



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 03:14 am BST

PDB ID : 7OYD / pdb_00007oyd
EMDB ID : EMD-13114
Title : Cryo-EM structure of a rabbit 80S ribosome with zebrafish Dap1b
Authors : Leesch, F.; Lorenzo-Orts, L.; Grishkovskaya, I.; Kandolf, S.; Belacic, K.; Meinhart, A.; Haselbach, D.; Pauli, A.
Deposited on : 2021-06-24
Resolution : 2.30 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:

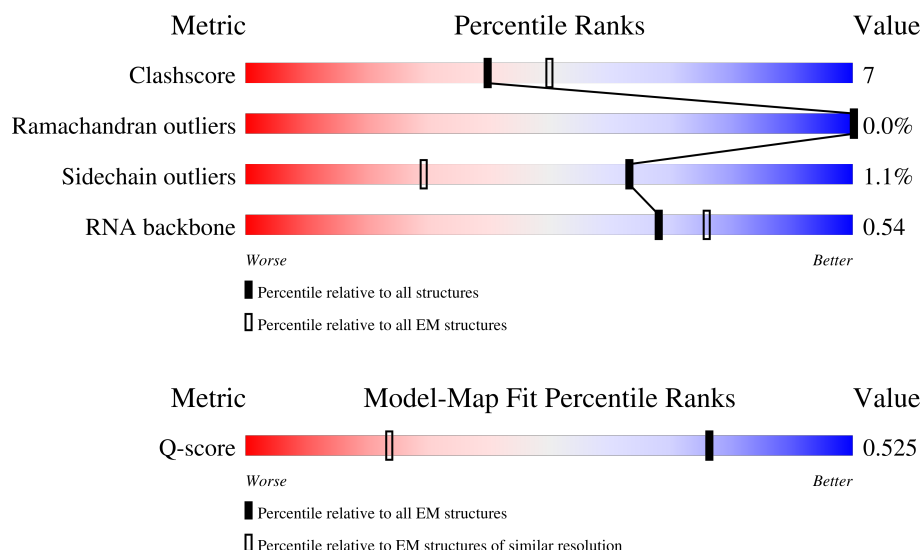
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.30 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.



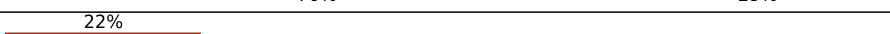
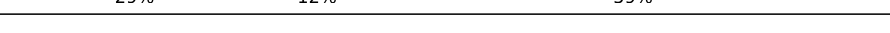
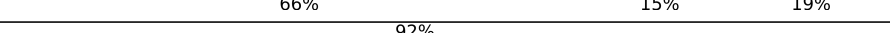
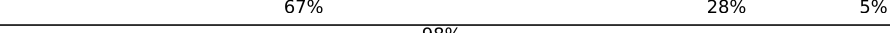
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	x	217	42% 59% 15% 25%
2	5	3740	63% 21% 5% 10%
3	8	156	73% 17% 8%

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Mol	Chain	Length	Quality of chain
4	9	1786	
5	A	257	
6	AA	295	
7	Aa	115	
8	B	403	
9	BB	264	
10	Bb	84	
11	C	413	
12	CC	293	
13	Cc	69	
14	D	297	
15	DD	243	
16	Dd	56	
17	E	291	
18	EE	263	
19	Ee	133	
20	F	249	
21	FF	204	
22	G	266	
23	GG	249	
24	Gg	317	
25	H	192	
26	HH	432	
27	I	214	
28	II	208	

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Mol	Chain	Length	Quality of chain
29	J	178	
30	JJ	194	
31	K	120	
32	KK	165	
33	L	211	
34	LL	158	
35	M	218	
36	N	204	
37	NN	151	
38	O	203	
39	OO	151	
40	P	187	
41	PP	145	
42	Q	188	
43	QQ	146	
44	R	196	
45	RR	135	
46	S	224	
47	SS	152	
48	T	160	
49	TT	145	
50	U	141	
51	UU	119	
52	V	140	
53	VV	83	

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Mol	Chain	Length	Quality of chain
54	W	157	
55	WW	130	
56	X	156	
57	XX	143	
58	Y	145	
59	YY	133	
60	Z	136	
61	ZZ	124	
62	a	148	
63	b	245	
64	c	115	
65	d	125	
66	e	157	
67	f	110	
68	g	117	
69	h	123	
70	i	105	
71	j	97	
72	k	70	
73	l	51	
74	m	128	
75	n	25	
76	o	106	
77	p	92	
78	r	137	

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Mol	Chain	Length	Quality of chain
79	s	318	43%48%13%38%
80	s1	109	16%83%
81	t	154	13%65%16%18%
82	v	858	39%67%17%15%
83	w	407	5%92%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 213014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	163	Total	C	N	O	S	0	0
			1291	832	225	228	6		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	3358	Total	C	N	O	P	0	0
			72165	32204	13226	23377	3358		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	144	Total	C	N	O	P	0	0
			3072	1370	547	1011	144		

- Molecule 4 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	247	Total	C	N	O	S	0	0
			1891	1185	388	312	6		

- Molecule 6 is a protein called 40S ribosomal protein SA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a protein called 40S ribosomal protein S26-like.

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

- Molecule 8 is a protein called Ribosomal protein L3.

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

- Molecule 9 is a protein called 40S ribosomal protein S3a.

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

- Molecule 10 is a protein called 40S ribosomal protein S27.

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

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	358	Total	C	N	O	S	0	0
			2856	1797	572	473	14		

- Molecule 12 is a protein called 40S ribosomal protein S2.

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

- Molecule 13 is a protein called 40S ribosomal protein S28.

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

- Molecule 14 is a protein called 60S ribosomal protein L5.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 15 is a protein called Ribosomal protein S3.

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

- Molecule 16 is a protein called 40S ribosomal protein S29.

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

- Molecule 17 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	213	Total	C	N	O	S	0	0
			1710	1103	325	279	3		

- Molecule 18 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	EE	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
EE	25	GLY	SER	conflict	UNP G1TK17

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

- Molecule 19 is a protein called 40S ribosomal protein S30.

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

- Molecule 20 is a protein called 60S ribosomal protein L7.

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

- Molecule 21 is a protein called Ribosomal protein S5.

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

- Molecule 22 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	215	Total	C	N	O	S	0	0
			1747	1115	337	291	4		

- Molecule 23 is a protein called 40S ribosomal protein S6.

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

- Molecule 24 is a protein called RACK1.

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

- Molecule 25 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	H	186	Total	C	N	O	S	0	0
			1484	933	277	268	6		

- Molecule 26 is a protein called 40S ribosomal protein S7.

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

- Molecule 27 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	202	Total	C	N	O	S	0	0
			1640	1041	317	269	13		

- Molecule 28 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 29 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	168	Total	C	N	O	S	0	0
			1344	850	251	237	6		

- Molecule 30 is a protein called 40S ribosomal protein S9.

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

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

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

- Molecule 32 is a protein called S10_pectin domain-containing protein.

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

- Molecule 33 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	205	Total	C	N	O	S	0	0
			1658	1037	346	271	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 34 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 35 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	M	135	Total	C	N	O	S	0	0
			1117	715	217	178	7		

- Molecule 36 is a protein called Ribosomal protein L15.

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

- Molecule 37 is a protein called 40S ribosomal protein S13.

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

- Molecule 38 is a protein called 60S ribosomal protein L13a.

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

- Molecule 39 is a protein called 40S ribosomal protein S14-like.

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

- Molecule 40 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	152	Total	C	N	O	S	0	0
			1233	772	240	212	9		

- Molecule 41 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	PP	125	Total	C	N	O	S	0	0
			1025	652	192	174	7		

- Molecule 42 is a protein called Ribosomal protein L18.

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

- Molecule 43 is a protein called Ribosomal protein S16.

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

- Molecule 44 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	R	166	Total	C	N	O	S	0	0
			1383	859	298	217	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 45 is a protein called 40S ribosomal protein eS17.

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

- Molecule 46 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S	176	Total	C	N	O	S	0	0
			1456	927	282	236	11		

- Molecule 47 is a protein called 40S ribosomal protein uS13.

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

- Molecule 48 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	158	Total	C	N	O	S	0	0
			1292	820	251	215	6		

- Molecule 49 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	TT	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
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 50 is a protein called 60S ribosomal protein L22-like.

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

- Molecule 51 is a protein called 40S ribosomal protein uS10.

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

- Molecule 52 is a protein called Ribosomal protein L23.

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

- Molecule 53 is a protein called 40S ribosomal protein S21.

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

- Molecule 54 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 55 is a protein called Ribosomal protein S15a.

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

- Molecule 56 is a protein called 60S ribosomal protein L23a.

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

- Molecule 57 is a protein called 40S ribosomal protein S23.

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

- Molecule 58 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 59 is a protein called 40S ribosomal protein S24.

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

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

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

- Molecule 61 is a protein called 40S ribosomal protein S25.

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

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b	98	Total	C	N	O	S	0	0
			806	498	182	123	3		

- Molecule 64 is a protein called 60S ribosomal protein L30.

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

- Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	d	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 66 is a protein called 60S ribosomal protein L32.

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

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	g	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 69 is a protein called 60S ribosomal protein L35.

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

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	i	101	Total	C	N	O	S	0	0
			821	514	174	128	5		

- Molecule 71 is a protein called Ribosomal protein L37.

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

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 73 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 74 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	m	51	Total	C	N	O	S	0	0
			420	261	88	65	6		

- Molecule 75 is a protein called 60s ribosomal protein l41.

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

- Molecule 76 is a protein called 60S ribosomal protein L36a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	o	102	Total	C	N	O	S	0	0
			834	522	171	135	6		

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	r	123	Total	C	N	O	S	0	0
			986	611	204	166	5		

- Molecule 79 is a protein called 60S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	s	196	Total	C	N	O	S	0	0
			1501	953	263	276	9		

- Molecule 80 is a protein called Dap1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	s1	18	Total	C	N	O	S	0	0
			150	96	30	23	1		

- Molecule 81 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	t	126	Total	C	N	O	S	0	0
			961	603	168	182	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	36	SER	GLY	conflict	UNP P10160

- Molecule 82 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	v	726	Total	C	N	O	S	0	0
			5669	3611	972	1046	40		

- Molecule 83 is a protein called SERPINE1 mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	w	32	Total	C	N	O	0	0
			252	148	55	49		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	195	Total	Mg	0
			195	195	
84	8	2	Total	Mg	0
			2	2	
84	I	1	Total	Mg	0
			1	1	
84	P	1	Total	Mg	0
			1	1	
84	g	1	Total	Mg	0
			1	1	
84	v	1	Total	Mg	0
			1	1	

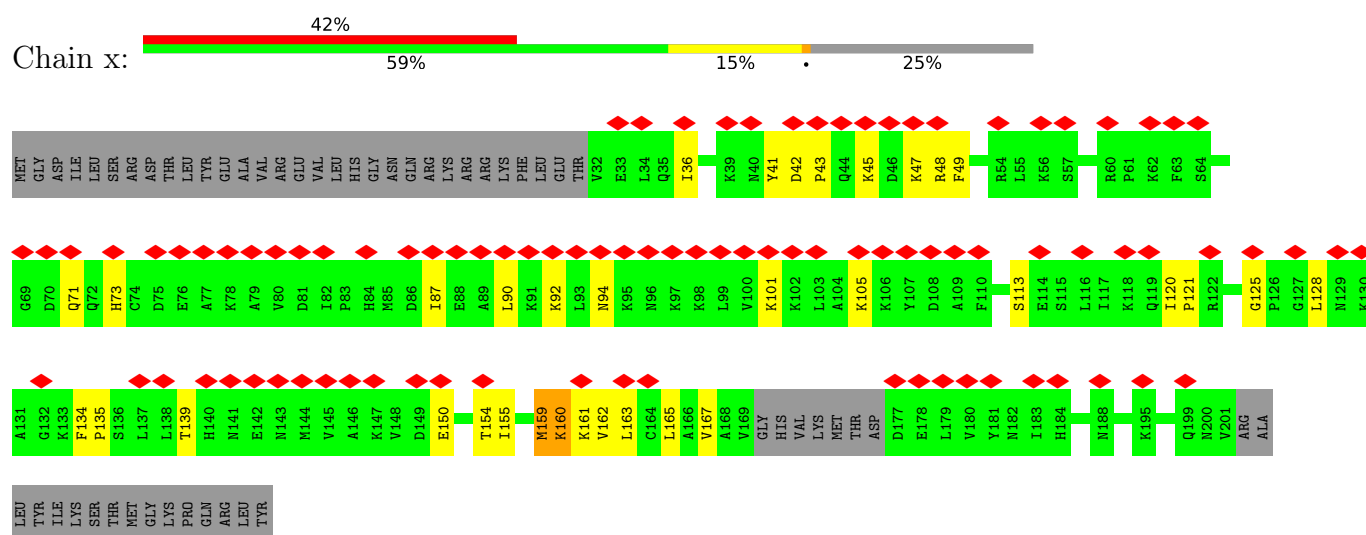
- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	Aa	1	Total	Zn	0
			1	1	
85	KK	1	Total	Zn	0
			1	1	
85	g	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	

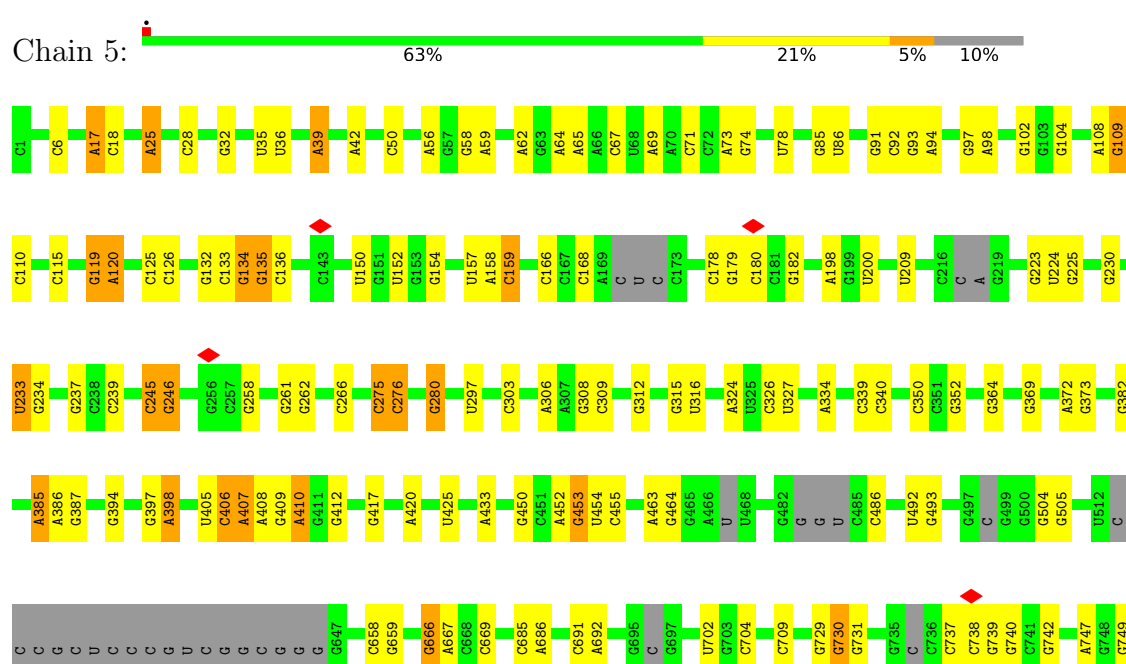
3 Residue-property plots

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

• Molecule 1: Ribosomal protein uL1



• Molecule 2: 28S rRNA

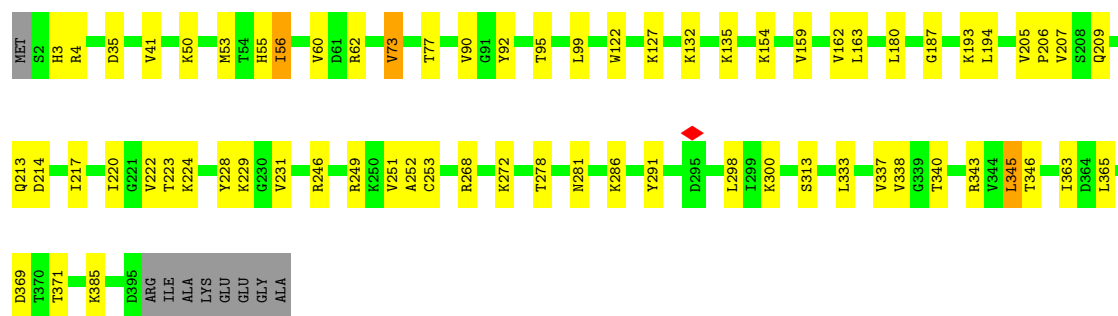






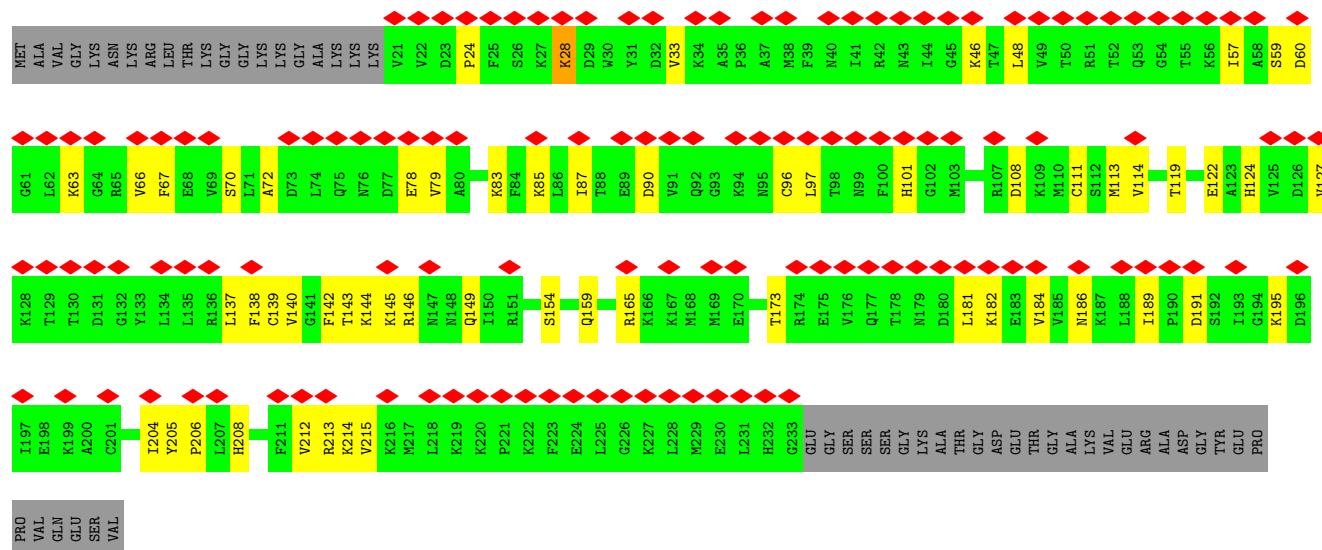


Chain B: 



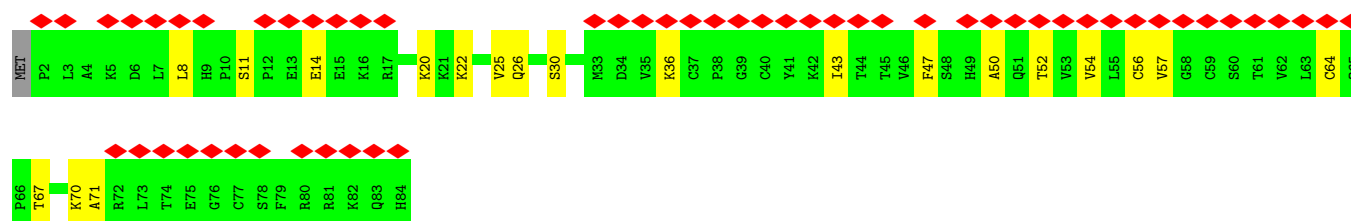
• Molecule 9: 40S ribosomal protein S3a

Chain BB: 



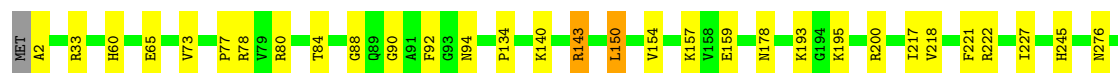
• Molecule 10: 40S ribosomal protein S27

Chain Bb: 

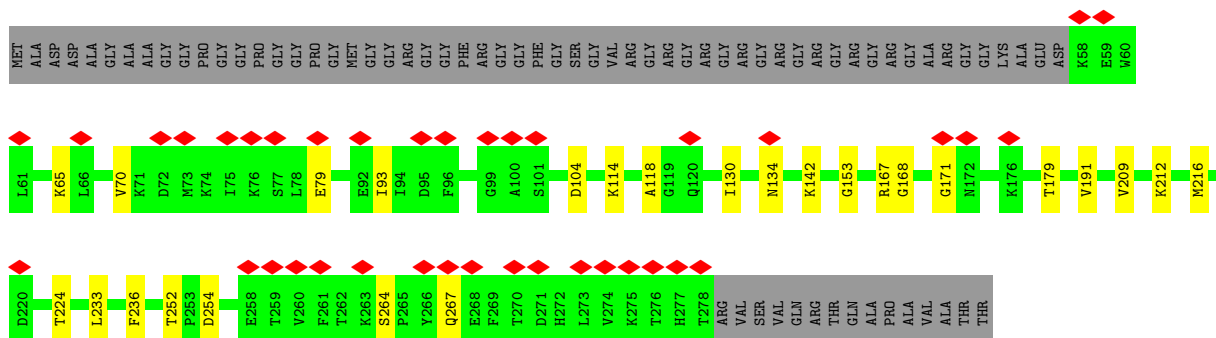


• Molecule 11: 60S ribosomal protein L4

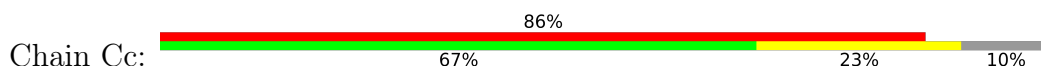
Chain C: 



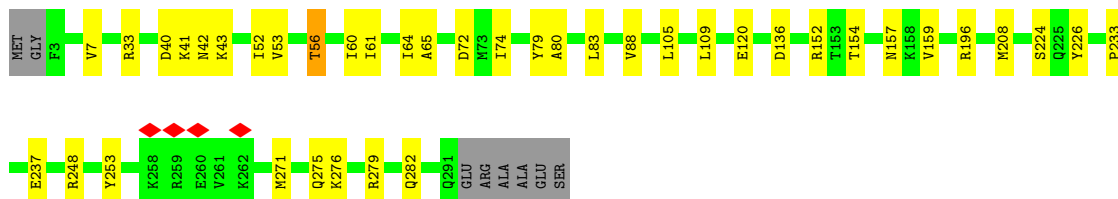
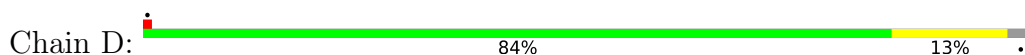
- Molecule 12: 40S ribosomal protein S2



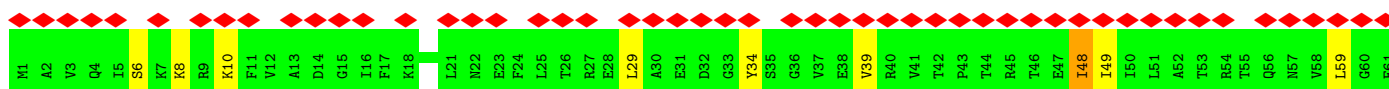
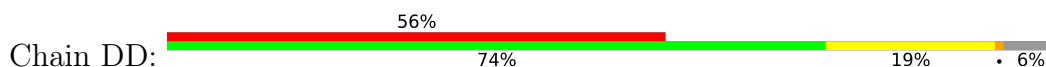
- Molecule 13: 40S ribosomal protein S28

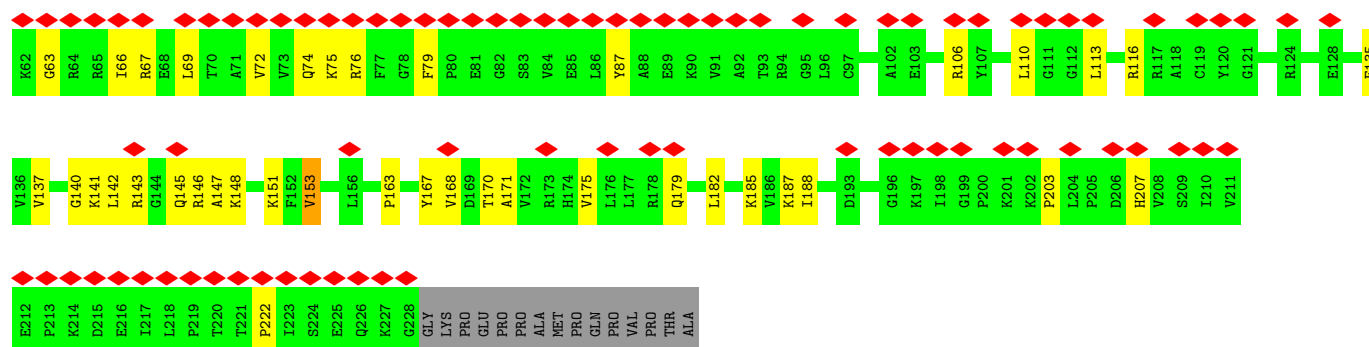


- Molecule 14: 60S ribosomal protein L5

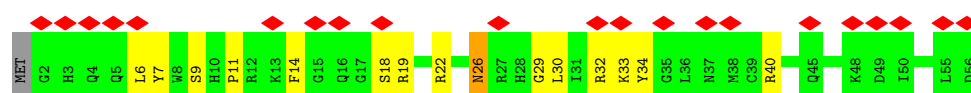
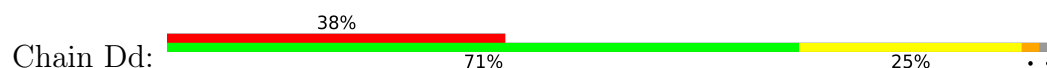


- Molecule 15: Ribosomal protein S3

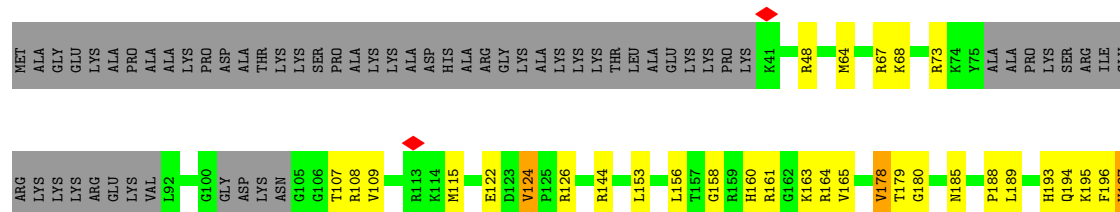




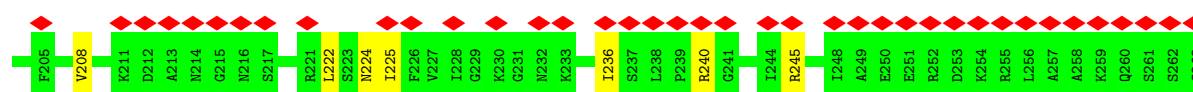
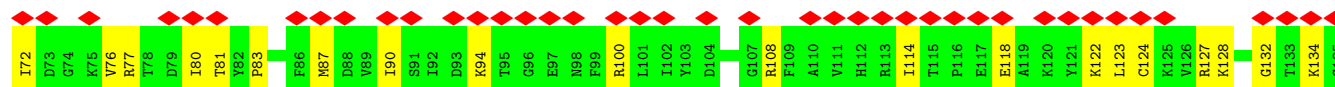
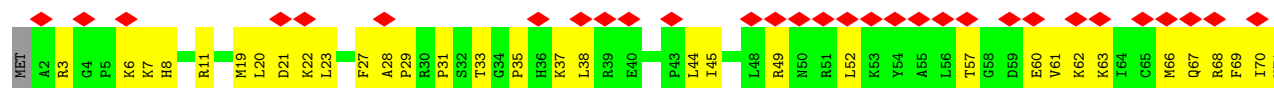
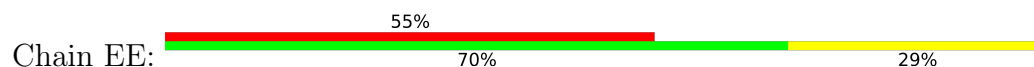
• Molecule 16: 40S ribosomal protein S29

