5MC	C5-C4	6.89	1.49	1.44
30	WA	1610	7MG	C5-N7	6.88	1.44	1.35
53	ZA	1374	5MC	C4-N3	6.83	1.45	1.34
53	ZA	1337	4AC	C6-C5	6.83	1.50	1.35
30	WA	3787	5MC	C4-N3	6.81	1.45	1.34
30	WA	4477	B8W	O6-C6	6.75	1.45	1.35
30	WA	4190	B8W	O6-C6	6.73	1.45	1.35
30	WA	2778	OMG	C4-N3	6.68	1.49	1.34
30	WA	3787	5MC	C5-C4	6.67	1.49	1.44
30	WA	4452	5MC	C4-N3	6.66	1.44	1.34
30	WA	4499	OMG	C4-N3	6.65	1.49	1.34
30	WA	4642	OMG	C4-N3	6.63	1.49	1.34
30	WA	1630	OMG	C4-N3	6.62	1.49	1.34
30	WA	4877	2MG	C4-N3	6.62	1.49	1.34
30	WA	1888	OMG	C4-N3	6.61	1.49	1.34
30	WA	3797	OMG	C4-N3	6.60	1.49	1.34
30	WA	2369	OMG	C4-N3	6.59	1.49	1.34
30	WA	1322	OMG	C4-N3	6.59	1.49	1.34
30	WA	4875	OMG	C4-N3	6.59	1.49	1.34
30	WA	4376	MHG	C2-N1	6.59	1.47	1.36
30	WA	4201	OMG	C4-N3	6.58	1.49	1.34
30	WA	2429	OMG	C4-N3	6.58	1.49	1.34
30	WA	1522	2MG	C4-N3	6.58	1.49	1.34
30	WA	4375	OMG	C4-N3	6.57	1.49	1.34
30	WA	2055	OMG	C4-N3	6.57	1.49	1.34
30	WA	4628	OMG	C4-N3	6.56	1.49	1.34
30	WA	2866	OMC	C2-N3	6.55	1.49	1.36
30	WA	2385	B8W	O6-C6	6.55	1.45	1.35
30	WA	373	OMG	C4-N3	6.54	1.49	1.34
30	WA	2427	OMC	C2-N3	6.54	1.49	1.36
30	WA	4534	B8W	O6-C6	6.53	1.45	1.35
30	WA	1527	OMG	C4-N3	6.53	1.49	1.34
30	WA	3706	OMC	C2-N3	6.52	1.49	1.36
30	WA	4134	B8W	O6-C6	6.52	1.45	1.35
30	WA	4541	OMC	C2-N3	6.47	1.49	1.36
30	WA	2370	OMC	C2-N3	6.45	1.49	1.36
30	WA	4676	B8T	C2-N3	6.45	1.49	1.36
30	WA	3892	OMC	C2-N3	6.43	1.49	1.36
30	WA	4488	B8T	C2-N3	6.43	1.49	1.36
30	WA	3902	B8K	C8-N9	6.41	1.50	1.45
30	WA	3914	OMC	C2-N3	6.39	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4452	5MC	C5-C4	6.38	1.48	1.44
30	WA	3874	OMC	C2-N3	6.37	1.49	1.36
30	WA	2809	OMC	C2-N3	6.35	1.49	1.36
30	WA	1354	P4U	C2-N3	6.34	1.48	1.36
30	WA	4199	I4U	C2-N3	6.29	1.48	1.36
30	WA	4340	5MC	C2-N3	6.28	1.48	1.36
30	WA	1664	I4U	C6-C5	6.26	1.49	1.35
30	WA	4199	I4U	C6-C5	6.26	1.49	1.35
30	WA	1664	I4U	C2-N3	6.26	1.48	1.36
30	WA	3787	5MC	C2-N3	6.25	1.48	1.36
53	ZA	1374	5MC	C2-N3	6.25	1.48	1.36
53	ZA	1219	JMH	C2-N1	6.22	1.47	1.38
30	WA	2791	B9H	C2-N1	6.21	1.47	1.38
30	WA	1354	P4U	C6-C5	6.19	1.49	1.35
30	WA	4452	5MC	C2-N3	6.17	1.48	1.36
30	WA	3885	P7G	C4-N9	6.14	1.45	1.35
30	WA	4676	B8T	C6-C5	6.13	1.49	1.35
30	WA	4488	B8T	C6-C5	6.10	1.49	1.35
30	WA	4695	B8K	C4-N3	6.08	1.48	1.34
30	WA	1914	P7G	C4-N9	6.07	1.45	1.35
30	WA	3902	B8K	C4-N3	6.05	1.48	1.34
30	WA	1461	JMH	C2-N1	6.05	1.46	1.38
53	ZA	1337	4AC	C4-N4	6.03	1.48	1.39
30	WA	4376	MHG	C4-N9	6.03	1.45	1.37
30	WA	3706	OMC	C6-C5	6.01	1.49	1.35
30	WA	4541	OMC	C6-C5	6.00	1.49	1.35
30	WA	3874	OMC	C6-C5	6.00	1.49	1.35
30	WA	3892	OMC	C6-C5	5.99	1.49	1.35
30	WA	4535	UR3	C6-C5	5.99	1.49	1.35
30	WA	3914	OMC	C6-C5	5.99	1.48	1.35
30	WA	2427	OMC	C6-C5	5.98	1.48	1.35
30	WA	2370	OMC	C6-C5	5.98	1.48	1.35
30	WA	2809	OMC	C6-C5	5.98	1.48	1.35
30	WA	2302	E7G	C2-N3	5.97	1.47	1.33
30	WA	2866	OMC	C6-C5	5.95	1.48	1.35
53	ZA	1219	JMH	C6-C5	5.95	1.48	1.35
30	WA	4602	UR3	C6-C5	5.93	1.48	1.35
30	WA	3904	BGH	C2-N3	5.93	1.47	1.33
30	WA	1871	UR3	C6-C5	5.92	1.48	1.35
30	WA	1461	JMH	C6-C5	5.91	1.48	1.35
30	WA	1802	E7G	C2-N3	5.90	1.47	1.33
30	WA	3902	B8K	C2-N3	5.88	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	2527	7MG	C2-N3	5.88	1.47	1.33
30	WA	4695	B8K	C2-N3	5.88	1.47	1.33
53	ZA	1248	B8N	C2-N1	5.88	1.56	1.39
30	WA	1610	7MG	C2-N3	5.87	1.47	1.33
30	WA	2759	B9B	C2-N2	5.87	1.45	1.33
30	WA	3904	BGH	C4-N3	5.86	1.47	1.34
30	WA	3902	B8K	C4-N9	5.85	1.45	1.37
30	WA	237	B9B	C2-N2	5.84	1.45	1.33
30	WA	1579	B9B	C2-N2	5.84	1.45	1.33
30	WA	4555	7MG	C2-N3	5.82	1.47	1.33
30	WA	4360	E6G	C2-N2	5.80	1.45	1.33
30	WA	4641	PSU	C6-N1	5.75	1.45	1.36
30	WA	4695	B8K	C4-N9	5.66	1.44	1.37
30	WA	4311	OMU	C6-C5	5.65	1.48	1.35
30	WA	4625	OMU	C6-C5	5.63	1.48	1.35
53	ZA	1248	B8N	C6-C5	5.60	1.43	1.35
30	WA	3885	P7G	C2-N1	5.56	1.46	1.33
30	WA	4695	B8K	C2-N2	5.55	1.47	1.34
30	WA	3904	BGH	O4'-C1'	-5.54	1.29	1.42
30	WA	1914	P7G	C2-N1	5.53	1.46	1.33
30	WA	2778	OMG	C2-N3	5.53	1.46	1.33
32	YA	14	OMU	C6-C5	5.53	1.47	1.35
30	WA	1888	OMG	C2-N3	5.50	1.46	1.33
30	WA	4642	OMG	C2-N3	5.50	1.46	1.33
30	WA	4499	OMG	C2-N3	5.49	1.46	1.33
30	WA	3902	B8K	C2-N2	5.49	1.47	1.34
30	WA	1630	OMG	C2-N3	5.46	1.46	1.33
30	WA	3797	OMG	C2-N3	5.46	1.46	1.33
30	WA	4875	OMG	C2-N3	5.44	1.46	1.33
30	WA	2429	OMG	C2-N3	5.44	1.46	1.33
30	WA	2369	OMG	C2-N3	5.43	1.46	1.33
30	WA	4375	OMG	C2-N3	5.43	1.46	1.33
30	WA	1322	OMG	C2-N3	5.43	1.46	1.33
53	ZA	1678	A2M	C6-N6	5.42	1.48	1.34
30	WA	2055	OMG	C2-N3	5.42	1.46	1.33
30	WA	2302	E7G	C4-N9	5.41	1.44	1.37
30	WA	4628	OMG	C2-N3	5.40	1.46	1.33
30	WA	4201	OMG	C2-N3	5.39	1.46	1.33
51	v	715	DDE	CBI-NAD	5.38	1.45	1.32
30	WA	3872	A2M	C6-N6	5.38	1.48	1.34
30	WA	398	A2M	C6-N6	5.38	1.47	1.34
30	WA	1527	OMG	C2-N3	5.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	3723	A2M	C6-N6	5.38	1.47	1.34
30	WA	3728	A2M	C6-N6	5.37	1.47	1.34
30	WA	1529	A2M	C6-N6	5.37	1.47	1.34
30	WA	4528	A2M	C6-N6	5.36	1.47	1.34
30	WA	373	OMG	C2-N3	5.36	1.46	1.33
30	WA	4576	A2M	C6-N6	5.35	1.47	1.34
30	WA	1876	A2M	C6-N6	5.35	1.47	1.34
30	WA	2406	A2M	C6-N6	5.35	1.47	1.34
30	WA	1461	JMH	C4-N4	5.34	1.49	1.27
30	WA	1539	A2M	C6-N6	5.34	1.47	1.34
30	WA	3830	A2M	C6-N6	5.34	1.47	1.34
30	WA	1332	A2M	C6-N6	5.34	1.47	1.34
30	WA	2368	A2M	C6-N6	5.34	1.47	1.34
30	WA	1529	A2M	C2'-C1'	5.33	1.66	1.53
30	WA	2427	OMC	C4-N3	5.33	1.45	1.34
53	ZA	1219	JMH	C4-N4	5.33	1.49	1.27
30	WA	3706	OMC	C4-N3	5.31	1.45	1.34
53	ZA	1219	JMH	C2-N3	5.31	1.49	1.39
30	WA	3892	OMC	C4-N3	5.30	1.45	1.34
30	WA	2866	OMC	C4-N3	5.28	1.45	1.34
30	WA	3904	BGH	C4-N9	5.27	1.44	1.37
30	WA	3728	A2M	C2'-C1'	5.26	1.66	1.53
30	WA	2370	OMC	C4-N3	5.25	1.44	1.34
30	WA	4576	A2M	C2'-C1'	5.24	1.66	1.53
30	WA	4541	OMC	C4-N3	5.23	1.44	1.34
30	WA	1610	7MG	C4-N9	5.23	1.44	1.37
30	WA	3874	OMC	C4-N3	5.22	1.44	1.34
30	WA	2809	OMC	C4-N3	5.21	1.44	1.34
30	WA	3914	OMC	C4-N3	5.21	1.44	1.34
30	WA	4555	7MG	C4-N9	5.20	1.44	1.37
30	WA	2527	7MG	C4-N9	5.20	1.44	1.37
30	WA	1461	JMH	C2-N3	5.20	1.49	1.39
30	WA	3734	PSU	C6-N1	5.19	1.44	1.36
30	WA	3885	P7G	C2-N2	5.19	1.46	1.34
30	WA	3790	A2M	C6-N6	5.19	1.47	1.34
30	WA	2406	A2M	C2'-C1'	5.18	1.65	1.53
30	WA	1914	P7G	C2-N2	5.18	1.46	1.34
30	WA	4602	UR3	C2-N3	5.17	1.49	1.39
30	WA	1682	PSU	C6-N1	5.17	1.44	1.36
30	WA	4535	UR3	C2-N3	5.14	1.49	1.39
30	WA	398	A2M	C2'-C1'	5.14	1.65	1.53
30	WA	2513	PSU	C6-N1	5.14	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	ZA	1243	PSU	C6-N1	5.14	1.44	1.36
30	WA	4536	PSU	C6-N1	5.14	1.44	1.36
30	WA	1802	E7G	C4-N9	5.13	1.44	1.37
30	WA	4298	PSU	C6-N1	5.12	1.44	1.36
30	WA	3769	PSU	C6-N1	5.11	1.44	1.36
30	WA	3723	A2M	C2'-C1'	5.11	1.65	1.53
30	WA	3720	PSU	C6-N1	5.11	1.44	1.36
30	WA	4633	PSU	C6-N1	5.09	1.44	1.36
30	WA	1871	UR3	C2-N3	5.09	1.49	1.39
30	WA	4505	PSU	C6-N1	5.07	1.44	1.36
30	WA	1688	PSU	C6-N1	5.06	1.44	1.36
30	WA	4455	PSU	C6-N1	5.06	1.44	1.36
30	WA	1587	PSU	C6-N1	5.05	1.44	1.36
53	ZA	1678	A2M	C2'-C1'	5.04	1.65	1.53
30	WA	4447	PSU	C6-N1	5.04	1.44	1.36
30	WA	4528	A2M	C2'-C1'	5.04	1.65	1.53
53	ZA	1337	4AC	C2-N1	5.00	1.50	1.40
30	WA	4408	PSU	C6-N1	5.00	1.44	1.36
30	WA	3872	A2M	C2'-C1'	4.99	1.65	1.53
30	WA	2368	A2M	C2'-C1'	4.99	1.65	1.53
30	WA	1876	A2M	C2'-C1'	4.97	1.65	1.53
30	WA	1865	B8H	C1'-C5	-4.94	1.39	1.50
30	WA	1332	A2M	C2'-C1'	4.94	1.65	1.53
30	WA	2778	OMG	C2-N2	4.93	1.45	1.34
30	WA	1539	A2M	C2'-C1'	4.92	1.65	1.53
30	WA	4875	OMG	C2-N2	4.92	1.45	1.34
30	WA	2429	OMG	C2-N2	4.91	1.45	1.34
30	WA	1888	OMG	C2-N2	4.90	1.45	1.34
30	WA	4499	OMG	C2-N2	4.90	1.45	1.34
30	WA	3767	B8H	C2-N3	4.89	1.46	1.38
30	WA	1522	2MG	C2-N1	4.89	1.44	1.36
30	WA	3797	OMG	C2-N2	4.88	1.45	1.34
30	WA	1322	OMG	C2-N2	4.87	1.45	1.34
30	WA	1527	OMG	C2-N2	4.87	1.45	1.34
30	WA	3790	A2M	C2'-C1'	4.87	1.65	1.53
30	WA	4375	OMG	C2-N2	4.87	1.45	1.34
30	WA	373	OMG	C2-N2	4.86	1.45	1.34
30	WA	4642	OMG	C2-N2	4.86	1.45	1.34
30	WA	2369	OMG	C2-N2	4.86	1.45	1.34
30	WA	2055	OMG	C2-N2	4.86	1.45	1.34
30	WA	4088	5MU	C2-N3	4.86	1.46	1.38
30	WA	3904	BGH	C2-N2	4.85	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4628	OMG	C2-N2	4.85	1.45	1.34
30	WA	4301	B8H	C1'-C5	-4.85	1.39	1.50
30	WA	1630	OMG	C2-N2	4.85	1.45	1.34
30	WA	4201	OMG	C2-N2	4.84	1.45	1.34
30	WA	4301	B8H	C2-N3	4.84	1.46	1.38
30	WA	3830	A2M	C2'-C1'	4.84	1.65	1.53
30	WA	1865	B8H	C2-N3	4.84	1.46	1.38
30	WA	2302	E7G	C2-N2	4.84	1.45	1.34
30	WA	2866	OMC	C2-N1	4.82	1.50	1.40
30	WA	1802	E7G	C2-N2	4.82	1.45	1.34
30	WA	3767	B8H	C1'-C5	-4.80	1.39	1.50
30	WA	4877	2MG	C2-N1	4.79	1.44	1.36
30	WA	2527	7MG	C2-N2	4.79	1.45	1.34
30	WA	1610	7MG	C2-N2	4.79	1.45	1.34
30	WA	730	2MG	C2-N1	4.76	1.44	1.36
30	WA	4555	7MG	C2-N2	4.75	1.45	1.34
30	WA	2427	OMC	C4-N4	4.72	1.45	1.33
30	WA	4541	OMC	C4-N4	4.71	1.45	1.33
30	WA	3892	OMC	C4-N4	4.71	1.45	1.33
30	WA	2866	OMC	C4-N4	4.70	1.45	1.33
30	WA	3874	OMC	C4-N4	4.70	1.45	1.33
30	WA	2809	OMC	C4-N4	4.69	1.45	1.33
30	WA	2370	OMC	C4-N4	4.69	1.45	1.33
30	WA	3914	OMC	C4-N4	4.68	1.45	1.33
30	WA	3706	OMC	C4-N4	4.67	1.45	1.33
30	WA	3790	A2M	O4'-C1'	-4.67	1.31	1.42
30	WA	3885	P7G	C2-N3	4.67	1.49	1.37
30	WA	2427	OMC	C2-N1	4.66	1.49	1.40
30	WA	4488	B8T	C4-N4	4.61	1.45	1.36
30	WA	4541	OMC	C2-N1	4.61	1.49	1.40
30	WA	4676	B8T	C4-N4	4.59	1.45	1.36
30	WA	3892	OMC	C2-N1	4.58	1.49	1.40
30	WA	4452	5MC	C6-N1	4.58	1.45	1.38
30	WA	1914	P7G	C2-N3	4.56	1.48	1.37
53	ZA	1678	A2M	O4'-C1'	-4.55	1.31	1.42
53	ZA	1374	5MC	C6-N1	4.53	1.45	1.38
30	WA	2370	OMC	C2-N1	4.53	1.49	1.40
30	WA	3914	OMC	C2-N1	4.53	1.49	1.40
30	WA	2809	OMC	C2-N1	4.52	1.49	1.40
30	WA	3706	OMC	C2-N1	4.52	1.49	1.40
30	WA	2385	B8W	C2-N2	4.50	1.42	1.33
30	WA	4134	B8W	C2-N2	4.49	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	1539	A2M	O4'-C1'	-4.49	1.31	1.42
30	WA	3874	OMC	C2-N1	4.48	1.49	1.40
30	WA	4340	5MC	C6-N1	4.47	1.45	1.38
30	WA	4477	B8W	C2-N2	4.45	1.42	1.33
30	WA	4190	B8W	C2-N2	4.45	1.42	1.33
53	ZA	1374	5MC	C4-N4	4.43	1.45	1.34
30	WA	1529	A2M	O4'-C1'	-4.43	1.31	1.42
30	WA	4340	5MC	C4-N4	4.43	1.45	1.34
30	WA	4534	B8W	C2-N2	4.42	1.42	1.33
30	WA	3787	5MC	C6-N1	4.41	1.45	1.38
30	WA	4452	5MC	C4-N4	4.41	1.45	1.34
30	WA	4488	B8T	C2-N1	4.39	1.49	1.40
30	WA	1354	P4U	C2-N1	4.38	1.49	1.40
30	WA	2406	A2M	O4'-C1'	-4.38	1.31	1.42
30	WA	3872	A2M	O4'-C1'	-4.38	1.31	1.42
30	WA	3787	5MC	C4-N4	4.37	1.45	1.34
30	WA	1332	A2M	O4'-C1'	-4.36	1.31	1.42
30	WA	4576	A2M	O4'-C1'	-4.35	1.31	1.42
30	WA	2368	A2M	O4'-C1'	-4.35	1.32	1.42
53	ZA	1374	5MC	C2-N1	4.34	1.49	1.40
30	WA	3787	5MC	C2-N1	4.33	1.49	1.40
30	WA	4676	B8T	C2-N1	4.33	1.49	1.40
30	WA	4528	A2M	O4'-C1'	-4.30	1.32	1.42
30	WA	4340	5MC	C2-N1	4.30	1.49	1.40
30	WA	4569	M7A	C6-N6	4.29	1.45	1.34
30	WA	3728	A2M	O4'-C1'	-4.29	1.32	1.42
30	WA	3830	A2M	O4'-C1'	-4.26	1.32	1.42
53	ZA	1337	4AC	C5-C4	4.26	1.50	1.41
30	WA	3902	B8K	C5-C6	4.23	1.54	1.43
30	WA	398	A2M	O4'-C1'	-4.23	1.32	1.42
30	WA	4695	B8K	C5-C6	4.22	1.54	1.43
30	WA	1876	A2M	O4'-C1'	-4.22	1.32	1.42
30	WA	3723	A2M	O4'-C1'	-4.22	1.32	1.42
30	WA	4452	5MC	C2-N1	4.21	1.48	1.40
30	WA	4625	OMU	C4-N3	4.19	1.45	1.38
30	WA	1664	I4U	C2-N1	4.16	1.48	1.40
30	WA	4311	OMU	C4-N3	4.13	1.45	1.38
30	WA	3769	PSU	C4-N3	4.12	1.46	1.38
30	WA	1354	P4U	O4-C4	4.11	1.40	1.35
30	WA	1871	UR3	O4-C4	-4.10	1.14	1.23
32	YA	14	OMU	C4-N3	4.10	1.45	1.38
30	WA	4199	I4U	C2-N1	4.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4695	B8K	C2-N1	4.09	1.47	1.37
30	WA	3902	B8K	C2-N1	4.07	1.47	1.37
30	WA	4535	UR3	O4-C4	-4.07	1.14	1.23
30	WA	4536	PSU	C4-N3	4.07	1.46	1.38
30	WA	4569	M7A	C5-N7	4.07	1.48	1.39
30	WA	4298	PSU	C4-N3	4.07	1.46	1.38
30	WA	3734	PSU	C4-N3	4.06	1.46	1.38
30	WA	4602	UR3	O4-C4	-4.05	1.15	1.23
53	ZA	1243	PSU	C4-N3	4.04	1.46	1.38
30	WA	4447	PSU	C4-N3	4.03	1.46	1.38
30	WA	1587	PSU	C4-N3	4.03	1.46	1.38
30	WA	4408	PSU	C4-N3	4.02	1.46	1.38
30	WA	4505	PSU	C4-N3	4.01	1.46	1.38
30	WA	3720	PSU	C4-N3	4.01	1.46	1.38
30	WA	4641	PSU	C4-N3	4.00	1.46	1.38
30	WA	1682	PSU	C4-N3	4.00	1.46	1.38
30	WA	1688	PSU	C4-N3	3.99	1.46	1.38
30	WA	2513	PSU	C4-N3	3.99	1.46	1.38
30	WA	3904	BGH	C5-C6	3.99	1.53	1.43
30	WA	4633	PSU	C4-N3	3.97	1.46	1.38
30	WA	4455	PSU	C4-N3	3.92	1.46	1.38
53	ZA	1337	4AC	C7-N4	3.90	1.45	1.37
30	WA	1610	7MG	C2-N1	3.88	1.47	1.37
30	WA	4420	1MA	C5-C6	3.84	1.53	1.43
30	WA	2527	7MG	C2-N1	3.82	1.46	1.37
30	WA	4420	1MA	C2-N1	3.80	1.43	1.35
30	WA	4376	MHG	C8-N7	3.79	1.52	1.45
30	WA	4360	E6G	O6-C6	3.77	1.40	1.34
30	WA	4555	7MG	C2-N1	3.76	1.46	1.37
30	WA	1328	1MA	C2-N1	3.75	1.43	1.35
30	WA	1328	1MA	C5-C6	3.74	1.53	1.43
30	WA	1802	E7G	C2-N1	3.73	1.46	1.37
30	WA	2302	E7G	C2-N1	3.71	1.46	1.37
51	v	715	DDE	CG-ND1	-3.70	1.31	1.38
30	WA	4190	B8W	C5-C4	-3.69	1.32	1.39
30	WA	4534	B8W	C5-C4	-3.67	1.32	1.39
30	WA	1914	P7G	C6-N1	3.66	1.44	1.38
30	WA	4676	B8T	C5-C4	3.65	1.49	1.41
30	WA	237	B9B	O6-C6	3.64	1.40	1.34
30	WA	4376	MHG	C5-C6	3.64	1.52	1.43
30	WA	4477	B8W	C5-C4	-3.63	1.32	1.39
30	WA	3904	BGH	C6-N1	3.63	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	3790	A2M	C4-N9	-3.63	1.30	1.37
30	WA	2385	B8W	C5-C4	-3.63	1.32	1.39
30	WA	4488	B8T	C5-C4	3.62	1.49	1.41
30	WA	4134	B8W	C5-C4	-3.61	1.32	1.39
30	WA	1529	A2M	C5'-C4'	-3.61	1.40	1.51
30	WA	3885	P7G	C6-N1	3.60	1.44	1.38
30	WA	3904	BGH	C2-N1	3.60	1.46	1.37
30	WA	2302	E7G	C5-C6	3.58	1.52	1.43
30	WA	3904	BGH	C5-N7	3.58	1.46	1.39
30	WA	1802	E7G	C5-C6	3.58	1.52	1.43
30	WA	4576	A2M	C5'-C4'	-3.57	1.40	1.51
30	WA	4695	B8K	C5-N7	3.55	1.46	1.39
30	WA	3830	A2M	C5'-C4'	-3.55	1.40	1.51
30	WA	2759	B9B	O6-C6	3.54	1.40	1.34
30	WA	1876	A2M	C4-N9	-3.53	1.30	1.37
30	WA	1579	B9B	O6-C6	3.53	1.40	1.34
30	WA	1332	A2M	C5'-C4'	-3.49	1.41	1.51
30	WA	3790	A2M	C5'-C4'	-3.48	1.41	1.51
30	WA	4695	B8K	C6-N1	3.48	1.45	1.38
30	WA	3872	A2M	C5'-C4'	-3.47	1.41	1.51
30	WA	1876	A2M	C5'-C4'	-3.47	1.41	1.51
30	WA	4528	A2M	C5'-C4'	-3.47	1.41	1.51
30	WA	4528	A2M	C4-N9	-3.47	1.30	1.37
30	WA	2406	A2M	C5'-C4'	-3.47	1.41	1.51
30	WA	4555	7MG	C5-C6	3.47	1.52	1.43
53	ZA	1678	A2M	C5'-C4'	-3.46	1.41	1.51
30	WA	3902	B8K	C5-N7	3.46	1.46	1.39
30	WA	4477	B8W	C8-N9	-3.46	1.31	1.37
30	WA	2527	7MG	C5-C6	3.45	1.52	1.43
30	WA	2368	A2M	C4-N9	-3.45	1.30	1.37
30	WA	2368	A2M	C5'-C4'	-3.44	1.41	1.51
30	WA	1610	7MG	C5-C6	3.44	1.52	1.43
30	WA	3728	A2M	C5'-C4'	-3.44	1.41	1.51
30	WA	3904	BGH	O2'-C2'	-3.43	1.34	1.42
30	WA	398	A2M	C5'-C4'	-3.43	1.41	1.51
30	WA	1332	A2M	C4-N9	-3.42	1.30	1.37
30	WA	3830	A2M	C4-N9	-3.41	1.30	1.37
30	WA	1914	P7G	C8-N7	3.41	1.52	1.45
30	WA	3723	A2M	C5'-C4'	-3.41	1.41	1.51
30	WA	4576	A2M	C4-N9	-3.41	1.30	1.37
30	WA	3723	A2M	C4-N9	-3.39	1.30	1.37
30	WA	398	A2M	C4-N9	-3.38	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	ZA	1678	A2M	C4-N9	-3.38	1.30	1.37
30	WA	2406	A2M	C4-N9	-3.37	1.30	1.37
30	WA	1539	A2M	C5'-C4'	-3.37	1.41	1.51
30	WA	3872	A2M	C4-N9	-3.36	1.30	1.37
30	WA	3902	B8K	C6-N1	3.36	1.45	1.38
30	WA	3885	P7G	C8-N7	3.34	1.51	1.45
30	WA	4190	B8W	C8-N9	-3.33	1.31	1.37
30	WA	3892	OMC	C6-N1	3.32	1.46	1.38
30	WA	1529	A2M	C4-N9	-3.31	1.30	1.37
30	WA	1539	A2M	C4-N9	-3.31	1.30	1.37
30	WA	3874	OMC	C6-N1	3.30	1.46	1.38
30	WA	2427	OMC	C6-N1	3.30	1.45	1.38
30	WA	4541	OMC	C6-N1	3.29	1.45	1.38
30	WA	2370	OMC	C6-N1	3.28	1.45	1.38
30	WA	3790	A2M	C3'-C4'	3.28	1.61	1.53
30	WA	2809	OMC	C6-N1	3.28	1.45	1.38
30	WA	4134	B8W	C8-N9	-3.27	1.32	1.37
30	WA	3706	OMC	C6-N1	3.26	1.45	1.38
30	WA	2385	B8W	C8-N9	-3.26	1.32	1.37
30	WA	2866	OMC	C6-N1	3.25	1.45	1.38
30	WA	3914	OMC	C6-N1	3.24	1.45	1.38
30	WA	1802	E7G	C8-N7	3.22	1.51	1.45
30	WA	3904	BGH	C71-N7	3.21	1.46	1.39
30	WA	4534	B8W	C8-N9	-3.20	1.32	1.37
30	WA	1610	7MG	C6-N1	3.20	1.44	1.38
30	WA	4576	A2M	O2'-C2'	3.20	1.50	1.42
30	WA	4535	UR3	C5-C4	3.19	1.51	1.43
30	WA	2527	7MG	C6-N1	3.18	1.44	1.38
30	WA	4199	I4U	C6-N1	3.18	1.45	1.38
30	WA	1664	I4U	C6-N1	3.17	1.45	1.38
53	ZA	1678	A2M	C3'-C4'	3.17	1.61	1.53
30	WA	3728	A2M	C4-N9	-3.15	1.31	1.37
30	WA	1914	P7G	C5-C4	3.15	1.44	1.36
30	WA	1664	I4U	O4-C41	-3.15	1.40	1.47
30	WA	4488	B8T	C6-N1	3.15	1.45	1.38
30	WA	2302	E7G	C8-N7	3.15	1.51	1.45
53	ZA	1678	A2M	O2'-C2'	3.12	1.50	1.42
51	v	715	DDE	CBW-NCB	-3.12	1.47	1.54
30	WA	4676	B8T	C6-N1	3.11	1.45	1.38
30	WA	3885	P7G	C5-C4	3.11	1.44	1.36
30	WA	4555	7MG	C6-N1	3.10	1.44	1.38
30	WA	4199	I4U	O4-C41	-3.10	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4602	UR3	C5-C4	3.10	1.51	1.43
30	WA	3728	A2M	C3'-C4'	3.08	1.60	1.53
30	WA	4376	MHG	C6-N1	3.08	1.44	1.38
30	WA	1802	E7G	C6-N1	3.08	1.44	1.38
30	WA	3728	A2M	O2'-C2'	3.08	1.50	1.42
53	ZA	1337	4AC	C6-N1	3.08	1.45	1.38
30	WA	1871	UR3	C5-C4	3.07	1.51	1.43
30	WA	3872	A2M	C3'-C4'	3.07	1.60	1.53
30	WA	1354	P4U	C6-N1	3.07	1.45	1.38
30	WA	1539	A2M	C3'-C4'	3.07	1.60	1.53
30	WA	2302	E7G	C6-N1	3.06	1.44	1.38
30	WA	1332	A2M	C3'-C4'	3.06	1.60	1.53
30	WA	4528	A2M	C3'-C4'	3.05	1.60	1.53
30	WA	1332	A2M	O2'-C2'	3.03	1.50	1.42
30	WA	4225	6MZ	C5-C4	-3.03	1.33	1.39
53	ZA	1219	JMH	C5-C4	3.02	1.49	1.42
30	WA	1529	A2M	O2'-C2'	3.02	1.50	1.42
30	WA	1461	JMH	C5-C4	3.01	1.49	1.42
30	WA	2368	A2M	C3'-C4'	3.00	1.60	1.53
30	WA	3723	A2M	O2'-C2'	3.00	1.50	1.42
30	WA	730	2MG	C5-N7	-3.00	1.33	1.39
30	WA	398	A2M	O2'-C2'	3.00	1.50	1.42
30	WA	4311	OMU	O4-C4	-2.99	1.18	1.24
30	WA	2406	A2M	O2'-C2'	2.98	1.50	1.42
30	WA	4576	A2M	C3'-C4'	2.98	1.60	1.53
30	WA	4625	OMU	O4-C4	-2.98	1.18	1.24
30	WA	1579	B9B	C5-C4	-2.97	1.33	1.39
30	WA	3723	A2M	C3'-C4'	2.96	1.60	1.53
30	WA	3830	A2M	O2'-C2'	2.96	1.49	1.42
32	YA	14	OMU	O4-C4	-2.95	1.18	1.24
30	WA	4877	2MG	C5-N7	-2.95	1.33	1.39
30	WA	2368	A2M	O2'-C2'	2.95	1.49	1.42
30	WA	398	A2M	C3'-C4'	2.94	1.60	1.53
30	WA	2406	A2M	C3'-C4'	2.94	1.60	1.53
30	WA	1522	2MG	C5-N7	-2.93	1.33	1.39
30	WA	1876	A2M	C3'-C4'	2.93	1.60	1.53
30	WA	4452	5MC	O2-C2	-2.92	1.18	1.23
30	WA	3723	A2M	C5-N7	-2.92	1.33	1.39
30	WA	2759	B9B	C5-C4	-2.92	1.33	1.39
30	WA	1539	A2M	C5-N7	-2.91	1.33	1.39
30	WA	3914	OMC	O2-C2	-2.91	1.18	1.23
30	WA	1332	A2M	C5-N7	-2.91	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	3790	A2M	O2'-C2'	2.91	1.49	1.42
30	WA	4528	A2M	O2'-C2'	2.90	1.49	1.42
30	WA	1876	A2M	O2'-C2'	2.90	1.49	1.42
30	WA	3830	A2M	C3'-C4'	2.90	1.60	1.53
30	WA	3872	A2M	C5-N7	-2.89	1.33	1.39
30	WA	237	B9B	C5-C4	-2.89	1.33	1.39
30	WA	2368	A2M	C5-N7	-2.89	1.33	1.39
30	WA	3728	A2M	C5-N7	-2.89	1.33	1.39
30	WA	1876	A2M	C5-N7	-2.88	1.33	1.39
30	WA	1529	A2M	C5-N7	-2.88	1.33	1.39
30	WA	3885	P7G	O6-C6	-2.87	1.18	1.23
30	WA	4875	OMG	C2-N1	2.87	1.44	1.37
30	WA	3872	A2M	O2'-C2'	2.87	1.49	1.42
30	WA	373	OMG	C2-N1	2.86	1.44	1.37
30	WA	4628	OMG	C2-N1	2.86	1.44	1.37
30	WA	2778	OMG	C2-N1	2.86	1.44	1.37
30	WA	3830	A2M	C5-N7	-2.85	1.33	1.39
53	ZA	1678	A2M	C5-N7	-2.85	1.33	1.39
30	WA	4528	A2M	C5-N7	-2.85	1.33	1.39
30	WA	4576	A2M	C5-N7	-2.84	1.33	1.39
30	WA	3790	A2M	O3'-C3'	2.84	1.50	1.43
30	WA	3797	OMG	C2-N1	2.83	1.44	1.37
30	WA	3797	OMG	C5-N7	-2.83	1.33	1.39
30	WA	4360	E6G	C5-C4	-2.83	1.34	1.39
30	WA	398	A2M	C5-N7	-2.83	1.33	1.39
30	WA	3790	A2M	C5-N7	-2.83	1.33	1.39
30	WA	1529	A2M	C3'-C4'	2.83	1.60	1.53
30	WA	1322	OMG	C2-N1	2.83	1.44	1.37
30	WA	2055	OMG	C2-N1	2.82	1.44	1.37
30	WA	1322	OMG	C5-N7	-2.82	1.33	1.39
30	WA	1888	OMG	C2-N1	2.82	1.44	1.37
30	WA	2429	OMG	C2-N1	2.82	1.44	1.37
30	WA	1914	P7G	O6-C6	-2.82	1.18	1.23
30	WA	1888	OMG	C5-N7	-2.82	1.33	1.39
30	WA	2406	A2M	C5-N7	-2.82	1.33	1.39
30	WA	4642	OMG	C5-N7	-2.82	1.33	1.39
30	WA	4375	OMG	C2-N1	2.81	1.44	1.37
30	WA	4642	OMG	C2-N1	2.81	1.44	1.37
30	WA	1539	A2M	O2'-C2'	2.80	1.49	1.42
30	WA	4201	OMG	C2-N1	2.80	1.44	1.37
30	WA	4695	B8K	O6-C6	-2.80	1.18	1.23
30	WA	4311	OMU	C6-N1	2.80	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	2369	OMG	C2-N1	2.80	1.44	1.37
30	WA	3723	A2M	O4'-C4'	2.80	1.51	1.45
30	WA	1630	OMG	C2-N1	2.80	1.44	1.37
30	WA	2055	OMG	C5-N7	-2.79	1.33	1.39
30	WA	1527	OMG	C2-N1	2.79	1.44	1.37
30	WA	1876	A2M	O4'-C4'	2.79	1.51	1.45
30	WA	4535	UR3	C6-N1	2.78	1.44	1.38
30	WA	4499	OMG	C2-N1	2.78	1.44	1.37
30	WA	1630	OMG	C5-N7	-2.78	1.33	1.39
30	WA	3728	A2M	O4'-C4'	2.78	1.51	1.45
30	WA	3723	A2M	O3'-C3'	2.78	1.49	1.43
30	WA	2369	OMG	C5-N7	-2.77	1.33	1.39
53	ZA	1337	4AC	O7-C7	-2.77	1.17	1.23
30	WA	398	A2M	O3'-C3'	2.77	1.49	1.43
30	WA	4499	OMG	C5-N7	-2.77	1.33	1.39
30	WA	2406	A2M	O3'-C3'	2.76	1.49	1.43
30	WA	3830	A2M	O4'-C4'	2.76	1.51	1.45
30	WA	2778	OMG	C5-N7	-2.76	1.33	1.39
30	WA	398	A2M	O4'-C4'	2.75	1.51	1.45
30	WA	1871	UR3	C6-N1	2.75	1.44	1.38
30	WA	4576	A2M	O3'-C3'	2.75	1.49	1.43
30	WA	3790	A2M	O4'-C4'	2.74	1.51	1.45
53	ZA	1678	A2M	O3'-C3'	2.74	1.49	1.43
30	WA	1664	I4U	O2-C2	-2.74	1.18	1.23
30	WA	4625	OMU	C6-N1	2.74	1.44	1.38
30	WA	4201	OMG	C5-N7	-2.73	1.33	1.39
30	WA	1539	A2M	O3'-C3'	2.73	1.49	1.43
30	WA	4628	OMG	C5-N7	-2.73	1.33	1.39
30	WA	2429	OMG	C5-N7	-2.72	1.33	1.39
30	WA	4225	6MZ	C5-N7	-2.72	1.34	1.39
30	WA	4375	OMG	C5-N7	-2.72	1.33	1.39
30	WA	4541	OMC	O2-C2	-2.72	1.18	1.23
30	WA	373	OMG	C5-N7	-2.72	1.33	1.39
30	WA	3728	A2M	O3'-C3'	2.72	1.49	1.43
30	WA	4676	B8T	O2-C2	-2.71	1.18	1.23
30	WA	3872	A2M	O3'-C3'	2.71	1.49	1.43
30	WA	1527	OMG	C5-N7	-2.71	1.33	1.39
30	WA	3874	OMC	O2-C2	-2.71	1.18	1.23
30	WA	4528	A2M	O3'-C3'	2.71	1.49	1.43
30	WA	4199	I4U	O2-C2	-2.71	1.18	1.23
30	WA	3830	A2M	O3'-C3'	2.71	1.49	1.43
30	WA	4602	UR3	C6-N1	2.71	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	1579	B9B	C5-N7	-2.71	1.34	1.39
30	WA	4528	A2M	O4'-C4'	2.71	1.51	1.45
30	WA	1332	A2M	O4'-C4'	2.71	1.51	1.45
30	WA	2385	B8W	C5-N7	-2.70	1.34	1.39
30	WA	4695	B8K	C71-N7	2.70	1.45	1.39
30	WA	1876	A2M	O3'-C3'	2.70	1.49	1.43
30	WA	3902	B8K	O6-C6	-2.70	1.18	1.23
30	WA	2809	OMC	O2-C2	-2.70	1.18	1.23
30	WA	2368	A2M	O3'-C3'	2.70	1.49	1.43
30	WA	1354	P4U	O2-C2	-2.70	1.18	1.23
30	WA	4488	B8T	O2-C2	-2.70	1.18	1.23
30	WA	2759	B9B	C5-N7	-2.70	1.34	1.39
30	WA	2427	OMC	O2-C2	-2.70	1.18	1.23
30	WA	1539	A2M	O4'-C4'	2.69	1.51	1.45
30	WA	4134	B8W	C4-N3	2.69	1.37	1.34
30	WA	2370	OMC	O2-C2	-2.69	1.18	1.23
32	YA	14	OMU	C6-N1	2.69	1.44	1.38
30	WA	3904	BGH	O3'-C3'	2.69	1.49	1.43
30	WA	3872	A2M	O4'-C4'	2.69	1.51	1.45
30	WA	4534	B8W	C4-N3	2.68	1.37	1.34
30	WA	1610	7MG	O6-C6	-2.67	1.18	1.23
30	WA	1888	OMG	O6-C6	-2.67	1.18	1.23
30	WA	4875	OMG	C5-N7	-2.67	1.33	1.39
30	WA	4534	B8W	C5-N7	-2.67	1.34	1.39
30	WA	1332	A2M	O3'-C3'	2.67	1.49	1.43
30	WA	4134	B8W	C5-N7	-2.67	1.34	1.39
30	WA	3892	OMC	O2-C2	-2.66	1.18	1.23
30	WA	2385	B8W	C4-N3	2.66	1.37	1.34
30	WA	4555	7MG	O6-C6	-2.66	1.18	1.23
30	WA	2866	OMC	O2-C2	-2.66	1.18	1.23
53	ZA	1219	JMH	C6-N1	2.65	1.44	1.38
30	WA	4477	B8W	C5-N7	-2.65	1.34	1.39
30	WA	2527	7MG	O6-C6	-2.65	1.18	1.23
51	v	715	DDE	OAG-CBI	-2.64	1.19	1.23
30	WA	4477	B8W	C4-N3	2.64	1.37	1.34
30	WA	4576	A2M	O4'-C4'	2.64	1.50	1.45
30	WA	4360	E6G	C5-N7	-2.64	1.34	1.39
30	WA	3904	BGH	O6-C6	-2.64	1.18	1.23
53	ZA	1248	B8N	C4-C5	-2.64	1.41	1.47
30	WA	1328	1MA	C5-N7	-2.63	1.33	1.39
30	WA	2406	A2M	O4'-C4'	2.63	1.50	1.45
30	WA	4190	B8W	C5-N7	-2.63	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	237	B9B	C5-N7	-2.63	1.34	1.39
30	WA	1529	A2M	O3'-C3'	2.63	1.49	1.43
30	WA	4190	B8W	C4-N3	2.63	1.37	1.34
30	WA	2368	A2M	O4'-C4'	2.63	1.50	1.45
30	WA	4088	5MU	O4-C4	-2.63	1.18	1.23
53	ZA	1374	5MC	O2-C2	-2.62	1.18	1.23
30	WA	3706	OMC	O2-C2	-2.62	1.18	1.23
30	WA	4340	5MC	O2-C2	-2.61	1.18	1.23
30	WA	4420	1MA	C5-N7	-2.59	1.33	1.39
30	WA	1865	B8H	O4-C4	-2.59	1.18	1.23
30	WA	1802	E7G	O6-C6	-2.58	1.18	1.23
30	WA	1461	JMH	C6-N1	2.57	1.44	1.38
30	WA	4499	OMG	O6-C6	-2.56	1.18	1.23
30	WA	3787	5MC	O2-C2	-2.56	1.18	1.23
30	WA	2302	E7G	O6-C6	-2.54	1.18	1.23
30	WA	4642	OMG	O6-C6	-2.54	1.18	1.23
30	WA	3797	OMG	O6-C6	-2.54	1.18	1.23
30	WA	373	OMG	O6-C6	-2.53	1.18	1.23
30	WA	1630	OMG	O6-C6	-2.53	1.18	1.23
30	WA	4301	B8H	O4-C4	-2.53	1.18	1.23
30	WA	1322	OMG	O6-C6	-2.53	1.18	1.23
30	WA	4628	OMG	O6-C6	-2.52	1.18	1.23
30	WA	1522	2MG	O6-C6	-2.52	1.18	1.23
30	WA	4375	OMG	O6-C6	-2.51	1.18	1.23
30	WA	1527	OMG	O6-C6	-2.51	1.18	1.23
30	WA	2055	OMG	O6-C6	-2.51	1.18	1.23
30	WA	4088	5MU	O2-C2	-2.51	1.18	1.23
30	WA	373	OMG	C6-N1	2.51	1.43	1.38
30	WA	3767	B8H	O4-C4	-2.50	1.18	1.23
30	WA	4875	OMG	O6-C6	-2.50	1.18	1.23
30	WA	3902	B8K	C71-N7	2.49	1.45	1.39
30	WA	2429	OMG	O6-C6	-2.49	1.18	1.23
30	WA	2778	OMG	O6-C6	-2.48	1.18	1.23
30	WA	3892	OMC	C5-C4	2.48	1.48	1.42
30	WA	2369	OMG	O6-C6	-2.48	1.18	1.23
30	WA	4201	OMG	O6-C6	-2.48	1.18	1.23
30	WA	4877	2MG	C5-C6	2.47	1.53	1.44
30	WA	4628	OMG	C6-N1	2.47	1.43	1.38
30	WA	4201	OMG	C5-C6	2.47	1.53	1.44
30	WA	4877	2MG	O6-C6	-2.47	1.18	1.23
30	WA	3706	OMC	C5-C4	2.47	1.48	1.42
30	WA	730	2MG	O6-C6	-2.47	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	4298	PSU	C1'-C5	2.46	1.55	1.50
30	WA	4875	OMG	C5-C6	2.46	1.53	1.44
30	WA	2778	OMG	C5-C6	2.46	1.53	1.44
30	WA	2778	OMG	C6-N1	2.46	1.43	1.38
30	WA	1522	2MG	C5-C6	2.46	1.53	1.44
30	WA	4875	OMG	C6-N1	2.45	1.43	1.38
30	WA	4628	OMG	C5-C6	2.45	1.53	1.44
30	WA	1527	OMG	C5-C6	2.45	1.53	1.44
30	WA	3874	OMC	C5-C4	2.45	1.48	1.42
30	WA	3914	OMC	C5-C4	2.45	1.48	1.42
30	WA	2429	OMG	C5-C6	2.44	1.53	1.44
30	WA	4375	OMG	C5-C6	2.44	1.53	1.44
30	WA	2370	OMC	C5-C4	2.44	1.48	1.42
30	WA	4541	OMC	C5-C4	2.44	1.48	1.42
30	WA	2791	B9H	C6-N1	2.44	1.43	1.38
30	WA	730	2MG	C5-C6	2.44	1.53	1.44
30	WA	3797	OMG	C5-C6	2.44	1.53	1.44
30	WA	4311	OMU	O2-C2	-2.43	1.18	1.23
30	WA	4201	OMG	C6-N1	2.43	1.43	1.38
30	WA	1527	OMG	C6-N1	2.43	1.43	1.38
30	WA	2055	OMG	C5-C6	2.43	1.53	1.44
30	WA	2427	OMC	C5-C4	2.42	1.48	1.42
30	WA	3790	A2M	C5-C4	-2.42	1.34	1.39
30	WA	2369	OMG	C5-C6	2.42	1.53	1.44
30	WA	1630	OMG	C5-C6	2.42	1.53	1.44
30	WA	2809	OMC	C5-C4	2.41	1.48	1.42
30	WA	2369	OMG	C6-N1	2.41	1.43	1.38
30	WA	4642	OMG	C5-C6	2.41	1.53	1.44
30	WA	2429	OMG	C6-N1	2.41	1.43	1.38
30	WA	1322	OMG	C5-C6	2.41	1.53	1.44
30	WA	4642	OMG	C6-N1	2.41	1.43	1.38
30	WA	4625	OMU	O2-C2	-2.41	1.18	1.23
30	WA	373	OMG	C5-C6	2.41	1.53	1.44
30	WA	4499	OMG	C5-C6	2.40	1.53	1.44
30	WA	1630	OMG	C6-N1	2.39	1.43	1.38
30	WA	3797	OMG	C6-N1	2.39	1.43	1.38
30	WA	4641	PSU	C1'-C5	2.39	1.55	1.50
30	WA	2055	OMG	C6-N1	2.39	1.43	1.38
30	WA	3767	B8H	O2-C2	-2.39	1.18	1.23
30	WA	4375	OMG	C6-N1	2.39	1.43	1.38
32	YA	14	OMU	O2-C2	-2.39	1.18	1.23
30	WA	4447	PSU	C1'-C5	2.38	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	2866	OMC	C5-C4	2.38	1.48	1.42
30	WA	1322	OMG	C6-N1	2.37	1.43	1.38
30	WA	1865	B8H	O2-C2	-2.37	1.18	1.23
30	WA	1888	OMG	C6-N1	2.37	1.43	1.38
30	WA	4301	B8H	O2-C2	-2.37	1.18	1.23
30	WA	1664	I4U	C5-C4	2.37	1.49	1.43
53	ZA	1678	A2M	O4'-C4'	2.37	1.50	1.45
30	WA	1888	OMG	C5-C6	2.36	1.53	1.44
30	WA	1529	A2M	O4'-C4'	2.36	1.50	1.45
30	WA	4602	UR3	O2-C2	-2.36	1.18	1.22
30	WA	4535	UR3	O2-C2	-2.36	1.18	1.22
30	WA	1871	UR3	O2-C2	-2.36	1.18	1.22
30	WA	4499	OMG	C6-N1	2.36	1.43	1.38
30	WA	1522	2MG	C6-N1	2.35	1.43	1.38
30	WA	1587	PSU	C1'-C5	2.34	1.55	1.50
30	WA	4877	2MG	C6-N1	2.33	1.43	1.38
30	WA	3720	PSU	C1'-C5	2.32	1.55	1.50
30	WA	4376	MHG	O6-C6	-2.32	1.19	1.23
30	WA	4311	OMU	C5-C4	2.30	1.48	1.43
30	WA	3769	PSU	C1'-C5	2.30	1.55	1.50
30	WA	4625	OMU	C5-C4	2.29	1.48	1.43
30	WA	3734	PSU	C1'-C5	2.29	1.55	1.50
30	WA	373	OMG	C4-N9	-2.29	1.32	1.38
30	WA	4199	I4U	C5-C4	2.28	1.49	1.43
30	WA	4408	PSU	C1'-C5	2.27	1.55	1.50
30	WA	4528	A2M	C5-C4	-2.27	1.35	1.39
30	WA	4360	E6G	C8-N9	-2.26	1.33	1.37
30	WA	1876	A2M	C5-C4	-2.25	1.35	1.39
30	WA	1332	A2M	C5-C4	-2.25	1.35	1.39
30	WA	1579	B9B	C8-N9	-2.25	1.33	1.37
30	WA	4376	MHG	C5-C4	2.24	1.44	1.37
30	WA	3904	BGH	C5-C4	2.24	1.44	1.37
30	WA	2406	A2M	C5-C4	-2.23	1.35	1.39
30	WA	2368	A2M	C5-C4	-2.23	1.35	1.39
53	ZA	1243	PSU	C1'-C5	2.23	1.55	1.50
53	ZA	1678	A2M	C5-C4	-2.21	1.35	1.39
51	v	715	DDE	CD2-NE2	-2.21	1.31	1.36
30	WA	4536	PSU	C1'-C5	2.21	1.55	1.50
30	WA	1354	P4U	C5-C4	2.21	1.49	1.43
30	WA	4225	6MZ	C8-N9	-2.21	1.33	1.37
30	WA	2759	B9B	C8-N9	-2.19	1.33	1.37
30	WA	237	B9B	C8-N9	-2.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	WA	3830	A2M	C5-C4	-2.19	1.35	1.39
30	WA	4628	OMG	C4-N9	-2.19	1.32	1.38
30	WA	1527	OMG	C4-N9	-2.18	1.32	1.38
30	WA	2513	PSU	C1'-C5	2.18	1.55	1.50
30	WA	3872	A2M	C5-C4	-2.18	1.35	1.39
30	WA	1539	A2M	C5-C4	-2.17	1.35	1.39
30	WA	398	A2M	C5-C4	-2.17	1.35	1.39
30	WA	4576	A2M	C5-C4	-2.17	1.35	1.39
30	WA	730	2MG	C6-N1	2.17	1.42	1.38
30	WA	4535	UR3	C4-N3	2.16	1.45	1.40
30	WA	1529	A2M	C5-C4	-2.15	1.35	1.39
30	WA	1688	PSU	C1'-C5	2.14	1.55	1.50
30	WA	1579	B9B	C5-C6	-2.14	1.37	1.41
30	WA	3902	B8K	C5-C4	2.14	1.44	1.37
32	YA	14	OMU	C5-C4	2.14	1.48	1.43
30	WA	1871	UR3	C4-N3	2.14	1.44	1.40
30	WA	2055	OMG	C4-N9	-2.14	1.32	1.38
30	WA	4602	UR3	C4-N3	2.14	1.44	1.40
30	WA	1888	OMG	C4-N9	-2.14	1.32	1.38
30	WA	4633	PSU	C1'-C5	2.13	1.55	1.50
30	WA	1682	PSU	C1'-C5	2.13	1.55	1.50
30	WA	4505	PSU	C1'-C5	2.13	1.55	1.50
30	WA	3728	A2M	C5-C4	-2.13	1.35	1.39
30	WA	3723	A2M	C5-C4	-2.13	1.35	1.39
30	WA	1322	OMG	C4-N9	-2.12	1.32	1.38
30	WA	3797	OMG	C4-N9	-2.12	1.32	1.38
30	WA	4875	OMG	C4-N9	-2.12	1.32	1.38
30	WA	2429	OMG	C4-N9	-2.10	1.32	1.38
30	WA	1522	2MG	C4-N9	-2.10	1.32	1.38
30	WA	2369	OMG	C4-N9	-2.10	1.32	1.38
30	WA	4201	OMG	C4-N9	-2.09	1.32	1.38
30	WA	4375	OMG	C4-N9	-2.08	1.32	1.38
30	WA	4602	UR3	C3U-N3	-2.07	1.43	1.47
30	WA	4695	B8K	C5-C4	2.07	1.44	1.37
30	WA	4642	OMG	C4-N9	-2.07	1.32	1.38
30	WA	1610	7MG	C5-C4	2.06	1.44	1.37
30	WA	4499	OMG	C4-N9	-2.06	1.32	1.38
30	WA	1802	E7G	C5-C4	2.06	1.44	1.37
30	WA	2302	E7G	C5-C4	2.06	1.44	1.37
30	WA	1630	OMG	C4-N9	-2.06	1.32	1.38
30	WA	2527	7MG	C5-C4	2.04	1.44	1.37
30	WA	1587	PSU	O4-C4	-2.04	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	ZA	1248	B8N	O4-C4	-2.04	1.18	1.23
30	WA	2778	OMG	C4-N9	-2.02	1.32	1.38
30	WA	2791	B9H	O2-C2	-2.02	1.18	1.22
30	WA	4408	PSU	O4'-C1'	-2.01	1.41	1.43
30	WA	4455	PSU	C1'-C5	2.01	1.54	1.50
30	WA	4420	1MA	C6-N6	-2.01	1.23	1.28
30	WA	1682	PSU	O4-C4	-2.01	1.19	1.23
30	WA	4298	PSU	O4-C4	-2.00	1.19	1.23
30	WA	4555	7MG	C5-C4	2.00	1.43	1.37