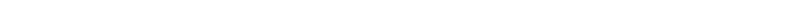


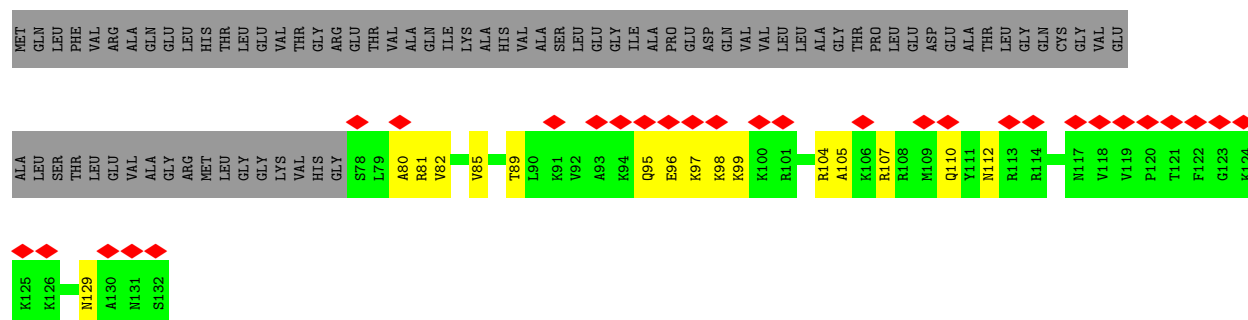
• Molecule 17: 60S ribosomal protein L6



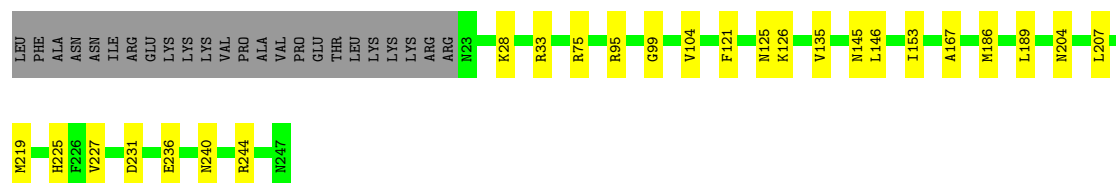
• Molecule 18: 40S ribosomal protein S4

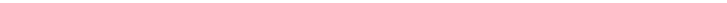


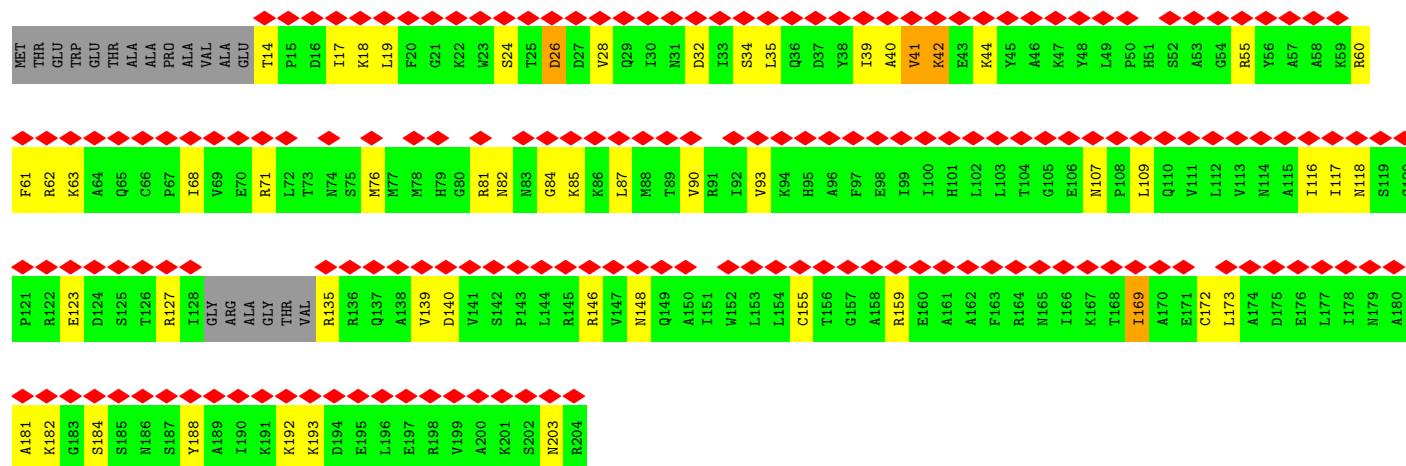
- Chain Ee: 

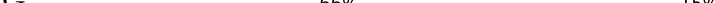


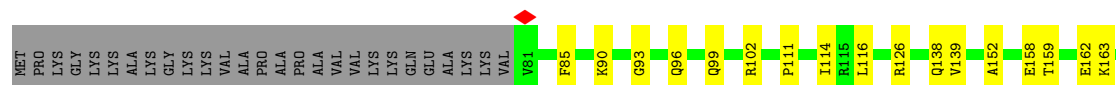
- Chain F: 80% 10% 10%

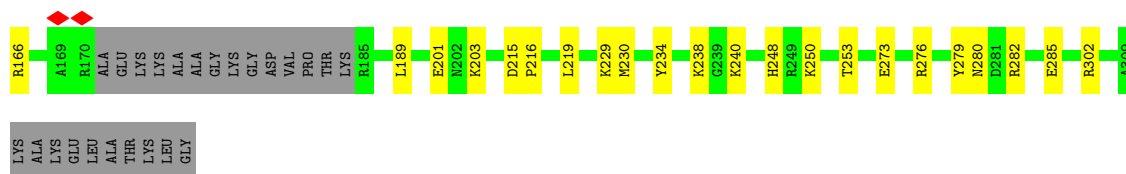


- Chain FF:  86% 64% 25% 9%

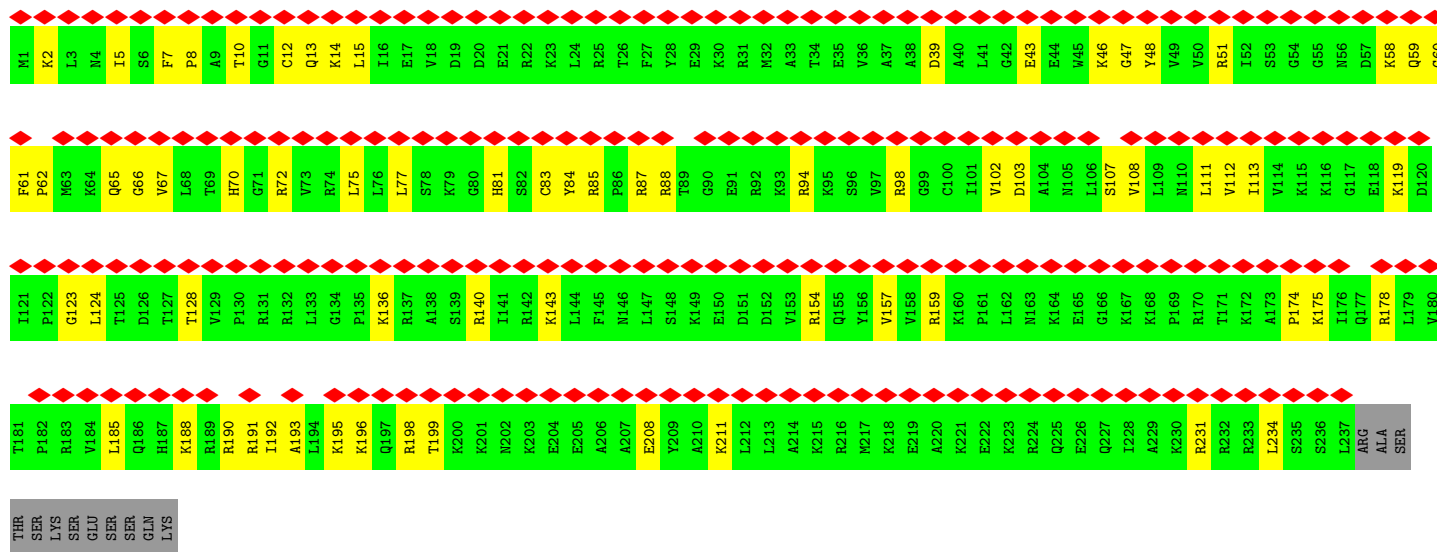


- Chain G:  66% 15% 19%

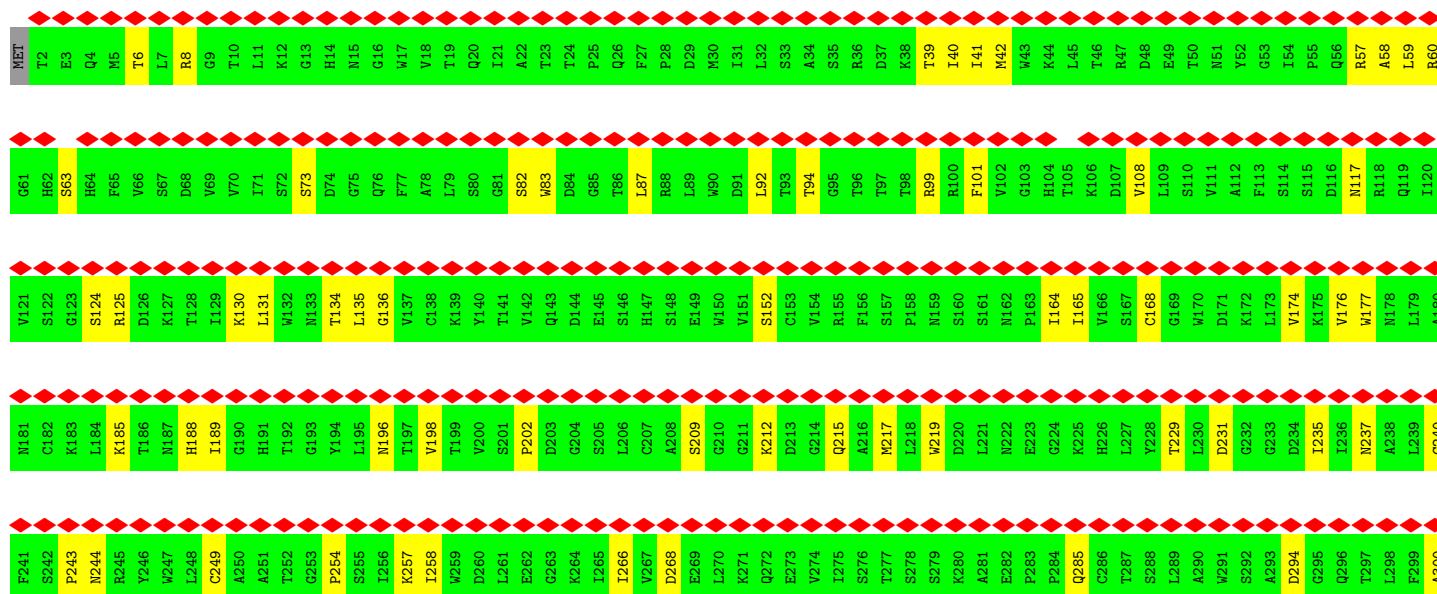
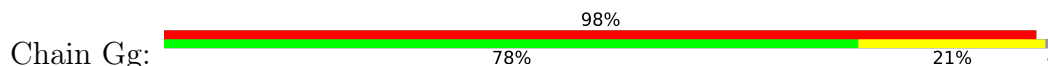


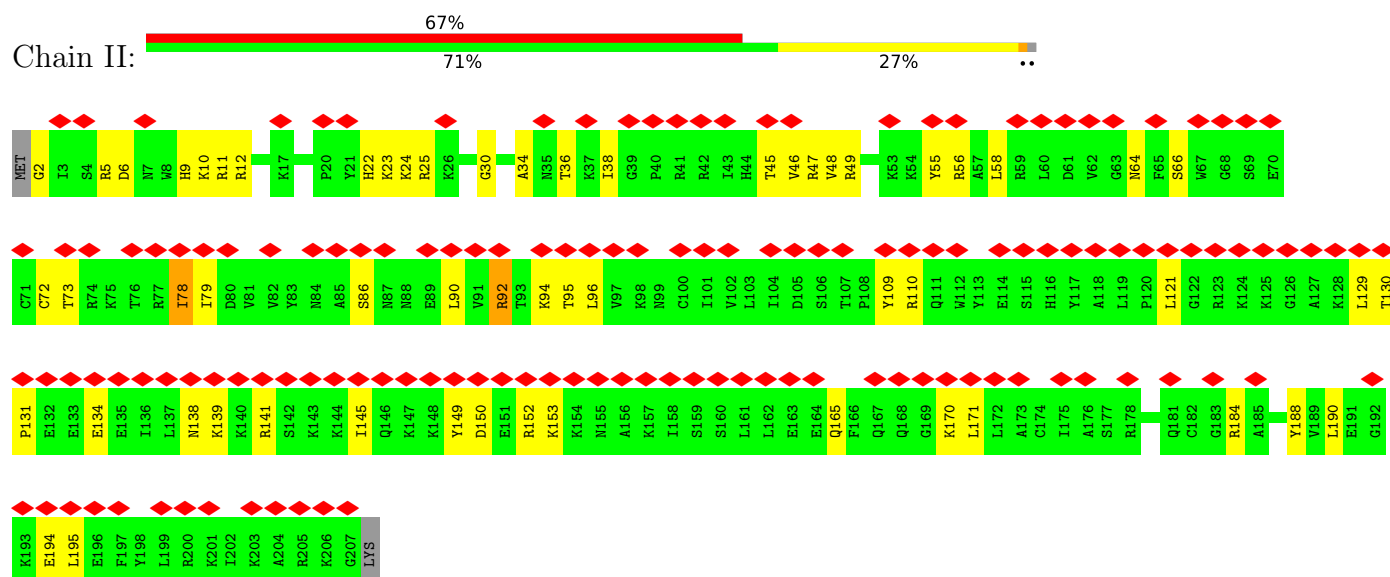


• Molecule 23: 40S ribosomal protein S6

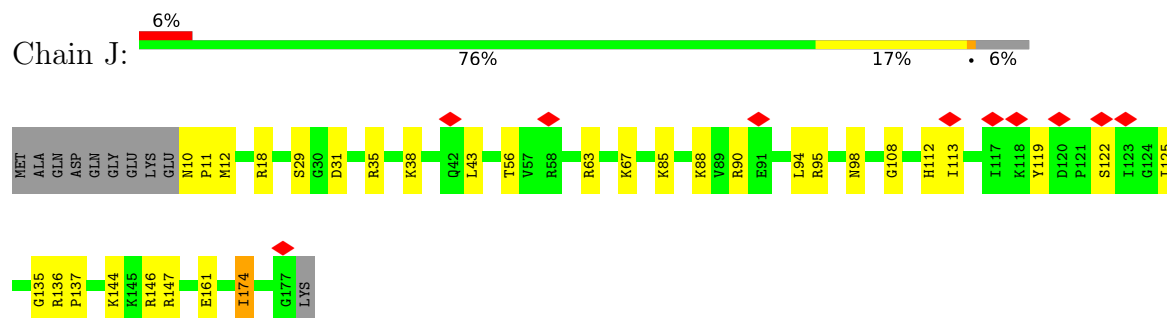


• Molecule 24: RACK1

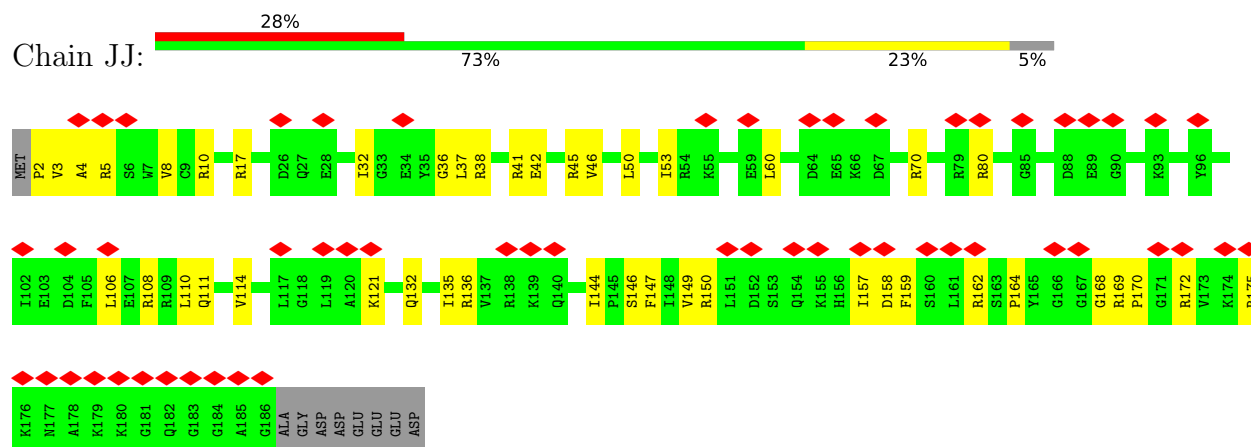




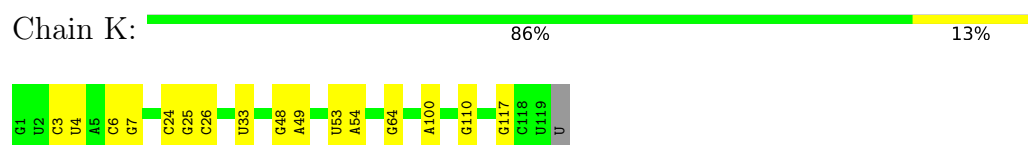
- Molecule 29: 60S ribosomal protein L11



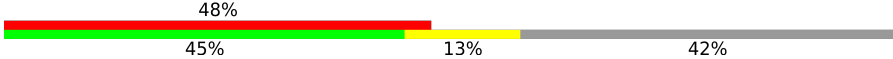
- Molecule 30: 40S ribosomal protein S9

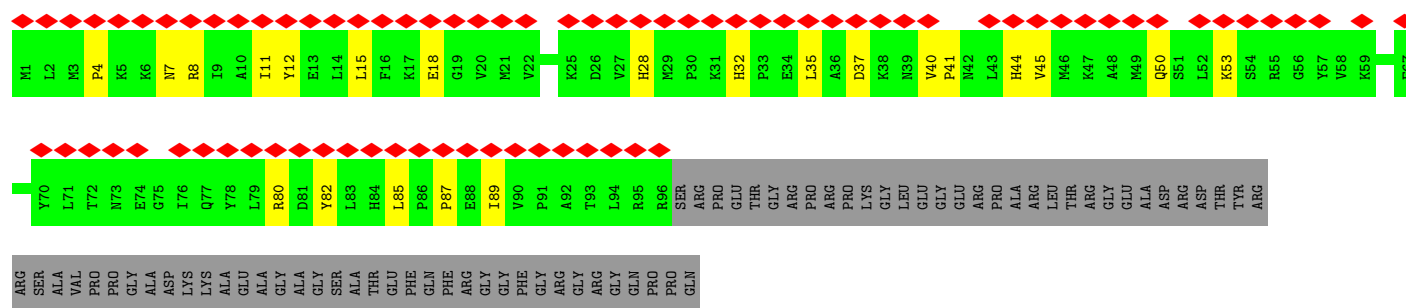


- Molecule 31: 5S rRNA



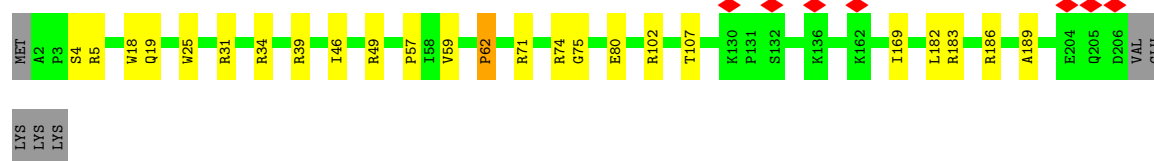
- Molecule 32: S10_ plectin domain-containing protein

Chain KK: 



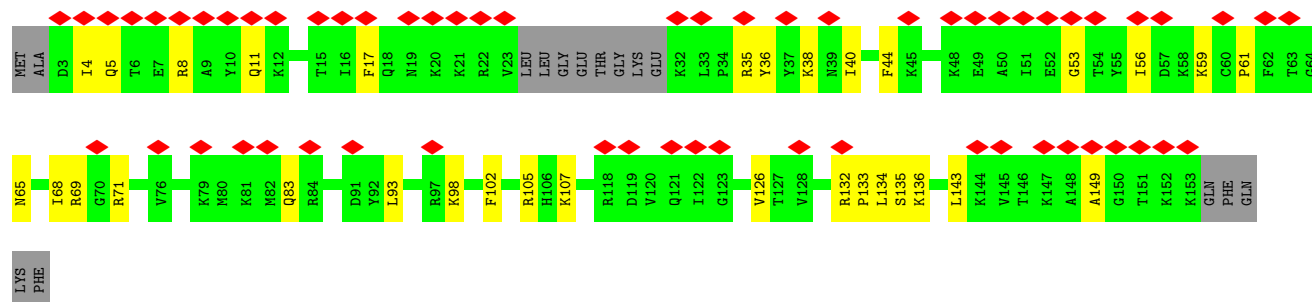
- Molecule 33: 60S ribosomal protein L13

Chain L: 



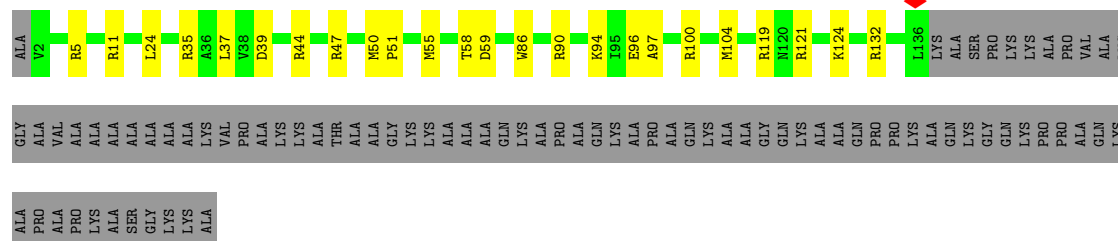
- Molecule 34: 40S ribosomal protein S11

Chain LL: 



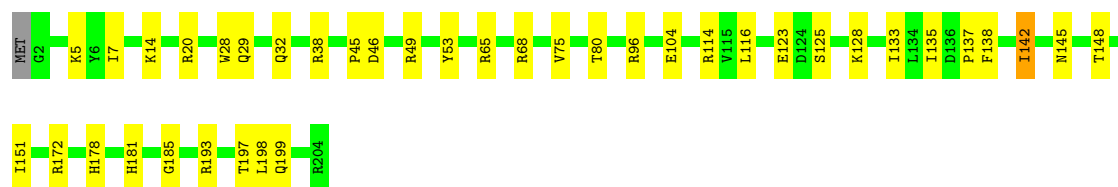
- Molecule 35: 60S ribosomal protein L14

Chain M: 



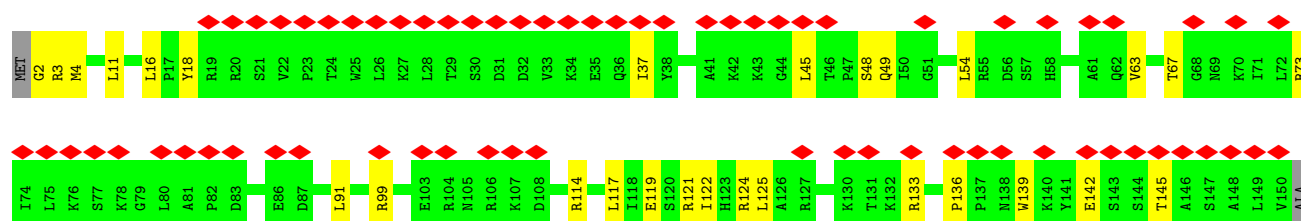
- Molecule 36: Ribosomal protein L15

Chain N:  80% 19%



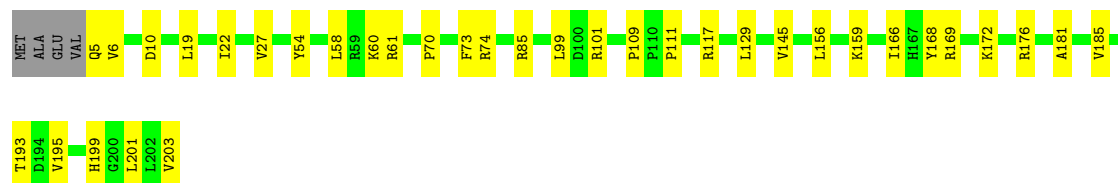
- Molecule 37: 40S ribosomal protein S13

Chain NN:  45% 80% 19%



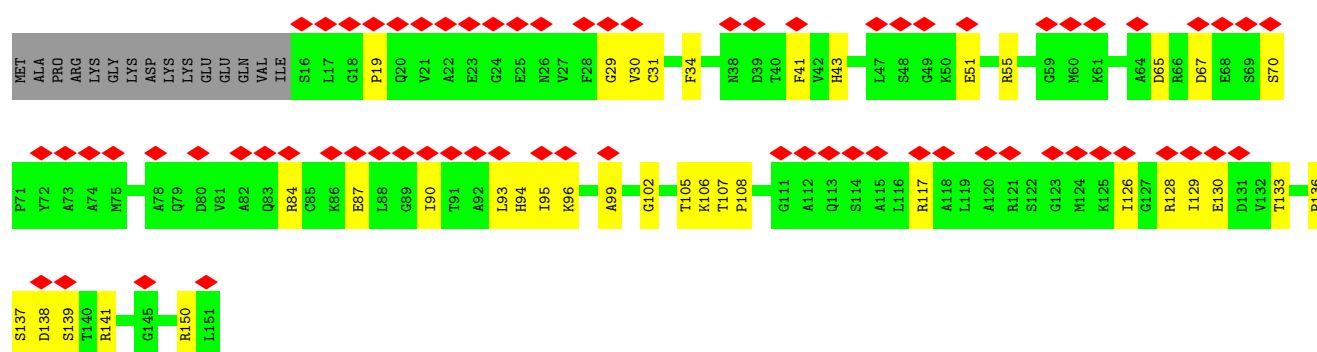
- Molecule 38: 60S ribosomal protein L13a

Chain O:  81% 17%



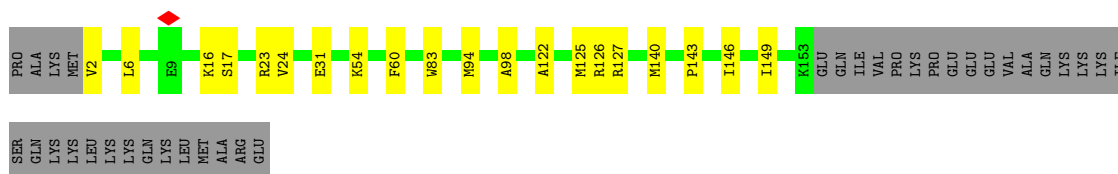
- Molecule 39: 40S ribosomal protein S14-like

Chain OO:  46% 66% 25% 10%

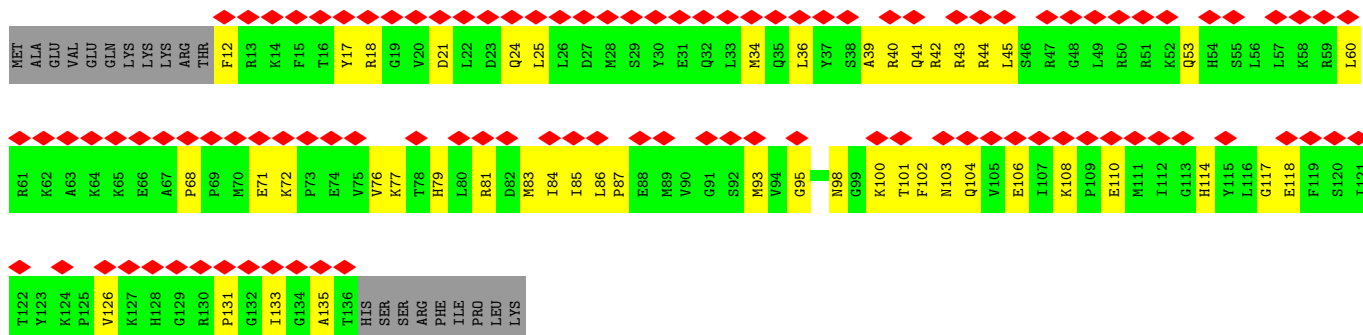
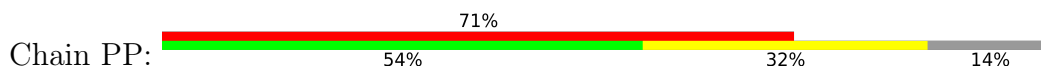


- Molecule 40: 60S ribosomal protein L17

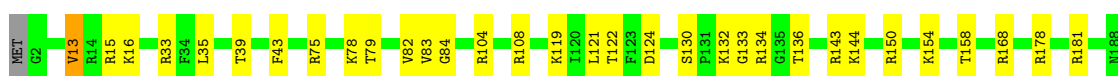
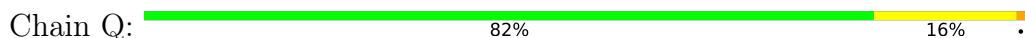
Chain P:  71% 11% 19%



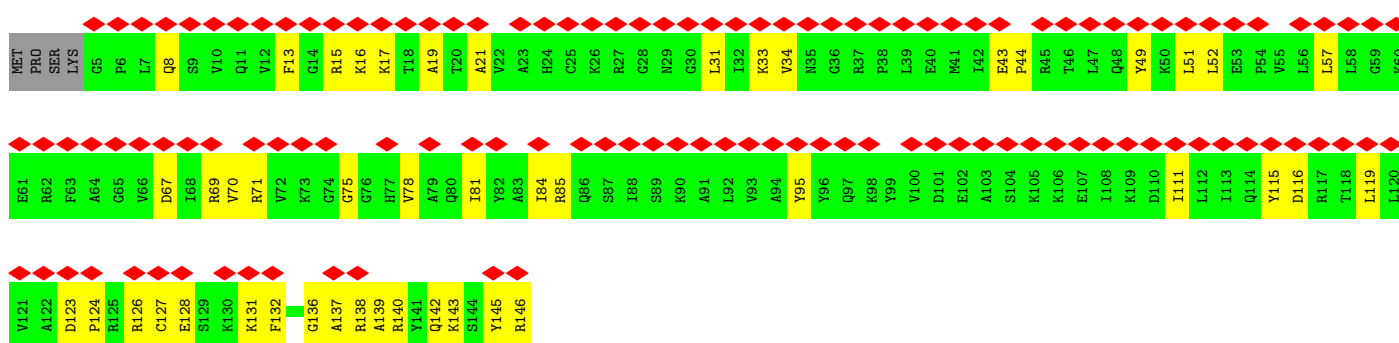
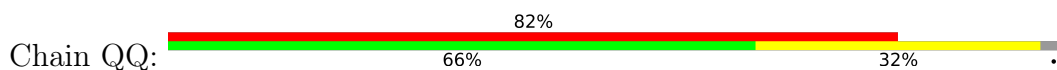
- Molecule 41: 40S ribosomal protein uS19