All (795) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	4569	M7A	C5-C6-N6	14.83	148.94	123.75
30	WA	4569	M7A	N6-C6-N1	-12.28	91.02	118.38
30	WA	4088	5MU	C5-C4-N3	10.30	124.28	115.32
30	WA	4088	5MU	C5-C6-N1	-9.05	113.48	123.31
30	WA	4641	PSU	N1-C2-N3	8.71	124.36	115.17
30	WA	4134	B8W	N2-C2-N3	8.64	130.17	117.22
30	WA	4534	B8W	N2-C2-N3	8.54	130.03	117.22
30	WA	2385	B8W	N2-C2-N3	8.53	130.01	117.22
30	WA	4190	B8W	N2-C2-N3	8.52	130.00	117.22
30	WA	4477	B8W	N2-C2-N3	8.43	129.87	117.22
30	WA	4534	B8W	O6-C6-N1	8.40	130.13	118.96
30	WA	2385	B8W	O6-C6-N1	8.26	129.94	118.96
30	WA	4134	B8W	O6-C6-N1	8.26	129.94	118.96
30	WA	4477	B8W	O6-C6-N1	8.23	129.91	118.96
30	WA	4190	B8W	O6-C6-N1	8.20	129.87	118.96
30	WA	4633	PSU	N1-C2-N3	8.02	123.63	115.17
30	WA	4455	PSU	N1-C2-N3	8.01	123.62	115.17
30	WA	1688	PSU	N1-C2-N3	7.99	123.59	115.17
30	WA	2513	PSU	N1-C2-N3	7.85	123.45	115.17
30	WA	4505	PSU	N1-C2-N3	7.85	123.45	115.17
30	WA	4376	MHG	C2-N3-C4	7.85	121.81	112.00
53	ZA	1243	PSU	N1-C2-N3	7.84	123.44	115.17
30	WA	1682	PSU	N1-C2-N3	7.84	123.44	115.17
30	WA	3769	PSU	N1-C2-N3	7.81	123.41	115.17
30	WA	3720	PSU	N1-C2-N3	7.77	123.36	115.17
30	WA	4536	PSU	N1-C2-N3	7.75	123.35	115.17
30	WA	4408	PSU	N1-C2-N3	7.75	123.35	115.17
30	WA	4641	PSU	C6-N1-C2	-7.73	115.52	122.69
30	WA	3734	PSU	N1-C2-N3	7.68	123.27	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1664	I4U	O4-C4-C5	7.67	120.89	115.45
30	WA	4447	PSU	N1-C2-N3	7.57	123.16	115.17
30	WA	1587	PSU	N1-C2-N3	7.56	123.14	115.17
30	WA	4298	PSU	N1-C2-N3	7.45	123.02	115.17
30	WA	2759	B9B	C5-C4-N3	-7.27	119.52	127.18
30	WA	1579	B9B	C5-C4-N3	-7.11	119.69	127.18
30	WA	4134	B8W	C5-C4-N3	-7.11	119.69	127.18
30	WA	2385	B8W	C5-C4-N3	-7.06	119.74	127.18
30	WA	4534	B8W	C5-C4-N3	-7.03	119.78	127.18
30	WA	4360	E6G	C5-C4-N3	-6.99	119.81	127.18
30	WA	237	B9B	C5-C4-N3	-6.92	119.89	127.18
30	WA	4190	B8W	C5-C4-N3	-6.86	119.95	127.18
30	WA	4477	B8W	C5-C4-N3	-6.83	119.98	127.18
30	WA	4088	5MU	C4-N3-C2	-6.75	118.49	127.34
30	WA	1865	B8H	C4-N3-C2	-6.70	118.56	127.34
30	WA	4301	B8H	C4-N3-C2	-6.67	118.60	127.34
30	WA	4455	PSU	C4-N3-C2	-6.60	117.28	126.37
30	WA	1682	PSU	C4-N3-C2	-6.56	117.33	126.37
30	WA	730	2MG	C2-N3-C4	6.55	120.19	112.00
30	WA	1688	PSU	C4-N3-C2	-6.54	117.36	126.37
30	WA	4376	MHG	C4-C5-N7	6.52	110.23	104.94
30	WA	2513	PSU	C4-N3-C2	-6.50	117.42	126.37
30	WA	3767	B8H	C4-N3-C2	-6.50	118.82	127.34
30	WA	4633	PSU	C4-N3-C2	-6.48	117.45	126.37
30	WA	1802	E7G	C4-C5-N7	6.46	110.18	104.94
30	WA	4505	PSU	C4-N3-C2	-6.46	117.48	126.37
53	ZA	1243	PSU	C4-N3-C2	-6.45	117.48	126.37
30	WA	2302	E7G	C4-C5-N7	6.44	110.16	104.94
30	WA	4536	PSU	C4-N3-C2	-6.41	117.55	126.37
30	WA	4408	PSU	C4-N3-C2	-6.41	117.55	126.37
30	WA	3734	PSU	C4-N3-C2	-6.37	117.60	126.37
30	WA	3720	PSU	C4-N3-C2	-6.36	117.61	126.37
30	WA	4199	I4U	O4-C4-C5	6.36	119.96	115.45
30	WA	1522	2MG	C2-N3-C4	6.35	119.95	112.00
30	WA	4877	2MG	C2-N3-C4	6.35	119.94	112.00
30	WA	4301	B8H	N3-C2-N1	6.30	121.31	115.22
30	WA	1587	PSU	C4-N3-C2	-6.28	117.72	126.37
30	WA	3769	PSU	C4-N3-C2	-6.27	117.73	126.37
30	WA	3767	B8H	N3-C2-N1	6.27	121.28	115.22
30	WA	4447	PSU	C4-N3-C2	-6.25	117.76	126.37
30	WA	1865	B8H	N3-C2-N1	6.24	121.25	115.22
30	WA	4298	PSU	C4-N3-C2	-6.15	117.90	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1354	P4U	O4-C4-C5	6.06	119.75	115.45
30	WA	4534	B8W	O6-C6-C5	-6.05	109.87	117.17
53	ZA	1248	B8N	C4-N3-C2	-5.97	118.27	125.62
30	WA	4134	B8W	O6-C6-C5	-5.90	110.06	117.17
30	WA	4641	PSU	C4-N3-C2	-5.88	118.27	126.37
30	WA	3769	PSU	C6-N1-C2	-5.85	117.26	122.69
30	WA	2385	B8W	O6-C6-C5	-5.82	110.15	117.17
30	WA	4633	PSU	C6-N1-C2	-5.80	117.31	122.69
30	WA	4528	A2M	N3-C2-N1	-5.73	119.90	128.58
53	ZA	1678	A2M	N3-C2-N1	-5.73	119.91	128.58
30	WA	3728	A2M	N3-C2-N1	-5.72	119.93	128.58
30	WA	2302	E7G	C2-N3-C4	5.69	122.10	112.30
30	WA	2406	A2M	N3-C2-N1	-5.68	119.98	128.58
30	WA	4298	PSU	C6-N1-C2	-5.66	117.44	122.69
30	WA	4311	OMU	C4-N3-C2	-5.65	119.60	126.61
30	WA	1688	PSU	C6-N1-C2	-5.65	117.45	122.69
30	WA	4555	7MG	C2-N3-C4	5.64	122.02	112.30
30	WA	1610	7MG	C2-N3-C4	5.64	122.02	112.30
30	WA	3790	A2M	N3-C2-N1	-5.64	120.05	128.58
30	WA	2527	7MG	C2-N3-C4	5.64	122.01	112.30
30	WA	3720	PSU	C6-N1-C2	-5.64	117.46	122.69
30	WA	4576	A2M	N3-C2-N1	-5.63	120.05	128.58
30	WA	1876	A2M	N3-C2-N1	-5.63	120.06	128.58
30	WA	4225	6MZ	N1-C2-N3	-5.63	120.06	128.58
30	WA	4569	M7A	N3-C4-N9	5.62	133.91	126.88
30	WA	4455	PSU	C6-N1-C2	-5.61	117.48	122.69
30	WA	4535	UR3	C4-N3-C2	-5.61	120.06	124.58
30	WA	1802	E7G	C2-N3-C4	5.61	121.96	112.30
30	WA	398	A2M	N3-C2-N1	-5.60	120.10	128.58
30	WA	4695	B8K	C5-C6-N1	5.60	120.80	110.94
30	WA	4505	PSU	C6-N1-C2	-5.60	117.50	122.69
30	WA	4190	B8W	O6-C6-C5	-5.58	110.44	117.17
30	WA	1529	A2M	N3-C2-N1	-5.57	120.15	128.58
30	WA	3790	A2M	N9-C8-N7	-5.57	106.04	113.94
30	WA	1332	A2M	N3-C2-N1	-5.56	120.17	128.58
30	WA	3830	A2M	N3-C2-N1	-5.55	120.18	128.58
53	ZA	1243	PSU	C6-N1-C2	-5.55	117.54	122.69
30	WA	4477	B8W	O6-C6-C5	-5.55	110.48	117.17
30	WA	4536	PSU	C6-N1-C2	-5.53	117.56	122.69
30	WA	2368	A2M	N3-C2-N1	-5.52	120.22	128.58
30	WA	730	2MG	C5-C4-N3	-5.52	119.60	128.39
30	WA	3734	PSU	C6-N1-C2	-5.52	117.57	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	2513	PSU	C6-N1-C2	-5.49	117.59	122.69
30	WA	1682	PSU	C6-N1-C2	-5.48	117.61	122.69
30	WA	4408	PSU	C6-N1-C2	-5.47	117.61	122.69
30	WA	4625	OMU	C4-N3-C2	-5.47	119.82	126.61
30	WA	4569	M7A	N3-C2-N1	-5.45	120.33	128.58
53	ZA	1678	A2M	N9-C8-N7	-5.44	106.22	113.94
30	WA	1539	A2M	N3-C2-N1	-5.44	120.35	128.58
30	WA	1587	PSU	C6-N1-C2	-5.42	117.66	122.69
30	WA	3872	A2M	N3-C2-N1	-5.42	120.37	128.58
30	WA	3723	A2M	N3-C2-N1	-5.40	120.41	128.58
30	WA	4420	1MA	N1-C2-N3	-5.39	119.59	126.00
32	YA	14	OMU	C4-N3-C2	-5.38	119.93	126.61
30	WA	4528	A2M	N9-C8-N7	-5.38	106.30	113.94
30	WA	4447	PSU	C6-N1-C2	-5.38	117.70	122.69
30	WA	3902	B8K	C5-C6-N1	5.36	120.38	110.94
30	WA	2406	A2M	N9-C8-N7	-5.36	106.33	113.94
30	WA	3904	BGH	C5-C6-N1	5.36	120.37	110.94
30	WA	2368	A2M	N9-C8-N7	-5.34	106.36	113.94
30	WA	1876	A2M	N9-C8-N7	-5.31	106.40	113.94
30	WA	4576	A2M	N9-C8-N7	-5.31	106.41	113.94
30	WA	1332	A2M	N9-C8-N7	-5.30	106.42	113.94
30	WA	1328	1MA	N1-C2-N3	-5.29	119.71	126.00
30	WA	3830	A2M	N9-C8-N7	-5.27	106.46	113.94
30	WA	398	A2M	N9-C8-N7	-5.26	106.47	113.94
30	WA	4088	5MU	N3-C2-N1	5.24	121.72	114.89
30	WA	4134	B8W	N2-C2-N1	-5.23	109.38	117.22
30	WA	3872	A2M	N9-C8-N7	-5.22	106.54	113.94
30	WA	1529	A2M	N9-C8-N7	-5.21	106.54	113.94
30	WA	4877	2MG	C5-C4-N3	-5.21	120.10	128.39
30	WA	4695	B8K	C4-C5-N7	5.16	109.10	104.93
30	WA	1871	UR3	C4-N3-C2	-5.15	120.43	124.58
30	WA	4602	UR3	C4-N3-C2	-5.13	120.45	124.58
30	WA	1539	A2M	N9-C8-N7	-5.12	106.68	113.94
53	ZA	1248	B8N	C5-C4-N3	5.11	125.44	116.15
30	WA	4534	B8W	N2-C2-N1	-5.10	109.58	117.22
30	WA	4376	MHG	C2-N1-C6	-5.09	118.40	124.55
30	WA	2385	B8W	N2-C2-N1	-5.07	109.62	117.22
30	WA	4420	1MA	C2-N3-C4	5.06	122.46	112.53
30	WA	3723	A2M	N9-C8-N7	-5.06	106.75	113.94
30	WA	1914	P7G	C4-C5-N7	5.06	110.12	106.71
30	WA	4190	B8W	N2-C2-N1	-5.06	109.64	117.22
30	WA	3728	A2M	N9-C8-N7	-5.01	106.82	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	4455	PSU	C6-C5-C4	5.01	121.56	118.17
30	WA	1522	2MG	C5-C4-N3	-5.01	120.42	128.39
30	WA	3728	A2M	C5-C4-N3	-4.99	119.84	126.72
30	WA	4642	OMG	C5-C4-N3	-4.98	120.46	128.39
30	WA	4360	E6G	C4-C5-C6	4.95	120.08	115.22
30	WA	3797	OMG	C5-C4-N3	-4.94	120.52	128.39
30	WA	1630	OMG	C5-C4-N3	-4.94	120.52	128.39
30	WA	2778	OMG	C5-C4-N3	-4.94	120.53	128.39
30	WA	4499	OMG	C5-C4-N3	-4.94	120.53	128.39
30	WA	4477	B8W	N2-C2-N1	-4.93	109.83	117.22
30	WA	3904	BGH	C4-C5-N7	4.92	108.91	104.93
30	WA	3902	B8K	C4-C5-N7	4.90	108.89	104.93
30	WA	1888	OMG	C5-C4-N3	-4.89	120.61	128.39
30	WA	2369	OMG	C5-C4-N3	-4.86	120.65	128.39
30	WA	4134	B8W	C4-C5-C6	4.86	120.00	115.22
30	WA	1328	1MA	C2-N3-C4	4.86	122.05	112.53
30	WA	4375	OMG	C5-C4-N3	-4.86	120.66	128.39
30	WA	1579	B9B	C4-C5-C6	4.85	119.98	115.22
30	WA	4201	OMG	C5-C4-N3	-4.85	120.67	128.39
30	WA	2385	B8W	C4-C5-C6	4.85	119.98	115.22
30	WA	1322	OMG	C5-C4-N3	-4.84	120.68	128.39
30	WA	3885	P7G	C4-C5-N7	4.84	109.97	106.71
30	WA	4225	6MZ	C5-C4-N3	-4.83	120.06	126.72
30	WA	2759	B9B	C4-C5-C6	4.83	119.97	115.22
30	WA	2055	OMG	C5-C4-N3	-4.80	120.75	128.39
30	WA	1539	A2M	C5-C4-N3	-4.80	120.11	126.72
30	WA	4695	B8K	C2-N3-C4	4.79	120.56	112.30
30	WA	4477	B8W	C4-C5-C6	4.79	119.93	115.22
30	WA	2429	OMG	C5-C4-N3	-4.78	120.78	128.39
30	WA	4190	B8W	C4-C5-C6	4.78	119.91	115.22
30	WA	4505	PSU	C6-C5-C4	4.77	121.39	118.17
30	WA	4534	B8W	C4-C5-C6	4.76	119.90	115.22
30	WA	1527	OMG	C5-C4-N3	-4.76	120.81	128.39
30	WA	1529	A2M	C5-C4-N3	-4.75	120.18	126.72
30	WA	4875	OMG	C5-C4-N3	-4.74	120.84	128.39
30	WA	4628	OMG	C5-C4-N3	-4.74	120.85	128.39
30	WA	1682	PSU	C6-C5-C4	4.73	121.37	118.17
30	WA	3790	A2M	C4-N9-C8	4.73	110.70	105.74
30	WA	730	2MG	C1'-N9-C8	-4.71	113.35	126.73
30	WA	3872	A2M	C5-C4-N3	-4.70	120.24	126.72
30	WA	3723	A2M	C5-C4-N3	-4.67	120.29	126.72
30	WA	2406	A2M	C5-C4-N3	-4.66	120.30	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	237	B9B	C4-C5-C6	4.66	119.80	115.22
30	WA	2513	PSU	C6-C5-C4	4.63	121.30	118.17
30	WA	2368	A2M	C5-C4-N3	-4.62	120.35	126.72
30	WA	3902	B8K	C2-N3-C4	4.62	120.26	112.30
30	WA	1688	PSU	C6-C5-C4	4.62	121.29	118.17
30	WA	4633	PSU	C6-C5-C4	4.60	121.28	118.17
30	WA	3769	PSU	O2-C2-N1	-4.60	118.05	122.79
30	WA	398	A2M	C5-C4-N3	-4.60	120.38	126.72
53	ZA	1678	A2M	C5-C4-N3	-4.59	120.40	126.72
30	WA	4088	5MU	C5M-C5-C6	-4.58	116.66	122.85
30	WA	1332	A2M	C5-C4-N3	-4.57	120.43	126.72
30	WA	3830	A2M	C5-C4-N3	-4.56	120.44	126.72
53	ZA	1678	A2M	C4-N9-C8	4.56	110.52	105.74
30	WA	2778	OMG	C1'-N9-C8	-4.55	113.80	126.73
30	WA	4576	A2M	C5-C4-N3	-4.55	120.45	126.72
30	WA	373	OMG	C5-C4-N3	-4.55	121.15	128.39
30	WA	4536	PSU	C6-C5-C4	4.54	121.24	118.17
30	WA	3797	OMG	C1'-N9-C8	-4.51	113.92	126.73
30	WA	4505	PSU	O2-C2-N1	-4.51	118.14	122.79
30	WA	4536	PSU	O2-C2-N1	-4.50	118.15	122.79
30	WA	2369	OMG	C1'-N9-C8	-4.49	113.97	126.73
30	WA	3904	BGH	C2-N3-C4	4.49	120.03	112.30
30	WA	1688	PSU	O2-C2-N1	-4.49	118.16	122.79
30	WA	2302	E7G	C5-C6-N1	4.48	118.83	110.94
30	WA	1630	OMG	C1'-N9-C8	-4.48	114.01	126.73
30	WA	4633	PSU	O2-C2-N1	-4.48	118.17	122.79
30	WA	1802	E7G	C5-C6-N1	4.47	118.80	110.94
30	WA	4528	A2M	C5-C4-N3	-4.47	120.57	126.72
30	WA	1876	A2M	C5-C4-N3	-4.46	120.57	126.72
30	WA	3720	PSU	O2-C2-N1	-4.43	118.22	122.79
30	WA	4420	1MA	C5-C4-N3	-4.43	120.75	127.27
30	WA	4376	MHG	C5-C6-N1	4.41	118.70	110.94
30	WA	1579	B9B	N3-C4-N9	4.41	132.59	126.99
30	WA	4455	PSU	O2-C2-N1	-4.41	118.24	122.79
30	WA	1527	OMG	C2-N3-C4	4.40	119.87	112.30
53	ZA	1243	PSU	O2-C2-N1	-4.39	118.26	122.79
30	WA	4695	B8K	C72-C71-N7	4.39	125.27	118.80
30	WA	4447	PSU	O2-C2-N1	-4.39	118.27	122.79
30	WA	2778	OMG	C2-N3-C4	4.38	119.85	112.30
30	WA	4642	OMG	C2-N3-C4	4.38	119.84	112.30
30	WA	4499	OMG	C2-N3-C4	4.37	119.83	112.30
30	WA	4201	OMG	C2-N3-C4	4.37	119.83	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	2527	7MG	C5-C6-N1	4.37	118.63	110.94
30	WA	3797	OMG	C2-N3-C4	4.36	119.81	112.30
30	WA	1630	OMG	C2-N3-C4	4.36	119.81	112.30
30	WA	2513	PSU	O2-C2-N1	-4.36	118.30	122.79
30	WA	3790	A2M	C5-C4-N3	-4.36	120.72	126.72
30	WA	1610	7MG	C5-C6-N1	4.36	118.61	110.94
30	WA	1682	PSU	O2-C2-N1	-4.35	118.30	122.79
30	WA	1876	A2M	C4-N9-C8	4.35	110.31	105.74
30	WA	1888	OMG	C2-N3-C4	4.35	119.79	112.30
53	ZA	1243	PSU	C6-C5-C4	4.35	121.11	118.17
30	WA	4528	A2M	C4-N9-C8	4.35	110.30	105.74
30	WA	4499	OMG	C1'-N9-C8	-4.35	114.38	126.73
30	WA	4576	A2M	C4-N9-C8	4.35	110.30	105.74
30	WA	2406	A2M	C4-N9-C8	4.34	110.29	105.74
30	WA	4875	OMG	C2-N3-C4	4.34	119.77	112.30
30	WA	4555	7MG	C5-C6-N1	4.34	118.57	110.94
30	WA	2368	A2M	C4-N9-C8	4.34	110.29	105.74
30	WA	2369	OMG	C2-N3-C4	4.33	119.75	112.30
30	WA	2429	OMG	C2-N3-C4	4.33	119.75	112.30
30	WA	1332	A2M	C4-N9-C8	4.33	110.28	105.74
30	WA	4628	OMG	C2-N3-C4	4.32	119.75	112.30
30	WA	4408	PSU	C6-C5-C4	4.32	121.09	118.17
30	WA	4408	PSU	O2-C2-N1	-4.32	118.34	122.79
30	WA	4375	OMG	C2-N3-C4	4.31	119.73	112.30
30	WA	3734	PSU	O2-C2-N1	-4.31	118.34	122.79
30	WA	4642	OMG	C1'-N9-C8	-4.31	114.49	126.73
30	WA	1322	OMG	C2-N3-C4	4.30	119.70	112.30
30	WA	2055	OMG	C2-N3-C4	4.29	119.69	112.30
30	WA	1888	OMG	C1'-N9-C8	-4.29	114.54	126.73
30	WA	1529	A2M	C4-N9-C8	4.29	110.24	105.74
30	WA	1322	OMG	C1'-N9-C8	-4.27	114.59	126.73
30	WA	4190	B8W	N9-C8-N7	-4.26	107.89	113.94
30	WA	3830	A2M	C4-N9-C8	4.26	110.21	105.74
30	WA	1587	PSU	O2-C2-N1	-4.26	118.39	122.79
30	WA	398	A2M	C4-N9-C8	4.26	110.21	105.74
30	WA	2759	B9B	N3-C4-N9	4.25	132.39	126.99
30	WA	373	OMG	C2-N3-C4	4.25	119.62	112.30
30	WA	4134	B8W	N3-C4-N9	4.23	132.36	126.99
30	WA	4877	2MG	C2-N1-C6	-4.23	119.44	124.55
30	WA	4201	OMG	C1'-N9-C8	-4.23	114.72	126.73
30	WA	1328	1MA	C5-C4-N3	-4.22	121.06	127.27
30	WA	2055	OMG	C1'-N9-C8	-4.22	114.75	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	3769	PSU	C6-C5-C4	4.21	121.02	118.17
30	WA	4641	PSU	C6-C5-C4	4.20	121.01	118.17
30	WA	237	B9B	N3-C4-N9	4.20	132.32	126.99
30	WA	4534	B8W	N3-C4-N9	4.18	132.30	126.99
30	WA	4298	PSU	O2-C2-N1	-4.18	118.48	122.79
30	WA	3720	PSU	C6-C5-C4	4.17	120.99	118.17
30	WA	4360	E6G	N9-C8-N7	-4.16	108.04	113.94
30	WA	4641	PSU	O2-C2-N1	-4.16	118.50	122.79
30	WA	3872	A2M	C4-N9-C8	4.16	110.10	105.74
30	WA	2527	7MG	C4-C5-N7	4.14	110.27	105.38
30	WA	3734	PSU	C6-C5-C4	4.14	120.97	118.17
30	WA	4360	E6G	N3-C4-N9	4.13	132.23	126.99
30	WA	237	B9B	N9-C8-N7	-4.12	108.09	113.94
30	WA	4534	B8W	N9-C8-N7	-4.12	108.09	113.94
30	WA	4875	OMG	C1'-N9-C8	-4.11	115.06	126.73
30	WA	1876	A2M	C2'-C1'-N9	-4.11	107.00	113.75
30	WA	1610	7MG	C4-C5-N7	4.09	110.21	105.38
30	WA	3902	B8K	C72-C71-N7	4.09	124.83	118.80
30	WA	2429	OMG	C1'-N9-C8	-4.08	115.13	126.73
30	WA	4477	B8W	N9-C8-N7	-4.08	108.14	113.94
30	WA	4375	OMG	C1'-N9-C8	-4.08	115.14	126.73
30	WA	1579	B9B	N9-C8-N7	-4.07	108.16	113.94
30	WA	1522	2MG	C2-N1-C6	-4.07	119.64	124.55
30	WA	4628	OMG	C1'-N9-C8	-4.05	115.22	126.73
30	WA	730	2MG	C1'-N9-C4	4.04	138.43	126.49
30	WA	4225	6MZ	N9-C8-N7	-4.03	108.22	113.94
30	WA	4477	B8W	N3-C4-N9	4.01	132.09	126.99
30	WA	3723	A2M	C4-N9-C8	4.01	109.95	105.74
30	WA	2385	B8W	N3-C4-N9	4.00	132.07	126.99
30	WA	4555	7MG	C4-C5-N7	4.00	110.10	105.38
30	WA	2791	B9H	C31-N3-C2	4.00	122.20	117.29
30	WA	4877	2MG	C1'-N9-C8	-3.99	115.40	126.73
30	WA	1539	A2M	C4-N9-C8	3.98	109.92	105.74
30	WA	2385	B8W	N9-C8-N7	-3.98	108.29	113.94
30	WA	1527	OMG	C1'-N9-C8	-3.97	115.45	126.73
30	WA	4134	B8W	N9-C8-N7	-3.96	108.32	113.94
30	WA	4311	OMU	N3-C2-N1	3.96	120.04	114.89
30	WA	2759	B9B	N9-C8-N7	-3.93	108.36	113.94
30	WA	4190	B8W	N3-C4-N9	3.93	131.98	126.99
30	WA	4088	5MU	O4-C4-C5	-3.91	120.45	124.92
30	WA	4088	5MU	C5M-C5-C4	3.90	122.94	118.78
30	WA	3728	A2M	C4-N9-C8	3.90	109.83	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1322	OMG	N9-C8-N7	-3.88	106.20	113.40
30	WA	1527	OMG	N9-C8-N7	-3.87	106.22	113.40
30	WA	2302	E7G	C2-N1-C6	-3.85	118.12	125.11
32	YA	14	OMU	N3-C2-N1	3.85	119.90	114.89
30	WA	373	OMG	N9-C8-N7	-3.83	106.30	113.40
30	WA	2302	E7G	C5-C4-N3	-3.83	120.95	128.13
30	WA	4447	PSU	C6-C5-C4	3.82	120.75	118.17
30	WA	373	OMG	C1'-N9-C8	-3.82	115.89	126.73
30	WA	4695	B8K	C5-C4-N9	3.80	111.20	106.33
30	WA	4625	OMU	N3-C2-N1	3.79	119.82	114.89
30	WA	1802	E7G	C2-N1-C6	-3.78	118.26	125.11
30	WA	4875	OMG	N9-C8-N7	-3.78	106.39	113.40
30	WA	1610	7MG	C2-N1-C6	-3.76	118.30	125.11
30	WA	4555	7MG	C2-N1-C6	-3.75	118.30	125.11
30	WA	2527	7MG	C2-N1-C6	-3.74	118.32	125.11
30	WA	4628	OMG	N9-C8-N7	-3.74	106.47	113.40
30	WA	1522	2MG	C1'-N9-C8	-3.73	116.13	126.73
30	WA	4499	OMG	N9-C8-N7	-3.73	106.49	113.40
30	WA	4642	OMG	N9-C8-N7	-3.73	106.49	113.40
30	WA	3728	A2M	N3-C4-N9	3.71	133.48	127.17
30	WA	1630	OMG	N9-C8-N7	-3.70	106.55	113.40
30	WA	4360	E6G	N2-C2-N3	3.69	122.76	117.22
30	WA	1461	JMH	C5-C6-N1	-3.69	115.84	121.84
30	WA	4555	7MG	C5-C4-N3	-3.69	121.21	128.13
30	WA	4225	6MZ	C4-C5-C6	3.68	119.84	116.78
30	WA	2369	OMG	N9-C8-N7	-3.68	106.58	113.40
30	WA	237	B9B	O6-C6-C5	3.67	121.58	116.73
30	WA	4375	OMG	N9-C8-N7	-3.67	106.59	113.40
30	WA	3904	BGH	C5-C4-N9	3.67	111.04	106.33
30	WA	3904	BGH	C72-C71-N7	3.67	124.22	118.80
30	WA	1610	7MG	C5-C4-N3	-3.67	121.24	128.13
30	WA	4201	OMG	N9-C8-N7	-3.67	106.60	113.40
30	WA	1888	OMG	N9-C8-N7	-3.66	106.61	113.40
30	WA	2429	OMG	N9-C8-N7	-3.66	106.61	113.40
30	WA	3902	B8K	C5-C4-N9	3.66	111.02	106.33
30	WA	730	2MG	N9-C4-N3	3.66	133.27	125.95
30	WA	2778	OMG	N9-C8-N7	-3.66	106.62	113.40
30	WA	3797	OMG	N9-C8-N7	-3.65	106.63	113.40
30	WA	1865	B8H	C5-C4-N3	3.65	124.59	116.55
30	WA	2527	7MG	C5-C4-N3	-3.65	121.28	128.13
30	WA	2055	OMG	N9-C8-N7	-3.64	106.65	113.40
30	WA	4535	UR3	C5-C4-N3	3.64	119.83	115.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1802	E7G	C5-C4-N3	-3.64	121.31	128.13
30	WA	4199	I4U	C5-C4-N3	-3.63	119.53	124.86
30	WA	730	2MG	C2-N1-C6	-3.62	120.17	124.55
30	WA	4301	B8H	C5-C4-N3	3.61	124.51	116.55
30	WA	3902	B8K	C5-C4-N3	-3.61	121.35	128.13
30	WA	1587	PSU	C6-C5-C4	3.60	120.60	118.17
30	WA	1529	A2M	N3-C4-N9	3.59	133.28	127.17
30	WA	1664	I4U	C5-C4-N3	-3.58	119.61	124.86
30	WA	4376	MHG	C5-C4-N3	-3.57	121.44	128.13
30	WA	2759	B9B	O6-C6-C5	3.56	121.44	116.73
30	WA	1871	UR3	C5-C4-N3	3.56	119.73	115.04
30	WA	1522	2MG	N1-C2-N2	3.55	120.19	116.56
30	WA	4311	OMU	C5-C4-N3	3.55	119.77	114.80
30	WA	4602	UR3	C5-C4-N3	3.55	119.71	115.04
53	ZA	1678	A2M	N3-C4-N9	3.54	133.20	127.17
30	WA	3767	B8H	C5-C4-N3	3.52	124.30	116.55
30	WA	3767	B8H	O2-C2-N1	-3.51	119.23	122.78
30	WA	3728	A2M	C2-N3-C4	3.51	120.39	111.83
53	ZA	1219	JMH	C5-C6-N1	-3.50	116.14	121.84
30	WA	4695	B8K	C5-C4-N3	-3.50	121.55	128.13
30	WA	4625	OMU	C5-C4-N3	3.50	119.70	114.80
30	WA	4499	OMG	N9-C4-N3	3.50	132.95	125.95
30	WA	1888	OMG	N9-C4-N3	3.50	132.95	125.95
30	WA	3904	BGH	C2'-C1'-N9	-3.49	107.04	114.14
30	WA	4642	OMG	N9-C4-N3	3.49	132.93	125.95
30	WA	2778	OMG	N9-C4-N3	3.48	132.91	125.95
30	WA	237	B9B	N3-C2-N1	-3.47	120.16	125.48
30	WA	1630	OMG	N9-C4-N3	3.46	132.87	125.95
30	WA	3872	A2M	N3-C4-N9	3.46	133.05	127.17
30	WA	1539	A2M	N3-C4-N9	3.44	133.01	127.17
30	WA	2406	A2M	N3-C4-N9	3.43	133.01	127.17
30	WA	2369	OMG	N9-C4-N3	3.42	132.80	125.95
30	WA	4534	B8W	C61-O6-C6	-3.42	114.00	117.20
30	WA	1332	A2M	N3-C4-N9	3.42	132.98	127.17
30	WA	3902	B8K	N9-C8-N7	3.41	107.81	103.31
30	WA	3797	OMG	N9-C4-N3	3.41	132.78	125.95
30	WA	4360	E6G	N3-C2-N1	-3.41	120.26	125.48
30	WA	1354	P4U	C5-C4-N3	-3.40	119.87	124.86
30	WA	4225	6MZ	C9-N6-C6	-3.40	119.70	122.85
30	WA	1322	OMG	N9-C4-N3	3.40	132.74	125.95
30	WA	2368	A2M	N3-C4-N9	3.39	132.93	127.17
30	WA	2759	B9B	N3-C2-N1	-3.39	120.29	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	398	A2M	N3-C4-N9	3.38	132.92	127.17
30	WA	4477	B8W	N1-C2-N3	-3.38	120.30	125.48
30	WA	4877	2MG	C1'-N9-C4	3.38	136.47	126.49
30	WA	4576	A2M	N3-C4-N9	3.37	132.91	127.17
30	WA	4301	B8H	O2-C2-N1	-3.37	119.37	122.78
30	WA	3723	A2M	N3-C4-N9	3.37	132.90	127.17
30	WA	1865	B8H	O2-C2-N1	-3.37	119.37	122.78
30	WA	2406	A2M	C2-N3-C4	3.37	120.06	111.83
30	WA	3904	BGH	C5-C4-N3	-3.36	121.82	128.13
30	WA	1579	B9B	N3-C2-N1	-3.36	120.33	125.48
30	WA	3830	A2M	N3-C4-N9	3.34	132.85	127.17
30	WA	4190	B8W	N1-C2-N3	-3.34	120.36	125.48
30	WA	4225	6MZ	C2-N3-C4	3.34	119.98	111.83
30	WA	2385	B8W	N1-C2-N3	-3.33	120.37	125.48
53	ZA	1678	A2M	C2-N3-C4	3.33	119.97	111.83
30	WA	2759	B9B	N2-C2-N3	3.33	122.21	117.22
30	WA	2791	B9H	C4-N3-C2	-3.33	116.01	122.00
30	WA	4534	B8W	N1-C2-N3	-3.32	120.40	125.48
30	WA	4375	OMG	N9-C4-N3	3.31	132.58	125.95
30	WA	1529	A2M	C2-N3-C4	3.31	119.92	111.83
30	WA	4528	A2M	C2-N3-C4	3.30	119.90	111.83
30	WA	4877	2MG	N1-C2-N2	3.30	119.93	116.56
30	WA	4201	OMG	N9-C4-N3	3.30	132.55	125.95
30	WA	1539	A2M	C2-N3-C4	3.30	119.89	111.83
30	WA	3790	A2M	N3-C4-N9	3.29	132.77	127.17
30	WA	398	A2M	C2-N3-C4	3.29	119.87	111.83
30	WA	4576	A2M	C2-N3-C4	3.29	119.87	111.83
53	ZA	1248	B8N	C1'-C5-C4	3.28	122.59	117.61
30	WA	4695	B8K	N9-C8-N7	3.28	107.64	103.31
30	WA	4134	B8W	N1-C2-N3	-3.28	120.45	125.48
30	WA	4528	A2M	N3-C4-N9	3.27	132.73	127.17
30	WA	2778	OMG	C1'-N9-C4	3.27	136.14	126.49
30	WA	2368	A2M	C2-N3-C4	3.27	119.82	111.83
32	YA	14	OMU	C5-C4-N3	3.27	119.38	114.80
30	WA	2429	OMG	N9-C4-N3	3.27	132.49	125.95
30	WA	2055	OMG	N9-C4-N3	3.26	132.48	125.95
53	ZA	1678	A2M	C5-N7-C8	3.26	108.58	103.45
30	WA	4569	M7A	C2-N3-C4	3.26	119.78	111.83
30	WA	3830	A2M	C2-N3-C4	3.26	119.78	111.83
30	WA	1876	A2M	N3-C4-N9	3.25	132.70	127.17
30	WA	4298	PSU	C6-C5-C4	3.25	120.37	118.17
30	WA	3790	A2M	C2-N3-C4	3.25	119.77	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1332	A2M	C2-N3-C4	3.25	119.76	111.83
30	WA	3872	A2M	C2-N3-C4	3.24	119.75	111.83
30	WA	2406	A2M	C5-N7-C8	3.24	108.55	103.45
30	WA	1876	A2M	C2-N3-C4	3.24	119.75	111.83
30	WA	3797	OMG	C1'-N9-C4	3.24	136.05	126.49
30	WA	237	B9B	N2-C2-N3	3.24	122.08	117.22
30	WA	4875	OMG	N9-C4-N3	3.23	132.42	125.95
30	WA	2368	A2M	C5-N7-C8	3.23	108.52	103.45
30	WA	3723	A2M	C2-N3-C4	3.22	119.70	111.83
30	WA	3787	5MC	C5-C6-N1	-3.22	119.82	123.31
30	WA	4376	MHG	N1-C2-N2	3.22	119.84	116.56
30	WA	4528	A2M	C5-N7-C8	3.21	108.50	103.45
30	WA	2385	B8W	C61-O6-C6	-3.21	114.20	117.20
30	WA	4628	OMG	N9-C4-N3	3.21	132.37	125.95
30	WA	1527	OMG	N9-C4-N3	3.21	132.37	125.95
30	WA	3790	A2M	C5-N7-C8	3.19	108.46	103.45
30	WA	1579	B9B	O6-C6-C5	3.19	120.94	116.73
30	WA	2369	OMG	C1'-N9-C4	3.19	135.90	126.49
30	WA	1630	OMG	C1'-N9-C4	3.19	135.90	126.49
30	WA	4576	A2M	C5-N7-C8	3.18	108.45	103.45
30	WA	1529	A2M	C5-N7-C8	3.18	108.44	103.45
30	WA	3872	A2M	C5-N7-C8	3.17	108.44	103.45
30	WA	398	A2M	C5-N7-C8	3.17	108.44	103.45
30	WA	1539	A2M	C5-N7-C8	3.17	108.44	103.45
30	WA	3830	A2M	C5-N7-C8	3.17	108.43	103.45
30	WA	1332	A2M	C5-N7-C8	3.16	108.42	103.45
30	WA	1876	A2M	C5-N7-C8	3.16	108.42	103.45
53	ZA	1374	5MC	C5-C6-N1	-3.15	119.89	123.31
30	WA	4528	A2M	C2'-C1'-N9	-3.15	108.57	113.75
30	WA	1579	B9B	N2-C2-N3	3.13	121.92	117.22
30	WA	4340	5MC	C5-C6-N1	-3.11	119.94	123.31
30	WA	3723	A2M	C5-N7-C8	3.11	108.33	103.45
30	WA	373	OMG	N9-C4-N3	3.10	132.16	125.95
30	WA	3728	A2M	C5-N7-C8	3.10	108.32	103.45
30	WA	1522	2MG	C1'-N9-C4	3.09	135.62	126.49
30	WA	1888	OMG	C2-N1-C6	-3.09	119.51	125.11
30	WA	3790	A2M	C2'-C1'-N9	-3.08	108.68	113.75
30	WA	4642	OMG	C2-N1-C6	-3.08	119.53	125.11
30	WA	2406	A2M	C2'-C1'-N9	-3.07	108.70	113.75
30	WA	3767	B8H	O4-C4-N3	-3.05	114.37	120.11
30	WA	4499	OMG	C2-N1-C6	-3.05	119.59	125.11
30	WA	4360	E6G	C5-N7-C8	3.04	108.22	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	ZA	1337	4AC	C6-C5-C4	3.03	120.65	117.00
30	WA	4499	OMG	C1'-N9-C4	3.03	135.43	126.49
30	WA	4477	B8W	C2-N1-C6	3.03	120.17	115.96
30	WA	4452	5MC	C5-C6-N1	-3.03	120.03	123.31
30	WA	4877	2MG	N9-C4-N3	3.02	132.00	125.95
30	WA	4642	OMG	C1'-N9-C4	3.01	135.38	126.49
32	YA	14	OMU	O4-C4-C5	-3.00	119.98	125.16
30	WA	1630	OMG	C2-N1-C6	-3.00	119.66	125.11
30	WA	4628	OMG	C2-N1-C6	-2.99	119.69	125.11
30	WA	3904	BGH	N9-C8-N7	2.99	107.25	103.31
30	WA	3723	A2M	C2'-C1'-N9	-2.99	108.84	113.75
30	WA	1522	2MG	N9-C8-N7	-2.98	107.87	113.40
30	WA	3797	OMG	C2-N1-C6	-2.98	119.70	125.11
30	WA	4201	OMG	C1'-N9-C4	2.98	135.29	126.49
30	WA	1527	OMG	C2-N1-C6	-2.98	119.71	125.11
30	WA	2055	OMG	C2-N1-C6	-2.98	119.71	125.11
30	WA	2055	OMG	C1'-N9-C4	2.98	135.28	126.49
30	WA	2369	OMG	C2-N1-C6	-2.97	119.72	125.11
30	WA	4201	OMG	C2-N1-C6	-2.97	119.72	125.11
30	WA	4375	OMG	C2-N1-C6	-2.97	119.72	125.11
30	WA	1888	OMG	C1'-N9-C4	2.97	135.25	126.49
30	WA	4555	7MG	C5-C4-N9	2.96	110.13	106.33
30	WA	4190	B8W	C5-N7-C8	2.96	108.11	103.45
30	WA	2778	OMG	C2-N1-C6	-2.96	119.74	125.11
51	v	715	DDE	OAG-CBI-NAD	-2.96	117.81	123.04
30	WA	1322	OMG	C2-N1-C6	-2.95	119.76	125.11
30	WA	4360	E6G	C2-N1-C6	2.95	120.06	115.96
30	WA	4190	B8W	C2-N1-C6	2.94	120.04	115.96
30	WA	4875	OMG	C2-N1-C6	-2.93	119.79	125.11
53	ZA	1337	4AC	N4-C4-N3	2.92	118.61	113.87
30	WA	1328	1MA	N9-C8-N7	-2.91	108.00	113.40
30	WA	4877	2MG	N9-C8-N7	-2.91	108.00	113.40
30	WA	4569	M7A	C5-C4-N3	-2.91	119.84	126.56
30	WA	4477	B8W	C5-N7-C8	2.91	108.02	103.45
30	WA	4477	B8W	C5-C6-N1	-2.90	119.61	123.49
30	WA	4625	OMU	O4-C4-C5	-2.90	120.16	125.16
30	WA	373	OMG	C2-N1-C6	-2.90	119.86	125.11
30	WA	1322	OMG	C1'-N9-C4	2.90	135.04	126.49
30	WA	2429	OMG	C2-N1-C6	-2.89	119.87	125.11
30	WA	4088	5MU	C6-C5-C4	2.89	120.40	118.02
30	WA	4088	5MU	O2-C2-N1	-2.88	119.05	122.80
30	WA	1461	JMH	C6-N1-C2	-2.87	119.45	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1610	7MG	C5-C4-N9	2.87	110.01	106.33
53	ZA	1248	B8N	O4-C4-N3	-2.86	115.35	119.99
30	WA	4311	OMU	O4-C4-C5	-2.85	120.24	125.16
30	WA	1802	E7G	C5-C4-N9	2.85	109.99	106.33
53	ZA	1219	JMH	C6-N1-C2	-2.85	119.47	121.80
30	WA	4375	OMG	C1'-N9-C4	2.84	134.88	126.49
53	ZA	1248	B8N	C31-N3-C4	2.84	121.20	117.18
30	WA	4190	B8W	C5-C6-N1	-2.84	119.69	123.49
30	WA	1328	1MA	C1'-N9-C4	-2.84	118.10	126.49
32	YA	14	OMU	C1'-N1-C2	2.84	122.69	117.59
30	WA	4225	6MZ	N3-C4-N9	2.83	131.99	127.17
30	WA	237	B9B	C2-N1-C6	2.83	119.90	115.96
30	WA	237	B9B	C5-N7-C8	2.83	107.90	103.45
30	WA	2429	OMG	C1'-N9-C4	2.83	134.84	126.49
30	WA	4420	1MA	N9-C8-N7	-2.83	108.16	113.40
30	WA	2759	B9B	C5-N7-C8	2.83	107.89	103.45
30	WA	2385	B8W	C2-N1-C6	2.82	119.88	115.96
30	WA	1522	2MG	N9-C4-N3	2.82	131.59	125.95
30	WA	4376	MHG	C5-C4-N9	2.81	109.93	106.33
30	WA	2385	B8W	C5-N7-C8	2.81	107.86	103.45
30	WA	4534	B8W	C5-N7-C8	2.81	107.86	103.45
30	WA	1579	B9B	C5-N7-C8	2.80	107.86	103.45
30	WA	4134	B8W	C5-N7-C8	2.80	107.85	103.45
30	WA	2527	7MG	C5-C4-N9	2.79	109.91	106.33
30	WA	4875	OMG	C1'-N9-C4	2.79	134.74	126.49
30	WA	1865	B8H	O4-C4-N3	-2.78	114.88	120.11
30	WA	3904	BGH	C6-C5-C4	-2.78	117.52	122.40
30	WA	4695	B8K	C6-C5-C4	-2.77	117.52	122.40
30	WA	4534	B8W	C2-N1-C6	2.77	119.81	115.96
30	WA	4628	OMG	C1'-N9-C4	2.77	134.66	126.49
30	WA	2302	E7G	C5-C4-N9	2.77	109.88	106.33
30	WA	4134	B8W	C2-N1-C6	2.76	119.81	115.96
30	WA	730	2MG	N9-C8-N7	-2.76	108.28	113.40
30	WA	4360	E6G	C5-C6-N1	-2.76	119.80	123.49
30	WA	1888	OMG	C5-C6-N1	2.75	120.26	113.25
30	WA	4225	6MZ	C5-N7-C8	2.75	107.77	103.45
30	WA	4499	OMG	C5-C6-N1	2.73	120.20	113.25
30	WA	4376	MHG	O6-C6-C5	-2.71	120.97	127.62
30	WA	4695	B8K	C2-N1-C6	-2.71	120.20	125.11
30	WA	1802	E7G	O6-C6-C5	-2.70	120.99	127.62
30	WA	4642	OMG	C5-C6-N1	2.70	120.12	113.25
53	ZA	1219	JMH	C31-N3-C2	2.70	122.03	117.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	2302	E7G	O6-C6-C5	-2.69	121.02	127.62
30	WA	1888	OMG	O6-C6-C5	-2.68	119.45	126.53
30	WA	2385	B8W	C5-C6-N1	-2.68	119.91	123.49
30	WA	3902	B8K	C2-N1-C6	-2.68	120.26	125.11
30	WA	4420	1MA	C1'-N9-C4	-2.68	118.58	126.49
30	WA	1871	UR3	C6-N1-C2	-2.67	119.61	121.80
30	WA	4360	E6G	C61-O6-C6	-2.67	114.92	117.57
30	WA	1527	OMG	C5-C6-N1	2.67	120.04	113.25
30	WA	4641	PSU	O2-C2-N3	-2.66	117.14	121.86
30	WA	1610	7MG	O6-C6-C5	-2.66	121.09	127.62
30	WA	1630	OMG	C5-C6-N1	2.66	120.01	113.25
30	WA	4628	OMG	C5-C6-N1	2.65	120.00	113.25
30	WA	2791	B9H	C6-N1-C2	-2.65	119.63	121.80
30	WA	4877	2MG	C5-C6-N1	2.65	119.99	113.25
30	WA	2778	OMG	C5-C6-N1	2.65	119.99	113.25
30	WA	1871	UR3	C1'-N1-C2	2.65	121.37	117.04
30	WA	4875	OMG	C5-C6-N1	2.64	119.97	113.25
30	WA	1522	2MG	C5-C6-N1	2.64	119.97	113.25
30	WA	398	A2M	C2'-C1'-N9	-2.64	109.41	113.75
30	WA	2369	OMG	C5-C6-N1	2.64	119.96	113.25
30	WA	2055	OMG	C5-C6-N1	2.64	119.96	113.25
30	WA	4201	OMG	C5-C6-N1	2.64	119.96	113.25
30	WA	2527	7MG	O6-C6-C5	-2.64	121.15	127.62
30	WA	1527	OMG	C1'-N9-C4	2.63	134.26	126.49
30	WA	3797	OMG	C5-C6-N1	2.63	119.94	113.25
30	WA	4301	B8H	O4-C4-N3	-2.63	115.17	120.11
30	WA	4375	OMG	C5-C6-N1	2.62	119.93	113.25
30	WA	373	OMG	C5-C6-N1	2.62	119.91	113.25
30	WA	4134	B8W	C5-C6-N1	-2.61	119.99	123.49
30	WA	4534	B8W	C5-C6-N1	-2.61	119.99	123.49
30	WA	2429	OMG	C5-C6-N1	2.61	119.90	113.25
30	WA	4499	OMG	O6-C6-C5	-2.60	119.67	126.53
30	WA	1322	OMG	C5-C6-N1	2.60	119.87	113.25
30	WA	730	2MG	C5-C6-N1	2.60	119.86	113.25
30	WA	4642	OMG	O6-C6-C5	-2.59	119.69	126.53
30	WA	1461	JMH	C31-N3-C2	2.59	121.85	117.33
30	WA	2759	B9B	C2-N1-C6	2.59	119.56	115.96
30	WA	1579	B9B	C2-N1-C6	2.58	119.55	115.96
30	WA	4088	5MU	O4-C4-N3	-2.57	115.27	120.11
30	WA	3790	A2M	C4-N9-C1'	-2.56	120.65	126.63
30	WA	1630	OMG	O6-C6-C5	-2.56	119.78	126.53
30	WA	373	OMG	O6-C6-C5	-2.54	119.82	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1914	P7G	N9-C8-N7	2.54	106.97	103.37
30	WA	4555	7MG	O6-C6-C5	-2.54	121.39	127.62
30	WA	2369	OMG	O6-C6-C5	-2.54	119.84	126.53
30	WA	2302	E7G	N9-C4-N3	2.53	129.17	125.46
30	WA	1322	OMG	C8-N7-C5	2.53	108.77	104.26
30	WA	4628	OMG	O6-C6-C5	-2.53	119.84	126.53
30	WA	4602	UR3	C6-N1-C2	-2.53	119.73	121.80
30	WA	2368	A2M	C2'-C1'-N9	-2.53	109.60	113.75
30	WA	2759	B9B	C2-N3-C4	2.51	120.24	113.51
30	WA	1579	B9B	C61-O6-C6	-2.51	113.29	117.66
30	WA	2778	OMG	O6-C6-C5	-2.51	119.92	126.53
30	WA	1610	7MG	N9-C8-N7	2.51	106.92	103.37
30	WA	4190	B8W	C4-C5-N7	-2.51	107.72	110.58
30	WA	4875	OMG	O6-C6-C5	-2.51	119.92	126.53
30	WA	3902	B8K	C6-C5-C4	-2.50	118.00	122.40
30	WA	3904	BGH	C2-N1-C6	-2.50	120.58	125.11
30	WA	4528	A2M	C4-N9-C1'	-2.50	120.79	126.63
30	WA	3797	OMG	O6-C6-C5	-2.49	119.95	126.53
30	WA	237	B9B	C5-C6-N1	-2.49	120.16	123.49
30	WA	1527	OMG	O6-C6-C5	-2.48	119.98	126.53
30	WA	2055	OMG	O6-C6-C5	-2.48	119.98	126.53
30	WA	4375	OMG	O6-C6-C5	-2.48	120.00	126.53
30	WA	2791	B9H	O2-C2-N3	-2.47	118.93	122.10
30	WA	1527	OMG	C8-N7-C5	2.47	108.67	104.26
30	WA	4569	M7A	C71-N7-C5	-2.47	113.13	123.44
30	WA	1522	2MG	O6-C6-C5	-2.47	120.01	126.53
30	WA	4201	OMG	O6-C6-C5	-2.47	120.01	126.53
30	WA	4360	E6G	C4-C5-N7	-2.47	107.76	110.58
30	WA	4477	B8W	C4-C5-N7	-2.47	107.76	110.58
30	WA	4877	2MG	O6-C6-C5	-2.47	120.01	126.53
30	WA	2429	OMG	O6-C6-C5	-2.47	120.02	126.53
30	WA	4534	B8W	C2-N3-C4	2.47	120.12	113.51
30	WA	1322	OMG	O6-C6-C5	-2.47	120.02	126.53
30	WA	2385	B8W	C2-N3-C4	2.47	120.12	113.51
30	WA	1876	A2M	C4-N9-C1'	-2.46	120.88	126.63
30	WA	1579	B9B	C2-N3-C4	2.46	120.09	113.51
30	WA	237	B9B	C2-N3-C4	2.45	120.08	113.51
30	WA	373	OMG	C1'-N9-C4	2.45	133.73	126.49
30	WA	4134	B8W	C2-N3-C4	2.45	120.07	113.51
30	WA	2791	B9H	C1'-N1-C2	2.45	121.05	117.04
30	WA	4676	B8T	C6-C5-C4	2.44	119.94	117.00
30	WA	4190	B8W	C2-N3-C4	2.44	120.04	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1328	1MA	C1'-N9-C8	2.43	133.64	126.73
30	WA	4477	B8W	C2-N3-C4	2.43	120.01	113.51
30	WA	4360	E6G	C2-N3-C4	2.42	119.99	113.51
30	WA	4875	OMG	C8-N7-C5	2.41	108.55	104.26
30	WA	4642	OMG	C8-N7-C5	2.40	108.54	104.26
30	WA	730	2MG	O6-C6-C5	-2.40	120.20	126.53
30	WA	2385	B8W	C4-C5-N7	-2.39	107.85	110.58
30	WA	1630	OMG	C8-N7-C5	2.39	108.51	104.26
30	WA	4628	OMG	C8-N7-C5	2.38	108.50	104.26
30	WA	1802	E7G	N9-C8-N7	2.38	106.73	103.37
30	WA	4375	OMG	C8-N7-C5	2.37	108.49	104.26
53	ZA	1337	4AC	C5-C4-N3	-2.37	118.89	122.60
30	WA	2302	E7G	N9-C8-N7	2.37	106.72	103.37
30	WA	4499	OMG	C8-N7-C5	2.36	108.47	104.26
30	WA	730	2MG	N1-C2-N3	-2.36	119.70	123.68
30	WA	4190	B8W	C4-N9-C8	2.36	108.22	105.74
30	WA	4535	UR3	C6-N1-C2	-2.36	119.87	121.80
30	WA	4201	OMG	C8-N7-C5	2.36	108.47	104.26
30	WA	3797	OMG	C8-N7-C5	2.36	108.46	104.26
30	WA	2778	OMG	C8-N7-C5	2.35	108.45	104.26
30	WA	1579	B9B	C5-C6-N1	-2.35	120.35	123.49
30	WA	373	OMG	C8-N7-C5	2.34	108.43	104.26
30	WA	2429	OMG	C8-N7-C5	2.33	108.41	104.26
30	WA	4488	B8T	C6-C5-C4	2.33	119.81	117.00
30	WA	4420	1MA	C1'-N9-C8	2.33	133.34	126.73
30	WA	2055	OMG	C8-N7-C5	2.32	108.40	104.26
30	WA	373	OMG	C8-N9-C4	2.32	110.37	106.03
30	WA	1322	OMG	C8-N9-C4	2.32	110.37	106.03
30	WA	2369	OMG	C8-N7-C5	2.32	108.39	104.26
53	ZA	1337	4AC	CM7-C7-N4	2.31	119.00	115.27
53	ZA	1219	JMH	C1'-N1-C2	2.31	120.82	117.04
30	WA	4477	B8W	C4-N9-C8	2.30	108.15	105.74
30	WA	730	2MG	CM2-N2-C2	-2.29	118.72	123.65
30	WA	2759	B9B	C5-C6-N1	-2.29	120.42	123.49
30	WA	4134	B8W	C4-C5-N7	-2.29	107.96	110.58
30	WA	2527	7MG	N9-C8-N7	2.29	106.61	103.37
30	WA	2527	7MG	N9-C4-N3	2.28	128.81	125.46
30	WA	4555	7MG	N9-C8-N7	2.28	106.60	103.37
30	WA	3885	P7G	N9-C8-N7	2.27	106.59	103.37
30	WA	1527	OMG	C8-N9-C4	2.27	110.28	106.03
30	WA	1888	OMG	C8-N7-C5	2.27	108.30	104.26
30	WA	2759	B9B	C4-C5-N7	-2.27	107.99	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	4340	5MC	CM5-C5-C6	-2.26	119.79	122.85
30	WA	4695	B8K	O6-C6-C5	-2.26	122.08	127.62
30	WA	237	B9B	C4-N9-C8	2.26	108.11	105.74
30	WA	1610	7MG	N9-C4-N3	2.25	128.75	125.46
30	WA	3830	A2M	C4-N9-C1'	-2.25	121.38	126.63
30	WA	4625	OMU	O2-C2-N1	-2.24	119.88	122.80
30	WA	4534	B8W	C4-N9-C8	2.24	108.09	105.74
30	WA	4311	OMU	O2-C2-N1	-2.24	119.89	122.80
30	WA	4534	B8W	C4-C5-N7	-2.23	108.04	110.58
30	WA	4875	OMG	C8-N9-C4	2.22	110.19	106.03
30	WA	4499	OMG	C8-N9-C4	2.22	110.19	106.03
30	WA	1888	OMG	C8-N9-C4	2.21	110.18	106.03
30	WA	1802	E7G	N9-C4-N3	2.21	128.70	125.46
30	WA	1579	B9B	C4-N9-C8	2.20	108.05	105.74
30	WA	1332	A2M	C4-N9-C1'	-2.19	121.50	126.63
30	WA	4642	OMG	C8-N9-C4	2.19	110.12	106.03
30	WA	1539	A2M	C4-C5-N7	-2.18	108.09	110.58
30	WA	4628	OMG	C8-N9-C4	2.18	110.12	106.03
30	WA	4555	7MG	N9-C4-N3	2.18	128.66	125.46
30	WA	4360	E6G	C4-N9-C8	2.18	108.03	105.74
30	WA	2385	B8W	C5-C4-N9	2.18	108.19	105.81
30	WA	2369	OMG	C8-N9-C4	2.18	110.11	106.03
30	WA	2406	A2M	C4-N9-C1'	-2.18	121.54	126.63
30	WA	2368	A2M	C4-N9-C1'	-2.17	121.55	126.63
30	WA	1630	OMG	C8-N9-C4	2.17	110.10	106.03
53	ZA	1219	JMH	O2-C2-N3	-2.17	118.33	121.33
30	WA	4408	PSU	O4'-C1'-C2'	2.16	108.15	105.15
30	WA	2368	A2M	C4-C5-N7	-2.16	108.11	110.58
30	WA	4376	MHG	N9-C4-N3	2.16	128.63	125.46
30	WA	4420	1MA	N9-C4-N3	2.16	131.83	126.90
30	WA	237	B9B	C4-C5-N7	-2.16	108.11	110.58
30	WA	730	2MG	N1-C2-N2	2.16	118.77	116.56
30	WA	4695	B8K	N1-C2-N3	-2.16	119.37	123.32
30	WA	4376	MHG	N9-C8-N7	2.16	106.42	103.37
53	ZA	1248	B8N	O4'-C1'-C2'	2.16	108.13	105.15
30	WA	4602	UR3	C1'-N1-C2	2.15	120.56	117.04
30	WA	3872	A2M	C4-N9-C1'	-2.15	121.61	126.63
30	WA	2778	OMG	C8-N9-C4	2.15	110.05	106.03
30	WA	2406	A2M	C4-C5-N7	-2.14	108.13	110.58
30	WA	398	A2M	C4-N9-C1'	-2.14	121.62	126.63
30	WA	2429	OMG	C8-N9-C4	2.14	110.03	106.03
30	WA	3797	OMG	C8-N9-C4	2.13	110.02	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1876	A2M	C4-C5-N7	-2.13	108.15	110.58
30	WA	1522	2MG	N1-C2-N3	-2.13	120.10	123.68
30	WA	4225	6MZ	C4-C5-N7	-2.12	108.15	110.58
30	WA	3723	A2M	C4-C5-N7	-2.12	108.16	110.58
30	WA	4201	OMG	C8-N9-C4	2.11	109.99	106.03
30	WA	4576	A2M	C4-N9-C1'	-2.11	121.70	126.63
30	WA	4375	OMG	C8-N9-C4	2.11	109.98	106.03
30	WA	1328	1MA	C8-N7-C5	2.10	108.01	104.26
30	WA	2759	B9B	C61-O6-C6	-2.10	114.00	117.66
30	WA	398	A2M	C4-C5-N7	-2.10	108.18	110.58
30	WA	4877	2MG	CM2-N2-C2	-2.10	119.14	123.65
30	WA	4455	PSU	O2-C2-N3	-2.09	118.14	121.86
30	WA	4420	1MA	C8-N7-C5	2.09	107.99	104.26
30	WA	3830	A2M	C4-C5-N7	-2.09	108.19	110.58
30	WA	3787	5MC	CM5-C5-C6	-2.09	120.02	122.85
30	WA	2055	OMG	C8-N9-C4	2.09	109.94	106.03
30	WA	4528	A2M	C4-C5-N7	-2.09	108.19	110.58
30	WA	2759	B9B	C5-C4-N9	2.08	108.08	105.81
30	WA	4576	A2M	C4-C5-N7	-2.08	108.20	110.58
30	WA	4376	MHG	N1-C2-N3	-2.08	120.17	123.68
30	WA	4877	2MG	C8-N7-C5	2.08	107.96	104.26
30	WA	1579	B9B	C4-C5-N7	-2.08	108.21	110.58
30	WA	4576	A2M	C2'-C1'-N9	-2.07	110.34	113.75
30	WA	4190	B8W	C4-N9-C1'	-2.07	121.78	126.63
30	WA	1539	A2M	C3'-C2'-C1'	-2.07	98.84	102.81
30	WA	3872	A2M	C4-C5-N7	-2.07	108.21	110.58
30	WA	4134	B8W	C4-N9-C8	2.07	107.91	105.74
30	WA	1522	2MG	C8-N7-C5	2.07	107.95	104.26
30	WA	4190	B8W	C5-C4-N9	2.07	108.07	105.81
30	WA	4633	PSU	O2-C2-N3	-2.06	118.20	121.86
30	WA	4225	6MZ	C4-N9-C8	2.06	107.90	105.74
30	WA	4447	PSU	O4'-C1'-C2'	2.06	108.00	105.15
30	WA	3902	B8K	O6-C6-C5	-2.05	122.58	127.62
30	WA	1529	A2M	C4-C5-N7	-2.05	108.24	110.58
30	WA	3723	A2M	C4-N9-C1'	-2.04	121.85	126.63
30	WA	1539	A2M	C4-N9-C1'	-2.04	121.86	126.63
30	WA	1328	1MA	N9-C4-N3	2.04	131.54	126.90
30	WA	1688	PSU	O2-C2-N3	-2.04	118.24	121.86
30	WA	2513	PSU	O2-C2-N3	-2.03	118.25	121.86
30	WA	2866	OMC	O2-C2-N3	-2.03	119.13	122.33
53	ZA	1374	5MC	CM5-C5-C6	-2.03	120.10	122.85
30	WA	3790	A2M	O4'-C1'-N9	2.03	111.98	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	WA	1682	PSU	O2-C2-N3	-2.03	118.26	121.86
30	WA	3904	BGH	O6-C6-C5	-2.02	122.65	127.62
53	ZA	1678	A2M	C4-C5-N7	-2.02	108.27	110.58
30	WA	3830	A2M	C2'-C1'-N9	-2.02	110.43	113.75
30	WA	1682	PSU	O4'-C1'-C2'	2.02	107.94	105.15
30	WA	4134	B8W	C61-O6-C6	-2.01	115.32	117.20
30	WA	3790	A2M	C4-C5-N7	-2.01	108.28	110.58
30	WA	1522	2MG	CM2-N2-C2	-2.01	119.33	123.65
30	WA	1332	A2M	C4-C5-N7	-2.01	108.29	110.58
53	ZA	1243	PSU	O2-C2-N3	-2.00	118.30	121.86