- Molecule 42: Ribosomal protein L18

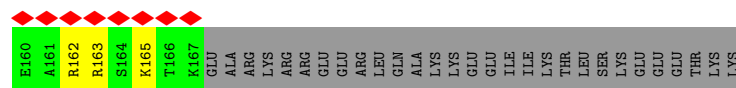


- Molecule 43: Ribosomal protein S16

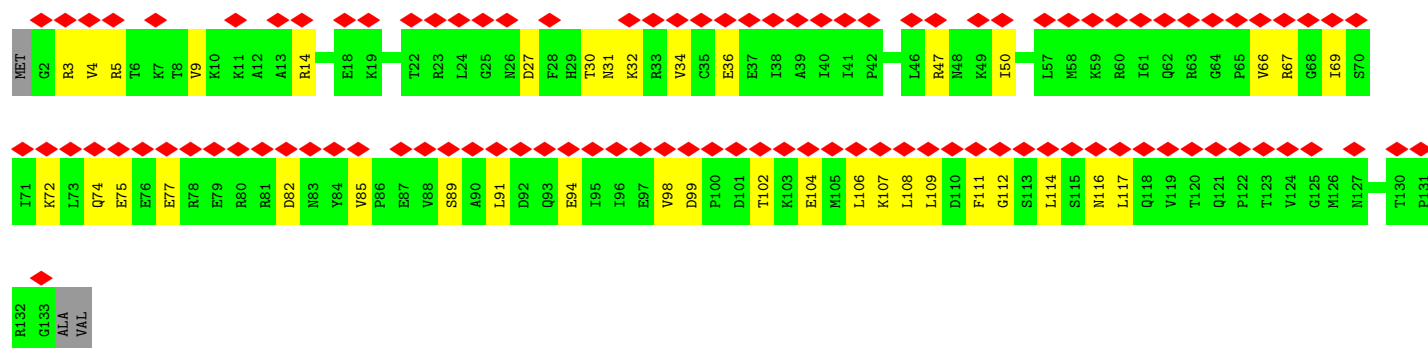
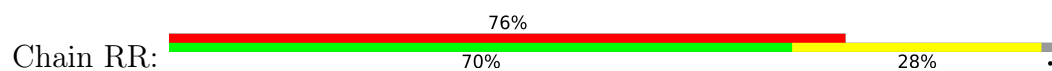


- Molecule 44: Ribosomal protein L19

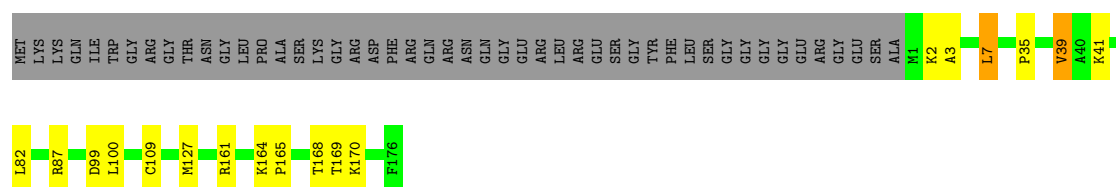




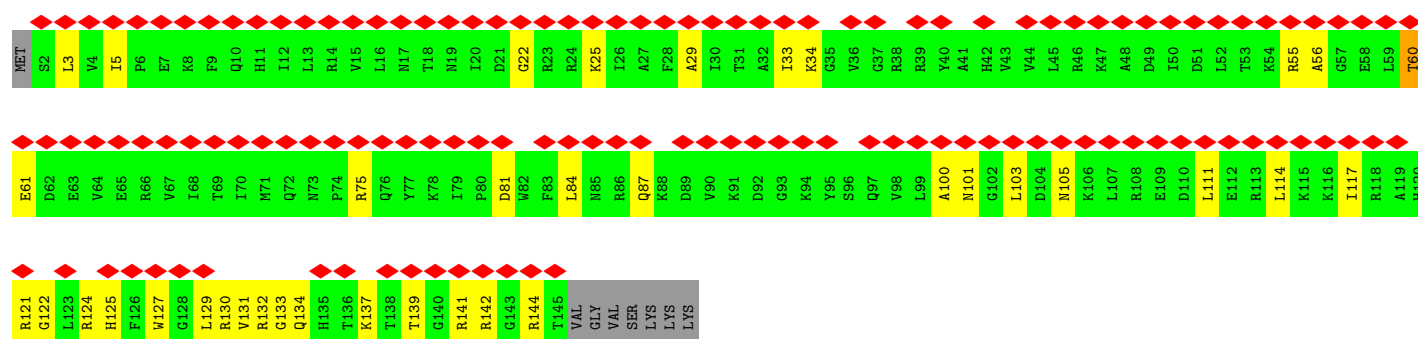
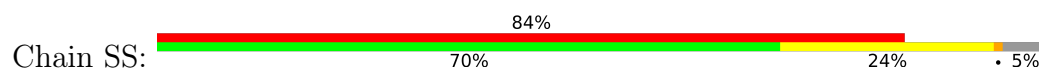
- Molecule 45: 40S ribosomal protein eS17



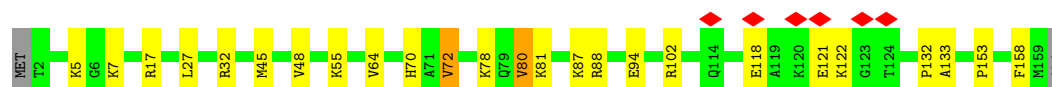
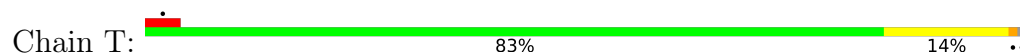
- Molecule 46: 60S ribosomal protein L18a



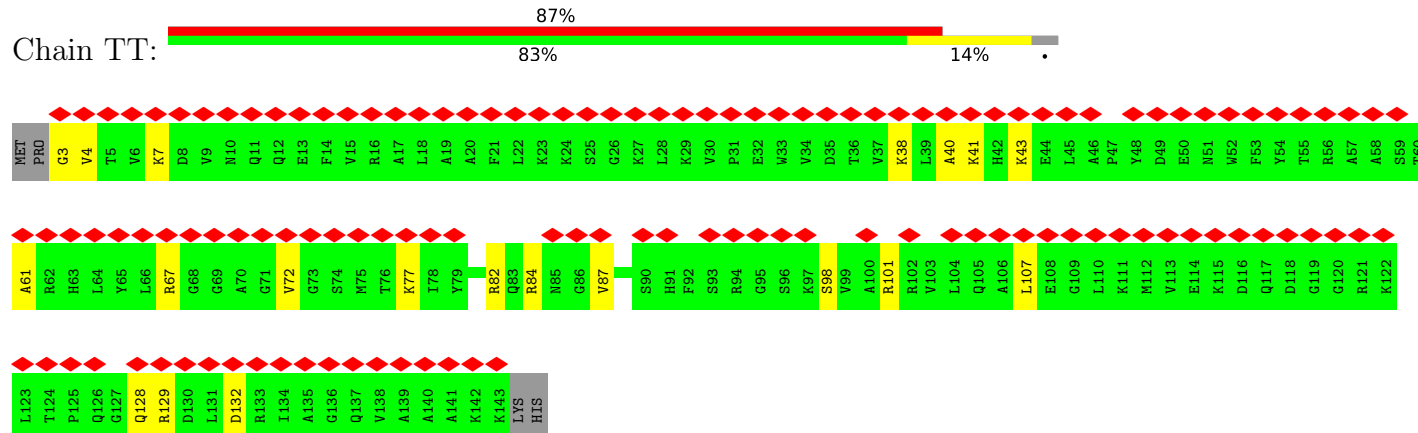
- Molecule 47: 40S ribosomal protein uS13



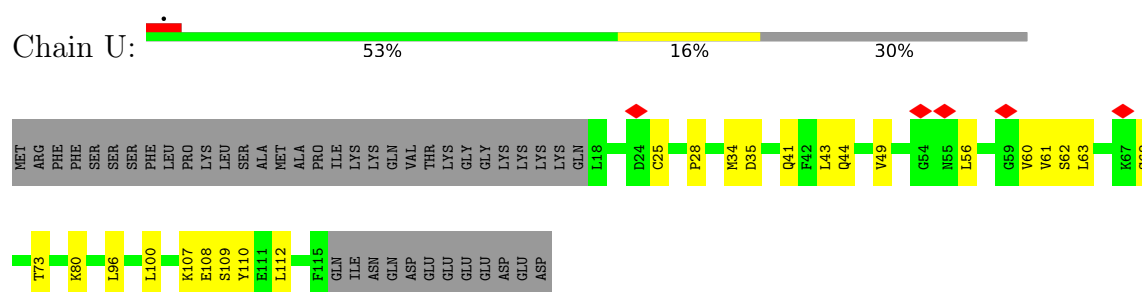
- Molecule 48: 60S ribosomal protein L21



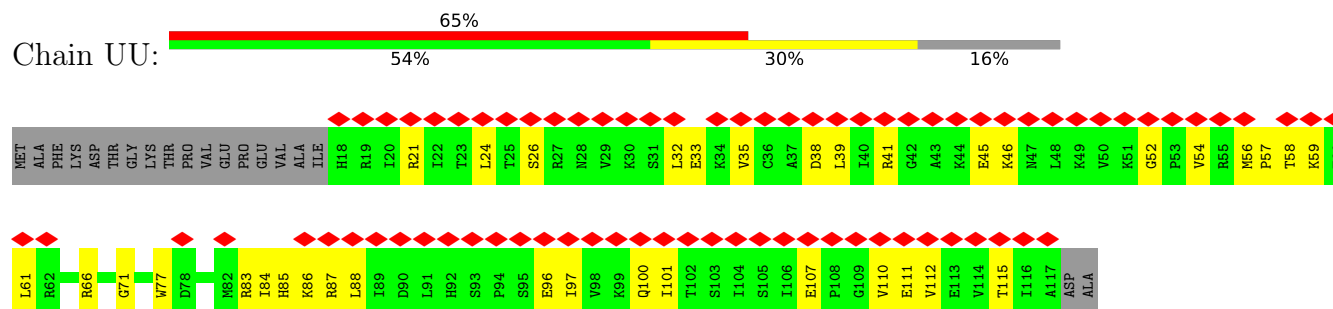
- Molecule 49: 40S ribosomal protein S19



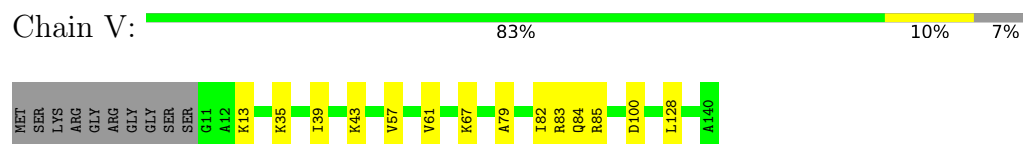
- Molecule 50: 60S ribosomal protein L22-like



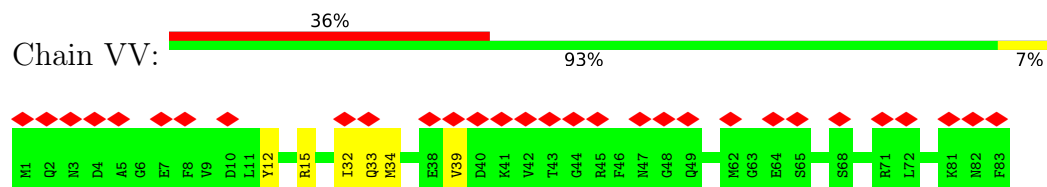
- Molecule 51: 40S ribosomal protein uS10



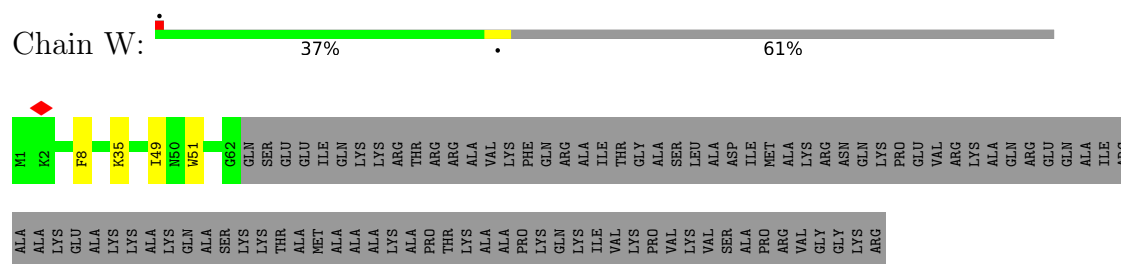
- Molecule 52: Ribosomal protein L23



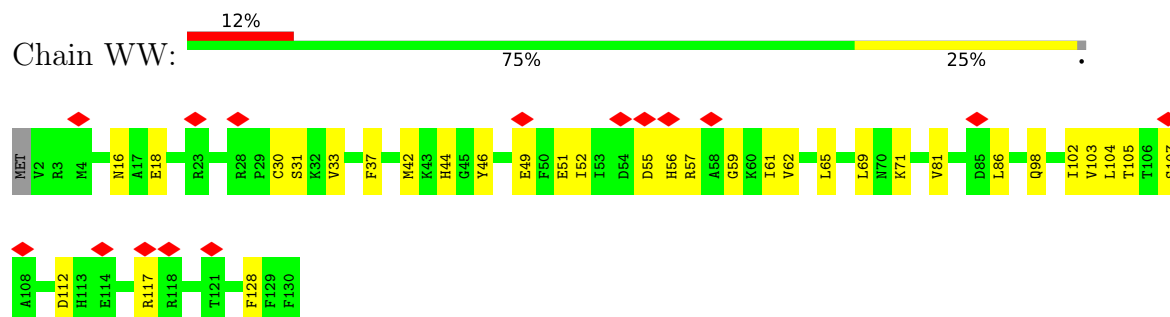
- Molecule 53: 40S ribosomal protein S21



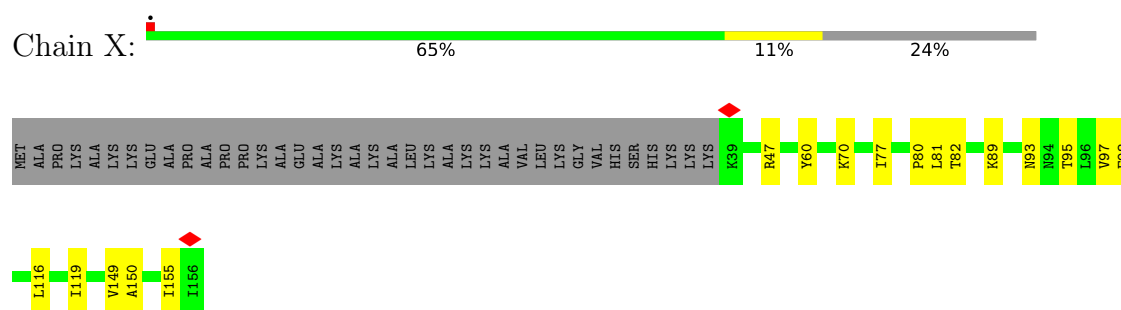
- Molecule 54: Ribosomal protein L24



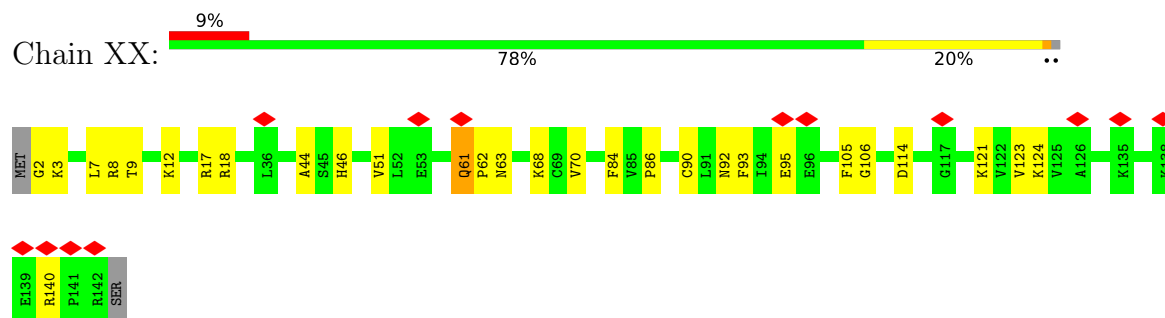
- Molecule 55: Ribosomal protein S15a



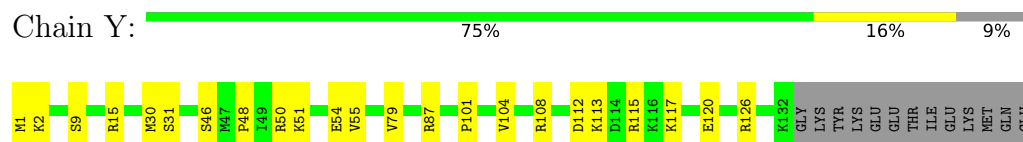
- Molecule 56: 60S ribosomal protein L23a



- Molecule 57: 40S ribosomal protein S23



- Molecule 58: Ribosomal protein L26

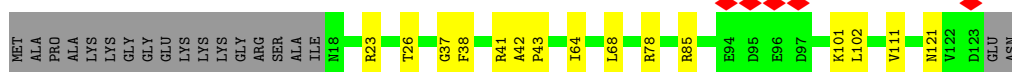


- | |
|------|
| MET |
| A2 |
| T8 |
| T9 |
| H10 |
| R18 |
| E30 |
| D36 |
| F39 |
| L40 |
| R41 |
| R68 |
| A69 |
| E70 |
| ALA |
| ILE |
| LYS |
| LYS |
| ALA |
| LEU |
| VAL |
| LYS |
| PRO |
| PRO |
| LYS |
| GLU |
| VAL |
| LYS |
| PRO |
| THR |
| ILE |
| PRO |
| LYS |
| GLY |
| V89 |
| H101 |
| P102 |
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| L104 |
| R17 |
| LEU |
| SER |
| ARG |
| PRO |
| GLN |
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| LYS |
| THR |
| GLU |

- Molecule 64: 60S ribosomal protein L30



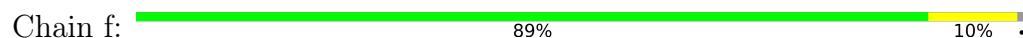
- Molecule 65: 60S ribosomal protein L31



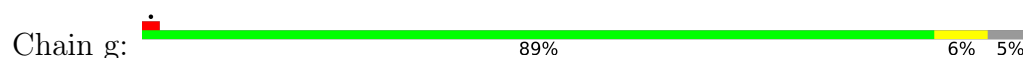
- Molecule 66: 60S ribosomal protein L32



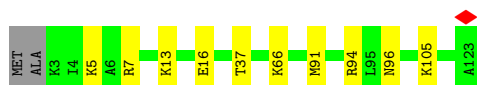
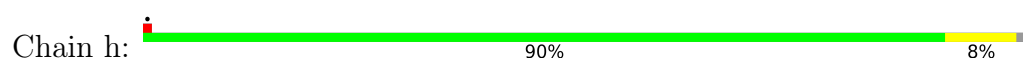
- Molecule 67: 60S ribosomal protein L35a



- Molecule 68: 60S ribosomal protein L34

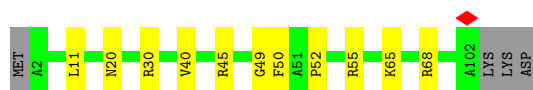


- Molecule 69: 60S ribosomal protein L35



- Molecule 70: 60S ribosomal protein L36

Chain i:  86% 10% .



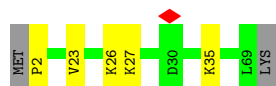
- Molecule 71: Ribosomal protein L37

Chain j:  73% 15% 11%



- Molecule 72: 60S ribosomal protein L38

Chain k:  90% 7% .



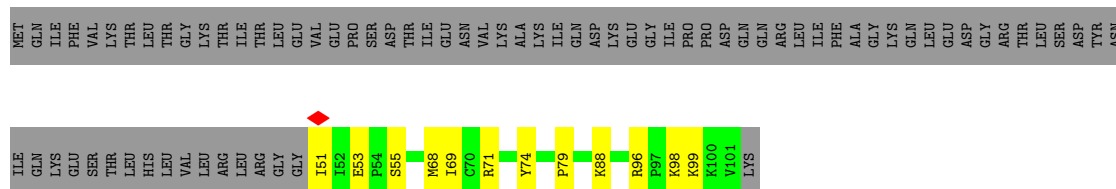
- Molecule 73: 60S ribosomal protein L39-like

Chain l:  86% 12% .



- Molecule 74: Ubiquitin-60S ribosomal protein L40

Chain m:  30% 9% 60%



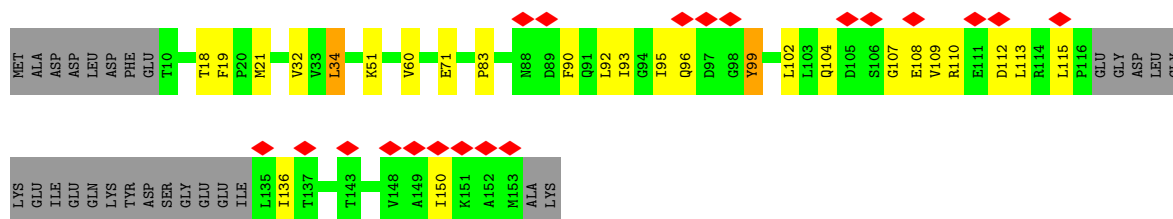
- Molecule 75: 60s ribosomal protein l41

Chain n:  80% 20%

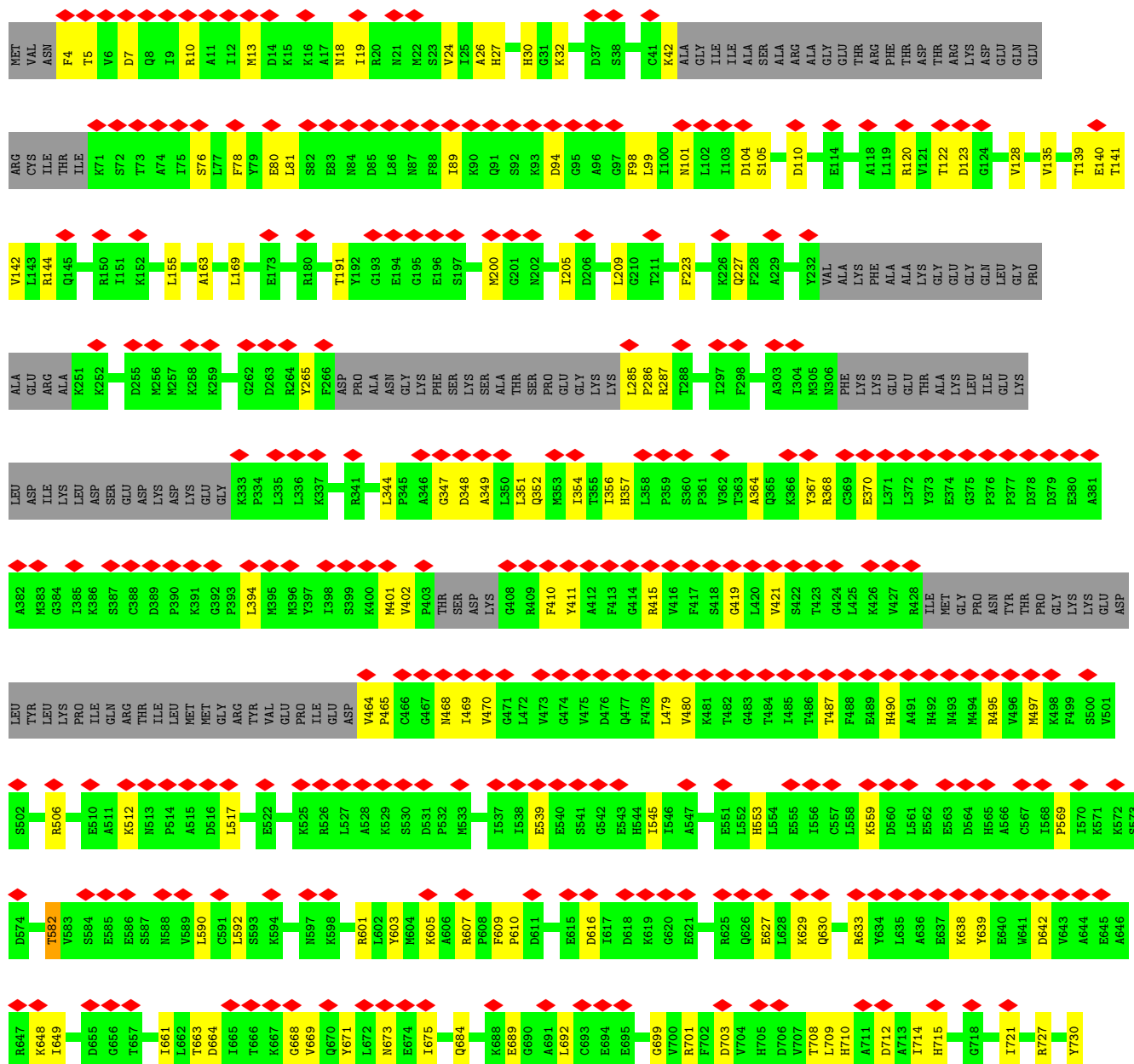
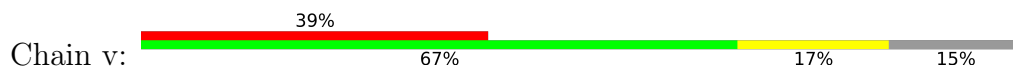


- Molecule 76: 60S ribosomal protein L36a-like

Chain o:  86% 9% . .



• Molecule 82: Elongation factor 2



- Molecule 83: SERPINE1 mRNA binding protein 1

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	479754	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.432	Depositor
Minimum map value	-1.954	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	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: B8W, 5MC, M7A, B8K, PSU, P7G, OMG, B9B, P4U, 1MA, A2M, MA6, MHG, OMC, 2MG, 7MG, 5CT, ZN, DDE, E7G, I4U, B8H, MLZ, OMU, B9H, 5MU, 4AC, E3C, E6G, B8Q, 6MZ, MG, UR3, BGH, B8T, B8N

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	x	0.32	0/1311	0.44	0/1762
2	5	0.13	2/78172 (0.0%)	0.21	0/121809
3	8	0.13	0/3406	0.17	0/5301
4	9	0.33	0/39723	0.44	1/61870 (0.0%)
5	A	0.12	0/1929	0.32	0/2586
6	AA	0.36	0/1747	0.66	0/2374
7	Aa	0.32	0/828	0.61	0/1109
8	B	0.11	0/3240	0.30	0/4339
9	BB	0.31	0/1756	0.71	0/2350
10	Bb	0.29	0/665	0.59	0/891
11	C	0.12	0/2899	0.31	0/3895
12	CC	0.40	0/1753	0.65	0/2369
13	Cc	0.25	0/490	0.52	0/656
14	D	0.10	0/2407	0.26	0/3224
15	DD	0.33	0/1796	0.67	0/2417
16	Dd	0.32	0/470	0.62	0/623
17	E	0.11	0/1743	0.30	0/2337
18	EE	0.34	0/2118	0.68	0/2849
19	Ee	0.30	0/447	0.58	0/587
20	F	0.11	0/1911	0.29	0/2549
21	FF	0.30	0/1492	0.76	5/2005 (0.2%)
22	G	0.11	0/1778	0.28	0/2397
23	GG	0.27	0/1946	0.73	1/2590 (0.0%)
24	Gg	0.26	0/2493	0.60	0/3394
25	H	0.09	0/1502	0.26	0/2020
26	HH	0.32	0/1510	0.66	0/2022
27	I	0.11	0/1678	0.28	0/2239
28	II	0.36	1/1715 (0.1%)	0.68	0/2287
29	J	0.09	0/1367	0.27	0/1829
30	JJ	0.36	0/1550	0.67	2/2069 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	K	0.09	0/2836	0.15	0/4421
32	KK	0.32	0/834	0.67	0/1125
33	L	0.12	0/1689	0.32	0/2261
34	LL	0.37	0/1195	0.61	0/1597
35	M	0.11	0/1138	0.29	0/1521
36	N	0.30	0/1746	0.41	0/2338
37	NN	0.31	0/1226	0.55	0/1649
38	O	0.11	0/1662	0.29	0/2222
39	OO	0.28	0/1029	0.64	0/1380
40	P	0.11	0/1259	0.30	0/1688
41	PP	0.29	0/1045	0.68	0/1396
42	Q	0.12	0/1539	0.33	0/2054
43	QQ	0.26	0/1146	0.64	0/1534
44	R	0.11	0/1399	0.31	0/1851
45	RR	0.27	0/1082	0.62	0/1452
46	S	0.12	0/1495	0.32	0/2005
47	SS	0.29	0/1208	0.71	0/1618
48	T	0.11	0/1320	0.27	0/1763
49	TT	0.24	0/1115	0.60	0/1493
50	U	0.09	0/814	0.25	0/1092
51	UU	0.29	0/805	0.63	0/1081
52	V	0.10	0/987	0.28	0/1324
53	VV	0.39	0/643	0.63	0/860
54	W	0.11	0/532	0.30	0/708
55	WW	0.44	0/1051	0.72	0/1406
56	X	0.10	0/984	0.28	0/1323
57	XX	0.41	0/1116	0.66	0/1490
58	Y	0.11	0/1119	0.29	0/1488
59	YY	0.26	0/1028	0.64	0/1366
60	Z	0.10	0/1130	0.27	0/1507
61	ZZ	0.27	0/604	0.68	0/810
62	a	0.11	0/1191	0.30	0/1590
63	b	0.10	0/819	0.29	0/1081
64	c	0.09	0/742	0.24	0/995
65	d	0.11	0/894	0.28	0/1204
66	e	0.11	0/1071	0.30	0/1429
67	f	0.12	0/895	0.32	0/1198
68	g	0.11	0/892	0.31	0/1189
69	h	0.10	0/1016	0.28	0/1341
70	i	0.11	0/832	0.30	0/1101
71	j	0.12	0/720	0.35	0/952
72	k	0.09	0/565	0.28	0/750
73	l	0.12	0/459	0.33	0/608

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	m	0.11	0/415	0.31	0/550
75	n	0.11	0/240	0.37	0/305
76	o	0.22	0/847	0.34	0/1117
77	p	0.11	0/718	0.29	0/953
78	r	0.12	0/1002	0.31	0/1344
79	s	0.10	0/1523	0.30	0/2055
80	s1	0.10	0/154	0.29	0/205
81	t	0.36	0/958	0.66	3/1288 (0.2%)
82	v	0.09	0/5758	0.27	0/7779
83	w	0.10	0/257	0.27	0/339
All	All	0.22	3/224586 (0.0%)	0.38	12/327945 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	AA	0	2
15	DD	0	1
18	EE	0	1
21	FF	0	1
24	Gg	0	1
28	II	0	1
41	PP	0	1
47	SS	0	1
51	UU	0	1
53	VV	0	1
57	XX	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	II	130	THR	C-N	7.42	1.40	1.33
2	5	3722	A2M	O3'-P	5.05	1.61	1.56
2	5	4527	A2M	O3'-P	5.03	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	t	108	GLU	N-CA-C	8.37	122.36	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	t	112	ASP	N-CA-C	7.09	120.05	111.82
23	GG	67	VAL	N-CA-C	-6.00	106.97	112.96
30	JJ	168	GLY	CA-C-N	5.65	128.51	120.49
30	JJ	168	GLY	C-N-CA	5.65	128.51	120.49
81	t	107	GLY	N-CA-C	5.33	121.05	110.77
21	FF	26	ASP	CA-C-N	5.22	131.51	121.54
21	FF	26	ASP	C-N-CA	5.22	131.51	121.54
21	FF	44	LYS	N-CA-C	-5.21	108.19	114.75
21	FF	42	LYS	CA-C-N	5.19	131.44	121.54
21	FF	42	LYS	C-N-CA	5.19	131.44	121.54
4	9	1394	G	C2'-C3'-O3'	5.11	121.36	113.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AA	42	LYS	Peptide
6	AA	43	SER	Peptide
15	DD	153	VAL	Peptide
18	EE	132	GLY	Peptide
21	FF	41	VAL	Peptide
24	Gg	135	LEU	Peptide
28	II	92	ARG	Peptide
41	PP	17	TYR	Peptide
47	SS	60	THR	Peptide
51	UU	107	GLU	Peptide
53	VV	32	ILE	Peptide
57	XX	61	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	x	1291	0	1374	45	0
2	5	72165	0	36223	482	0
3	8	3072	0	1559	17	0
4	9	36291	0	18323	870	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1891	0	1986	35	0
6	AA	1710	0	1708	39	0
7	Aa	814	0	863	14	0
8	B	3172	0	3310	44	0
9	BB	1729	0	1803	46	0
10	Bb	651	0	672	16	0
11	C	2856	0	3027	27	0
12	CC	1716	0	1806	17	0
13	Cc	488	0	514	15	0
14	D	2361	0	2395	27	0
15	DD	1768	0	1866	64	0
16	Dd	459	0	452	27	0
17	E	1710	0	1864	34	0
18	EE	2076	0	2177	85	0
19	Ee	443	0	492	16	0
20	F	1875	0	1995	18	0
21	FF	1471	0	1522	50	0
22	G	1747	0	1871	31	0
23	GG	1923	0	2089	138	0
24	Gg	2436	0	2393	38	0
25	H	1484	0	1552	14	0
26	HH	1488	0	1582	41	0
27	I	1640	0	1686	18	0
28	II	1686	0	1772	64	0
29	J	1344	0	1380	28	0
30	JJ	1525	0	1640	48	0
31	K	2538	0	1286	7	0
32	KK	810	0	836	14	0
33	L	1658	0	1766	21	0
34	LL	1175	0	1249	49	0
35	M	1117	0	1188	16	0
36	N	1701	0	1749	31	0
37	NN	1202	0	1289	33	0
38	O	1630	0	1778	21	0
39	OO	1016	0	1039	26	0
40	P	1233	0	1267	12	0
41	PP	1025	0	1074	54	0
42	Q	1515	0	1634	24	0
43	QQ	1128	0	1195	81	0
44	R	1383	0	1524	31	0
45	RR	1068	0	1121	35	0
46	S	1456	0	1497	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	SS	1190	0	1248	56	0
48	T	1292	0	1361	19	0
49	TT	1097	0	1132	38	0
50	U	800	0	825	12	0
51	UU	795	0	862	53	0
52	V	973	0	1032	10	0
53	VV	636	0	637	4	0
54	W	519	0	533	2	0
55	WW	1034	0	1080	29	0
56	X	967	0	1040	11	0
57	XX	1098	0	1167	33	0
58	Y	1102	0	1189	16	0
59	YY	1011	0	1083	38	0
60	Z	1107	0	1182	15	0
61	ZZ	598	0	656	14	0
62	a	1162	0	1209	19	0
63	b	806	0	866	9	0
64	c	732	0	767	8	0
65	d	879	0	923	8	0
66	e	1053	0	1147	15	0
67	f	876	0	912	11	0
68	g	882	0	972	7	0
69	h	1008	0	1142	10	0
70	i	821	0	901	8	0
71	j	705	0	737	12	0
72	k	559	0	624	4	0
73	l	447	0	480	4	0
74	m	420	0	454	8	0
75	n	239	0	286	19	0
76	o	834	0	902	8	0
77	p	708	0	756	8	0
78	r	986	0	1042	14	0
79	s	1501	0	1557	26	0
80	s1	150	0	156	1	0
81	t	961	0	985	17	0
82	v	5669	0	5721	96	0
83	w	252	0	223	52	0
84	5	195	0	0	0	0
84	8	2	0	0	0	0
84	I	1	0	0	0	0
84	P	1	0	0	0	0
84	g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	v	1	0	0	0	0
85	Aa	1	0	0	0	0
85	KK	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0
85	m	1	0	0	0	0
85	o	1	0	0	0	0
85	p	1	0	0	0	0
All	All	213014	0	161177	2543	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 7.