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	333	MLZ	CD-CE-NZ-CM
30	WA	237	B9B	C5-C6-O6-C61
30	WA	237	B9B	N1-C6-O6-C61
30	WA	237	B9B	O4'-C4'-C5'-O5'
30	WA	398	A2M	O4'-C4'-C5'-O5'
30	WA	398	A2M	C1'-C2'-O2'-CM'
30	WA	1332	A2M	C1'-C2'-O2'-CM'
30	WA	1354	P4U	N3-C4-O4-C41
30	WA	1354	P4U	C3'-C4'-C5'-O5'
30	WA	1354	P4U	O4'-C4'-C5'-O5'
30	WA	1579	B9B	C5-C6-O6-C61
30	WA	1579	B9B	N1-C6-O6-C61
30	WA	1865	B8H	C3'-C4'-C5'-O5'
30	WA	1865	B8H	O4'-C4'-C5'-O5'
30	WA	1871	UR3	O4'-C4'-C5'-O5'
30	WA	2055	OMG	C1'-C2'-O2'-CM2
30	WA	2369	OMG	C1'-C2'-O2'-CM2
30	WA	2385	B8W	C5-C6-O6-C61
30	WA	2429	OMG	O4'-C4'-C5'-O5'
30	WA	2429	OMG	C3'-C4'-C5'-O5'
30	WA	2778	OMG	O4'-C4'-C5'-O5'
30	WA	2778	OMG	C3'-C4'-C5'-O5'
30	WA	3706	OMC	C2'-C1'-N1-C2
30	WA	3706	OMC	C2'-C1'-N1-C6
30	WA	3767	B8H	C2'-C1'-C5-C4
30	WA	3767	B8H	O4'-C4'-C5'-O5'
30	WA	3797	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
30	WA	3830	A2M	C1'-C2'-O2'-CM'
30	WA	3872	A2M	C1'-C2'-O2'-CM'
30	WA	3885	P7G	O4'-C4'-C5'-O5'
30	WA	3902	B8K	O4'-C4'-C5'-O5'
30	WA	4134	B8W	C5-C6-O6-C61
30	WA	4134	B8W	N1-C6-O6-C61
30	WA	4190	B8W	C5-C6-O6-C61
30	WA	4190	B8W	N1-C6-O6-C61
30	WA	4360	E6G	C5-C6-O6-C61
30	WA	4360	E6G	N1-C6-O6-C61
30	WA	4376	MHG	C2'-C1'-N9-C8
30	WA	4420	1MA	C3'-C4'-C5'-O5'
30	WA	4452	5MC	C2'-C1'-N1-C2
30	WA	4452	5MC	C2'-C1'-N1-C6
30	WA	4477	B8W	C5-C6-O6-C61
30	WA	4477	B8W	N1-C6-O6-C61
30	WA	4505	PSU	C3'-C4'-C5'-O5'
30	WA	4576	A2M	C1'-C2'-O2'-CM'
30	WA	4625	OMU	C1'-C2'-O2'-CM2
30	WA	4642	OMG	C1'-C2'-O2'-CM2
30	WA	4875	OMG	O4'-C4'-C5'-O5'
30	WA	4875	OMG	C3'-C4'-C5'-O5'
32	YA	14	OMU	C1'-C2'-O2'-CM2
32	YA	14	OMU	O4'-C4'-C5'-O5'
44	LA	72	MLZ	CD-CE-NZ-CM
51	v	715	DDE	CAU-CBW-NCB-CAB
51	v	715	DDE	CAU-CBW-NCB-CAC
51	v	715	DDE	CAU-CBW-NCB-CAA
53	ZA	1243	PSU	C3'-C4'-C5'-O5'
53	ZA	1243	PSU	O4'-C4'-C5'-O5'
53	ZA	1248	B8N	C31-C32-C33-C34
53	ZA	1678	A2M	C1'-C2'-O2'-CM'
30	WA	237	B9B	C3'-C4'-C5'-O5'
30	WA	1587	PSU	C3'-C4'-C5'-O5'
30	WA	1587	PSU	O4'-C4'-C5'-O5'
30	WA	1871	UR3	C3'-C4'-C5'-O5'
30	WA	2302	E7G	C3'-C4'-C5'-O5'
30	WA	2302	E7G	O4'-C4'-C5'-O5'
30	WA	2369	OMG	O4'-C4'-C5'-O5'
30	WA	2385	B8W	C3'-C4'-C5'-O5'
30	WA	2385	B8W	O4'-C4'-C5'-O5'
30	WA	3728	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
30	WA	3734	PSU	O4'-C4'-C5'-O5'
30	WA	3797	OMG	C3'-C4'-C5'-O5'
30	WA	3892	OMC	C3'-C4'-C5'-O5'
30	WA	4298	PSU	C3'-C4'-C5'-O5'
30	WA	4420	1MA	O4'-C4'-C5'-O5'
30	WA	4505	PSU	O4'-C4'-C5'-O5'
30	WA	4641	PSU	C3'-C4'-C5'-O5'
30	WA	4642	OMG	O4'-C4'-C5'-O5'
30	WA	2385	B8W	N1-C6-O6-C61
30	WA	1802	E7G	O4'-C4'-C5'-O5'
30	WA	3728	A2M	C3'-C4'-C5'-O5'
30	WA	3885	P7G	C3'-C4'-C5'-O5'
30	WA	4298	PSU	O4'-C4'-C5'-O5'
30	WA	4455	PSU	C3'-C4'-C5'-O5'
30	WA	4455	PSU	O4'-C4'-C5'-O5'
30	WA	4641	PSU	O4'-C4'-C5'-O5'
51	v	715	DDE	CE1-CAT-CAU-CBW
30	WA	3767	B8H	C3'-C4'-C5'-O5'
30	WA	3902	B8K	C3'-C4'-C5'-O5'
30	WA	398	A2M	C3'-C4'-C5'-O5'
30	WA	1539	A2M	C3'-C4'-C5'-O5'
30	WA	4555	7MG	C3'-C4'-C5'-O5'
30	WA	1539	A2M	O4'-C4'-C5'-O5'
30	WA	3734	PSU	C3'-C4'-C5'-O5'
30	WA	3872	A2M	C3'-C4'-C5'-O5'
30	WA	3892	OMC	O4'-C4'-C5'-O5'
30	WA	4199	I4U	O4'-C4'-C5'-O5'
30	WA	4555	7MG	O4'-C4'-C5'-O5'
32	YA	14	OMU	C3'-C4'-C5'-O5'
30	WA	4376	MHG	C75-C73-C74-C76
30	WA	2369	OMG	C3'-C4'-C5'-O5'
30	WA	4376	MHG	O4'-C4'-C5'-O5'
30	WA	4642	OMG	C3'-C4'-C5'-O5'
30	WA	4676	B8T	C2'-C1'-N1-C6
30	WA	1354	P4U	O4-C41-C42-C43
30	WA	3787	5MC	O4'-C4'-C5'-O5'
30	WA	3872	A2M	O4'-C4'-C5'-O5'
30	WA	4505	PSU	C4'-C5'-O5'-P
30	WA	4452	5MC	O4'-C1'-N1-C6
30	WA	1322	OMG	C1'-C2'-O2'-CM2
30	WA	4452	5MC	O4'-C1'-N1-C2
30	WA	1802	E7G	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
30	WA	4301	B8H	C3'-C4'-C5'-O5'
30	WA	4301	B8H	O4'-C4'-C5'-O5'
30	WA	4199	I4U	C42-C41-O4-C4
3	C	333	MLZ	C-CA-CB-CG
30	WA	4199	I4U	C3'-C4'-C5'-O5'
3	C	333	MLZ	N-CA-CB-CG
30	WA	2791	B9H	O4'-C4'-C5'-O5'
30	WA	4528	A2M	C3'-C4'-C5'-O5'
30	WA	4676	B8T	O4'-C1'-N1-C6
30	WA	3872	A2M	C4'-C5'-O5'-P
32	YA	14	OMU	C2'-C1'-N1-C2
32	YA	14	OMU	C2'-C1'-N1-C6
30	WA	3790	A2M	O4'-C4'-C5'-O5'
30	WA	3902	B8K	C4'-C5'-O5'-P
30	WA	4875	OMG	C4'-C5'-O5'-P
30	WA	4455	PSU	O4'-C1'-C5-C4
53	ZA	1248	B8N	O4'-C1'-C5-C4
30	WA	3790	A2M	C3'-C4'-C5'-O5'
3	C	333	MLZ	CG-CD-CE-NZ
30	WA	1630	OMG	C4'-C5'-O5'-P
30	WA	4340	5MC	C4'-C5'-O5'-P
53	ZA	1248	B8N	C4'-C5'-O5'-P
30	WA	4360	E6G	C62-C61-O6-C6
30	WA	4340	5MC	C3'-C4'-C5'-O5'
30	WA	3706	OMC	O4'-C1'-N1-C6
30	WA	1888	OMG	C3'-C2'-O2'-CM2
30	WA	3790	A2M	C3'-C2'-O2'-CM'
30	WA	373	OMG	C4'-C5'-O5'-P
30	WA	2759	B9B	C4'-C5'-O5'-P
30	WA	3830	A2M	C3'-C4'-C5'-O5'
30	WA	4376	MHG	C72-C73-C74-C76
30	WA	4376	MHG	C2'-C1'-N9-C4
30	WA	3728	A2M	C4'-C5'-O5'-P
30	WA	1522	2MG	O4'-C4'-C5'-O5'
30	WA	4877	2MG	O4'-C4'-C5'-O5'
30	WA	4676	B8T	C2'-C1'-N1-C2
30	WA	1328	1MA	C2'-C1'-N9-C8
30	WA	1914	P7G	C72-C71-N7-C5
30	WA	2809	OMC	C1'-C2'-O2'-CM2
30	WA	3790	A2M	C1'-C2'-O2'-CM'
30	WA	4676	B8T	C4'-C5'-O5'-P
30	WA	4676	B8T	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
30	WA	4360	E6G	C3'-C4'-C5'-O5'
30	WA	3706	OMC	O4'-C1'-N1-C2
30	WA	4199	I4U	C43-C41-O4-C4
30	WA	1328	1MA	C2'-C1'-N9-C4
30	WA	1529	A2M	O4'-C1'-N9-C8
30	WA	4360	E6G	O4'-C4'-C5'-O5'
30	WA	2759	B9B	C5-C6-O6-C61
30	WA	1579	B9B	C4'-C5'-O5'-P
30	WA	3892	OMC	C4'-C5'-O5'-P
30	WA	2866	OMC	C2'-C1'-N1-C2
30	WA	4376	MHG	C71-C72-C73-C75