All (2543) 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)
2:5:1864:B8H:C4	2:5:1864:B8H:C5	1.83	1.56
2:5:1864:B8H:C6	2:5:1864:B8H:N1	1.67	1.56
4:9:142:C:C4	23:GG:185:LEU:CD1	1.76	1.56
2:5:4300:B8H:C6	2:5:4300:B8H:N1	1.68	1.52
2:5:4300:B8H:C4	2:5:4300:B8H:C5	1.83	1.51
4:9:142:C:C4	23:GG:185:LEU:HD13	1.02	1.50
4:9:142:C:N4	23:GG:185:LEU:CD1	1.76	1.46
4:9:1706:G:H4'	75:n:1:MET:CE	1.45	1.46
4:9:142:C:N4	23:GG:185:LEU:HD11	1.29	1.41
4:9:1745:A:O2'	23:GG:66:GLY:CA	1.68	1.39
4:9:1172:U:H4'	75:n:10:MET:CE	1.57	1.33
4:9:1745:A:O2'	23:GG:66:GLY:HA2	1.14	1.31
4:9:142:C:C5	23:GG:185:LEU:HD13	1.65	1.30
15:DD:143:ARG:CD	83:w:216:HIS:O	1.80	1.29
2:5:2367:A2M:C1'	2:5:2367:A2M:O4'	1.63	1.29
4:9:1031:A2M:C1'	4:9:1031:A2M:O4'	1.63	1.27
4:9:907:G:C5'	44:R:165:LYS:CE	2.13	1.27
4:9:1425:G:OP1	43:QQ:69:ARG:NH2	1.63	1.26
4:9:1416:C:O2'	49:TT:4:VAL:O	1.53	1.25
4:9:1678:A2M:C1'	4:9:1678:A2M:O4'	1.63	1.24
2:5:3903:BGH:O4'	2:5:3903:BGH:C4'	1.67	1.24
2:5:4575:A2M:C1'	2:5:4575:A2M:O4'	1.63	1.24
4:9:144:U:OP2	23:GG:178:ARG:NH1	1.69	1.24
4:9:1647:A:OP1	43:QQ:138:ARG:NH1	1.71	1.22
4:9:163:U:OP2	23:GG:87:ARG:NH2	1.71	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:398:A2M:C1'	2:5:398:A2M:O4'	1.63	1.20
4:9:142:C:OP2	23:GG:188:LYS:NZ	1.71	1.20
2:5:3722:A2M:C1'	2:5:3722:A2M:O4'	1.63	1.20
2:5:3829:A2M:C1'	2:5:3829:A2M:O4'	1.63	1.20
4:9:126:G:OP1	23:GG:198:ARG:CD	1.90	1.19
2:5:4527:A2M:C1'	2:5:4527:A2M:O4'	1.63	1.19
4:9:166:A2M:C1'	4:9:166:A2M:O4'	1.64	1.19
4:9:1408:U:OP1	43:QQ:71:ARG:NH2	1.74	1.18
2:5:3727:A2M:C1'	2:5:3727:A2M:O4'	1.63	1.18
4:9:1790:A:H4'	23:GG:81:HIS:CE1	1.80	1.15
4:9:1650:A:H5''	43:QQ:139:ALA:CB	1.76	1.15
2:5:1875:A2M:C1'	2:5:1875:A2M:O4'	1.63	1.14
4:9:159:A2M:C1'	4:9:159:A2M:O4'	1.64	1.14
4:9:1706:G:C4'	75:n:1:MET:CE	2.25	1.14
4:9:1408:U:P	43:QQ:71:ARG:HH22	1.71	1.13
4:9:1706:G:H4'	75:n:1:MET:HE2	1.28	1.13
1:x:159:MET:HA	1:x:159:MET:HE3	1.27	1.13
4:9:1706:G:C5'	75:n:1:MET:HE3	1.78	1.13
2:5:1538:A2M:C1'	2:5:1538:A2M:O4'	1.63	1.13
4:9:907:G:H5'	44:R:165:LYS:HE3	1.19	1.12
2:5:2405:A2M:C1'	2:5:2405:A2M:O4'	1.63	1.11
4:9:1540:G:OP1	49:TT:43:LYS:HE3	1.48	1.10
4:9:1650:A:H5''	43:QQ:139:ALA:HB2	1.13	1.10
15:DD:143:ARG:HD2	83:w:216:HIS:O	1.37	1.10
4:9:1489:A:C5'	83:w:195:ARG:HD3	1.79	1.10
4:9:1634:A:H4'	47:SS:142:ARG:CZ	1.83	1.09
4:9:1489:A:C5'	83:w:195:ARG:CD	2.24	1.09
4:9:331:C:H5'	23:GG:196:LYS:NZ	1.67	1.08
4:9:126:G:OP1	23:GG:198:ARG:HD3	1.50	1.08
4:9:875:A:H1'	26:HH:114:GLN:NE2	1.70	1.07
4:9:916:A:C5	37:NN:73:ARG:HD3	1.89	1.07
4:9:1706:G:H4'	75:n:1:MET:HE1	1.35	1.06
4:9:331:C:H5'	23:GG:196:LYS:HZ3	1.13	1.06
4:9:331:C:C5'	23:GG:196:LYS:NZ	2.18	1.06
4:9:1650:A:C5'	43:QQ:139:ALA:HB2	1.84	1.06
4:9:907:G:H5''	44:R:165:LYS:CE	1.80	1.06
4:9:1745:A:O2'	23:GG:66:GLY:HA3	1.56	1.05
4:9:1791:A:H4'	23:GG:75:LEU:HD11	1.38	1.05
4:9:1563:G:OP2	49:TT:72:VAL:HG22	1.55	1.05
4:9:1791:A:H5''	23:GG:75:LEU:HD12	1.34	1.05
4:9:1746:U:H4'	23:GG:65:GLN:CG	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1610:G:N7	47:SS:132:ARG:NH2	2.04	1.04
4:9:1417:C:N1	49:TT:3:GLY:N	2.05	1.04
4:9:164:A:H5''	23:GG:83:CYS:HA	1.05	1.03
4:9:142:C:N3	23:GG:185:LEU:HD13	1.71	1.02
4:9:523:A:OP2	30:JJ:38:ARG:HD3	1.58	1.02
4:9:164:A:C5'	23:GG:83:CYS:HA	1.87	1.02
4:9:1522:A:N6	41:PP:131:PRO:HG3	1.73	1.02
15:DD:146:ARG:HB3	83:w:206:HIS:ND1	1.73	1.02
4:9:1535:U:C6	21:FF:82:ASN:ND2	2.26	1.01
4:9:1745:A:C2'	23:GG:66:GLY:HA3	1.91	1.01
4:9:1172:U:H4'	75:n:10:MET:HE2	1.03	1.01
4:9:1649:U:H4'	43:QQ:138:ARG:HG2	1.38	1.01
4:9:913:A:H2'	26:HH:120:ARG:NH2	1.75	1.00
4:9:1647:A:H5''	43:QQ:138:ARG:NH2	1.75	1.00
4:9:142:C:C5	23:GG:185:LEU:HD22	1.96	1.00
15:DD:116:ARG:HB3	83:w:219:GLY:HA3	1.43	1.00
4:9:495:U:O2'	18:EE:27:PHE:O	1.78	0.99
4:9:1397:U:O4	43:QQ:13:PHE:CD1	2.14	0.99
4:9:1254:C:O2'	51:UU:71:GLY:O	1.80	0.99
4:9:907:G:C5'	44:R:165:LYS:HE3	1.85	0.99
4:9:1417:C:C2	49:TT:3:GLY:N	2.30	0.99
4:9:1016:U:O2	10:Bb:30:SER:OG	1.81	0.99
4:9:1172:U:C4'	75:n:10:MET:HE2	1.92	0.98
4:9:1617:G:H4'	16:Dd:14:PHE:CE1	1.99	0.98
4:9:197:U:H3	4:9:202:G:H1	0.98	0.98
4:9:1298:G:O4'	41:PP:79:HIS:ND1	1.95	0.98
15:DD:143:ARG:HD3	83:w:217:ASN:HB2	1.44	0.97
4:9:1331:C:N4	83:w:196:HIS:O	1.95	0.97
2:5:3771:C:O2'	4:9:1828:C:H4'	1.62	0.97
4:9:126:G:OP1	23:GG:198:ARG:HD2	1.58	0.97
4:9:1414:A:O2'	49:TT:128:GLN:OE1	1.82	0.97
15:DD:143:ARG:CG	83:w:216:HIS:O	2.13	0.97
4:9:386:C:H5''	28:II:10:LYS:HD3	1.47	0.96
4:9:1591:C:H5'	21:FF:85:LYS:NZ	1.80	0.96
15:DD:10:LYS:NZ	51:UU:111:GLU:OE1	1.98	0.96
4:9:1320:G:O3'	82:v:629:LYS:NZ	1.98	0.96
4:9:1416:C:C4'	49:TT:132:ASP:OD2	2.13	0.95
15:DD:143:ARG:HD3	83:w:217:ASN:CB	1.97	0.95
15:DD:146:ARG:O	83:w:206:HIS:CE1	2.20	0.95
4:9:1522:A:C6	41:PP:131:PRO:HG3	2.02	0.95
4:9:913:A:N6	26:HH:119:SER:O	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1706:G:H5'	75:n:1:MET:HE3	1.47	0.95
47:SS:3:LEU:O	61:ZZ:49:LEU:HD12	1.66	0.94
4:9:629:A:H1'	83:w:210:ARG:NH2	1.82	0.94
4:9:1587:G:H21	49:TT:77:LYS:HZ2	1.11	0.94
4:9:819:G:OP2	30:JJ:80:ARG:NH2	2.00	0.94
4:9:1745:A:HO2'	23:GG:66:GLY:HA2	1.28	0.94
4:9:916:A:O2'	37:NN:73:ARG:NH1	2.01	0.93
4:9:142:C:H41	23:GG:185:LEU:HD11	1.26	0.93
4:9:1609:C:H5''	47:SS:131:VAL:HB	1.49	0.93
4:9:164:A:H5''	23:GG:83:CYS:CA	1.96	0.92
47:SS:5:ILE:HG13	61:ZZ:49:LEU:HB2	1.47	0.92
4:9:1549:U:OP1	16:Dd:34:TYR:OH	1.86	0.92
18:EE:94:LYS:HZ3	59:YY:16:ARG:HB3	1.33	0.92
4:9:1706:G:C5'	75:n:1:MET:CE	2.45	0.92
4:9:1397:U:H3	43:QQ:13:PHE:HE1	1.03	0.91
4:9:144:U:P	23:GG:178:ARG:HH11	1.92	0.91
4:9:1489:A:C8	83:w:204:LEU:HD11	2.05	0.91
4:9:1617:G:H4'	16:Dd:14:PHE:CZ	2.05	0.91
4:9:1608:U:H4'	47:SS:130:ARG:CD	2.00	0.91
29:J:88:LYS:HB3	41:PP:12:PHE:CD1	2.04	0.91
4:9:907:G:H5''	44:R:165:LYS:HE2	1.48	0.91
4:9:1591:C:H5'	21:FF:85:LYS:HZ3	1.31	0.91
4:9:331:C:O5'	23:GG:196:LYS:NZ	2.02	0.90
4:9:907:G:H5'	44:R:165:LYS:CE	1.84	0.90
15:DD:116:ARG:CB	83:w:219:GLY:HA3	2.01	0.90
4:9:873:G:O4'	44:R:162:ARG:HD3	1.70	0.90
4:9:1609:C:OP1	47:SS:131:VAL:N	2.05	0.90
4:9:304:C:O3'	28:II:184:ARG:NH2	2.05	0.89
1:x:159:MET:HA	1:x:159:MET:CE	2.02	0.89
4:9:114:G:OP1	34:LL:69:ARG:NH1	2.05	0.89
4:9:1236:G:H4'	41:PP:133:ILE:HG23	1.54	0.89
4:9:916:A:C4	37:NN:73:ARG:HD3	2.08	0.88
4:9:1252:C:N4	43:QQ:146:ARG:OXT	2.06	0.88
4:9:1408:U:P	43:QQ:71:ARG:NH2	2.43	0.88
4:9:1580:A:C4	51:UU:57:PRO:HG3	2.07	0.88
4:9:561:A:O2'	30:JJ:132:GLN:OE1	1.89	0.88
4:9:502:C:N4	18:EE:67:GLN:OE1	2.06	0.88
4:9:1416:C:H4'	49:TT:132:ASP:CG	1.98	0.88
4:9:1230:C:H3'	47:SS:139:THR:HG21	1.56	0.88
4:9:1443:C:H5''	43:QQ:15:ARG:NH2	1.88	0.88
4:9:1790:A:H4'	23:GG:81:HIS:HE1	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:331:C:C5'	23:GG:196:LYS:HZ2	1.81	0.87
4:9:1122:A:H4'	9:BB:205:TYR:CD1	2.08	0.87
4:9:1580:A:C8	51:UU:57:PRO:HD2	2.09	0.87
4:9:1535:U:C6	21:FF:82:ASN:CG	2.52	0.87
4:9:380:G:H1'	28:II:5:ARG:HH12	1.39	0.87
4:9:65:C:C4	23:GG:136:LYS:HD2	2.09	0.87
4:9:1417:C:C1'	49:TT:3:GLY:N	2.38	0.86
4:9:628:A:C6	83:w:216:HIS:NE2	2.43	0.86
4:9:1443:C:H5''	43:QQ:15:ARG:HH22	1.40	0.86
4:9:1535:U:C5	21:FF:82:ASN:ND2	2.43	0.86
4:9:1580:A:C8	51:UU:57:PRO:CD	2.58	0.86
4:9:1649:U:H4'	43:QQ:138:ARG:CG	2.04	0.86
4:9:1647:A:C5'	43:QQ:138:ARG:NH2	2.38	0.86
4:9:383:G:O2'	34:LL:133:PRO:O	1.92	0.85
4:9:145:G:OP2	23:GG:178:ARG:NH1	2.08	0.85
4:9:422:U:OP1	34:LL:98:LYS:NZ	2.10	0.85
4:9:121:OMU:HM21	18:EE:35:PRO:HB3	1.58	0.85
4:9:110:U:H3	4:9:351:G:H1	1.24	0.85
4:9:1613:G:O5'	41:PP:39:ALA:HB2	1.75	0.84
4:9:1608:U:H5'	47:SS:130:ARG:NH1	1.92	0.84
2:5:2469:C:H1'	2:5:3676:G:H22	1.42	0.84
2:5:3770:A:N1	4:9:1827:U:O2'	2.10	0.84
2:5:4300:B8H:N1	2:5:4300:B8H:C5	2.38	0.84
4:9:580:U:O3'	59:YY:64:PHE:CD1	2.31	0.84
4:9:1746:U:H4'	23:GG:65:GLN:HG2	1.56	0.84
6:AA:19:LEU:HD21	45:RR:106:LEU:HD11	1.57	0.84
4:9:1416:C:O4'	49:TT:132:ASP:OD2	1.96	0.84
47:SS:5:ILE:CG1	61:ZZ:49:LEU:HB2	2.06	0.84
4:9:1332:A:O2'	15:DD:145:GLN:O	1.95	0.83
15:DD:146:ARG:HG2	83:w:206:HIS:HB2	1.59	0.83
4:9:1397:U:N3	43:QQ:13:PHE:HE1	1.77	0.83
4:9:307:G:H1'	28:II:45:THR:HG22	1.59	0.83
15:DD:143:ARG:HG3	83:w:216:HIS:O	1.76	0.83
4:9:581:U:OP1	59:YY:64:PHE:CE1	2.31	0.83
4:9:1023:A:H5''	37:NN:4:MET:HE2	1.59	0.82
18:EE:94:LYS:NZ	59:YY:16:ARG:HB3	1.93	0.82
4:9:1256:G:H21	16:Dd:29:GLY:HA2	1.45	0.82
29:J:88:LYS:HB3	41:PP:12:PHE:HD1	1.42	0.82
4:9:1172:U:H4'	75:n:10:MET:HE3	1.59	0.81
4:9:1791:A:C5'	23:GG:75:LEU:HD12	2.10	0.81
4:9:522:A:N6	30:JJ:41:ARG:HH22	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1331:C:H5	83:w:198:GLY:N	1.77	0.81
4:9:1661:A:OP2	16:Dd:32:ARG:NH1	2.13	0.81
4:9:1746:U:H4'	23:GG:65:GLN:CD	2.05	0.81
4:9:77:A:C2	23:GG:175:LYS:HE3	2.16	0.81
47:SS:5:ILE:HG13	61:ZZ:49:LEU:CB	2.11	0.81
4:9:1489:A:N6	83:w:197:SER:OG	2.12	0.81
4:9:65:C:C2	23:GG:174:PRO:HB3	2.16	0.81
4:9:1122:A:H4'	9:BB:205:TYR:CE1	2.15	0.81
4:9:1256:G:N2	16:Dd:29:GLY:HA2	1.96	0.81
4:9:1706:G:C4'	75:n:1:MET:HE2	2.01	0.81
4:9:1791:A:H4'	23:GG:75:LEU:CD1	2.11	0.81
1:x:48:ARG:HH11	1:x:160:LYS:HA	1.46	0.81
1:x:71:GLN:NE2	29:J:38:LYS:NZ	2.29	0.81
4:9:142:C:C5	23:GG:185:LEU:CD1	2.41	0.80
4:9:1652:G:H1	4:9:1672:U:H3	1.27	0.80
4:9:190:G:H5''	28:II:145:ILE:HD13	1.63	0.80
4:9:331:C:P	23:GG:196:LYS:HZ2	2.03	0.80
4:9:628:A:OP1	15:DD:179:GLN:OE1	1.99	0.80
4:9:1333:U:OP1	15:DD:146:ARG:HD2	1.82	0.80
4:9:1466:G:H5'	45:RR:4:VAL:HG22	1.64	0.80
34:LL:93:LEU:HD11	57:XX:8:ARG:HH22	1.44	0.79
4:9:142:C:C5	23:GG:185:LEU:CD2	2.65	0.79
4:9:367:U:OP1	28:II:11:ARG:NH2	2.16	0.79
4:9:1417:C:H1'	49:TT:3:GLY:HA3	1.65	0.79
4:9:1489:A:H5'	83:w:195:ARG:HD3	1.62	0.79
29:J:88:LYS:HD2	41:PP:12:PHE:CE1	2.17	0.79
4:9:331:C:C5'	23:GG:196:LYS:HZ3	1.84	0.79
4:9:1653:U:H3	4:9:1671:G:H1	1.26	0.79
4:9:875:A:H1'	26:HH:114:GLN:CD	2.07	0.79
4:9:1608:U:H4'	47:SS:130:ARG:NE	1.98	0.78
18:EE:94:LYS:NZ	59:YY:16:ARG:O	2.15	0.78
4:9:1791:A:C4'	23:GG:75:LEU:HD11	2.12	0.78
1:x:73:HIS:HD1	1:x:113:SER:HG	1.31	0.78
4:9:151:C:OP1	59:YY:119:GLY:HA2	1.84	0.78
4:9:580:U:O3'	59:YY:64:PHE:HD1	1.67	0.78
4:9:1608:U:H4'	47:SS:130:ARG:HD2	1.65	0.78
4:9:1609:C:H5''	47:SS:131:VAL:CB	2.13	0.78
4:9:314:U:OP2	23:GG:191:ARG:NH2	2.17	0.78
4:9:572:U:OP1	59:YY:60:PHE:N	2.17	0.77
2:5:2651:A:H62	2:5:2690:G:H8	1.33	0.77
4:9:1489:A:H5''	83:w:195:ARG:HD3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:78:C:H1'	23:GG:175:LYS:HD2	1.64	0.77
13:Cc:49:PRO:HB2	21:FF:61:PHE:CZ	2.19	0.77
4:9:660:C:O5'	57:XX:2:GLY:N	2.16	0.77
2:5:3696:A:H62	2:5:3827:G:H21	1.30	0.76
4:9:144:U:OP2	23:GG:178:ARG:CZ	2.32	0.76
4:9:1416:C:H4'	49:TT:132:ASP:OD2	1.84	0.76
1:x:42:ASP:HB3	1:x:45:LYS:HB2	1.68	0.76
4:9:387:C:OP2	28:II:10:LYS:NZ	2.19	0.76
4:9:1587:G:H21	49:TT:77:LYS:NZ	1.84	0.76
4:9:1503:C:H4'	82:v:669:VAL:O	1.86	0.75
4:9:1618:C:C6	16:Dd:11:PRO:HG2	2.22	0.75
4:9:380:G:C4	28:II:5:ARG:NH2	2.55	0.75
4:9:380:G:H1'	28:II:5:ARG:NH1	2.01	0.75
4:9:65:C:N4	23:GG:136:LYS:HD2	2.01	0.75
4:9:190:G:OP1	28:II:149:TYR:OH	2.03	0.75
4:9:583:A:OP1	30:JJ:162:ARG:NH2	2.19	0.75
4:9:875:A:C1'	26:HH:114:GLN:NE2	2.49	0.75
4:9:1669:G:OP1	43:QQ:132:PHE:HB3	1.87	0.75
4:9:1647:A:H5''	43:QQ:138:ARG:HH22	1.49	0.75
1:x:161:LYS:HG2	1:x:161:LYS:O	1.86	0.74
4:9:380:G:N3	28:II:5:ARG:NH2	2.35	0.74
4:9:1580:A:N7	51:UU:57:PRO:HD3	2.01	0.74
1:x:71:GLN:HE21	29:J:38:LYS:NZ	1.85	0.74
4:9:506:G:OP1	59:YY:108:LYS:NZ	2.20	0.74
4:9:687:C:N3	26:HH:118:ARG:NH2	2.35	0.74
4:9:77:A:N3	23:GG:175:LYS:HG3	2.03	0.74
2:5:1284:C:O2'	11:C:321:ASN:ND2	2.21	0.73
4:9:689:U:O2	26:HH:122:LEU:HD11	1.88	0.73
4:9:921:G:H1'	37:NN:11:LEU:HD21	1.70	0.73
4:9:448:A:H8	28:II:24:LYS:O	1.72	0.73
4:9:1609:C:H5''	47:SS:131:VAL:CG2	2.18	0.73
4:9:1332:A:HO2'	15:DD:145:GLN:C	1.95	0.73
4:9:1608:U:C5'	47:SS:130:ARG:NH1	2.51	0.73
4:9:1320:G:O5'	82:v:629:LYS:HD2	1.88	0.73
15:DD:148:LYS:HB2	83:w:206:HIS:CD2	2.24	0.73
4:9:616:A:OP1	57:XX:68:LYS:NZ	2.21	0.72
4:9:1568:C:H4'	49:TT:41:LYS:CE	2.19	0.72
6:AA:42:LYS:HE2	45:RR:99:ASP:CG	2.13	0.72
2:5:2642:G:H1	2:5:2701:A:H61	1.36	0.72
4:9:1417:C:H1'	49:TT:3:GLY:CA	2.19	0.72
4:9:503:C:OP1	18:EE:62:LYS:NZ	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:282:ARG:NH1	22:G:285:GLU:OE1	2.22	0.72
15:DD:143:ARG:CD	83:w:217:ASN:HB2	2.18	0.72
2:5:2461:G:H21	2:5:3676:G:H21	1.36	0.72
4:9:126:G:H2'	23:GG:199:THR:HG22	1.70	0.72
4:9:1397:U:O4	43:QQ:13:PHE:CE1	2.42	0.72
2:5:1355:G:OP1	11:C:33:ARG:NH1	2.23	0.71
4:9:1634:A:H4'	47:SS:142:ARG:NH1	2.04	0.71
4:9:1479:G:O2'	43:QQ:131:LYS:HE3	1.89	0.71
1:x:48:ARG:NH1	1:x:161:LYS:H	1.88	0.71
4:9:509:OMG:H5''	30:JJ:2:PRO:O	1.88	0.71
4:9:1869:A:N6	9:BB:114:VAL:O	2.24	0.71
4:9:1255:G:O4'	51:UU:71:GLY:HA3	1.89	0.71
4:9:1610:G:OP1	47:SS:121:ARG:NE	2.16	0.71
29:J:88:LYS:HD2	41:PP:12:PHE:HE1	1.55	0.71
6:AA:126:ASP:O	6:AA:130:ASP:HB2	1.91	0.71
4:9:294:U:C4	34:LL:65:ASN:HB2	2.25	0.71
4:9:1336:C:OP2	15:DD:185:LYS:NZ	2.24	0.71
4:9:142:C:H5'	23:GG:188:LYS:HE3	1.73	0.71
2:5:4639:A:H2	2:5:4667:G:H21	1.35	0.71
4:9:114:G:OP2	34:LL:132:ARG:HD2	1.91	0.71
4:9:1230:C:O5'	47:SS:139:THR:HB	1.90	0.71
4:9:1486:A:H4'	12:CC:118:ALA:HB2	1.72	0.71
4:9:1535:U:H6	21:FF:82:ASN:OD1	1.73	0.71
2:5:4550:A:N7	5:A:215:ASN:ND2	2.39	0.70
4:9:502:C:C5	18:EE:66:MET:HB3	2.26	0.70
4:9:1661:A:P	16:Dd:19:ARG:HH22	2.13	0.70
41:PP:110:GLU:HG3	47:SS:117:ILE:HD13	1.72	0.70
4:9:509:OMG:OP1	30:JJ:2:PRO:HD2	1.90	0.70
1:x:121:PRO:HA	1:x:125:GLY:HA3	1.72	0.70
4:9:658:U:H1'	57:XX:17:ARG:NH2	2.05	0.70
2:5:1506:G:H22	62:a:77:LYS:HD3	1.56	0.70
4:9:1544:C:O2'	43:QQ:75:GLY:O	2.08	0.70
2:5:3645:U:OP2	2:5:3650:A:N6	2.24	0.70
4:9:522:A:OP1	30:JJ:146:SER:OG	2.08	0.70
26:HH:148:LEU:HD12	55:WW:49:GLU:HB3	1.73	0.70
4:9:1706:G:H5''	75:n:1:MET:HE3	1.74	0.70
4:9:1587:G:N2	49:TT:77:LYS:HZ2	1.89	0.70
62:a:76:ASP:HB3	62:a:115:GLY:HA3	1.73	0.70
70:i:65:LYS:HD3	70:i:68:ARG:HD2	1.74	0.69
76:o:98:LYS:O	76:o:99:ARG:HD3	1.91	0.69
2:5:1665:C:OP1	66:e:36:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:3655:A:OP2	5:A:200:ARG:NH1	2.26	0.69
2:5:4527:A2M:H5''	2:5:4528:G:H5'	1.73	0.69
4:9:294:U:N3	34:LL:65:ASN:HB2	2.06	0.69
2:5:1864:B8H:C6	2:5:1864:B8H:C2	2.67	0.69
37:NN:18:TYR:CZ	55:WW:56:HIS:CE1	2.81	0.69
82:v:13:MET:SD	82:v:468:ASN:ND2	2.66	0.69
4:9:1489:A:H5''	83:w:195:ARG:CD	2.19	0.69
4:9:1643:U:H4'	43:QQ:143:LYS:O	1.91	0.69
11:C:221:PHE:HB3	11:C:227:ILE:HG21	1.75	0.69
38:O:85:ARG:HG3	38:O:99:LEU:HD11	1.74	0.69
4:9:629:A:H1'	83:w:210:ARG:HH22	1.57	0.69
4:9:1331:C:C5	83:w:198:GLY:N	2.60	0.69
82:v:110:ASP:HB2	82:v:553:HIS:HB2	1.74	0.69
4:9:1643:U:H5''	43:QQ:145:TYR:CD2	2.28	0.69
2:5:4300:B8H:C6	2:5:4300:B8H:C2	2.67	0.69
4:9:65:C:N4	23:GG:136:LYS:CD	2.56	0.69
4:9:143:U:O4	23:GG:188:LYS:HB2	1.93	0.69
34:LL:149:ALA:O	37:NN:133:ARG:NH2	2.26	0.68
61:ZZ:60:LYS:HG3	61:ZZ:61:GLU:HG2	1.74	0.68
82:v:42:LYS:HD3	82:v:347:GLY:HA3	1.73	0.68
4:9:75:G:C2	23:GG:159:ARG:NH2	2.61	0.68
2:5:3900:C:O2'	8:B:268:ARG:NH2	2.26	0.68
2:5:4128:G:N2	22:G:96:GLN:O	2.26	0.68
56:X:81:LEU:HD13	56:X:97:VAL:HG12	1.75	0.68
2:5:1864:B8H:C6	2:5:1864:B8H:CN1	2.70	0.68
4:9:1236:G:C4'	41:PP:133:ILE:HG23	2.24	0.68
2:5:5051:C:O2'	2:5:5054:C:OP2	2.12	0.68
4:9:821:G:C6	30:JJ:150:ARG:HG3	2.29	0.68
1:x:121:PRO:HG3	81:t:93:ILE:CD1	2.24	0.68
2:5:1357:G:N7	42:Q:104:ARG:NH2	2.42	0.68
4:9:873:G:H5''	44:R:162:ARG:HB3	1.76	0.68
4:9:1790:A:C4'	23:GG:81:HIS:HE1	2.07	0.68
11:C:143:ARG:HG2	11:C:178:ASN:HB3	1.76	0.68
18:EE:222:LEU:HA	18:EE:225:ILE:HD12	1.75	0.68
4:9:571:U:O3'	59:YY:60:PHE:O	2.12	0.68
23:GG:5:ILE:HD13	23:GG:124:LEU:HD22	1.76	0.68
4:9:1398:G:H1'	24:Gg:63:SER:OG	1.95	0.67
4:9:1489:A:C8	83:w:204:LEU:CD1	2.77	0.67
2:5:972:C:H42	2:5:2099:A:H61	1.42	0.67
4:9:78:C:H1'	23:GG:175:LYS:CD	2.24	0.67
4:9:871:U:O2'	44:R:163:ARG:NE	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:120:GLU:O	14:D:248:ARG:NH2	2.24	0.67
2:5:4755:G:H1	2:5:4952:C:H5	1.40	0.67
4:9:142:C:N3	23:GG:185:LEU:CD1	2.44	0.67
2:5:2815:G:N1	2:5:2818:C:OP2	2.26	0.67
4:9:1623:A:H5''	47:SS:133:GLY:HA3	1.76	0.67
2:5:2587:C:OP2	68:g:76:ARG:NH2	2.28	0.67
4:9:496:C:O3'	18:EE:29:PRO:HA	1.93	0.67
4:9:1332:A:O2'	15:DD:145:GLN:HB3	1.94	0.67
4:9:1553:C:H42	15:DD:76:ARG:HH22	1.43	0.67
2:5:245:C:O2'	2:5:246:G:OP2	2.11	0.67
4:9:522:A:H62	30:JJ:41:ARG:HH22	1.42	0.67
4:9:1535:U:C6	21:FF:82:ASN:OD1	2.47	0.67
29:J:90:ARG:NH2	29:J:108:GLY:O	2.27	0.67
28:II:149:TYR:HB3	28:II:153:LYS:HZ3	1.60	0.67
4:9:1556:A:N6	16:Dd:18:SER:HB2	2.10	0.67
17:E:189:LEU:H	17:E:253:GLN:HE22	1.42	0.67
4:9:495:U:H4'	18:EE:11:ARG:NH2	2.10	0.66
15:DD:146:ARG:CB	83:w:206:HIS:ND1	2.53	0.66
4:9:1568:C:H4'	49:TT:41:LYS:HE3	1.77	0.66
33:L:31:ARG:HG2	33:L:34:ARG:HH12	1.60	0.66
4:9:332:G:OP2	23:GG:193:ALA:CB	2.44	0.66
4:9:1580:A:C5	51:UU:57:PRO:HD3	2.31	0.66
23:GG:2:LYS:HB2	23:GG:108:VAL:HG22	1.76	0.66
25:H:114:ILE:HB	25:H:124:ARG:HB2	1.77	0.66
4:9:1643:U:H5''	43:QQ:145:TYR:CE2	2.30	0.66
82:v:370:GLU:O	82:v:495:ARG:NH2	2.29	0.66
4:9:1522:A:N6	41:PP:131:PRO:CG	2.56	0.66
82:v:141:THR:HG22	82:v:144:ARG:HH21	1.60	0.66
39:OO:67:ASP:HB2	39:OO:70:SER:HB3	1.77	0.66
2:5:1496:G:O2'	63:b:41:ARG:NH1	2.29	0.66
4:9:658:U:O2	57:XX:17:ARG:NH2	2.29	0.66
23:GG:208:GLU:HA	23:GG:211:LYS:HZ1	1.60	0.66
82:v:89:ILE:HG22	82:v:356:ILE:HG23	1.77	0.66
2:5:1559:G:O6	77:p:4:ARG:NH1	2.27	0.66
2:5:3771:C:HO2'	4:9:1828:C:H4'	1.58	0.66
4:9:1426:U:OP1	43:QQ:33:LYS:HD2	1.96	0.65
9:BB:138:PHE:HB2	9:BB:214:LYS:O	1.96	0.65
2:5:2841:U:OP1	8:B:249:ARG:NH1	2.28	0.65
2:5:4674:C:O2'	2:5:4676:A:OP2	2.13	0.65
4:9:190:G:O2'	4:9:209:A:N6	2.29	0.65
29:J:136:ARG:NH2	29:J:161:GLU:OE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1608:G:H2'	2:5:1609:7MG:H82	1.77	0.65
4:9:47:G:H1	4:9:479:C:H42	1.43	0.65
35:M:104:MET:HE2	38:O:199:HIS:HB3	1.78	0.65
4:9:374:G:H1'	34:LL:83:GLN:NE2	2.12	0.65
4:9:448:A:H3'	28:II:23:LYS:HD2	1.77	0.65
2:5:2525:G:H2'	2:5:2526:7MG:H82	1.77	0.65
26:HH:144:ILE:HD11	26:HH:152:ARG:HD3	1.78	0.65
82:v:351:LEU:HD23	82:v:354:ILE:HD11	1.78	0.65
2:5:2093:G:H1	2:5:2103:C:H41	1.45	0.65
2:5:4529:C:OP1	8:B:246:ARG:NH1	2.29	0.65
4:9:1489:A:C5'	83:w:195:ARG:HD2	2.20	0.65
21:FF:135:ARG:HH12	21:FF:203:ASN:HB2	1.62	0.65
4:9:827:A:H4'	30:JJ:8:VAL:O	1.97	0.65
18:EE:68:ARG:HG3	18:EE:76:VAL:HG11	1.79	0.65
40:P:126:ARG:HG2	40:P:140:MET:HE1	1.77	0.65
19:Ee:80:ALA:HB1	82:v:684:GLN:HE22	1.62	0.65
2:5:1994:A:H3'	2:5:1995:A:H5''	1.78	0.64
2:5:4300:B8H:C6	2:5:4300:B8H:CN1	2.70	0.64
9:BB:124:HIS:HA	9:BB:137:LEU:O	1.97	0.64
10:Bb:26:GLN:HB3	55:WW:57:ARG:HH12	1.61	0.64
13:Cc:47:LYS:HB2	21:FF:139:VAL:CG1	2.27	0.64
15:DD:143:ARG:HD3	83:w:216:HIS:O	1.92	0.64
56:X:77:ILE:HD12	56:X:116:LEU:HD12	1.79	0.64
26:HH:73:GLN:HA	26:HH:76:GLN:HB2	1.78	0.64
2:5:4624:OMU:OP2	2:5:4674:C:N4	2.24	0.64
6:AA:185:MET:HE3	53:VV:39:VAL:HG22	1.79	0.64
17:E:115:MET:O	78:r:87:ARG:NH1	2.28	0.64
24:Gg:87:LEU:HB2	24:Gg:101:PHE:HB2	1.80	0.64
4:9:522:A:OP2	30:JJ:45:ARG:NH1	2.30	0.64
4:9:151:C:OP1	59:YY:119:GLY:CA	2.45	0.64
4:9:294:U:H3	34:LL:65:ASN:HB2	1.63	0.64
4:9:1647:A:OP1	43:QQ:138:ARG:CZ	2.45	0.64
24:Gg:257:LYS:HZ3	24:Gg:268:ASP:H	1.45	0.64
4:9:345:U:H5''	18:EE:37:LYS:HB3	1.79	0.64
4:9:1397:U:O4	43:QQ:13:PHE:HD1	1.77	0.64
2:5:4352:A:O2'	2:5:4354:C:OP2	2.15	0.64
4:9:1148:A:OP1	7:Aa:6:ARG:NH2	2.30	0.64
4:9:1613:G:H3'	41:PP:39:ALA:CB	2.28	0.64
17:E:64:MET:HG3	17:E:68:LYS:HE3	1.79	0.64
8:B:205:VAL:HG13	8:B:209:GLN:HE21	1.62	0.64
79:s:30:VAL:HG21	79:s:187:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:v:120:ARG:HE	82:v:497:MET:HG2	1.62	0.64
4:9:1023:A:OP2	37:NN:124:ARG:HD2	1.97	0.64
4:9:1396:A:O2'	4:9:1398:G:N7	2.31	0.64
4:9:1745:A:C2'	23:GG:66:GLY:CA	2.60	0.64
2:5:914:U:O4	2:5:919:C:N4	2.30	0.64
2:5:2762:G:O2'	2:5:2769:A:N3	2.31	0.64
4:9:526:A:H5'	19:Ee:104:ARG:NH1	2.13	0.64
4:9:1225:U:H1'	43:QQ:142:GLN:HE22	1.62	0.64
4:9:1634:A:H4'	47:SS:142:ARG:NE	2.11	0.63
2:5:2561:G:H1	2:5:2574:U:H3	1.47	0.63
4:9:1790:A:C4'	23:GG:81:HIS:CE1	2.70	0.63
2:5:4545:G:N2	2:5:4548:A:OP2	2.28	0.63
4:9:1333:U:H4'	15:DD:147:ALA:HB2	1.81	0.63
4:9:1677:U:H2'	4:9:1678:A2M:H8	1.79	0.63
39:OO:96:LYS:HA	39:OO:130:GLU:O	1.97	0.63
1:x:71:GLN:NE2	29:J:38:LYS:HZ1	1.96	0.63
1:x:71:GLN:OE1	29:J:35:ARG:HD3	1.99	0.63
4:9:1647:A:P	43:QQ:138:ARG:HH12	2.14	0.63
1:x:48:ARG:HH12	1:x:161:LYS:H	1.46	0.63
4:9:1255:G:C4'	51:UU:71:GLY:HA3	2.28	0.63
4:9:1791:A:H5''	23:GG:75:LEU:CD1	2.20	0.63
2:5:1886:U:OP2	66:e:46:ARG:NH1	2.32	0.63
4:9:687:C:C4	26:HH:118:ARG:NH2	2.66	0.63
6:AA:15:VAL:HG21	45:RR:111:PHE:CG	2.34	0.63
6:AA:33:GLN:HB3	6:AA:154:LEU:HD22	1.81	0.63
12:CC:264:SER:HB3	12:CC:267:GLN:HG3	1.80	0.63
17:E:156:LEU:HD11	17:E:198:ILE:HG13	1.79	0.63
2:5:115:C:O2'	2:5:276:C:OP1	2.17	0.63
4:9:1587:G:C2	49:TT:77:LYS:HD2	2.34	0.63
2:5:1077:G:H22	2:5:1242:A:H2	1.45	0.63
4:9:332:G:OP2	23:GG:193:ALA:HB1	1.99	0.63
4:9:448:A:C8	28:II:24:LYS:O	2.51	0.63
6:AA:203:PHE:HZ	45:RR:91:LEU:HD21	1.64	0.63
22:G:111:PRO:HD2	22:G:114:ILE:HD12	1.81	0.63
33:L:75:GLY:O	33:L:102:ARG:NH2	2.32	0.63
2:5:408:A:H4'	2:5:409:G:H3'	1.80	0.62
2:5:1080:C:O2	2:5:1239:G:N2	2.32	0.62
2:5:1398:G:OP1	33:L:186:ARG:NH2	2.32	0.62
2:5:2326:G:OP1	66:e:36:ARG:NH1	2.32	0.62
4:9:925:G:OP1	37:NN:121:ARG:NH2	2.32	0.62
4:9:1216:C:O2'	43:QQ:143:LYS:NZ	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:JJ:164:PRO:HB3	30:JJ:170:PRO:HA	1.81	0.62
2:5:2410:G:O2'	73:l:48:LYS:NZ	2.32	0.62
4:9:1298:G:H5'	41:PP:79:HIS:CE1	2.34	0.62
5:A:234:LYS:HG2	5:A:238:ILE:HD12	1.81	0.62
24:Gg:130:LYS:NZ	24:Gg:131:LEU:O	2.32	0.62
34:LL:4:ILE:HG12	34:LL:5:GLN:HG3	1.81	0.62
76:o:98:LYS:C	76:o:99:ARG:HD3	2.24	0.62
79:s:29:ILE:HB	79:s:191:GLN:HB3	1.81	0.62
4:9:142:C:OP2	23:GG:188:LYS:CE	2.46	0.62
4:9:1791:A:C4'	23:GG:75:LEU:CD1	2.74	0.62
14:D:83:LEU:HB3	14:D:88:VAL:HB	1.80	0.62
22:G:93:GLY:HA3	22:G:96:GLN:HE21	1.63	0.62
4:9:1320:G:H4'	82:v:629:LYS:HZ2	1.64	0.62
4:9:1614:A:OP2	41:PP:39:ALA:HB1	1.99	0.62
4:9:1705:C:H4'	75:n:1:MET:N	2.14	0.62
18:EE:11:ARG:NH1	18:EE:21:ASP:OD1	2.32	0.62
27:I:76:MET:HE3	27:I:138:ILE:HG21	1.80	0.62
39:OO:30:VAL:HG12	39:OO:94:HIS:HB2	1.81	0.62
2:5:1191:G:N2	2:5:1191:G:OP2	2.33	0.62
4:9:148:U:H2'	4:9:149:A:H8	1.65	0.62
79:s:36:GLY:H	79:s:39:GLN:HE21	1.48	0.62
4:9:502:C:C5	18:EE:66:MET:CB	2.83	0.62
4:9:503:C:P	18:EE:62:LYS:NZ	2.72	0.62
2:5:74:G:H5'	33:L:59:VAL:HB	1.81	0.62
4:9:581:U:P	59:YY:64:PHE:CE1	2.93	0.62
30:JJ:42:GLU:HA	30:JJ:45:ARG:HG2	1.81	0.62
32:KK:8:ARG:NH2	32:KK:12:TYR:OH	2.32	0.62
66:e:57:ASN:HD22	66:e:59:GLY:H	1.46	0.62
79:s:109:ALA:O	79:s:181:SER:OG	2.17	0.62
82:v:648:LYS:HB3	82:v:664:ASP:HB3	1.79	0.62
2:5:1441:C:H5''	2:5:1442:U:H5'	1.80	0.62
2:5:4876:2MG:OP2	35:M:94:LYS:NZ	2.33	0.62
2:5:4914:A:H4'	8:B:95:THR:HG22	1.81	0.62
4:9:502:C:C4	18:EE:67:GLN:OE1	2.52	0.62
6:AA:15:VAL:HG21	45:RR:111:PHE:CD1	2.34	0.62
12:CC:142:LYS:HD2	12:CC:153:GLY:HA3	1.82	0.62
55:WW:86:LEU:HD23	55:WW:117:ARG:HE	1.65	0.62
3:8:142:U:OP1	36:N:38:ARG:NH2	2.33	0.61
4:9:1613:G:H3'	41:PP:39:ALA:HB2	1.81	0.61
24:Gg:174:VAL:HG23	24:Gg:188:HIS:HB2	1.81	0.61
2:5:4080:G:OP1	22:G:126:ARG:NE	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1236:G:H4'	41:PP:133:ILE:O	2.00	0.61
50:U:107:LYS:HG2	50:U:108:GLU:HG3	1.81	0.61
4:9:77:A:C2	23:GG:175:LYS:CE	2.82	0.61
4:9:1550:G:H3'	4:9:1579:A:H61	1.64	0.61
11:C:140:LYS:HE2	11:C:245:HIS:HB2	1.82	0.61
37:NN:4:MET:SD	37:NN:124:ARG:NH2	2.73	0.61
59:YY:83:LYS:HE3	59:YY:96:LEU:HD23	1.82	0.61
4:9:1534:C:OP1	21:FF:81:ARG:NH1	2.26	0.61
4:9:1746:U:C4'	23:GG:65:GLN:CG	2.73	0.61
52:V:82:ILE:HG22	52:V:83:ARG:HG3	1.82	0.61
4:9:76:U:H1'	23:GG:154:ARG:HH12	1.66	0.61
27:I:189:ARG:NH1	27:I:200:ILE:O	2.33	0.61
51:UU:21:ARG:HB2	51:UU:115:THR:HB	1.82	0.61
2:5:1381:G:H21	2:5:1384:G:H5''	1.65	0.61
2:5:3872:G:H22	2:5:3904:G:H1'	1.66	0.61
4:9:495:U:H4'	18:EE:11:ARG:HH22	1.64	0.61
5:A:117:GLU:HG3	5:A:162:ASN:HB2	1.82	0.61
34:LL:11:GLN:HB3	34:LL:56:ILE:HD13	1.81	0.61
82:v:19:ILE:HG22	82:v:99:LEU:HB3	1.83	0.61
2:5:938:A:OP1	35:M:44:ARG:NH2	2.34	0.61
9:BB:66:VAL:HG22	9:BB:87:ILE:HG22	1.82	0.61
4:9:1650:A:C4'	43:QQ:139:ALA:HB2	2.30	0.61
18:EE:122:LYS:NZ	18:EE:124:CYS:SG	2.74	0.61
36:N:123:GLU:OE1	36:N:128:LYS:NZ	2.34	0.61
2:5:280:G:H5''	36:N:14:LYS:HE2	1.82	0.60
4:9:1397:U:C4	43:QQ:13:PHE:CE1	2.89	0.60
4:9:1608:U:C4'	47:SS:130:ARG:HD2	2.31	0.60
42:Q:16:LYS:O	42:Q:33:ARG:NH2	2.35	0.60
4:9:1608:U:H4'	47:SS:130:ARG:CZ	2.30	0.60
4:9:1650:A:OP1	43:QQ:137:ALA:N	2.35	0.60
18:EE:137:PRO:HB2	18:EE:150:PRO:HD2	1.84	0.60
2:5:1181:U:O2'	14:D:282:GLN:NE2	2.33	0.60
20:F:104:VAL:HG13	20:F:135:VAL:HG12	1.83	0.60
22:G:273:GLU:OE1	22:G:276:ARG:NH1	2.34	0.60
28:II:129:LEU:HD22	28:II:134:GLU:HB3	1.84	0.60
2:5:4435:U:OP2	27:I:3:ARG:NH1	2.35	0.60
2:5:4773:G:H5'	38:O:176:ARG:HD3	1.83	0.60
23:GG:231:ARG:HA	23:GG:234:LEU:HB2	1.83	0.60
28:II:139:LYS:HA	28:II:141:ARG:HH21	1.66	0.60
59:YY:86:GLU:OE2	59:YY:90:ARG:NH1	2.33	0.60
2:5:303:C:OP2	36:N:68:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2643:U:H2'	2:5:2698:G:H1	1.65	0.60
4:9:65:C:O2	23:GG:174:PRO:HB3	2.01	0.60
4:9:127:C:O2	18:EE:134:LYS:NZ	2.30	0.60
4:9:294:U:O4	34:LL:65:ASN:HB2	2.01	0.60
4:9:1578:U:H1'	15:DD:6:SER:HB2	1.84	0.60
4:9:1587:G:N2	49:TT:77:LYS:NZ	2.46	0.60
24:Gg:99:ARG:NH2	24:Gg:136:GLY:O	2.33	0.60
39:OO:102:GLY:O	39:OO:106:LYS:NZ	2.35	0.60
40:P:23:ARG:NH2	40:P:125:MET:SD	2.74	0.60
81:t:136:ILE:HG12	81:t:150:ILE:HG22	1.83	0.60
82:v:401:MET:HB3	82:v:410:PHE:HB3	1.83	0.60
2:5:2266:G:OP2	78:r:98:ARG:NH2	2.34	0.60
3:8:85:U:O4	58:Y:50:ARG:NH1	2.34	0.60
44:R:105:LEU:HD22	44:R:135:LYS:HG3	1.82	0.60
5:A:117:GLU:HB2	5:A:122:ASP:OD1	2.02	0.60
21:FF:188:TYR:O	21:FF:192:LYS:NZ	2.34	0.60
2:5:2536:C:O2'	56:X:93:ASN:ND2	2.34	0.60
8:B:291:TYR:HB3	8:B:298:LEU:HD11	1.83	0.60
3:8:153:C:OP1	22:G:238:LYS:NZ	2.35	0.60
4:9:925:G:H1	4:9:1017:U:H3	1.48	0.60
4:9:1256:G:C4	16:Dd:40:ARG:HD3	2.37	0.60
15:DD:137:VAL:HG22	15:DD:151:LYS:HG3	1.84	0.60
24:Gg:215:GLN:NE2	24:Gg:231:ASP:OD1	2.35	0.60
51:UU:33:GLU:OE2	51:UU:87:ARG:NH2	2.34	0.60
2:5:407:A:O2'	2:5:410:A:OP1	2.16	0.59
2:5:3663:G:H4'	5:A:227:ARG:HH22	1.67	0.59
4:9:924:G:OP2	37:NN:3:ARG:NE	2.31	0.59
4:9:1479:G:O2'	43:QQ:131:LYS:CE	2.49	0.59
15:DD:29:LEU:HB2	15:DD:34:TYR:HB2	1.83	0.59
30:JJ:136:ARG:NH1	30:JJ:159:PHE:O	2.35	0.59
35:M:119:ARG:NH2	38:O:193:THR:OG1	2.35	0.59
82:v:26:ALA:HB2	82:v:128:VAL:HB	1.83	0.59
2:5:4130:C:OP1	22:G:90:LYS:NZ	2.28	0.59
4:9:144:U:OP2	23:GG:178:ARG:NE	2.35	0.59
4:9:1417:C:H1'	49:TT:3:GLY:N	2.14	0.59
15:DD:146:ARG:O	83:w:206:HIS:HE1	1.80	0.59
82:v:209:LEU:O	82:v:357:HIS:NE2	2.34	0.59
2:5:1503:C:OP1	42:Q:150:ARG:NH2	2.35	0.59
4:9:142:C:C6	23:GG:185:LEU:HD22	2.35	0.59
4:9:1416:C:C4'	49:TT:132:ASP:CG	2.66	0.59
9:BB:122:GLU:O	9:BB:165:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:71:GLN:NE2	29:J:38:LYS:HZ2	1.99	0.59
2:5:3658:G:O2'	2:5:3697:U:OP1	2.16	0.59
2:5:4081:A:N1	2:5:4175:C:N4	2.50	0.59
51:UU:45:GLU:HG3	51:UU:46:LYS:HG3	1.84	0.59
4:9:1580:A:N7	51:UU:57:PRO:CD	2.61	0.59
4:9:109:U:O2'	34:LL:71:ARG:NH2	2.35	0.59
13:Cc:47:LYS:HB2	21:FF:139:VAL:HG11	1.84	0.59
15:DD:222:PRO:HA	24:Gg:189:ILE:O	2.02	0.59
78:r:28:GLU:OE2	78:r:31:ASN:ND2	2.36	0.59
82:v:630:GLN:OE1	82:v:633:ARG:NH2	2.36	0.59
2:5:972:C:HO2'	2:5:2263:G:H1	1.50	0.59
4:9:126:G:C2'	23:GG:199:THR:HG22	2.32	0.59
4:9:510:G:OP1	30:JJ:3:VAL:HA	2.02	0.59
4:9:1236:G:C5'	41:PP:133:ILE:HG23	2.32	0.59
4:9:1334:G:H5'	15:DD:140:GLY:HA2	1.85	0.59
4:9:1397:U:N3	43:QQ:13:PHE:CE1	2.62	0.59
4:9:1466:G:OP1	45:RR:4:VAL:HG13	2.03	0.59
4:9:1580:A:N9	51:UU:57:PRO:HG3	2.18	0.59
21:FF:182:LYS:HD3	21:FF:184:SER:HB2	1.85	0.59
25:H:118:LEU:HD11	25:H:167:VAL:HG22	1.85	0.59
32:KK:11:ILE:HD12	32:KK:45:VAL:HG23	1.84	0.59
39:OO:29:GLY:O	39:OO:93:LEU:HA	2.02	0.59
41:PP:100:LYS:HG3	41:PP:101:THR:HG23	1.83	0.59
43:QQ:116:ASP:HB3	43:QQ:119:LEU:HD23	1.85	0.59
2:5:1372:A:H1'	58:Y:1:MET:HE2	1.82	0.59
4:9:1224:G:H21	43:QQ:142:GLN:NE2	2.01	0.59
17:E:193:HIS:HD2	17:E:195:LYS:H	1.50	0.59
4:9:441:C:OP2	28:II:2:GLY:N	2.35	0.59
4:9:639:C:H2'	4:9:640:A:H8	1.68	0.59
4:9:1609:C:C5'	47:SS:131:VAL:HB	2.30	0.59
6:AA:200:ASP:OD2	45:RR:89:SER:HA	2.03	0.59
47:SS:127:TRP:O	47:SS:144:ARG:NH2	2.36	0.59
2:5:4419:1MA:N6	2:5:4431:G:HO2'	1.99	0.58
4:9:120:U:H1'	18:EE:33:THR:O	2.03	0.58
18:EE:63:LYS:O	18:EE:67:GLN:NE2	2.33	0.58
82:v:601:ARG:HH11	82:v:708:THR:HG21	1.67	0.58
2:5:1485:C:O2'	2:5:1486:G:O5'	2.22	0.58
2:5:3815:G:O2'	2:5:3818:U:OP2	2.18	0.58
4:9:386:C:H5''	28:II:10:LYS:CD	2.29	0.58
6:AA:80:ARG:NH2	6:AA:126:ASP:OD2	2.36	0.58
14:D:33:ARG:NH1	14:D:72:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LL:68:ILE:HG21	34:LL:143:LEU:HD21	1.86	0.58
47:SS:34:LYS:HB3	47:SS:100:ALA:HA	1.84	0.58
14:D:271:MET:O	14:D:276:LYS:NZ	2.36	0.58
18:EE:19:MET:HE1	18:EE:108:ARG:HH21	1.67	0.58
62:a:72:THR:HG22	62:a:110:LYS:HB3	1.85	0.58
78:r:28:GLU:HG2	78:r:31:ASN:HB2	1.85	0.58
2:5:2050:G:H5'	38:O:60:LYS:HE2	1.84	0.58
26:HH:40:LEU:HA	26:HH:43:LEU:HD22	1.86	0.58
82:v:766:LYS:HE3	82:v:796:PHE:HA	1.85	0.58
4:9:688:U:H2'	26:HH:103:LYS:HD2	1.85	0.58
4:9:923:G:H5''	37:NN:2:GLY:O	2.04	0.58
14:D:56:THR:HG21	31:K:26:C:H5''	1.85	0.58
3:8:41:A:H4'	71:j:59:THR:HG23	1.85	0.58
4:9:190:G:C5'	28:II:145:ILE:HD13	2.32	0.58
4:9:1402:A:C4'	51:UU:54:VAL:HG22	2.34	0.58
7:Aa:57:SER:HA	39:OO:126:ILE:O	2.04	0.58
21:FF:35:LEU:HD23	21:FF:146:ARG:HH21	1.68	0.58
46:S:164:LYS:HB3	46:S:165:PRO:HD3	1.84	0.58
49:TT:38:LYS:NZ	49:TT:40:ALA:O	2.37	0.58
81:t:104:GLN:HE21	81:t:110:ARG:HB3	1.68	0.58
4:9:70:G:O2'	4:9:79:A:N6	2.36	0.58
4:9:1447:G:OP1	51:UU:85:HIS:CE1	2.56	0.58
8:B:222:VAL:O	8:B:343:ARG:NH1	2.36	0.58
9:BB:146:ARG:HH21	9:BB:206:PRO:HG3	1.69	0.58
24:Gg:176:VAL:O	24:Gg:185:LYS:N	2.37	0.58
37:NN:99:ARG:NH2	37:NN:119:GLU:OE2	2.37	0.58
54:W:8:PHE:HZ	54:W:49:ILE:HD12	1.69	0.58
60:Z:99:ASP:OD1	60:Z:102:ARG:NH2	2.32	0.58
4:9:1791:A:C5'	23:GG:75:LEU:CD1	2.80	0.58
45:RR:94:GLU:O	45:RR:116:ASN:ND2	2.36	0.58
50:U:100:LEU:HD13	50:U:112:LEU:HD23	1.85	0.58
4:9:1402:A:H4'	51:UU:54:VAL:CG2	2.34	0.58
55:WW:30:CYS:SG	55:WW:31:SER:N	2.77	0.58
2:5:1874:C:H2'	2:5:1875:A2M:H8	1.84	0.58
4:9:1661:A:C8	16:Dd:14:PHE:HD2	2.22	0.58
4:9:1864:U:O2'	4:9:1866:A:N7	2.37	0.58
5:A:209:HIS:CE1	5:A:235:VAL:HG11	2.39	0.58
9:BB:119:THR:H	9:BB:143:THR:HG22	1.69	0.58
12:CC:134:ASN:OD1	12:CC:167:ARG:NH1	2.37	0.58
14:D:65:ALA:HB2	14:D:74:ILE:HD13	1.86	0.58
64:c:38:ILE:HD11	64:c:46:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:123:G:H4'	18:EE:146:THR:O	2.04	0.57
4:9:380:G:H1'	28:II:5:ARG:HH22	1.68	0.57
30:JJ:169:ARG:HE	30:JJ:175:ARG:HD3	1.69	0.57
4:9:76:U:H1'	23:GG:154:ARG:NH1	2.19	0.57
28:II:150:ASP:HA	28:II:153:LYS:HD3	1.85	0.57
42:Q:178:ARG:H	62:a:51:GLY:HA2	1.69	0.57
2:5:4236:U:H4'	2:5:4237:A:O5'	2.04	0.57
4:9:57:U:O2'	4:9:499:G:N3	2.37	0.57
4:9:190:G:H5''	28:II:145:ILE:CD1	2.33	0.57
4:9:872:A:O2'	4:9:874:G:OP2	2.22	0.57
82:v:627:GLU:HB3	82:v:630:GLN:HB3	1.86	0.57
2:5:2461:G:H21	2:5:3676:G:N2	2.03	0.57
4:9:91:A:N1	23:GG:88:ARG:NH2	2.52	0.57
4:9:637:U:O2	19:Ee:129:ASN:ND2	2.36	0.57
15:DD:59:LEU:HG	15:DD:66:ILE:HD11	1.85	0.57
32:KK:35:LEU:HD12	32:KK:40:VAL:HG21	1.84	0.57
58:Y:112:ASP:H	58:Y:115:ARG:HB3	1.69	0.57
82:v:727:ARG:NH1	82:v:853:ASN:O	2.37	0.57
4:9:122:G:H1'	18:EE:144:ALA:O	2.05	0.57
82:v:675:ILE:HG22	82:v:721:ILE:HD13	1.85	0.57
4:9:26:U:H2'	4:9:27:A2M:H8	1.87	0.57
4:9:355:G:H5''	34:LL:105:ARG:NH1	2.20	0.57
4:9:628:A:C6	83:w:216:HIS:CD2	2.92	0.57
4:9:916:A:C4	37:NN:73:ARG:CD	2.86	0.57
55:WW:46:TYR:HB3	55:WW:69:LEU:HB3	1.86	0.57
79:s:27:CYS:HB2	79:s:193:PHE:HB3	1.86	0.57
82:v:739:ARG:NH1	82:v:823:ASP:OD1	2.37	0.57
4:9:1298:G:O4'	41:PP:79:HIS:CE1	2.56	0.57
4:9:1647:A:H5'	43:QQ:138:ARG:CZ	2.35	0.57
13:Cc:7:GLN:OE1	13:Cc:10:LYS:NZ	2.38	0.57
45:RR:98:VAL:HG11	45:RR:117:LEU:HD12	1.86	0.57
51:UU:59:LYS:HB2	51:UU:84:ILE:HG22	1.86	0.57
1:x:92:LYS:O	1:x:94:ASN:ND2	2.37	0.57
2:5:67:C:OP2	2:5:312:G:N2	2.38	0.57
4:9:372:U:OP1	28:II:12:ARG:O	2.22	0.57
4:9:1865:C:O4'	7:Aa:5:ARG:HD2	2.05	0.57
38:O:166:ILE:HD13	38:O:169:ARG:HH12	1.70	0.57
64:c:99:PRO:HD3	64:c:105:ILE:HD12	1.86	0.57
82:v:607:ARG:HH21	82:v:701:ARG:HE	1.53	0.57
4:9:502:C:C6	18:EE:66:MET:HG3	2.39	0.56
4:9:694:G:H22	4:9:732:U:H3	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1121:G:O2'	9:BB:204:ILE:HG13	2.05	0.56
4:9:1454:A:H3'	45:RR:5:ARG:HH12	1.69	0.56
4:9:1489:A:H62	83:w:197:SER:CB	2.18	0.56
50:U:41:GLN:NE2	50:U:44:GLN:OE1	2.38	0.56
2:5:1373:C:OP2	2:5:1374:G:O2'	2.23	0.56
2:5:1891:G:OP2	67:f:19:ARG:NH2	2.38	0.56
2:5:4293:U:HO2'	2:5:4324:G:HO2'	1.47	0.56
4:9:126:G:O6	23:GG:196:LYS:HG2	2.06	0.56
4:9:385:G:H3'	34:LL:136:LYS:HB2	1.87	0.56
4:9:584:A:OP1	30:JJ:169:ARG:NH2	2.34	0.56
15:DD:135:GLU:HG3	15:DD:153:VAL:HG12	1.87	0.56
45:RR:74:GLN:HA	45:RR:77:GLU:HG2	1.87	0.56
51:UU:26:SER:HB2	51:UU:110:VAL:HA	1.87	0.56
65:d:64:ILE:HG23	65:d:68:LEU:HD23	1.87	0.56
82:v:5:THR:OG1	82:v:7:ASP:OD1	2.18	0.56
2:5:709:C:H1'	2:5:4946:C:H5	1.70	0.56
2:5:2547:A:H2	2:5:2777:OMG:HN21	1.52	0.56
2:5:2583:G:N2	2:5:2586:A:OP2	2.34	0.56
2:5:4306:U:H4'	48:T:5:LYS:HD2	1.86	0.56
4:9:1397:U:C4	43:QQ:13:PHE:CD1	2.91	0.56
11:C:78:ARG:HB3	11:C:88:GLY:HA2	1.87	0.56
21:FF:24:SER:O	21:FF:107:ASN:ND2	2.31	0.56
2:5:134:G:H4'	2:5:135:G:O5'	2.06	0.56
2:5:1507:A:H4'	2:5:1508:G:H5'	1.86	0.56
2:5:2605:A:N6	2:5:2748:A:OP2	2.39	0.56
4:9:555:A:H5'	19:Ee:98:LYS:HE3	1.88	0.56
4:9:1488:C:O2'	4:9:1490:G:OP2	2.21	0.56
9:BB:48:LEU:HB2	39:OO:51:GLU:HG2	1.86	0.56
82:v:671:TYR:HB2	82:v:709:LEU:HD12	1.88	0.56
4:9:75:G:N2	23:GG:159:ARG:HH21	2.04	0.56
34:LL:59:LYS:HD3	34:LL:134:LEU:HD23	1.88	0.56
2:5:154:G:H4'	69:h:105:LYS:HD3	1.87	0.56
2:5:1904:C:H5'	66:e:57:ASN:HD21	1.71	0.56
2:5:2469:C:H1'	2:5:3676:G:N2	2.18	0.56
4:9:913:A:H61	26:HH:119:SER:HB3	1.70	0.56
14:D:253:TYR:OH	31:K:117:G:OP1	2.21	0.56
17:E:196:PHE:HD2	67:f:106:TYR:HB2	1.71	0.56
24:Gg:217:MET:SD	24:Gg:219:TRP:NE1	2.79	0.56
36:N:137:PRO:HA	36:N:142:ILE:HD11	1.87	0.56
39:OO:95:ILE:HB	39:OO:129:ILE:HG22	1.87	0.56
4:9:78:C:C1'	23:GG:175:LYS:HD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:603:C:N4	4:9:620:G:O6	2.39	0.56
4:9:1646:C:H5''	43:QQ:138:ARG:HH11	1.70	0.56
28:II:36:THR:HG23	28:II:96:LEU:HB2	1.88	0.56
38:O:54:TYR:OH	38:O:73:PHE:O	2.23	0.56
60:Z:89:ILE:HG22	60:Z:91:LEU:HG	1.87	0.56
82:v:42:LYS:NZ	82:v:348:ASP:OD1	2.39	0.56
1:x:71:GLN:N	29:J:31:ASP:OD2	2.30	0.56
36:N:193:ARG:O	36:N:197:THR:OG1	2.21	0.56
61:ZZ:48:VAL:HG22	61:ZZ:80:ARG:HE	1.71	0.56
1:x:71:GLN:HB2	29:J:31:ASP:OD2	2.05	0.56
2:5:4126:G:H4'	68:g:90:ARG:HG2	1.86	0.56
18:EE:69:PHE:CD2	59:YY:17:LEU:HD22	2.41	0.56
70:i:50:PHE:O	70:i:55:ARG:NH2	2.39	0.56
4:9:522:A:H3'	30:JJ:38:ARG:NH2	2.21	0.55
4:9:628:A:C5	83:w:216:HIS:CE1	2.94	0.55
4:9:628:A:N1	83:w:216:HIS:CD2	2.74	0.55
11:C:65:GLU:HG3	11:C:80:ARG:HH21	1.70	0.55
13:Cc:49:PRO:HA	21:FF:60:ARG:NH2	2.21	0.55
15:DD:146:ARG:CG	83:w:206:HIS:HB2	2.32	0.55
24:Gg:99:ARG:NH1	24:Gg:134:THR:O	2.39	0.55
32:KK:85:LEU:HB3	32:KK:89:ILE:HD11	1.88	0.55
45:RR:104:GLU:HA	45:RR:107:LYS:HG2	1.86	0.55
58:Y:54:GLU:HB2	58:Y:108:ARG:HG2	1.88	0.55
79:s:127:ASN:ND2	79:s:153:GLU:OE1	2.39	0.55
30:JJ:108:ARG:NH2	30:JJ:149:VAL:O	2.39	0.55
32:KK:80:ARG:HD3	32:KK:85:LEU:HB2	1.88	0.55
61:ZZ:88:LEU:HG	61:ZZ:91:LEU:HD12	1.87	0.55
2:5:4931:G:OP2	2:5:4931:G:N2	2.30	0.55
4:9:164:A:H3'	4:9:165:G:H21	1.71	0.55
4:9:830:A:OP2	4:9:846:G:N2	2.38	0.55
4:9:1591:C:H5'	21:FF:85:LYS:HZ2	1.70	0.55
14:D:224:SER:HB3	31:K:49:A:H5''	1.89	0.55
21:FF:40:ALA:H	21:FF:68:ILE:HD11	1.70	0.55
24:Gg:58:ALA:HB1	24:Gg:60:ARG:HH12	1.72	0.55
78:r:26:SER:OG	78:r:28:GLU:OE1	2.23	0.55
82:v:820:LEU:HD12	82:v:821:PRO:HD2	1.88	0.55
2:5:1632:C:OP1	5:A:14:SER:OG	2.24	0.55
2:5:4680:G:OP1	8:B:281:ASN:ND2	2.39	0.55
4:9:913:A:C2'	26:HH:120:ARG:NH2	2.60	0.55
4:9:1520:G:OP1	47:SS:137:LYS:HB2	2.06	0.55
34:LL:102:PHE:H	57:XX:8:ARG:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Q:122:THR:OG1	42:Q:124:ASP:OD1	2.20	0.55
4:9:1643:U:O3'	43:QQ:143:LYS:HB3	2.05	0.55
15:DD:116:ARG:HB2	83:w:219:GLY:HA3	1.83	0.55
23:GG:12:CYS:SG	23:GG:13:GLN:N	2.80	0.55
59:YY:27:VAL:O	59:YY:68:LYS:HA	2.07	0.55
82:v:24:VAL:HG12	82:v:104:ASP:HA	1.87	0.55
3:8:96:C:H5''	69:h:66:LYS:HD2	1.89	0.55
4:9:1402:A:H4'	51:UU:54:VAL:HG22	1.88	0.55
4:9:1404:U:C2	51:UU:56:MET:CE	2.90	0.55
4:9:1513:C:H2'	4:9:1514:G:H8	1.71	0.55
9:BB:138:PHE:HD2	9:BB:214:LYS:HB3	1.72	0.55
1:x:47:LYS:O	1:x:159:MET:HB3	2.06	0.55
4:9:385:G:O2'	28:II:10:LYS:NZ	2.31	0.55
4:9:562:U:H1'	30:JJ:132:GLN:HG2	1.88	0.55
4:9:913:A:H2'	26:HH:120:ARG:HH21	1.69	0.55
9:BB:138:PHE:O	9:BB:213:ARG:N	2.39	0.55
24:Gg:99:ARG:HH12	24:Gg:136:GLY:HA3	1.71	0.55
29:J:85:LYS:HA	29:J:88:LYS:HE2	1.89	0.55
2:5:2839:A:O2'	8:B:228:TYR:O	2.23	0.55
4:9:1156:U:OP1	55:WW:71:LYS:NZ	2.30	0.55
4:9:1648:G:H3'	43:QQ:128:GLU:H	1.71	0.55
4:9:1650:A:OP1	43:QQ:136:GLY:HA3	2.07	0.55
19:Ee:104:ARG:HB3	30:JJ:38:ARG:HA	1.89	0.55
51:UU:96:GLU:HG2	51:UU:97:ILE:HG13	1.88	0.55
2:5:2093:G:OP2	11:C:294:LYS:NZ	2.34	0.55
2:5:3721:A:OP2	2:5:3739:G:N2	2.38	0.55
4:9:522:A:H62	30:JJ:41:ARG:NH2	2.05	0.55
4:9:1599:U:OP1	61:ZZ:80:ARG:NH2	2.39	0.55
20:F:126:LYS:HB2	48:T:133:ALA:HB3	1.88	0.55
21:FF:32:ASP:OD2	21:FF:146:ARG:NH2	2.40	0.55
21:FF:63:LYS:O	21:FF:71:ARG:NH1	2.40	0.55
21:FF:87:LEU:HA	21:FF:90:VAL:HG12	1.89	0.55
41:PP:53:GLN:HB2	41:PP:83:MET:HE1	1.89	0.55
2:5:1444:U:OP2	20:F:33:ARG:NH1	2.40	0.55
4:9:991:G:N7	7:Aa:7:ASN:ND2	2.55	0.55
4:9:1284:A:N6	4:9:1313:A:O2'	2.38	0.55
4:9:1417:C:C6	49:TT:3:GLY:N	2.74	0.55
47:SS:75:ARG:NH1	47:SS:81:ASP:OD1	2.40	0.55
50:U:25:CYS:O	50:U:68:SER:OG	2.24	0.55
2:5:364:G:O6	71:j:55:ARG:NH1	2.40	0.54
2:5:926:C:OP1	2:5:928:G:O2'	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:2:A:O2'	12:CC:224:THR:O	2.24	0.54
4:9:508:A:H3'	4:9:509:OMG:H8	1.71	0.54
4:9:636:C:OP1	19:Ee:97:LYS:NZ	2.32	0.54
4:9:1172:U:C4'	75:n:10:MET:CE	2.53	0.54
4:9:1718:G:O2'	4:9:1815:A:N6	2.40	0.54
47:SS:132:ARG:HB2	47:SS:134:GLN:HE22	1.72	0.54
4:9:1179:G:N2	4:9:1182:A:OP2	2.41	0.54
34:LL:35:ARG:NH1	34:LL:53:GLY:O	2.40	0.54
36:N:145:ASN:HB3	36:N:148:THR:HG22	1.90	0.54
41:PP:44:ARG:HH12	41:PP:53:GLN:HE22	1.54	0.54
50:U:28:PRO:HB2	50:U:34:MET:HG2	1.89	0.54
51:UU:26:SER:HB3	51:UU:32:LEU:HD23	1.89	0.54
4:9:1404:U:N3	51:UU:56:MET:HE2	2.22	0.54
4:9:1661:A:C8	16:Dd:14:PHE:CD2	2.94	0.54
10:Bb:54:VAL:HG12	10:Bb:64:CYS:HB2	1.90	0.54
24:Gg:6:THR:O	24:Gg:8:ARG:NH1	2.39	0.54
28:II:47:ARG:NH2	28:II:48:VAL:O	2.40	0.54
2:5:1522:A:OP1	62:a:27:LYS:NZ	2.30	0.54
15:DD:39:VAL:HG12	15:DD:48:ILE:HG22	1.90	0.54
23:GG:70:HIS:ND1	23:GG:103:ASP:OD2	2.41	0.54
2:5:406:C:O2'	2:5:407:A:OP1	2.25	0.54
2:5:737:C:H5	2:5:928:G:H1	1.55	0.54
2:5:4088:G:O6	5:A:72:ARG:NH2	2.41	0.54
4:9:77:A:O2'	23:GG:175:LYS:HA	2.08	0.54
4:9:92:A:O4'	18:EE:3:ARG:NH1	2.40	0.54
4:9:120:U:H1'	18:EE:33:THR:OG1	2.07	0.54
4:9:1320:G:H4'	82:v:629:LYS:NZ	2.22	0.54
9:BB:63:LYS:NZ	9:BB:90:ASP:OD1	2.40	0.54
28:II:138:ASN:O	28:II:141:ARG:NH2	2.41	0.54
4:9:380:G:H1'	28:II:5:ARG:NH2	2.22	0.54
4:9:1502:C:H4'	82:v:673:ASN:OD1	2.07	0.54
4:9:1668:U:H5'	51:UU:77:TRP:NE1	2.23	0.54
47:SS:124:ARG:HH21	47:SS:129:LEU:HG	1.73	0.54
50:U:62:SER:HB3	50:U:73:THR:HG23	1.89	0.54
79:s:160:LEU:HD21	79:s:174:LEU:HD22	1.90	0.54
1:x:120:ILE:HD12	1:x:135:PRO:HG3	1.89	0.54
4:9:1608:U:C5'	47:SS:130:ARG:HH11	2.20	0.54
14:D:271:MET:HB2	14:D:275:GLN:HE21	1.72	0.54
18:EE:23:LEU:O	30:JJ:4:ALA:HB1	2.08	0.54
18:EE:45:ILE:HD12	18:EE:61:VAL:HG21	1.89	0.54
25:H:91:LYS:HG2	25:H:145:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:XX:95:GLU:H	57:XX:140:ARG:HH12	1.55	0.54
58:Y:50:ARG:HB2	58:Y:115:ARG:HH22	1.73	0.54
3:8:47:C:H1'	3:8:61:A:H2'	1.90	0.54
4:9:446:G:H5''	28:II:49:ARG:HE	1.71	0.54
10:Bb:56:CYS:SG	10:Bb:57:VAL:N	2.80	0.54
14:D:40:ASP:HB2	14:D:43:LYS:HG2	1.89	0.54
24:Gg:196:ASN:ND2	24:Gg:237:ASN:OD1	2.41	0.54
4:9:1332:A:C2	15:DD:141:LYS:HE2	2.43	0.54
22:G:215:ASP:OD1	22:G:240:LYS:NZ	2.41	0.54
81:t:99:TYR:N	81:t:99:TYR:CD2	2.74	0.54
2:5:982:C:H4'	11:C:333:MLZ:HCM1	1.89	0.54
2:5:2592:C:OP1	2:5:2772:C:O2'	2.21	0.54
2:5:4212:U:OP1	2:5:4338:U:O2'	2.25	0.54
4:9:1053:C:H2'	4:9:1054:G:H8	1.73	0.54
6:AA:205:ARG:NH2	6:AA:213:GLU:OE2	2.41	0.54
9:BB:149:GLN:HE22	9:BB:154:SER:HB2	1.72	0.54
38:O:61:ARG:HA	38:O:70:PRO:HD2	1.90	0.54
57:XX:84:PHE:H	57:XX:121:LYS:HA	1.73	0.54
59:YY:18:LEU:HD12	59:YY:20:ARG:HH11	1.73	0.54
79:s:28:PHE:HB2	79:s:89:VAL:HB	1.89	0.54
82:v:122:THR:O	82:v:368:ARG:NH1	2.31	0.54
1:x:48:ARG:NH1	1:x:160:LYS:HA	2.20	0.53
2:5:71:C:H1'	33:L:62:PRO:O	2.08	0.53
2:5:973:G:OP1	2:5:2263:G:N2	2.37	0.53
2:5:1359:G:OP1	42:Q:108:ARG:NH1	2.39	0.53
2:5:4331:C:OP1	48:T:70:HIS:NE2	2.41	0.53
2:5:4940:G:O2'	2:5:4941:C:OP1	2.24	0.53
4:9:291:G:O4'	18:EE:202:PRO:HB3	2.08	0.53
4:9:919:A:O5'	37:NN:16:LEU:HD12	2.08	0.53
14:D:279:ARG:HA	14:D:282:GLN:HE21	1.73	0.53
21:FF:169:ILE:HA	21:FF:172:CYS:HB2	1.90	0.53
36:N:114:ARG:NH1	36:N:151:ILE:O	2.41	0.53
51:UU:32:LEU:HA	51:UU:35:VAL:HG22	1.89	0.53
59:YY:110:ARG:HH11	59:YY:126:GLY:HA3	1.72	0.53
10:Bb:11:SER:OG	10:Bb:14:GLU:OE1	2.24	0.53
20:F:153:ILE:HG22	20:F:186:MET:HE3	1.90	0.53
41:PP:98:ASN:ND2	41:PP:103:ASN:OD1	2.42	0.53
79:s:93:GLU:HB2	79:s:98:ILE:HD11	1.89	0.53
82:v:223:PHE:HB3	82:v:344:LEU:HD13	1.90	0.53
82:v:592:LEU:HD11	82:v:601:ARG:HB3	1.90	0.53
2:5:2482:C:N4	2:5:2483:G:O6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BB:33:VAL:HG21	9:BB:67:PHE:HE2	1.72	0.53
60:Z:54:THR:H	60:Z:57:MET:HE2	1.73	0.53
71:j:2:THR:O	71:j:7:SER:OG	2.23	0.53
2:5:4876:2MG:HM21	38:O:201:LEU:C	2.34	0.53
4:9:658:U:H1'	57:XX:17:ARG:HH21	1.72	0.53
4:9:1129:G:OP1	10:Bb:22:LYS:NZ	2.37	0.53
4:9:1540:G:OP1	49:TT:43:LYS:CE	2.40	0.53
4:9:1609:C:OP1	47:SS:134:GLN:OE1	2.27	0.53
9:BB:181:LEU:HA	9:BB:184:VAL:HG22	1.91	0.53
12:CC:252:THR:HG22	12:CC:254:ASP:H	1.73	0.53
43:QQ:34:VAL:HG12	43:QQ:70:VAL:HB	1.90	0.53
2:5:702:U:H5'	17:E:124:VAL:HG11	1.91	0.53
2:5:1870:UR3:H3U2	2:5:4409:G:C8	2.44	0.53
2:5:2038:G:OP1	46:S:87:ARG:HD3	2.08	0.53
2:5:4553:G:H2'	2:5:4554:7MG:H82	1.89	0.53
4:9:74:G:N2	4:9:77:A:OP2	2.41	0.53
4:9:126:G:O6	23:GG:196:LYS:HA	2.09	0.53
4:9:510:G:OP1	30:JJ:4:ALA:N	2.37	0.53
4:9:688:U:H5	26:HH:103:LYS:H	1.55	0.53
40:P:16:LYS:HG2	40:P:149:ILE:HG12	1.90	0.53
2:5:1659:C:OP2	62:a:26:ARG:NH1	2.41	0.53
3:8:102:G:OP2	3:8:104:A:O2'	2.26	0.53
6:AA:42:LYS:HD2	6:AA:48:ILE:HD11	1.91	0.53
13:Cc:15:THR:HG23	13:Cc:16:LYS:HG2	1.90	0.53
39:OO:99:ALA:H	39:OO:133:THR:HG22	1.74	0.53
43:QQ:49:TYR:HA	43:QQ:52:LEU:HB2	1.91	0.53
2:5:1324:U:O2'	2:5:1895:A:N1	2.42	0.53
2:5:2283:A:O2'	66:e:48:ARG:NH2	2.42	0.53
4:9:1617:G:N1	4:9:1620:A:OP2	2.41	0.53
27:I:53:VAL:HG11	48:T:158:PHE:HZ	1.74	0.53
39:OO:84:ARG:NH1	39:OO:87:GLU:OE2	2.41	0.53
76:o:6:LYS:HD2	76:o:93:LEU:HG	1.91	0.53
2:5:1520:G:O2'	33:L:18:TRP:NE1	2.41	0.53
2:5:4948:C:N4	67:f:58:VAL:O	2.42	0.53
4:9:358:C:P	57:XX:18:ARG:HD2	2.49	0.53
6:AA:24:HIS:HD2	45:RR:102:THR:HG21	1.72	0.53
6:AA:39:TYR:OH	45:RR:108:LEU:HD22	2.09	0.53
6:AA:85:ARG:NH2	45:RR:82:ASP:O	2.41	0.53
23:GG:8:PRO:HD2	23:GG:113:ILE:HG13	1.90	0.53
24:Gg:257:LYS:HE2	24:Gg:266:ILE:HG23	1.90	0.53
28:II:79:ILE:HG12	28:II:170:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:N:5:LYS:HG3	70:i:40:VAL:HG11	1.89	0.53
78:r:108:MET:HE3	78:r:112:ARG:HE	1.73	0.53
2:5:1581:G:C5	5:A:181:LYS:HB2	2.44	0.53
3:8:87:G:OP1	69:h:5:LYS:NZ	2.42	0.53
5:A:242:ARG:NH2	5:A:243:THR:O	2.42	0.53
11:C:159:GLU:HA	11:C:217:ILE:HB	1.91	0.53
29:J:29:SER:OG	29:J:67:LYS:O	2.23	0.53
73:l:24:PRO:HG2	73:l:27:ILE:HG12	1.90	0.53
4:9:1236:G:H4'	41:PP:133:ILE:CG2	2.35	0.52
4:9:1404:U:C2	51:UU:56:MET:HE2	2.44	0.52
4:9:1659:U:OP1	16:Dd:30:LEU:O	2.27	0.52
26:HH:165:ASN:O	26:HH:169:LYS:NZ	2.41	0.52
41:PP:114:HIS:ND1	41:PP:118:GLU:OE1	2.41	0.52
82:v:610:PRO:HG2	82:v:639:TYR:HB3	1.91	0.52
2:5:1330:A2M:OP2	2:5:4449:U:O2'	2.23	0.52
4:9:308:G:OP1	28:II:45:THR:HG21	2.09	0.52
4:9:1661:A:O4'	16:Dd:14:PHE:HB2	2.09	0.52
5:A:225:ILE:HD13	5:A:234:LYS:HA	1.91	0.52
13:Cc:26:GLN:NE2	21:FF:127:ARG:O	2.41	0.52
14:D:41:LYS:NZ	48:T:32:ARG:O	2.36	0.52
15:DD:143:ARG:HD3	83:w:217:ASN:CA	2.39	0.52
26:HH:9:VAL:HB	26:HH:44:ASN:HD21	1.74	0.52
59:YY:55:ILE:HG22	59:YY:75:ILE:HG23	1.90	0.52
2:5:1621:G:H1'	2:5:2517:A:N6	2.24	0.52
4:9:76:U:O2'	23:GG:154:ARG:NH1	2.42	0.52
4:9:292:A:H1'	34:LL:40:ILE:O	2.09	0.52
4:9:531:A:H61	4:9:553:U:H3	1.58	0.52
4:9:591:U:OP1	19:Ee:99:LYS:HE2	2.10	0.52
4:9:1668:U:H5'	51:UU:77:TRP:CE2	2.44	0.52
18:EE:44:LEU:HD11	18:EE:70:ILE:HG21	1.91	0.52
4:9:1745:A:H2'	23:GG:66:GLY:HA3	1.85	0.52
18:EE:87:MET:HE1	18:EE:236:ILE:HG21	1.92	0.52
36:N:7:ILE:HD11	36:N:46:ASP:HB3	1.92	0.52
41:PP:110:GLU:CG	47:SS:117:ILE:HD13	2.39	0.52
2:5:369:G:N2	2:5:372:A:OP2	2.33	0.52
2:5:737:C:H2'	2:5:739:G:H4'	1.92	0.52
4:9:22:A:H4'	30:JJ:17:ARG:HA	1.92	0.52
4:9:1298:G:C5'	41:PP:79:HIS:CE1	2.92	0.52
8:B:163:LEU:HG	8:B:180:LEU:HD11	1.91	0.52
21:FF:24:SER:OG	21:FF:26:ASP:OD1	2.27	0.52
22:G:163:LYS:HD2	22:G:166:ARG:HH22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SS:25:LYS:HA	47:SS:55:ARG:HA	1.91	0.52
2:5:1464:C:H5'	42:Q:144:LYS:HG2	1.90	0.52
2:5:4087:5MU:OP1	5:A:123:ARG:NH1	2.42	0.52
4:9:873:G:OP2	44:R:163:ARG:HD2	2.10	0.52
4:9:1256:G:C8	51:UU:66:ARG:CG	2.93	0.52
24:Gg:212:LYS:HG2	24:Gg:235:ILE:HD12	1.92	0.52
25:H:94:SER:HB2	25:H:142:ASP:HB3	1.91	0.52
82:v:421:VAL:O	82:v:464:VAL:N	2.42	0.52
82:v:609:PHE:HE1	82:v:701:ARG:HB2	1.74	0.52
4:9:496:C:O5'	18:EE:29:PRO:HD3	2.10	0.52
15:DD:75:LYS:HD2	32:KK:18:GLU:HG2	1.92	0.52
1:x:48:ARG:HH12	1:x:161:LYS:N	2.06	0.52
2:5:2848:A:O2'	2:5:4635:G:H4'	2.10	0.52
2:5:4300:B8H:C5	2:5:4300:B8H:C2	2.86	0.52
4:9:1580:A:O4'	51:UU:57:PRO:HG2	2.10	0.52
6:AA:77:ILE:HG23	6:AA:99:ILE:HD11	1.92	0.52
8:B:77:THR:HG21	8:B:337:VAL:HG22	1.92	0.52
23:GG:7:PHE:HB2	23:GG:124:LEU:HD12	1.92	0.52
49:TT:98:SER:OG	49:TT:101:ARG:NH2	2.42	0.52
51:UU:100:GLN:HG2	51:UU:101:ILE:HD12	1.91	0.52
79:s:102:LEU:HD22	79:s:187:LEU:HD22	1.90	0.52
1:x:161:LYS:O	1:x:162:VAL:HB	2.09	0.52
2:5:1178:G:H2'	2:5:1179:A:C8	2.44	0.52
2:5:4948:C:H1'	67:f:69:VAL:HG11	1.91	0.52
4:9:121:OMU:CM2	18:EE:144:ALA:HB3	2.39	0.52
4:9:628:A:N6	83:w:216:HIS:NE2	2.57	0.52
4:9:1538:C:OP1	49:TT:84:ARG:NH2	2.43	0.52
19:Ee:82:VAL:HG23	57:XX:92:ASN:HD21	1.74	0.52
26:HH:117:PRO:HG2	26:HH:120:ARG:HD3	1.91	0.52
63:b:36:ASP:HB3	63:b:39:PHE:HB3	1.92	0.52
82:v:191:THR:HG22	82:v:779:THR:HG22	1.90	0.52
2:5:2700:A:H5'	72:k:26:LYS:HE2	1.92	0.52
2:5:4526:G:O2'	2:5:4529:C:OP2	2.24	0.52
4:9:1025:U:O3'	4:9:1089:G:N2	2.43	0.52
14:D:42:ASN:H	14:D:42:ASN:HD22	1.58	0.52
18:EE:61:VAL:HG12	18:EE:80:ILE:HD12	1.92	0.52
19:Ee:80:ALA:CB	82:v:684:GLN:HE22	2.23	0.52
27:I:42:LYS:O	27:I:139:ARG:NH2	2.43	0.52
78:r:103:HIS:ND1	78:r:105:ASP:OD1	2.42	0.52
2:5:2330:G:OP1	66:e:108:ARG:NH1	2.43	0.51
4:9:380:G:C1'	28:II:5:ARG:HH22	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:660:C:O5'	57:XX:2:GLY:CA	2.59	0.51
4:9:885:U:O2	4:9:901:G:N2	2.38	0.51
4:9:1649:U:O2'	43:QQ:138:ARG:HB2	2.10	0.51
5:A:117:GLU:HB3	5:A:124:GLY:H	1.74	0.51
35:M:96:GLU:OE1	35:M:100:ARG:NE	2.42	0.51
2:5:233:U:O2'	2:5:2308:U:O4	2.24	0.51
2:5:1295:G:O2'	2:5:1296:C:OP1	2.27	0.51
2:5:4639:A:H8	2:5:5052:A:H61	1.57	0.51
4:9:380:G:H1'	28:II:5:ARG:CZ	2.40	0.51
4:9:1017:U:O2'	37:NN:48:SER:O	2.16	0.51
4:9:1416:C:OP1	49:TT:129:ARG:HG2	2.10	0.51
9:BB:146:ARG:HB3	9:BB:149:GLN:HB2	1.92	0.51
18:EE:57:THR:OG1	18:EE:60:GLU:OE1	2.25	0.51
18:EE:139:LEU:HD22	18:EE:150:PRO:HB3	1.92	0.51
47:SS:34:LYS:HG2	47:SS:103:LEU:HD22	1.92	0.51
60:Z:92:ASP:N	60:Z:92:ASP:OD1	2.42	0.51
1:x:73:HIS:ND1	1:x:113:SER:OG	2.30	0.51
2:5:102:G:OP1	33:L:71:ARG:NH2	2.39	0.51
2:5:667:A:N7	11:C:2:ALA:N	2.59	0.51
2:5:1333:G:H2'	2:5:3869:A:H5'	1.92	0.51
2:5:1965:G:O2'	2:5:2029:A:N6	2.42	0.51
4:9:851:C:O2'	4:9:852:G:N2	2.43	0.51
4:9:871:U:O2'	44:R:163:ARG:CZ	2.57	0.51
4:9:1231:C:O2'	4:9:1253:A:N6	2.43	0.51
4:9:1256:G:C5	16:Dd:40:ARG:HD3	2.46	0.51
4:9:1647:A:C5'	43:QQ:138:ARG:HH22	2.11	0.51
21:FF:90:VAL:HA	21:FF:93:VAL:HG12	1.90	0.51
24:Gg:152:SER:OG	24:Gg:168:CYS:SG	2.58	0.51
26:HH:154:ILE:HB	26:HH:185:VAL:HG22	1.92	0.51
29:J:56:THR:HG23	29:J:63:ARG:HA	1.92	0.51
65:d:26:THR:OG1	65:d:85:ARG:NH1	2.38	0.51
2:5:2366:U:H2'	2:5:2367:A2M:H8	1.92	0.51
2:5:5010:U:H4'	2:5:5011:A:H5'	1.91	0.51
4:9:502:C:P	18:EE:66:MET:HE2	2.51	0.51
15:DD:168:VAL:HA	15:DD:188:ILE:O	2.09	0.51
17:E:144:ARG:NH1	67:f:110:ILE:OXT	2.44	0.51
18:EE:191:ARG:HE	18:EE:245:ARG:HD3	1.75	0.51
23:GG:2:LYS:HD3	23:GG:15:LEU:HD21	1.92	0.51
26:HH:145:ARG:NH2	55:WW:51:GLU:OE2	2.43	0.51
28:II:165:GLN:HE22	28:II:171:LEU:HB2	1.76	0.51
51:UU:58:THR:OG1	51:UU:84:ILE:O	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Y:2:LYS:HE3	58:Y:9:SER:HB2	1.91	0.51
2:5:3892:G:O2'	2:5:3893:G:OP1	2.27	0.51
4:9:1568:C:H4'	49:TT:41:LYS:CD	2.40	0.51
5:A:120:PRO:HA	5:A:162:ASN:HB3	1.91	0.51
22:G:203:LYS:NZ	22:G:230:MET:O	2.44	0.51
67:f:50:VAL:HG22	67:f:69:VAL:HG12	1.91	0.51
2:5:394:G:N2	2:5:397:G:OP2	2.33	0.51
2:5:1201:C:H2'	2:5:1202:G:H8	1.75	0.51
2:5:1522:A:H61	33:L:19:GLN:HE22	1.59	0.51
2:5:4576:U:H2'	2:5:4577:G:C8	2.46	0.51
3:8:93:C:HO2'	3:8:94:G:H8	1.57	0.51
4:9:660:C:P	57:XX:2:GLY:N	2.82	0.51
13:Cc:30:VAL:HG21	13:Cc:50:VAL:HG11	1.93	0.51
60:Z:26:VAL:O	60:Z:93:LYS:NZ	2.43	0.51
2:5:109:G:OP2	33:L:74:ARG:NH2	2.40	0.51
2:5:921:C:H2'	2:5:922:G:C8	2.46	0.51
2:5:2424:A:OP2	40:P:127:ARG:NH1	2.38	0.51
2:5:2521:A:H5'	68:g:62:LYS:HE3	1.92	0.51
4:9:304:C:HO3'	28:II:184:ARG:NH2	2.09	0.51
4:9:1535:U:H6	21:FF:82:ASN:CG	2.09	0.51
4:9:1831:A:H2'	4:9:1832:6MZ:H8	1.92	0.51
18:EE:35:PRO:HD2	18:EE:83:PRO:HG2	1.92	0.51
21:FF:14:THR:OG1	21:FF:17:ILE:O	2.26	0.51
23:GG:14:LYS:HE2	23:GG:123:GLY:HA3	1.92	0.51
28:II:110:ARG:HG2	28:II:121:LEU:HB3	1.93	0.51
36:N:20:ARG:HH22	70:i:52:PRO:HG2	1.75	0.51
37:NN:114:ARG:HG2	37:NN:117:LEU:HD12	1.93	0.51
2:5:2742:C:O2'	2:5:2744:U:O2	2.26	0.51
21:FF:55:ARG:NH1	43:QQ:123:ASP:OD1	2.37	0.51
24:Gg:202:PRO:HG2	24:Gg:243:PRO:HA	1.93	0.51
36:N:45:PRO:O	36:N:49:ARG:HG3	2.11	0.51
41:PP:21:ASP:HB2	41:PP:24:GLN:HG2	1.92	0.51
82:v:692:LEU:HD11	82:v:738:PRO:HB2	1.93	0.51
2:5:2671:C:OP1	44:R:100:ARG:NE	2.34	0.51
4:9:294:U:OP1	34:LL:36:TYR:OH	2.27	0.51
4:9:873:G:O4'	44:R:162:ARG:CD	2.51	0.51
4:9:913:A:N6	26:HH:119:SER:HB3	2.25	0.51
4:9:1204:A:O2'	4:9:1700:C:OP2	2.27	0.51
21:FF:71:ARG:NH2	21:FF:148:ASN:OD1	2.44	0.51
21:FF:123:GLU:HG3	21:FF:140:ASP:HA	1.93	0.51
22:G:139:VAL:HG21	22:G:238:LYS:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:T:118:GLU:O	48:T:122:LYS:NZ	2.41	0.51
2:5:2012:U:O2	2:5:2016:A:N6	2.44	0.51
4:9:54:A:H3'	4:9:451:G:H22	1.75	0.51
4:9:72:C:O2'	4:9:74:G:OP2	2.29	0.51
4:9:1591:C:C5'	21:FF:85:LYS:HZ3	2.14	0.51
8:B:231:VAL:HG11	8:B:251:VAL:HG23	1.91	0.51
15:DD:170:THR:HG22	15:DD:187:LYS:HG2	1.92	0.51
17:E:48:ARG:HG2	17:E:67:ARG:HG2	1.92	0.51
24:Gg:257:LYS:NZ	24:Gg:258:ILE:O	2.44	0.51
37:NN:37:ILE:HG22	37:NN:54:LEU:HD11	1.92	0.51
59:YY:44:LEU:HD23	59:YY:55:ILE:HD13	1.93	0.51
60:Z:68:ILE:HD13	60:Z:119:GLU:HG2	1.92	0.51
76:o:26:TYR:HB3	76:o:67:VAL:HB	1.92	0.51
1:x:48:ARG:NH1	1:x:161:LYS:N	2.59	0.50
2:5:1695:G:H5'	42:Q:15:ARG:HG3	1.93	0.50
4:9:5:U:H2'	4:9:6:G:H8	1.75	0.50
4:9:123:G:O4'	18:EE:146:THR:HG23	2.11	0.50
21:FF:35:LEU:HD21	21:FF:117:ILE:HG22	1.92	0.50
26:HH:53:VAL:HG21	26:HH:172:THR:HA	1.93	0.50
2:5:1215:G:O2'	2:5:1216:G:OP1	2.26	0.50
4:9:1650:A:OP1	43:QQ:136:GLY:C	2.54	0.50
33:L:25:TRP:HE1	36:N:199:GLN:HE21	1.58	0.50
63:b:101:HIS:CD2	63:b:104:LEU:H	2.28	0.50
65:d:38:PHE:HB3	65:d:78:ARG:HG2	1.93	0.50
81:t:99:TYR:N	81:t:99:TYR:HD2	2.09	0.50
2:5:398:A2M:O5'	2:5:398:A2M:H8	2.11	0.50
2:5:1864:B8H:C5	2:5:1864:B8H:C2	2.86	0.50
2:5:2408:A:H61	2:5:2791:A:N6	2.09	0.50
4:9:1018:U:O4'	37:NN:48:SER:HA	2.11	0.50
9:BB:191:ASP:OD1	9:BB:195:LYS:NZ	2.40	0.50
15:DD:49:ILE:HG22	15:DD:87:TYR:HB2	1.92	0.50
22:G:99:GLN:HE21	22:G:102:ARG:HH12	1.58	0.50
42:Q:82:VAL:HG22	42:Q:84:GLY:H	1.77	0.50
69:h:91:MET:HB2	69:h:94:ARG:HE	1.76	0.50
79:s:41:GLN:O	79:s:45:MET:N	2.41	0.50
79:s:98:ILE:H	79:s:98:ILE:HD12	1.77	0.50
2:5:6:C:H5''	22:G:250:LYS:HB3	1.92	0.50
2:5:198:A:OP1	58:Y:126:ARG:NH2	2.44	0.50
2:5:1099:A:H61	2:5:1205:U:H3	1.58	0.50
4:9:27:A2M:HM'1	4:9:483:C:H1'	1.93	0.50
4:9:648:A:H5''	57:XX:106:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:27:ALA:O	5:A:128:ARG:NH1	2.39	0.50
8:B:41:VAL:HA	8:B:187:GLY:HA3	1.93	0.50
16:Dd:7:TYR:CE2	32:KK:28:HIS:HE1	2.30	0.50
61:ZZ:57:LYS:HA	61:ZZ:60:LYS:HG2	1.92	0.50
4:9:17:C:H2'	4:9:18:C:H6	1.76	0.50
4:9:123:G:H1'	18:EE:146:THR:CG2	2.41	0.50
4:9:1587:G:N2	49:TT:77:LYS:HD2	2.27	0.50
6:AA:79:SER:HA	6:AA:101:GLY:HA2	1.93	0.50
18:EE:87:MET:HE2	18:EE:123:LEU:HB3	1.93	0.50
2:5:1998:C:H2'	2:5:1999:G:H8	1.76	0.50
4:9:75:G:H22	23:GG:157:VAL:CG1	2.23	0.50
4:9:143:U:H5	23:GG:188:LYS:HD2	1.77	0.50
4:9:374:G:H1'	34:LL:83:GLN:HE21	1.77	0.50
4:9:1745:A:C1'	23:GG:66:GLY:HA3	2.42	0.50
23:GG:48:TYR:OH	23:GG:119:LYS:O	2.26	0.50
23:GG:81:HIS:HB2	23:GG:84:TYR:HE1	1.76	0.50
58:Y:50:ARG:HG2	58:Y:51:LYS:H	1.77	0.50
2:5:980:C:N3	11:C:323:ARG:NH1	2.59	0.50
4:9:587:A:H5'	4:9:592:C:H41	1.76	0.50
4:9:687:C:C2	26:HH:118:ARG:NH2	2.78	0.50
4:9:925:G:H5''	37:NN:91:LEU:HD21	1.93	0.50
4:9:1256:G:H8	51:UU:66:ARG:HG3	1.76	0.50
23:GG:59:GLN:HB2	23:GG:72:ARG:HH12	1.77	0.50
34:LL:40:ILE:HG21	34:LL:61:PRO:HB2	1.93	0.50
52:V:57:VAL:HG13	52:V:84:GLN:HG2	1.92	0.50
2:5:382:G:N1	2:5:385:A:OP2	2.40	0.50
2:5:4382:A:O2'	2:5:4383:A:H2'	2.12	0.50
4:9:1790:A:C5'	23:GG:81:HIS:HE1	2.24	0.50
9:BB:145:LYS:NZ	9:BB:149:GLN:O	2.42	0.50
17:E:164:ARG:O	17:E:185:ASN:ND2	2.44	0.50
17:E:196:PHE:CD2	67:f:106:TYR:HB2	2.47	0.50
27:I:36:LEU:HD13	27:I:69:ARG:HH21	1.77	0.50
44:R:99:MET:O	44:R:103:ARG:HG2	2.12	0.50
69:h:5:LYS:HD3	69:h:7:ARG:HH21	1.76	0.50
2:5:433:A:C2	2:5:3871:A2M:H4'	2.46	0.50
2:5:1887:OMG:HM22	2:5:2074:U:H3	1.77	0.50
4:9:1273:C:O2'	4:9:1506:A:N1	2.43	0.50
9:BB:182:LYS:O	9:BB:186:ASN:ND2	2.45	0.50
17:E:153:LEU:HD13	17:E:197:VAL:HG11	1.94	0.50
22:G:163:LYS:HZ2	22:G:166:ARG:HH12	1.57	0.50
25:H:44:GLU:HB3	25:H:58:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LL:61:PRO:HB3	34:LL:68:ILE:HD11	1.94	0.50
2:5:1400:G:N7	62:a:110:LYS:NZ	2.50	0.49
2:5:4396:G:N3	2:5:4451:5MC:HM52	2.27	0.49
4:9:124:U:OP1	18:EE:148:ARG:NE	2.45	0.49
4:9:355:G:OP1	34:LL:105:ARG:NH1	2.29	0.49
20:F:189:LEU:HD21	20:F:207:LEU:HD21	1.93	0.49
82:v:512:LYS:HG3	82:v:569:PRO:HB2	1.93	0.49
2:5:86:U:OP1	42:Q:168:ARG:NH1	2.45	0.49
2:5:3881:A:N3	2:5:4405:G:O2'	2.40	0.49
9:BB:33:VAL:HG23	9:BB:96:CYS:HB3	1.93	0.49
21:FF:18:LYS:NZ	21:FF:19:LEU:O	2.39	0.49
52:V:85:ARG:HH11	52:V:100:ASP:HA	1.76	0.49
56:X:89:LYS:HG3	56:X:95:THR:HB	1.93	0.49
2:5:4567:U:O4	2:5:4568:M7A:N6	2.45	0.49
4:9:65:C:N4	23:GG:136:LYS:HD3	2.26	0.49
4:9:156:G:O2'	23:GG:60:GLY:HA2	2.12	0.49
4:9:1228:A:H2'	4:9:1229:G:C8	2.47	0.49
4:9:1524:G:H1'	41:PP:135:ALA:O	2.12	0.49
6:AA:24:HIS:CD2	45:RR:102:THR:HG21	2.46	0.49
8:B:213:GLN:HE22	8:B:286:LYS:HA	1.77	0.49
33:L:169:ILE:HG12	62:a:123:ILE:HD11	1.93	0.49
37:NN:18:TYR:CE1	55:WW:56:HIS:CE1	2.99	0.49
41:PP:34:MET:HE2	41:PP:45:LEU:HG	1.93	0.49
82:v:227:GLN:NE2	82:v:352:GLN:OE1	2.45	0.49
2:5:3900:C:HO2'	8:B:268:ARG:HH22	1.55	0.49
2:5:4703:U:H1'	2:5:4704:A:H5''	1.93	0.49
4:9:77:A:H2	23:GG:175:LYS:CE	2.24	0.49
4:9:1013:U:OP1	4:9:1129:G:O2'	2.28	0.49
4:9:1521:C:H5'	41:PP:126:VAL:CG1	2.42	0.49
28:II:6:ASP:OD1	28:II:9:HIS:ND1	2.44	0.49
28:II:46:VAL:HG21	28:II:56:ARG:HE	1.77	0.49
30:JJ:144:ILE:HG22	30:JJ:146:SER:H	1.77	0.49
42:Q:79:THR:HB	42:Q:136:THR:HG22	1.94	0.49
45:RR:14:ARG:HD3	45:RR:67:ARG:HH21	1.78	0.49
59:YY:106:GLN:HA	59:YY:109:GLU:HG2	1.94	0.49
63:b:101:HIS:HD2	63:b:104:LEU:H	1.59	0.49
4:9:143:U:C5	23:GG:188:LYS:HD2	2.48	0.49
4:9:1256:G:N2	16:Dd:29:GLY:CA	2.70	0.49
4:9:1555:U:O4	16:Dd:19:ARG:HA	2.12	0.49
8:B:50:LYS:HB2	8:B:345:LEU:HD21	1.94	0.49
26:HH:148:LEU:HA	55:WW:42:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:WW:81:VAL:HG21	55:WW:104:LEU:HD22	1.95	0.49
2:5:78:U:H5''	36:N:185:GLY:HA2	1.95	0.49
4:9:520:A:O2'	4:9:825:A:N3	2.41	0.49
12:CC:191:VAL:HG11	12:CC:236:PHE:HA	1.94	0.49
15:DD:106:ARG:HG2	15:DD:175:VAL:HB	1.94	0.49
22:G:116:LEU:HD21	36:N:29:GLN:HG3	1.95	0.49
41:PP:81:ARG:NH2	41:PP:117:GLY:O	2.45	0.49
73:l:16:LYS:HG3	73:l:49:LEU:HD11	1.94	0.49
2:5:2049:G:O6	2:5:3874:C:O2'	2.30	0.49
4:9:383:G:H1'	34:LL:133:PRO:HG2	1.94	0.49
4:9:503:C:P	18:EE:62:LYS:HZ3	2.35	0.49
4:9:921:G:C2	10:Bb:22:LYS:HG2	2.47	0.49
4:9:1416:C:H5'	49:TT:132:ASP:OD1	2.13	0.49
4:9:1590:C:H5''	49:TT:82:ARG:NH1	2.28	0.49
8:B:132:LYS:HA	8:B:135:LYS:HE2	1.95	0.49
12:CC:79:GLU:HB2	53:VV:12:TYR:HB3	1.94	0.49
26:HH:30:LEU:O	26:HH:34:SER:HB3	2.12	0.49
74:m:69:ILE:HD13	74:m:98:LYS:HB2	1.95	0.49
2:5:2852:G:O2'	2:5:3842:U:O4	2.20	0.49
2:5:4423:U:OP1	2:5:4425:C:N4	2.46	0.49
4:9:303:C:H4'	28:II:64:ASN:HD21	1.77	0.49
4:9:388:U:H2'	4:9:389:A:H8	1.78	0.49
4:9:683:OMG:N1	4:9:1022:U:OP2	2.37	0.49
4:9:1395:C:O2'	4:9:1396:A:N3	2.36	0.49
4:9:1521:C:H5'	41:PP:126:VAL:HG11	1.95	0.49
17:E:193:HIS:CD2	17:E:195:LYS:H	2.30	0.49
18:EE:100:ARG:HH21	18:EE:118:GLU:HG2	1.77	0.49
21:FF:118:ASN:ND2	21:FF:181:ALA:O	2.45	0.49
38:O:27:VAL:HG13	38:O:101:ARG:HB2	1.95	0.49
45:RR:111:PHE:HB3	45:RR:114:LEU:HD21	1.95	0.49
46:S:35:PRO:HD2	46:S:39:VAL:HG21	1.94	0.49
58:Y:117:LYS:HA	58:Y:120:GLU:HG2	1.95	0.49
59:YY:26:ASP:OD1	59:YY:26:ASP:N	2.46	0.49
59:YY:97:TYR:HE2	59:YY:99:LYS:HD3	1.76	0.49
33:L:80:GLU:OE2	33:L:102:ARG:NH1	2.45	0.49
44:R:134:ASN:HB3	44:R:137:ILE:HG12	1.94	0.49
2:5:3694:U:O2'	2:5:3821:A:N3	2.40	0.49
4:9:502:C:OP1	18:EE:66:MET:HE2	2.13	0.49
4:9:962:A:N1	4:9:1055:A:O2'	2.46	0.49
17:E:107:THR:O	17:E:108:ARG:NH1	2.46	0.49