There are no ring outliers.

60 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	WA	4298	PSU	1	0
30	WA	1865	B8H	6	0
30	WA	2778	OMG	1	0
30	WA	4555	7MG	1	0
30	WA	1354	P4U	1	0
51	v	715	DDE	1	0
30	WA	1332	A2M	4	0
30	WA	4452	5MC	1	0
30	WA	4602	UR3	2	0
32	YA	14	OMU	3	0
30	WA	4360	E6G	2	0
30	WA	2369	OMG	1	0
30	WA	1527	OMG	1	0
30	WA	3872	A2M	2	0
53	ZA	1219	JMH	1	0
30	WA	2866	OMC	1	0
30	WA	1461	JMH	2	0
30	WA	3728	A2M	2	0
30	WA	4528	A2M	1	0
30	WA	1876	A2M	1	0
30	WA	4625	OMU	2	0
30	WA	4641	PSU	1	0
30	WA	1579	B9B	1	0
30	WA	3767	B8H	6	0
53	ZA	1337	4AC	4	0
30	WA	2055	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	WA	4695	B8K	1	0
30	WA	3723	A2M	3	0
30	WA	1914	P7G	1	0
30	WA	4877	2MG	3	0
30	WA	4199	I4U	1	0
30	WA	1630	OMG	1	0
30	WA	730	2MG	3	0
30	WA	4225	6MZ	3	0
30	WA	4088	5MU	5	0
30	WA	2368	A2M	1	0
30	WA	4134	B8W	1	0
30	WA	1888	OMG	1	0
30	WA	2427	OMC	1	0
30	WA	1322	OMG	1	0
30	WA	4477	B8W	2	0
53	ZA	1678	A2M	3	0
30	WA	4499	OMG	2	0
30	WA	3902	B8K	1	0
30	WA	3790	A2M	1	0
30	WA	398	A2M	1	0
30	WA	4628	OMG	2	0
30	WA	4576	A2M	1	0
30	WA	1871	UR3	3	0
30	WA	3830	A2M	1	0
30	WA	1539	A2M	1	0
30	WA	373	OMG	1	0
30	WA	2759	B9B	1	0
30	WA	4301	B8H	6	0
30	WA	2809	OMC	1	0
30	WA	2527	7MG	2	0
30	WA	4505	PSU	1	0
30	WA	3904	BGH	1	0
30	WA	4569	M7A	1	0
30	WA	1610	7MG	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 155 ligands modelled in this entry, 152 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
89	GDP	v	900	-	29,30,30	3.26	17 (58%)	45,47,47	2.14	11 (24%)
86	ANM	WA	5199	-	20,20,20	4.08	7 (35%)	24,27,27	1.42	3 (12%)
87	SPD	WA	5200	-	9,9,9	0.27	0	8,8,8	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	GDP	v	900	-	-	4/16/32/32	0/3/3/3
86	ANM	WA	5199	-	-	0/10/23/23	0/2/2/2
87	SPD	WA	5200	-	-	1/7/7/7	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	WA	5199	ANM	C3-C2	-11.84	1.32	1.53
86	WA	5199	ANM	C16-N1	-8.82	1.30	1.47
86	WA	5199	ANM	C2-C16	7.39	1.68	1.53
89	v	900	GDP	C4-N3	6.60	1.49	1.34
89	v	900	GDP	O4'-C4'	-6.26	1.31	1.45
89	v	900	GDP	C2-N3	5.63	1.46	1.33
89	v	900	GDP	C3'-C4'	5.43	1.66	1.53
89	v	900	GDP	PA-O3A	5.38	1.65	1.59
89	v	900	GDP	C1'-N9	-5.31	1.32	1.47
89	v	900	GDP	C2-N2	4.75	1.45	1.34
89	v	900	GDP	O4'-C1'	4.15	1.51	1.42
86	WA	5199	ANM	C4-C3	4.03	1.58	1.53
86	WA	5199	ANM	C4-N1	3.86	1.60	1.47
86	WA	5199	ANM	O2-C5	3.51	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	v	900	GDP	O2'-C2'	3.12	1.50	1.43
89	v	900	GDP	C2-N1	2.88	1.44	1.37
89	v	900	GDP	O6-C6	-2.54	1.18	1.23
89	v	900	GDP	C5-C6	2.51	1.53	1.44
89	v	900	GDP	C6-N1	2.51	1.43	1.38
86	WA	5199	ANM	C6-C5	2.41	1.57	1.49
89	v	900	GDP	C5-N7	-2.33	1.34	1.39
89	v	900	GDP	C2'-C1'	2.25	1.60	1.53
89	v	900	GDP	C4-N9	-2.22	1.32	1.38
89	v	900	GDP	O3'-C3'	2.07	1.48	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	v	900	GDP	C1'-N9-C8	-6.61	107.96	126.73
86	WA	5199	ANM	O2-C5-C6	4.99	119.99	111.09
89	v	900	GDP	N9-C8-N7	-4.89	104.34	113.40
89	v	900	GDP	C5-C4-N3	-4.47	121.28	128.39
89	v	900	GDP	C1'-N9-C4	4.22	138.97	126.49
89	v	900	GDP	C2-N3-C4	4.16	119.46	112.30
89	v	900	GDP	N9-C4-N3	4.01	133.97	125.95
89	v	900	GDP	C8-N9-C4	3.76	113.08	106.03
89	v	900	GDP	C2-N1-C6	-2.86	119.93	125.11
89	v	900	GDP	C8-N7-C5	2.75	109.15	104.26
89	v	900	GDP	C5-C6-N1	2.65	120.00	113.25
89	v	900	GDP	O6-C6-C5	-2.54	119.83	126.53
86	WA	5199	ANM	C12-C15-C16	-2.46	109.22	113.40
86	WA	5199	ANM	C2-O2-C5	-2.21	114.28	117.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

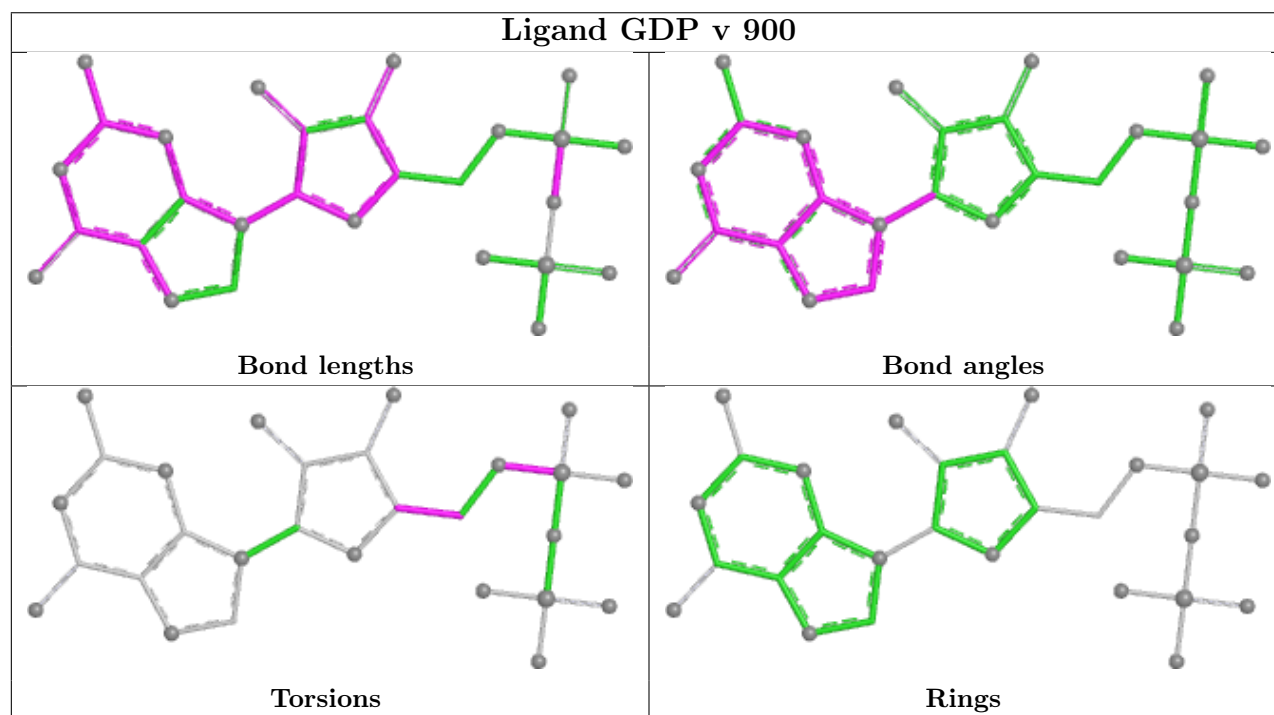
Mol	Chain	Res	Type	Atoms
89	v	900	GDP	C5'-O5'-PA-O3A
89	v	900	GDP	C5'-O5'-PA-O2A
87	WA	5200	SPD	N6-C7-C8-C9
89	v	900	GDP	O4'-C4'-C5'-O5'
89	v	900	GDP	C5'-O5'-PA-O1A