41:PP:72:LYS:HB3	41:PP:93:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Q:43:PHE:CD2	42:Q:133:GLY:HA3	2.48	0.49
42:Q:130:SER:OG	42:Q:134:ARG:N	2.45	0.49
52:V:57:VAL:HG22	52:V:84:GLN:HE21	1.77	0.49
66:e:7:LEU:HB2	66:e:93:LYS:HB3	1.95	0.49
77:p:30:GLU:HA	77:p:33:GLN:HE21	1.77	0.49
3:8:60:G:OP1	56:X:70:LYS:NZ	2.45	0.48
4:9:96:C:O2	4:9:473:A:O2'	2.31	0.48
4:9:821:G:O5'	30:JJ:150:ARG:NH2	2.44	0.48
4:9:996:A:H2'	4:9:997:A:C8	2.47	0.48
4:9:1609:C:OP1	47:SS:132:ARG:N	2.42	0.48
8:B:56:ILE:HD12	8:B:365:LEU:HD22	1.94	0.48
13:Cc:47:LYS:HB2	21:FF:139:VAL:HG12	1.95	0.48
32:KK:8:ARG:NH1	32:KK:82:TYR:OH	2.46	0.48
34:LL:5:GLN:NE2	34:LL:11:GLN:O	2.46	0.48
37:NN:142:GLU:HB3	37:NN:145:THR:HG22	1.95	0.48
44:R:70:ARG:HB3	44:R:76:MET:HE2	1.95	0.48
62:a:117:LEU:HD23	62:a:140:VAL:HG11	1.95	0.48
82:v:155:LEU:HD12	82:v:205:ILE:HG21	1.93	0.48
2:5:352:G:H2'	11:C:193:LYS:HE2	1.95	0.48
2:5:4384:A:OP1	76:o:58:LYS:NZ	2.42	0.48
4:9:1745:A:HO2'	23:GG:66:GLY:CA	2.00	0.48
6:AA:80:ARG:HG2	6:AA:82:THR:H	1.78	0.48
47:SS:137:LYS:O	47:SS:141:ARG:NH2	2.46	0.48
50:U:80:LYS:HE2	50:U:110:TYR:CZ	2.48	0.48
82:v:748:GLU:HG3	82:v:785:LYS:HG2	1.94	0.48
1:x:121:PRO:HG3	81:t:93:ILE:HD12	1.95	0.48
2:5:1629:OMG:N1	2:5:3922:G:OP1	2.43	0.48
4:9:498:C:H5''	18:EE:7:LYS:HD2	1.95	0.48
4:9:1331:C:C5	83:w:197:SER:HA	2.48	0.48
4:9:1553:C:C5	16:Dd:22:ARG:NH2	2.81	0.48
4:9:1616:U:OP2	41:PP:43:ARG:NH2	2.46	0.48
9:BB:139:CYS:HA	9:BB:212:VAL:HA	1.95	0.48
11:C:134:PRO:HB3	11:C:150:LEU:HD13	1.96	0.48
2:5:972:C:N4	2:5:2099:A:H61	2.09	0.48
2:5:1696:C:H4'	42:Q:143:ARG:HH22	1.78	0.48
2:5:1805:A:O3'	48:T:102:ARG:NH1	2.47	0.48
2:5:2012:U:H1'	2:5:2015:C:H41	1.78	0.48
2:5:2461:G:OP1	36:N:65:ARG:NH1	2.46	0.48
2:5:3700:C:O2'	2:5:3820:A:N1	2.40	0.48
4:9:1171:G:O2'	4:9:1187:G:O6	2.28	0.48
4:9:1256:G:C8	51:UU:66:ARG:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1609:C:OP2	47:SS:134:GLN:NE2	2.46	0.48
4:9:1618:C:C5	16:Dd:11:PRO:HG2	2.49	0.48
5:A:70:LYS:HD2	5:A:72:ARG:HH12	1.78	0.48
41:PP:77:LYS:HE3	41:PP:102:PHE:HD1	1.79	0.48
47:SS:60:THR:OG1	47:SS:61:GLU:N	2.46	0.48
51:UU:39:LEU:HD13	51:UU:101:ILE:HG22	1.94	0.48
60:Z:50:PRO:HD3	60:Z:68:ILE:HG13	1.95	0.48
2:5:1276:C:OP1	63:b:117:ARG:NH2	2.46	0.48
2:5:1333:G:O2'	2:5:1334:A:OP1	2.24	0.48
3:8:110:U:H5''	73:l:8:ARG:HH22	1.77	0.48
4:9:384:U:H4'	34:LL:135:SER:HA	1.95	0.48
4:9:844:U:OP2	18:EE:240:ARG:NH2	2.47	0.48
4:9:1228:A:H2'	4:9:1229:G:H8	1.79	0.48
4:9:1332:A:O2'	15:DD:145:GLN:CB	2.60	0.48
4:9:1745:A:H1'	23:GG:66:GLY:O	2.14	0.48
29:J:18:ARG:HD2	29:J:135:GLY:HA3	1.96	0.48
61:ZZ:74:SER:HA	61:ZZ:79:ILE:HG22	1.94	0.48
1:x:41:TYR:HB2	1:x:163:LEU:HD21	1.96	0.48
2:5:1899:G:OP1	20:F:95:ARG:NH2	2.46	0.48
2:5:2697:G:OP1	72:k:35:LYS:HE3	2.14	0.48
4:9:421:G:C5'	34:LL:98:LYS:HG3	2.43	0.48
4:9:924:G:P	37:NN:3:ARG:HE	2.36	0.48
4:9:1426:U:O2'	49:TT:7:LYS:HD2	2.14	0.48
4:9:1550:G:O2'	4:9:1558:C:O2	2.31	0.48
4:9:1664:A:O2'	4:9:1666:C:N4	2.44	0.48
4:9:1706:G:H5''	75:n:1:MET:CE	2.37	0.48
19:Ee:95:GLN:NE2	19:Ee:96:GLU:O	2.47	0.48
38:O:58:LEU:HD11	38:O:145:VAL:HG13	1.95	0.48
43:QQ:16:LYS:HG3	43:QQ:17:LYS:H	1.77	0.48
2:5:1876:G:O2'	2:5:4223:A:N3	2.46	0.48
2:5:4879:G:H2'	46:S:169:THR:HG22	1.96	0.48
4:9:78:C:O2'	23:GG:175:LYS:HD2	2.14	0.48
4:9:931:C:OP1	9:BB:159:GLN:HB2	2.14	0.48
4:9:1568:C:H4'	49:TT:41:LYS:HD2	1.95	0.48
4:9:1867:U:O2'	7:Aa:38:LYS:HG2	2.13	0.48
6:AA:164:ASN:O	6:AA:170:SER:OG	2.28	0.48
15:DD:69:LEU:HA	15:DD:72:VAL:HG22	1.96	0.48
18:EE:71:LYS:HB3	18:EE:76:VAL:HG22	1.96	0.48
82:v:663:THR:OG1	82:v:703:ASP:OD1	2.30	0.48
2:5:2330:G:OP2	66:e:101:HIS:ND1	2.43	0.48
4:9:844:U:OP2	18:EE:240:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1509:U:O4	82:v:668:GLY:HA2	2.13	0.48
23:GG:140:ARG:HA	23:GG:143:LYS:HG2	1.95	0.48
60:Z:41:ALA:HB2	60:Z:77:TYR:HE1	1.79	0.48
2:5:1218:C:H5''	2:5:1219:C:H5''	1.95	0.48
4:9:28:U:H2'	4:9:29:G:C8	2.49	0.48
4:9:1591:C:C5'	21:FF:85:LYS:NZ	2.67	0.48
6:AA:185:MET:HE2	6:AA:185:MET:HB3	1.74	0.48
9:BB:127:VAL:HG11	9:BB:173:THR:HA	1.95	0.48
17:E:211:ILE:HG23	17:E:215:LEU:HD12	1.95	0.48
22:G:201:GLU:HA	22:G:230:MET:HE3	1.96	0.48
28:II:66:SER:HA	28:II:73:THR:HB	1.95	0.48
38:O:5:GLN:HG3	38:O:6:VAL:HG23	1.95	0.48
60:Z:11:VAL:HG11	60:Z:80:LEU:HB3	1.96	0.48
4:9:180:G:H21	23:GG:195:LYS:HD3	1.79	0.48
33:L:107:THR:HG22	70:i:20:ASN:HB3	1.95	0.48
43:QQ:132:PHE:O	43:QQ:140:ARG:NH2	2.45	0.48
44:R:10:LEU:HB3	44:R:41:ILE:HG13	1.95	0.48
2:5:1695:G:H5''	42:Q:13:VAL:O	2.13	0.47
4:9:1232:U:H2'	4:9:1233:G:H8	1.78	0.47
4:9:1580:A:N9	51:UU:57:PRO:CG	2.77	0.47
4:9:1646:C:H5''	43:QQ:138:ARG:NH1	2.29	0.47
23:GG:39:ASP:OD1	23:GG:47:GLY:N	2.47	0.47
36:N:116:LEU:HD22	36:N:135:ILE:HD11	1.96	0.47
38:O:109:PRO:HB2	38:O:111:PRO:HD2	1.95	0.47
82:v:394:LEU:HB3	82:v:487:THR:HG22	1.95	0.47
2:5:666:G:OP2	78:r:67:ARG:NH2	2.46	0.47
2:5:1401:A:N1	2:5:1502:G:O2'	2.47	0.47
2:5:1459:G:O2'	2:5:1460:B8Q:OP1	2.29	0.47
2:5:1931:U:OP1	2:5:1953:U:O2'	2.28	0.47
2:5:3813:G:OP2	2:5:3813:G:N2	2.41	0.47
2:5:4278:A:H2'	2:5:4279:G:C8	2.49	0.47
2:5:4489:C:O2'	74:m:88:LYS:NZ	2.47	0.47
2:5:4562:U:OP2	8:B:246:ARG:NH2	2.42	0.47
4:9:77:A:C2	23:GG:175:LYS:HG3	2.48	0.47
4:9:448:A:C5'	28:II:25:ARG:HD3	2.44	0.47
4:9:1479:G:O2'	43:QQ:131:LYS:NZ	2.45	0.47
4:9:1479:G:O3'	43:QQ:131:LYS:HE2	2.15	0.47
5:A:97:ASN:OD1	5:A:100:ASN:ND2	2.47	0.47
8:B:300:LYS:HG2	8:B:313:SER:HB3	1.96	0.47
34:LL:40:ILE:HD11	34:LL:44:PHE:HB2	1.96	0.47
53:VV:15:ARG:HH11	53:VV:33:GLN:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Y:112:ASP:OD1	58:Y:113:LYS:N	2.43	0.47
74:m:53:GLU:HG2	74:m:55:SER:H	1.79	0.47
2:5:1206:C:H2'	2:5:1207:G:C8	2.50	0.47
2:5:1242:A:O2'	2:5:1243:C:OP1	2.27	0.47
2:5:4879:G:C8	46:S:169:THR:HG21	2.49	0.47
4:9:860:G:O2'	55:WW:107:SER:HB2	2.14	0.47
14:D:52:ILE:HD13	31:K:6:C:H4'	1.95	0.47
26:HH:148:LEU:CD1	55:WW:49:GLU:HB3	2.42	0.47
48:T:78:LYS:HD3	48:T:87:LYS:HD3	1.95	0.47
2:5:245:C:HO2'	2:5:246:G:P	2.35	0.47
2:5:4541:C:H2'	2:5:4542:G:C8	2.49	0.47
4:9:76:U:C1'	23:GG:154:ARG:NH1	2.77	0.47
4:9:142:C:C5'	23:GG:188:LYS:HE3	2.43	0.47
4:9:1013:U:H2'	4:9:1014:G:H8	1.78	0.47
6:AA:19:LEU:HD11	45:RR:106:LEU:HD21	1.97	0.47
6:AA:42:LYS:HE2	45:RR:99:ASP:OD2	2.14	0.47
6:AA:118:GLU:HG3	12:CC:65:LYS:HE3	1.96	0.47
27:I:59:GLN:HB3	27:I:126:VAL:HG11	1.97	0.47
33:L:46:ILE:HB	33:L:49:ARG:HB2	1.97	0.47
40:P:31:GLU:HG2	40:P:60:PHE:HA	1.95	0.47
52:V:39:ILE:HG12	52:V:61:VAL:HG11	1.96	0.47
59:YY:109:GLU:O	59:YY:113:ARG:NE	2.47	0.47
81:t:90:PHE:HB3	81:t:102:LEU:HB3	1.96	0.47
2:5:132:G:C2	2:5:133:C:H1'	2.49	0.47
2:5:1079:G:H1	2:5:1239:G:H1	1.63	0.47
2:5:2880:G:C8	77:p:16:THR:HG22	2.50	0.47
2:5:3696:A:H62	2:5:3827:G:N2	2.06	0.47
4:9:142:C:P	23:GG:188:LYS:HE3	2.54	0.47
4:9:916:A:C6	37:NN:73:ARG:HD3	2.46	0.47
5:A:2:GLY:N	5:A:207:VAL:O	2.47	0.47
7:Aa:68:TYR:HB2	9:BB:111:CYS:SG	2.54	0.47
15:DD:63:GLY:O	15:DD:67:ARG:NH2	2.47	0.47
17:E:144:ARG:NH2	17:E:194:GLN:O	2.47	0.47
24:Gg:42:MET:HE2	24:Gg:57:ARG:HB3	1.96	0.47
27:I:189:ARG:HH12	27:I:201:PRO:HA	1.78	0.47
33:L:189:ALA:HA	70:i:11:LEU:HD13	1.96	0.47
82:v:649:ILE:HG23	82:v:661:ILE:HG23	1.97	0.47
2:5:62:A:OP1	36:N:172:ARG:NH1	2.44	0.47
2:5:975:G:O2'	17:E:126:ARG:NH1	2.34	0.47
2:5:1903:G:O2'	66:e:57:ASN:ND2	2.47	0.47
2:5:4393:C:H2'	2:5:4394:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:482:G:N1	4:9:485:A:OP2	2.48	0.47
4:9:912:C:H3'	4:9:913:A:H3'	1.96	0.47
23:GG:43:GLU:O	23:GG:46:LYS:NZ	2.35	0.47
24:Gg:124:SER:OG	24:Gg:125:ARG:N	2.47	0.47
35:M:39:ASP:HB3	35:M:47:ARG:HD3	1.97	0.47
38:O:74:ARG:HD2	38:O:145:VAL:HG12	1.96	0.47
59:YY:20:ARG:NH2	59:YY:22:GLN:OE1	2.43	0.47
79:s:47:LEU:HD22	79:s:50:LYS:HE3	1.96	0.47
2:5:92:C:C2	62:a:55:LYS:HE2	2.50	0.47
2:5:966:G:HO2'	2:5:967:A:H8	1.63	0.47
2:5:3623:G:H4'	44:R:79:GLY:O	2.15	0.47
2:5:4450:U:O2'	2:5:4454:PSU:OP1	2.32	0.47
4:9:114:G:N7	34:LL:133:PRO:HD2	2.30	0.47
4:9:356:C:P	34:LL:105:ARG:HH22	2.37	0.47
4:9:379:C:O2'	28:II:30:GLY:HA2	2.14	0.47
4:9:522:A:H2'	30:JJ:38:ARG:NH2	2.29	0.47
4:9:913:A:N6	26:HH:119:SER:C	2.69	0.47
4:9:1502:C:H4'	82:v:673:ASN:CG	2.39	0.47
4:9:1865:C:C2	7:Aa:5:ARG:HG2	2.49	0.47
8:B:229:LYS:HG3	8:B:272:LYS:HD3	1.96	0.47
10:Bb:36:LYS:HB3	10:Bb:43:ILE:HG22	1.97	0.47
14:D:60:ILE:HB	14:D:80:ALA:HB2	1.95	0.47
18:EE:127:ARG:HB2	18:EE:140:VAL:HG23	1.96	0.47
24:Gg:240:CYS:N	24:Gg:249:CYS:SG	2.87	0.47
36:N:75:VAL:HG21	36:N:80:THR:HG22	1.97	0.47
61:ZZ:94:LYS:HG3	61:ZZ:96:LEU:HD13	1.95	0.47
2:5:1538:A2M:H8	2:5:1538:A2M:H5'	1.96	0.47
2:5:1637:G:H5'	2:5:1638:A:OP1	2.14	0.47
4:9:434:G:H2'	4:9:435:A:C8	2.49	0.47
4:9:624:C:H41	57:XX:63:ASN:ND2	2.13	0.47
4:9:661:U:OP2	57:XX:2:GLY:N	2.48	0.47
4:9:1616:U:O2'	4:9:1661:A:N3	2.40	0.47
4:9:1661:A:P	16:Dd:19:ARG:NH2	2.84	0.47
4:9:1673:U:O2'	21:FF:84:GLY:O	2.30	0.47
4:9:1714:U:H2'	4:9:1715:A:C8	2.50	0.47
4:9:1741:U:OP1	28:II:58:LEU:HD23	2.14	0.47
10:Bb:50:ALA:H	10:Bb:71:ALA:HB2	1.80	0.47
16:Dd:6:LEU:HA	16:Dd:9:SER:HB3	1.97	0.47
19:Ee:107:ARG:NH1	19:Ee:110:GLN:OE1	2.47	0.47
42:Q:75:ARG:HA	42:Q:78:LYS:HE2	1.97	0.47
81:t:102:LEU:HD12	81:t:113:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2599:C:H5''	5:A:71:LYS:HE2	1.97	0.47
2:5:3729:G:N2	2:5:3732:A:OP2	2.41	0.47
4:9:1332:A:H2	15:DD:141:LYS:HE2	1.80	0.47
23:GG:7:PHE:HB2	23:GG:124:LEU:HB2	1.97	0.47
36:N:96:ARG:NH1	36:N:104:GLU:OE2	2.46	0.47
48:T:80:VAL:HG12	48:T:81:LYS:H	1.79	0.47
66:e:23:HIS:HD2	66:e:43:ASN:HD21	1.62	0.47
82:v:163:ALA:HB1	82:v:169:LEU:HD12	1.96	0.47
1:x:159:MET:CE	1:x:159:MET:CA	2.86	0.47
2:5:1594:C:H4'	2:5:2861:A:H5'	1.96	0.47
2:5:2521:A:O2'	68:g:66:ARG:NH2	2.47	0.47
2:5:3881:A:OP2	2:5:3881:A:H2'	2.15	0.47
4:9:678:U:OP2	4:9:1026:C:N4	2.37	0.47
4:9:1224:G:N2	43:QQ:142:GLN:NE2	2.62	0.47
9:BB:28:LYS:HG3	9:BB:48:LEU:HB3	1.96	0.47
9:BB:137:LEU:HD13	9:BB:215:VAL:HG22	1.97	0.47
15:DD:143:ARG:HD3	83:w:217:ASN:CG	2.40	0.47
16:Dd:26:ASN:N	16:Dd:26:ASN:HD22	2.14	0.47
27:I:91:LEU:HD12	27:I:135:ILE:HG23	1.97	0.47
78:r:108:MET:O	78:r:112:ARG:HG2	2.15	0.47
4:9:123:G:C1'	18:EE:146:THR:HG23	2.44	0.46
4:9:1320:G:OP1	82:v:629:LYS:HB2	2.15	0.46
5:A:196:TRP:O	5:A:198:ARG:N	2.49	0.46
17:E:122:GLU:HG3	66:e:7:LEU:HD22	1.96	0.46
35:M:24:LEU:HD11	35:M:86:TRP:CG	2.49	0.46
36:N:53:TYR:HB2	36:N:133:ILE:HD13	1.96	0.46
79:s:91:THR:HG21	79:s:98:ILE:HG21	1.97	0.46
82:v:710:HIS:ND1	82:v:710:HIS:O	2.48	0.46
2:5:2524:C:H2'	2:5:2525:G:C8	2.51	0.46
2:5:3715:A:H2	2:5:3744:G:H1	1.63	0.46
4:9:1402:A:O2'	51:UU:54:VAL:CG1	2.63	0.46
6:AA:84:GLN:HA	6:AA:87:VAL:HG22	1.98	0.46
20:F:121:PHE:O	20:F:204:ASN:ND2	2.46	0.46
22:G:152:ALA:HB1	22:G:189:LEU:HD11	1.98	0.46
24:Gg:73:SER:H	24:Gg:117:ASN:HD21	1.63	0.46
29:J:112:HIS:CE1	29:J:125:ILE:HA	2.50	0.46
42:Q:154:LYS:HE3	42:Q:158:THR:HG21	1.97	0.46
77:p:37:TYR:HB2	77:p:47:MET:HB2	1.97	0.46
2:5:1560:C:O2'	2:5:2673:C:OP1	2.25	0.46
4:9:116:OMU:HM23	4:9:116:OMU:H1'	1.70	0.46
4:9:581:U:P	59:YY:64:PHE:CD1	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1643:U:H5''	43:QQ:145:TYR:HD2	1.77	0.46
4:9:1852:C:OP2	75:n:5:TRP:CD1	2.69	0.46
7:Aa:22:ARG:HH21	7:Aa:27:ALA:HB1	1.80	0.46
8:B:60:VAL:HG12	8:B:62:ARG:HG2	1.98	0.46
59:YY:7:ILE:HG22	59:YY:27:VAL:HG22	1.97	0.46
59:YY:21:LYS:HB2	59:YY:75:ILE:HB	1.95	0.46
82:v:123:ASP:OD1	82:v:415:ARG:NH1	2.39	0.46
2:5:984:C:OP2	17:E:68:LYS:HE2	2.14	0.46
2:5:3892:G:HO2'	2:5:3893:G:P	2.38	0.46
4:9:421:G:H5'	34:LL:98:LYS:HG3	1.96	0.46
4:9:848:U:H2'	4:9:849:A:H8	1.79	0.46
4:9:1580:A:C4	51:UU:57:PRO:CG	2.92	0.46
20:F:145:ASN:OD1	20:F:146:LEU:N	2.46	0.46
26:HH:51:ILE:HD11	26:HH:59:ALA:HB3	1.97	0.46
59:YY:44:LEU:HD21	59:YY:75:ILE:HD11	1.98	0.46
1:x:42:ASP:OD1	1:x:43:PRO:HD2	2.15	0.46
2:5:1853:U:H3'	33:L:5:ARG:HH12	1.81	0.46
2:5:4511:A:H2'	2:5:4512:C:C6	2.51	0.46
4:9:448:A:O5'	28:II:25:ARG:HD3	2.14	0.46
4:9:1016:U:H2'	10:Bb:47:PHE:CE1	2.51	0.46
4:9:1245:G:O2'	4:9:1492:U:OP1	2.29	0.46
4:9:1298:G:C5'	41:PP:79:HIS:HE1	2.28	0.46
4:9:1332:A:O2'	15:DD:145:GLN:C	2.51	0.46
7:Aa:48:ALA:HB1	39:OO:117:ARG:HE	1.80	0.46
8:B:92:TYR:HB3	8:B:99:LEU:HG	1.96	0.46
17:E:165:VAL:HG13	17:E:180:GLY:N	2.31	0.46
27:I:51:HIS:CD2	27:I:168:SER:HB2	2.51	0.46
35:M:5:ARG:NH2	35:M:59:ASP:OD1	2.37	0.46
74:m:71:ARG:HE	74:m:96:ARG:HB3	1.81	0.46
82:v:32:LYS:NZ	82:v:105:SER:O	2.49	0.46
2:5:1343:U:H2'	2:5:1344:C:C6	2.51	0.46
2:5:2461:G:HO2'	2:5:3676:G:HO2'	1.64	0.46
4:9:121:OMU:HM22	18:EE:144:ALA:HB3	1.98	0.46
4:9:1351:G:O2'	4:9:1378:A:N1	2.40	0.46
4:9:1553:C:O2'	4:9:1554:C:O4'	2.33	0.46
6:AA:52:LYS:HB2	45:RR:109:LEU:HD13	1.97	0.46
8:B:154:LYS:HG2	8:B:194:LEU:HD12	1.97	0.46
13:Cc:14:VAL:HA	13:Cc:32:VAL:HG12	1.98	0.46
26:HH:7:LYS:NZ	26:HH:40:LEU:O	2.38	0.46
46:S:161:ARG:HH11	46:S:164:LYS:HD2	1.80	0.46
48:T:121:GLU:HG3	48:T:122:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:t:95:ILE:HG22	81:t:96:GLN:O	2.15	0.46
82:v:609:PHE:CE1	82:v:701:ARG:HB2	2.50	0.46
2:5:4899:C:O3'	35:M:132:ARG:NH2	2.49	0.46
2:5:4911:G:H2'	2:5:4917:G:H21	1.80	0.46
4:9:921:G:H1'	37:NN:11:LEU:CD2	2.42	0.46
4:9:1740:C:O2	4:9:1795:G:N2	2.48	0.46
14:D:64:ILE:HD12	14:D:109:LEU:HD22	1.96	0.46
19:Ee:85:VAL:O	19:Ee:89:THR:HB	2.15	0.46
45:RR:114:LEU:HB2	45:RR:117:LEU:HD22	1.97	0.46
52:V:35:LYS:HD2	52:V:67:LYS:HE3	1.97	0.46
69:h:91:MET:HA	69:h:94:ARG:HG3	1.98	0.46
75:n:16:LYS:HA	75:n:19:LYS:HD3	1.98	0.46
4:9:355:G:P	34:LL:105:ARG:HH11	2.37	0.46
18:EE:31:PRO:HA	18:EE:81:THR:HB	1.96	0.46
35:M:97:ALA:HB2	38:O:203:VAL:HG13	1.96	0.46
55:WW:44:HIS:NE2	55:WW:112:ASP:OD2	2.49	0.46
62:a:71:PRO:HG2	62:a:108:TYR:HA	1.96	0.46
1:x:155:ILE:HD12	1:x:167:VAL:HG21	1.97	0.46
2:5:178:C:H2'	2:5:179:G:C8	2.51	0.46
2:5:4079:U:OP1	22:G:302:ARG:NH2	2.48	0.46
4:9:629:A:H4'	15:DD:143:ARG:HH22	1.81	0.46
5:A:36:GLU:HG3	5:A:91:GLY:HA2	1.97	0.46
8:B:56:ILE:O	8:B:73:VAL:HA	2.16	0.46
33:L:169:ILE:HD13	62:a:142:GLY:HA2	1.98	0.46
40:P:17:SER:HB2	40:P:98:ALA:HB2	1.98	0.46
46:S:127:MET:HA	48:T:153:PRO:HD2	1.97	0.46
59:YY:4:THR:HG23	59:YY:32:LYS:HZ2	1.79	0.46
2:5:2679:G:H1	64:c:33:GLN:NE2	2.14	0.46
4:9:493:A:H1'	4:9:574:A:H5'	1.98	0.46
4:9:552:G:H5''	19:Ee:112:ASN:CG	2.41	0.46
26:HH:70:LYS:HA	26:HH:73:GLN:HB2	1.98	0.46
50:U:56:LEU:HD23	50:U:61:VAL:HG23	1.97	0.46
55:WW:30:CYS:N	55:WW:59:GLY:O	2.44	0.46
65:d:37:GLY:O	65:d:41:ARG:HG3	2.15	0.46
79:s:51:ALA:HA	79:s:91:THR:HG22	1.98	0.46
81:t:60:VAL:HG22	81:t:71:GLU:HG2	1.98	0.46
82:v:200:MET:N	82:v:200:MET:SD	2.89	0.46
1:x:159:MET:HE3	1:x:159:MET:CA	2.17	0.45
2:5:239:C:OP1	58:Y:46:SER:OG	2.34	0.45
2:5:1622:G:H5''	71:j:13:ASN:HD21	1.80	0.45
2:5:4293:U:O2'	2:5:4324:G:O2'	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:4471:A:O2'	2:5:4514:A:N3	2.42	0.45
4:9:494:C:H5''	18:EE:57:THR:HB	1.99	0.45
4:9:1375:G:H2'	4:9:1376:A:H8	1.79	0.45
4:9:1649:U:OP1	43:QQ:128:GLU:HB3	2.17	0.45
4:9:1711:U:H2'	4:9:1712:A:H8	1.81	0.45
6:AA:50:ASN:HD21	6:AA:53:ARG:NH1	2.14	0.45
9:BB:72:ALA:HB3	39:OO:128:ARG:HH12	1.81	0.45
12:CC:168:GLY:N	12:CC:179:THR:O	2.33	0.45
22:G:158:GLU:OE1	22:G:166:ARG:NH2	2.49	0.45
47:SS:101:ASN:O	47:SS:105:ASN:OD1	2.34	0.45
58:Y:30:MET:HB3	58:Y:101:PRO:HG2	1.98	0.45
1:x:134:PHE:CE1	81:t:93:ILE:HD12	2.51	0.45
2:5:3763:A:H4'	4:9:1826:G:O2'	2.17	0.45
4:9:197:U:O4	4:9:202:G:O6	2.33	0.45
4:9:660:C:O5'	57:XX:2:GLY:HA3	2.16	0.45
36:N:28:TRP:O	36:N:32:GLN:HG2	2.16	0.45
38:O:156:LEU:HD23	38:O:159:LYS:HD3	1.97	0.45
39:OO:105:THR:HG22	39:OO:107:THR:H	1.81	0.45
39:OO:136:PRO:HG3	39:OO:139:SER:HB3	1.98	0.45
50:U:49:VAL:HG11	50:U:60:VAL:HG21	1.99	0.45
82:v:727:ARG:NH2	82:v:856:ASP:OD1	2.47	0.45
2:5:1332:G:O2'	2:5:2353:A:OP1	2.32	0.45
4:9:85:A:H2'	4:9:86:C:H6	1.81	0.45
4:9:928:G:H2'	4:9:929:G:C8	2.51	0.45
4:9:1854:U:OP1	39:OO:150:ARG:NH1	2.48	0.45
21:FF:55:ARG:HH12	43:QQ:124:PRO:HD2	1.82	0.45
34:LL:93:LEU:HD21	57:XX:8:ARG:NH2	2.31	0.45
36:N:96:ARG:HH12	36:N:104:GLU:CD	2.25	0.45
43:QQ:34:VAL:HG11	43:QQ:84:ILE:HD13	1.99	0.45
60:Z:108:ARG:HG2	60:Z:111:ARG:HH21	1.80	0.45
68:g:5:LEU:HD21	68:g:30:ILE:HG22	1.98	0.45
2:5:32:G:H21	2:5:50:C:H5	1.63	0.45
2:5:3749:U:H4'	5:A:242:ARG:HG3	1.98	0.45
2:5:4493:G:N3	2:5:4712:A:H2'	2.32	0.45
4:9:162:C:OP1	23:GG:87:ARG:NH2	2.50	0.45
4:9:301:A:O2'	28:IL:72:CYS:HA	2.16	0.45
4:9:520:A:H5'	30:JJ:10:ARG:O	2.16	0.45
4:9:1610:G:OP1	47:SS:131:VAL:HG11	2.15	0.45
4:9:1647:A:C5'	43:QQ:138:ARG:CZ	2.95	0.45
15:DD:203:PRO:HB2	15:DD:207:HIS:HE1	1.80	0.45
21:FF:34:SER:HB2	21:FF:146:ARG:HH22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:GG:10:THR:HG21	23:GG:128:THR:HG23	1.97	0.45
32:KK:80:ARG:HH11	32:KK:87:PRO:HA	1.82	0.45
47:SS:25:LYS:O	47:SS:29:ALA:HB2	2.17	0.45
56:X:119:ILE:HD13	56:X:149:VAL:HG11	1.98	0.45
82:v:81:LEU:HD21	82:v:98:PHE:HD1	1.80	0.45
2:5:364:G:O6	71:j:52:LYS:HE3	2.17	0.45
2:5:4264:U:H2'	2:5:4265:C:C6	2.52	0.45
2:5:4586:C:O2'	8:B:99:LEU:O	2.23	0.45
4:9:292:A:C2	34:LL:68:ILE:O	2.70	0.45
4:9:1298:G:H5'	41:PP:79:HIS:HE1	1.81	0.45
4:9:1325:G:O2'	4:9:1327:G:OP1	2.35	0.45
32:KK:41:PRO:HD2	32:KK:44:HIS:CD2	2.52	0.45
44:R:92:LYS:O	44:R:96:MET:HG3	2.16	0.45
51:UU:24:LEU:HB3	51:UU:112:VAL:HG12	1.98	0.45
57:XX:123:VAL:HG12	57:XX:124:LYS:HG3	1.98	0.45
2:5:17:A:OP2	56:X:60:TYR:OH	2.33	0.45
2:5:2621:G:OP2	44:R:64:ARG:NH2	2.50	0.45
2:5:3645:U:H5	2:5:3650:A:N7	2.15	0.45
2:5:4476:B8W:O2'	74:m:74:TYR:O	2.35	0.45
2:5:4608:G:N2	2:5:4611:A:OP2	2.49	0.45
4:9:963:A:OP1	39:OO:65:ASP:OD1	2.35	0.45
4:9:1284:A:OP1	4:9:1285:G:O2'	2.34	0.45
4:9:1299:A:O2'	4:9:1301:A:OP1	2.31	0.45
6:AA:37:TYR:HA	6:AA:53:ARG:HD2	1.98	0.45
38:O:168:TYR:CE2	38:O:172:LYS:HD2	2.52	0.45
43:QQ:78:VAL:HA	43:QQ:81:ILE:HG12	1.99	0.45
2:5:327:U:O2'	70:i:30:ARG:NH1	2.49	0.45
2:5:1203:G:H2'	2:5:1204:G:C8	2.52	0.45
2:5:1215:G:HO2'	2:5:1216:G:P	2.39	0.45
2:5:2873:U:O2'	2:5:2885:A:N7	2.42	0.45
2:5:3721:A:H2'	2:5:3722:A2M:C8	2.46	0.45
4:9:28:U:H2'	4:9:29:G:H8	1.80	0.45
4:9:104:A:H62	4:9:356:C:H5	1.65	0.45
4:9:648:A:H5''	57:XX:106:GLY:CA	2.47	0.45
4:9:1651:A:H2'	4:9:1652:G:H8	1.81	0.45
4:9:1746:U:H4'	23:GG:65:GLN:HG3	1.91	0.45
11:C:301:ALA:HB1	42:Q:132:LYS:HE2	1.99	0.45
15:DD:116:ARG:HB3	83:w:219:GLY:CA	2.31	0.45
18:EE:184:THR:N	18:EE:224:ASN:O	2.47	0.45
25:H:16:VAL:HG21	25:H:81:ILE:HG23	1.97	0.45
41:PP:95:GLY:HA2	41:PP:104:GLN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:4528:G:N3	8:B:252:ALA:HB1	2.32	0.45
4:9:331:C:OP1	23:GG:196:LYS:NZ	2.49	0.45
4:9:522:A:N6	30:JJ:41:ARG:NH2	2.58	0.45
4:9:1609:C:P	47:SS:131:VAL:H	2.38	0.45
14:D:61:ILE:HG23	14:D:79:TYR:CE1	2.52	0.45
24:Gg:198:VAL:HG23	24:Gg:209:SER:HB3	1.98	0.45
25:H:41:ILE:HG21	25:H:73:ILE:HD11	1.98	0.45
26:HH:157:HIS:HB3	26:HH:190:PRO:HG3	1.98	0.45
41:PP:106:GLU:OE1	41:PP:108:LYS:NZ	2.43	0.45
43:QQ:43:GLU:HA	43:QQ:44:PRO:HA	1.80	0.45
60:Z:88:ASP:O	60:Z:121:ARG:NH2	2.50	0.45
71:j:27:TYR:HA	71:j:34:CYS:HA	1.99	0.45
1:x:49:PHE:CD1	1:x:49:PHE:O	2.70	0.45
2:5:1977:G:H1	2:5:1997:C:H42	1.65	0.45
2:5:2605:A:N6	2:5:2747:A:H3'	2.32	0.45
2:5:4138:C:H2'	2:5:4139:G:C8	2.52	0.45
2:5:4462:C:H2'	2:5:4463:U:C6	2.52	0.45
7:Aa:45:VAL:HB	7:Aa:49:ALA:HB3	1.99	0.45
17:E:160:HIS:HB3	17:E:163:LYS:HD2	1.99	0.45
35:M:37:LEU:HD11	35:M:47:ARG:HD2	1.99	0.45
60:Z:76:ASN:OD1	60:Z:77:TYR:N	2.50	0.45
70:i:45:ARG:NH2	70:i:49:GLY:O	2.44	0.45
78:r:90:LEU:HG	78:r:111:