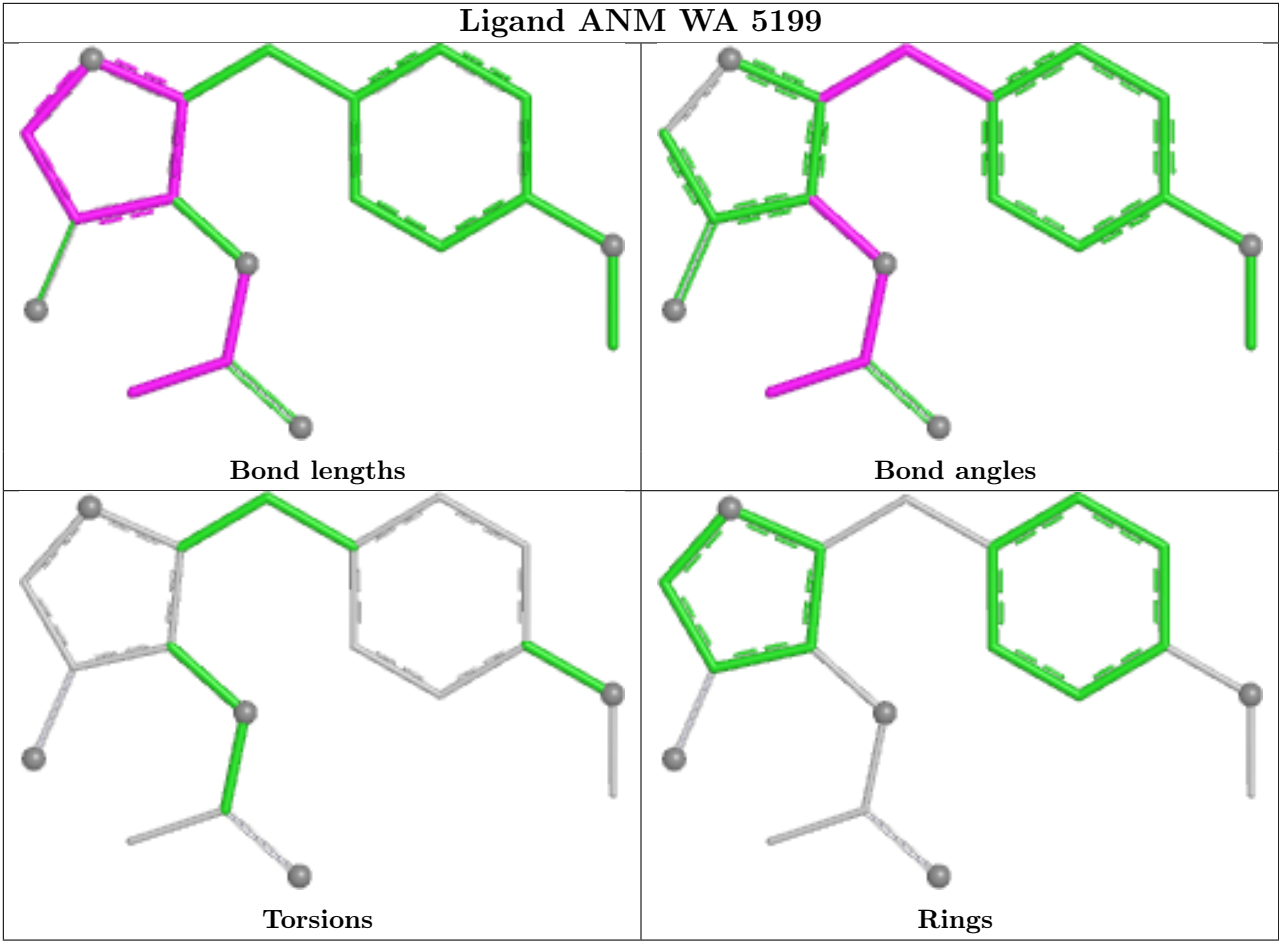
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	v	900	GDP	2	0
86	WA	5199	ANM	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	WA	19
52	w	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	221:VAL	C	282:THR	N	59.11
1	WA	2118:G	O3'	2263:C	P	40.34
1	WA	1258:C	O3'	1277:G	P	36.79
1	WA	2906:G	O3'	3602:G	P	19.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	WA	4106:C	O3'	4112:G	P	18.00
1	WA	4143:C	O3'	4151:G	P	17.00
1	WA	1701:C	O3'	1725:C	P	16.82
1	WA	524:C	O3'	639:G	P	15.75
1	WA	5027:U	O3'	5033:G	P	15.32
1	WA	762:G	O3'	906:C	P	14.57
1	WA	996:U	O3'	1070:G	P	14.49
1	WA	1370:U	O3'	1374:A	P	13.08
1	WA	182:G	O3'	189:G	P	11.43
1	WA	501:G	O3'	505:G	P	7.06
1	WA	4734:A	O3'	4740:G	P	6.15
1	WA	513:U	O3'	516:C	P	5.85
1	WA	4745:G	O3'	4748:G	P	5.74
1	WA	1245:C	O3'	1250:G	P	4.40
1	WA	3766:C	O3'	3767:B8H	P	4.01
1	WA	3767:B8H	O3'	3768:A	P	3.17

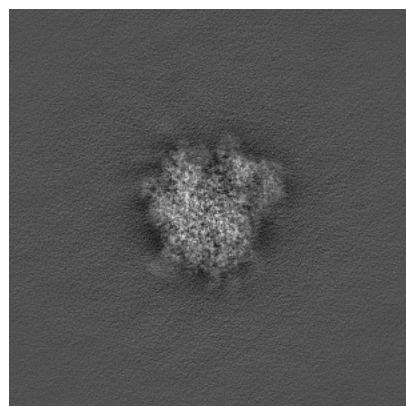
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43568. These allow visual inspection of the internal detail of the map and identification of artifacts.

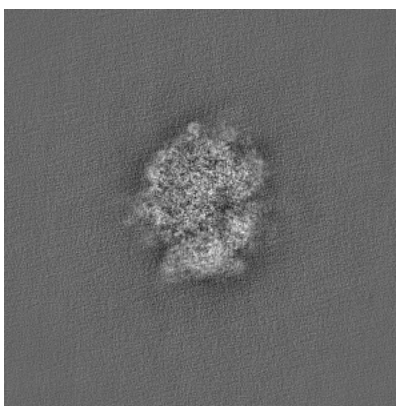
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

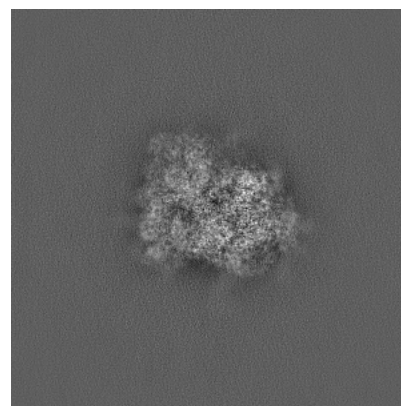
6.1.1 Primary map



X

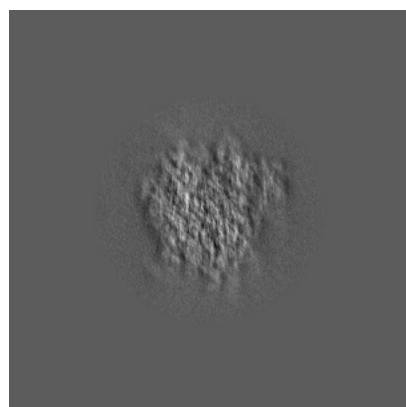


Y

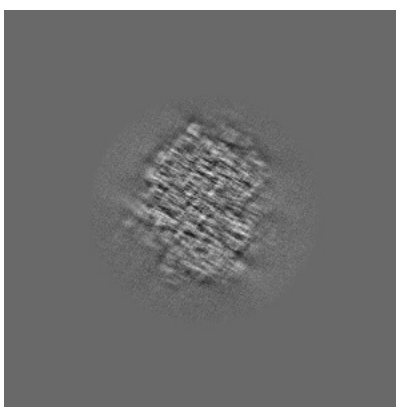


Z

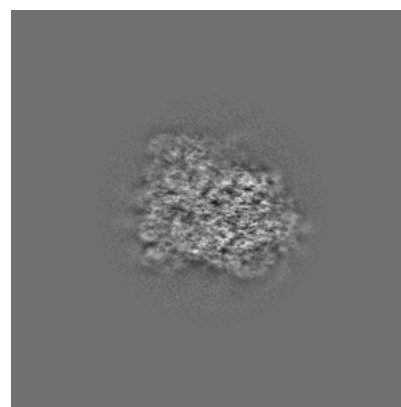
6.1.2 Raw map



X



Y

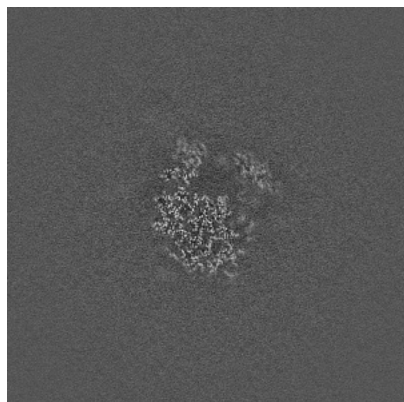


Z

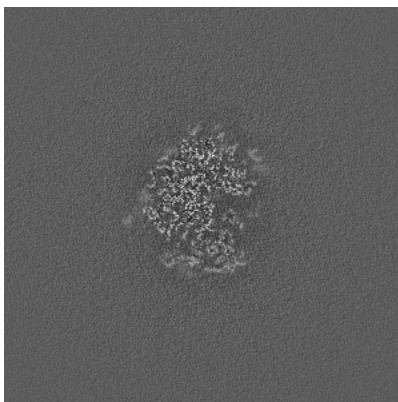
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

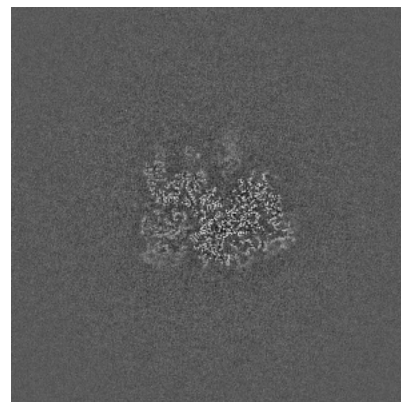
6.2.1 Primary map



X Index: 324

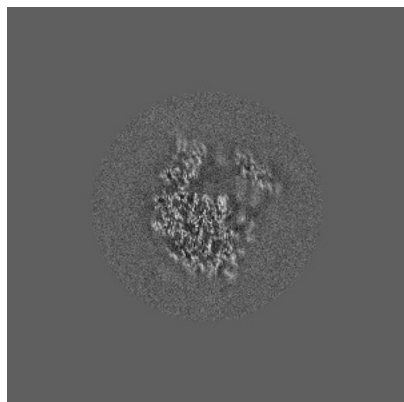


Y Index: 324

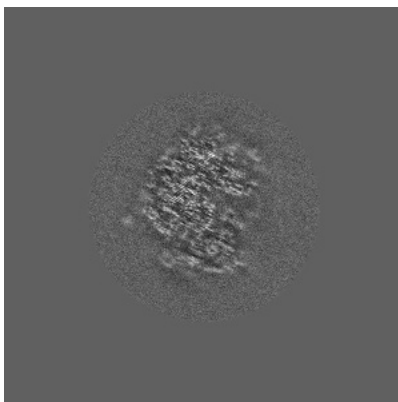


Z Index: 324

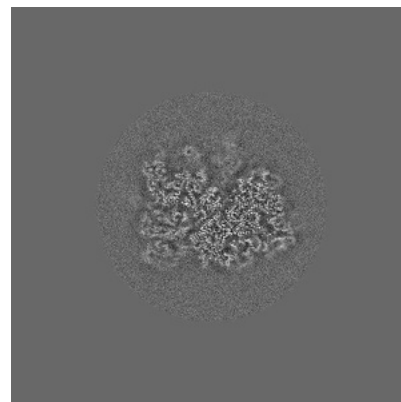
6.2.2 Raw map



X Index: 324



Y Index: 324

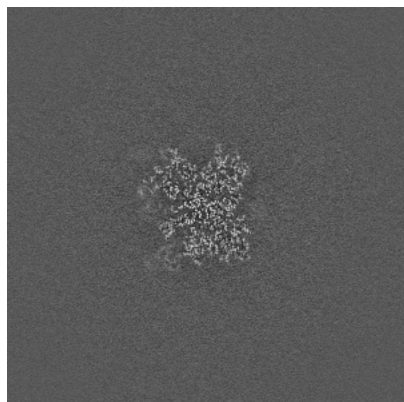


Z Index: 324

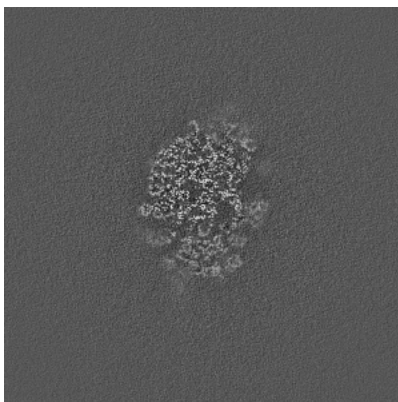
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

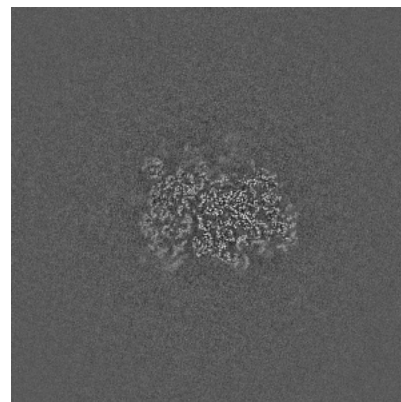
6.3.1 Primary map



X Index: 373

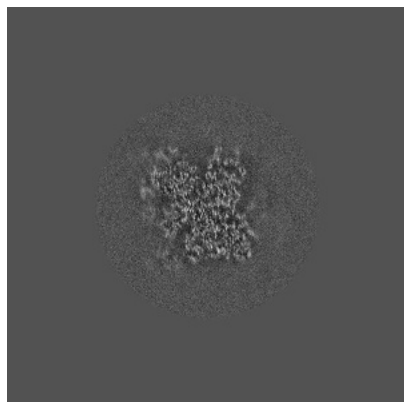


Y Index: 302

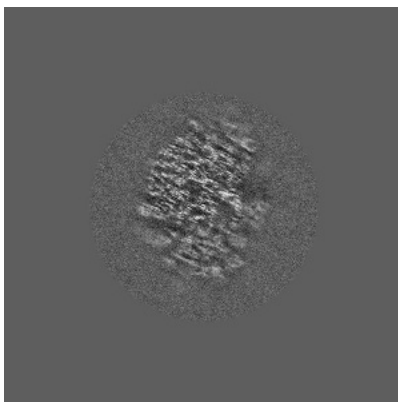


Z Index: 315

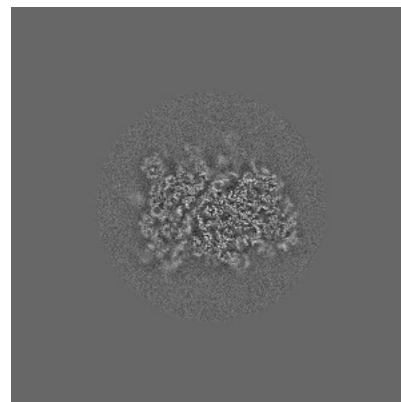
6.3.2 Raw map



X Index: 369



Y Index: 302

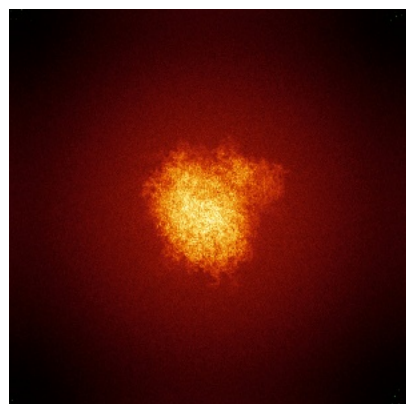


Z Index: 314

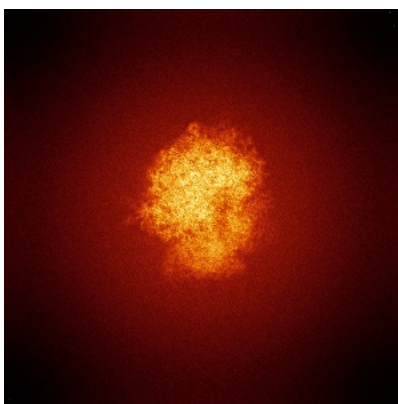
The images above show the largest variance slices of the map in three orthogonal directions.

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

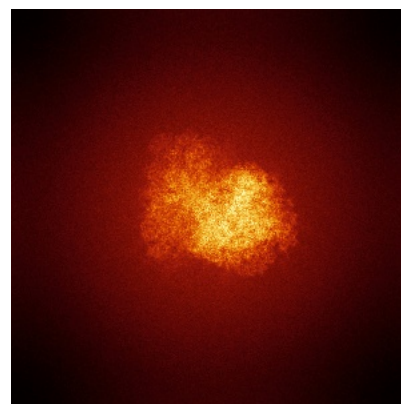
6.4.1 Primary map



X

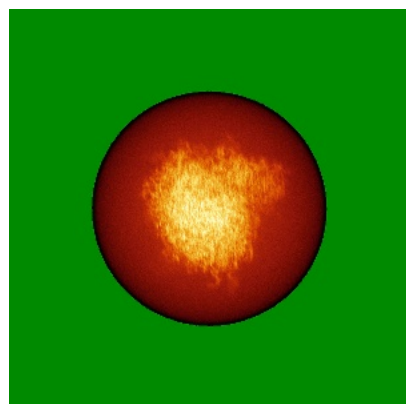


Y

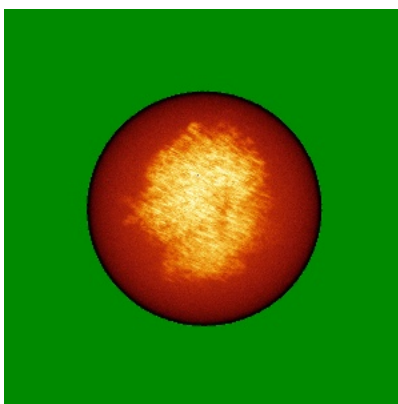


Z

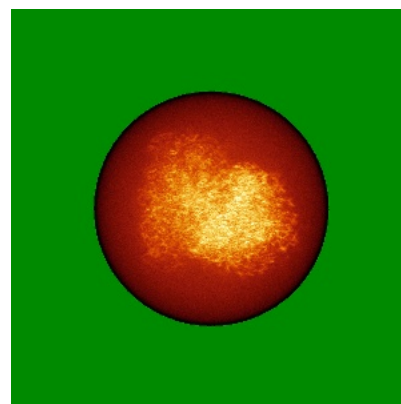
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

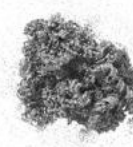
6.5.1 Primary map



X



Y



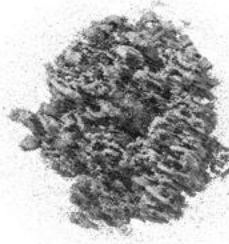
Z

The images above show the 3D surface view of the map at the recommended contour level 6.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

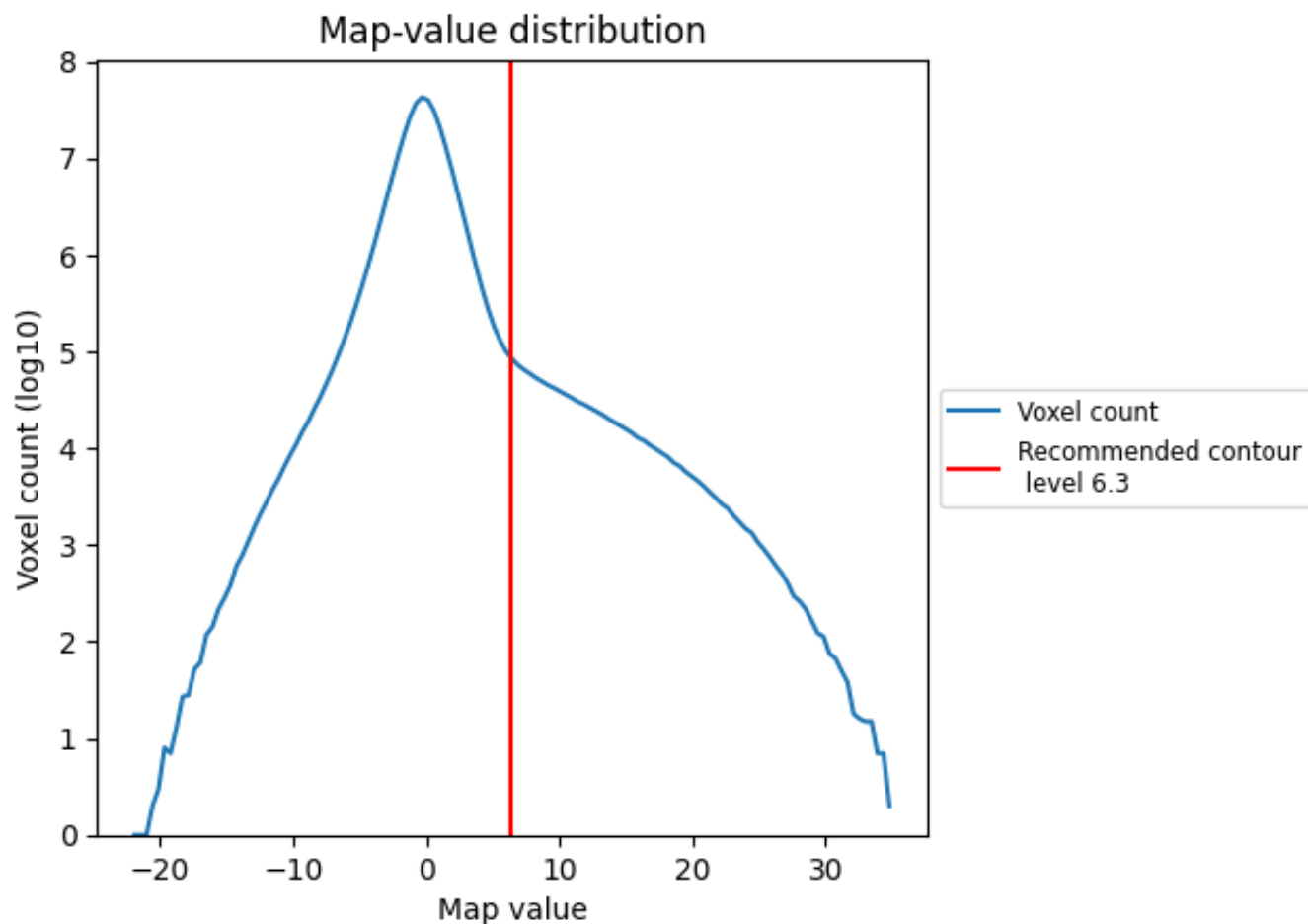
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

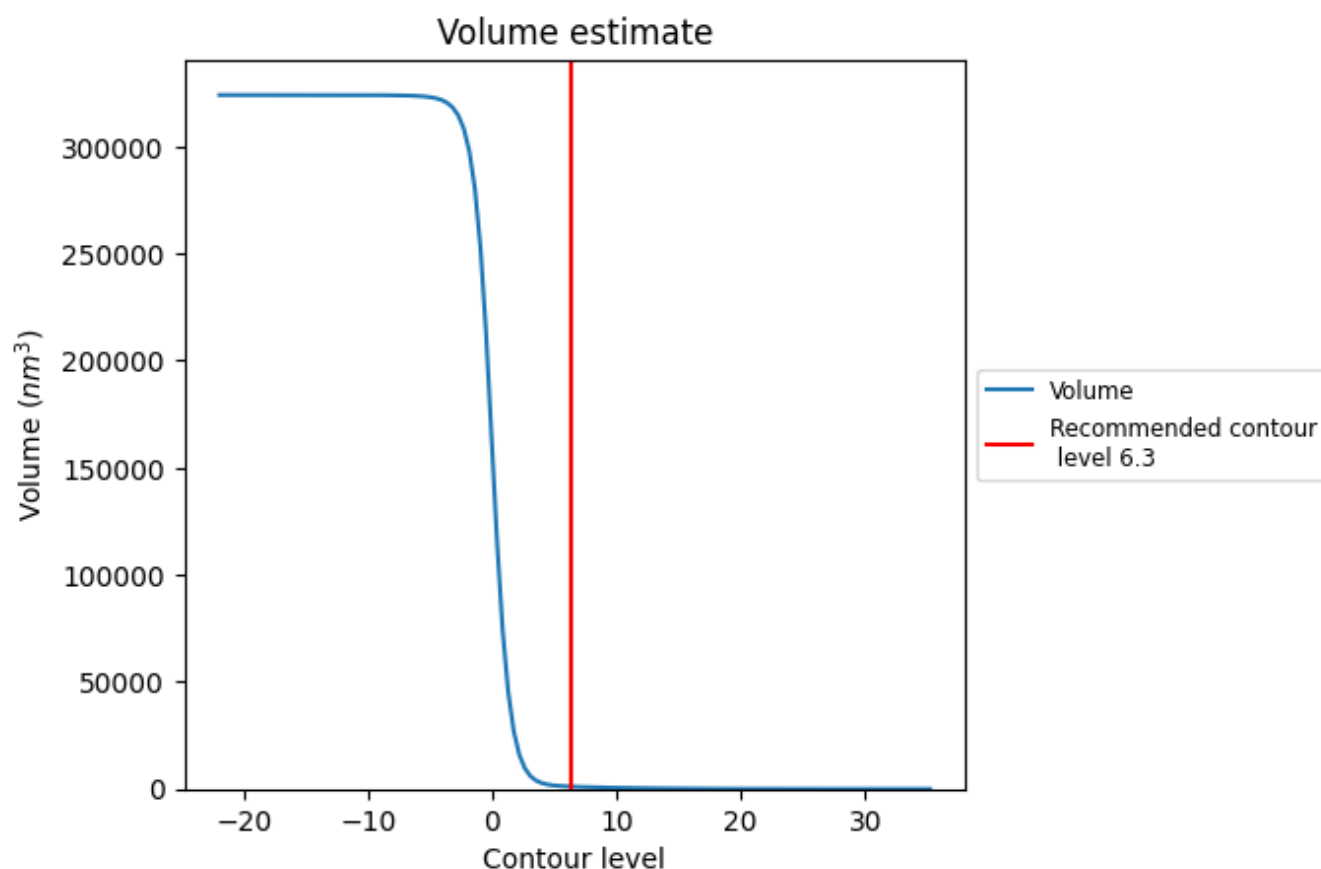
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

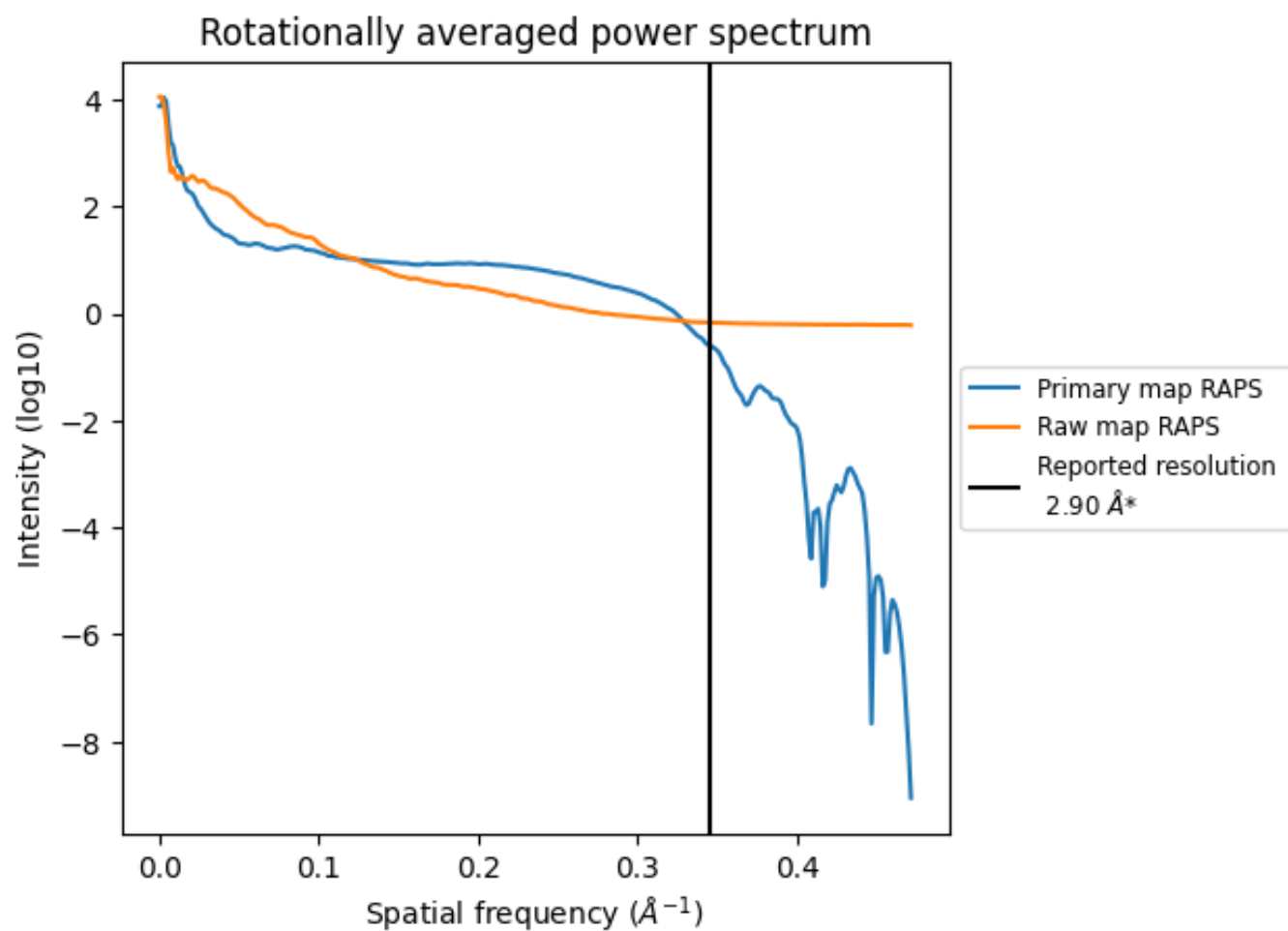
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1124 nm^3 ; this corresponds to an approximate mass of 1016 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

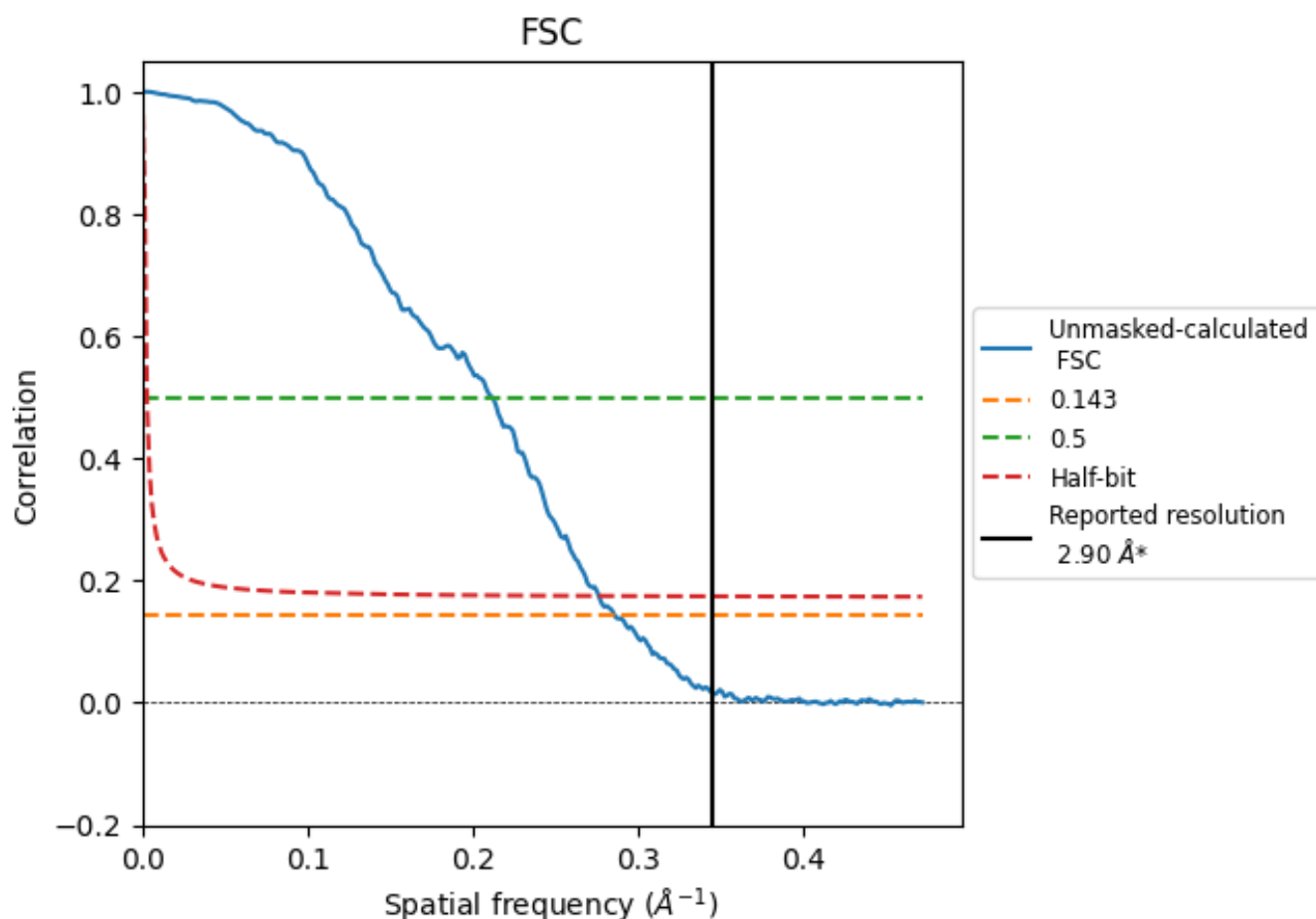


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

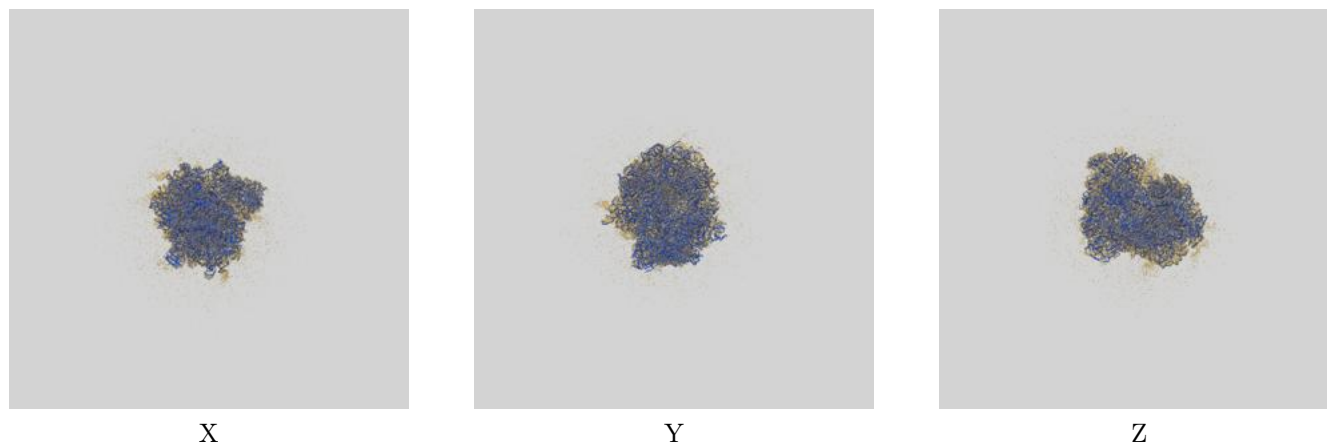
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	4.73	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.50 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

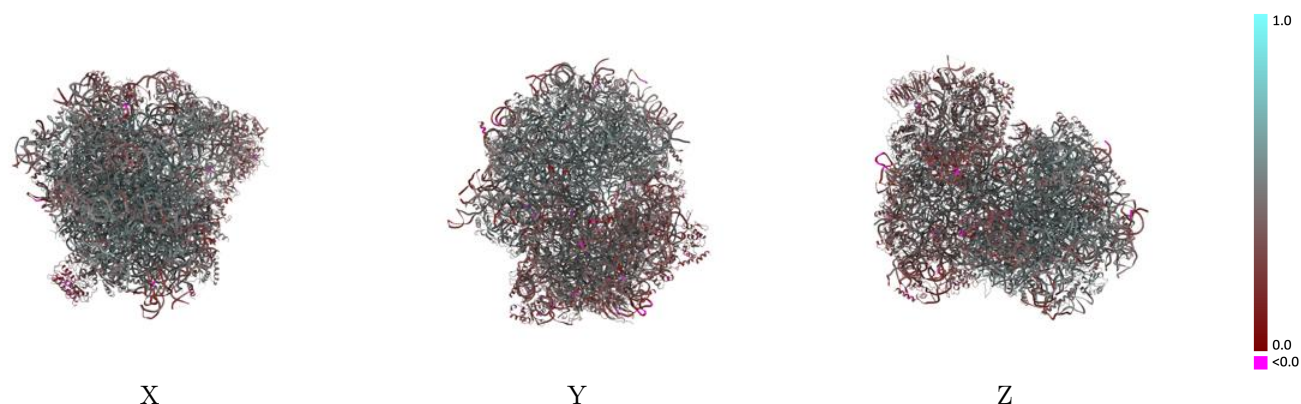
This section contains information regarding the fit between EMDB map EMD-43568 and PDB model 8VVT. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



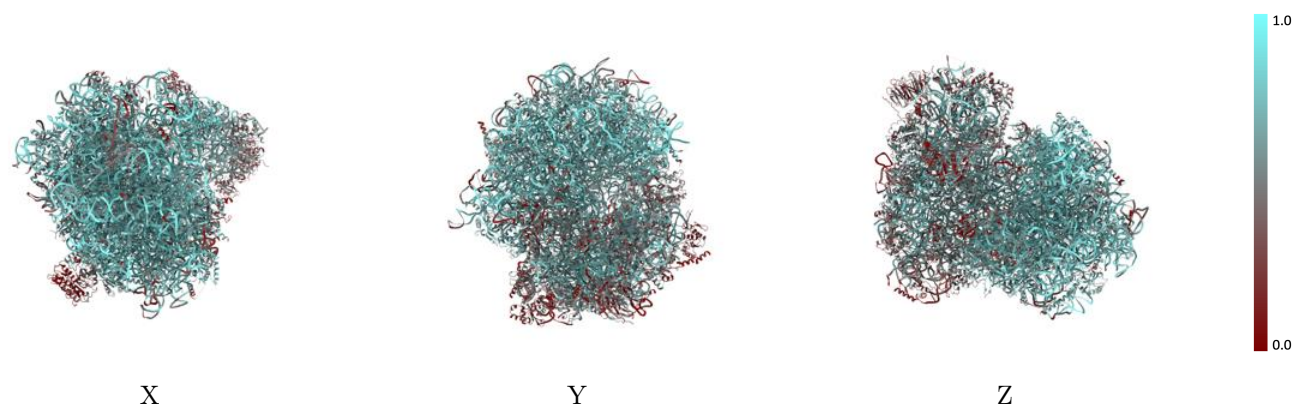
The images above show the 3D surface view of the map at the recommended contour level 6.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



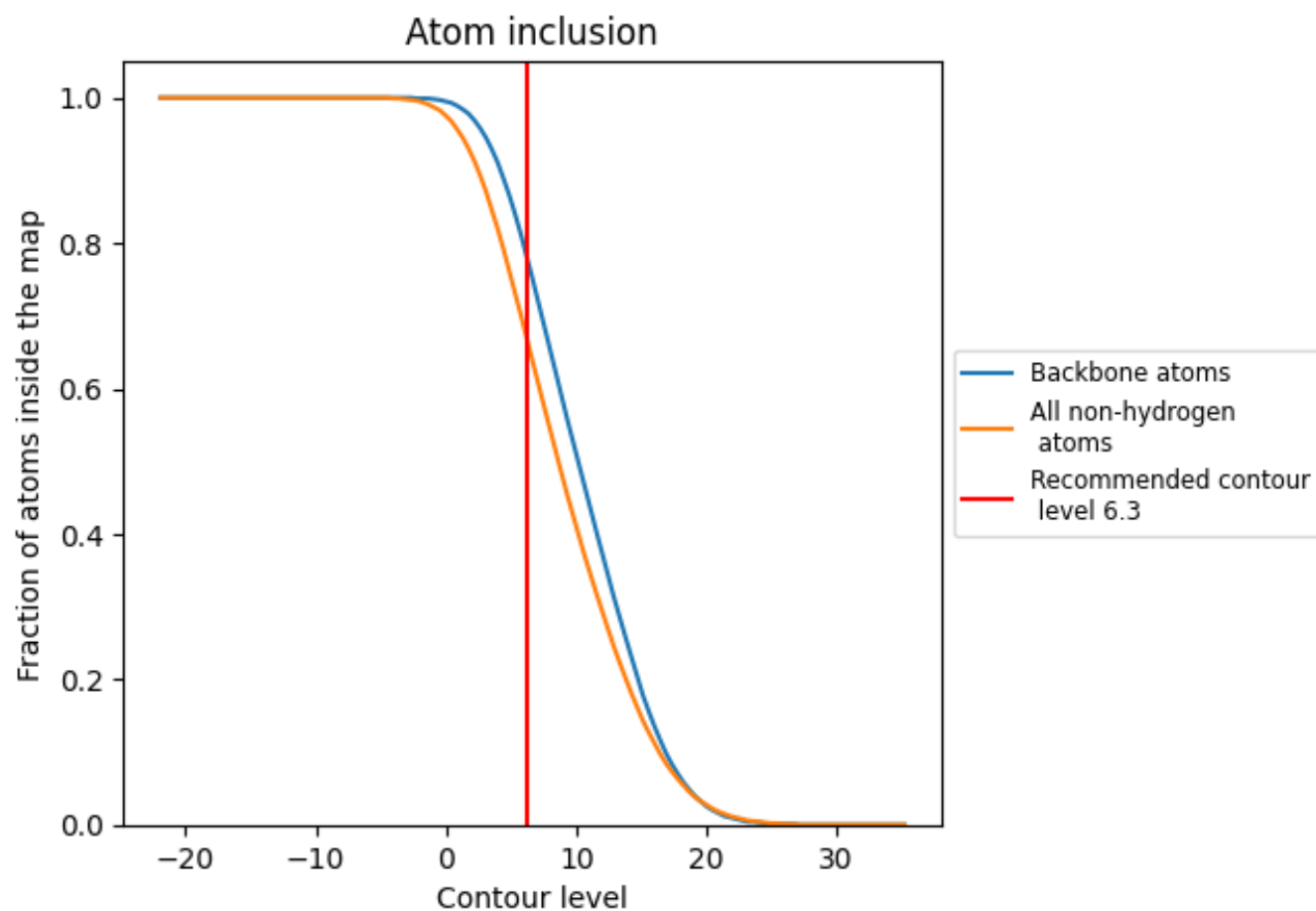
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 66% 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 (6.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.4450
A	 0.7030	 0.5280
AA	 0.6070	 0.4690
AB	 0.4930	 0.4000
AC	 0.5180	 0.4400
B	 0.7090	 0.5210
BA	 0.6500	 0.4650
BB	 0.3710	 0.3540
BC	 0.4080	 0.3690
C	 0.6840	 0.5120
CA	 0.6660	 0.4940
CB	 0.5770	 0.4450
CC	 0.3430	 0.3240
D	 0.7060	 0.4790
DA	 0.7090	 0.5320
DB	 0.5000	 0.4080
DC	 0.5750	 0.4240
E	 0.6630	 0.4880
EA	 0.7170	 0.5330
EB	 0.4640	 0.4010
EC	 0.4550	 0.4000
F	 0.6970	 0.5200
FA	 0.6840	 0.5080
FB	 0.3820	 0.3390
FC	 0.2130	 0.2950
G	 0.6390	 0.4500
GA	 0.6510	 0.4760
GB	 0.3000	 0.2970
GC	 0.3330	 0.3220
H	 0.6720	 0.4960
HA	 0.6860	 0.4700
HB	 0.3030	 0.3410
I	 0.6950	 0.5110
IA	 0.7490	 0.5330
IB	 0.3870	 0.3670



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Chain	Atom inclusion	Q-score
J	 0.6260	 0.4530
JA	 0.5980	 0.4450
JB	 0.5520	 0.4110
K	 0.6720	 0.4860
KA	 0.6590	 0.4890
KB	 0.4770	 0.3670
L	 0.7010	 0.4820
LA	 0.7100	 0.5090
LB	 0.4960	 0.4290
M	 0.7350	 0.5330
MA	 0.6010	 0.4850
MB	 0.1530	 0.2470
N	 0.7240	 0.5090
NA	 0.6780	 0.5150
NB	 0.4710	 0.4090
O	 0.7110	 0.5210
OA	 0.6780	 0.5170
OB	 0.4130	 0.3810
P	 0.7060	 0.5250
PA	 0.7170	 0.5130
PB	 0.5000	 0.3910
Q	 0.6180	 0.4650
QA	 0.4330	 0.3400
QB	 0.4220	 0.3680
R	 0.7050	 0.5180
RA	 0.2350	 0.2580
RB	 0.3420	 0.3540
S	 0.6830	 0.5080
SB	 0.4170	 0.3550
T	 0.6280	 0.4370
TB	 0.4560	 0.3660
U	 0.6770	 0.5230
UB	 0.4120	 0.3600
V	 0.5210	 0.4180
VB	 0.5260	 0.4070
W	 0.6890	 0.4960
WA	 0.7980	 0.4770
WB	 0.5440	 0.4550
X	 0.6770	 0.4910
XA	 0.8690	 0.5150
XB	 0.5600	 0.4650
Y	 0.6800	 0.4730

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Chain	Atom inclusion	Q-score
YA	 0.8030	 0.4820
YB	 0.4040	 0.3420
Z	 0.7460	 0.5270
ZA	 0.6580	 0.4000
ZB	 0.3430	 0.3220
b	 0.2020	 0.3040
v	 0.4930	 0.3890
w	 0.4460	 0.3970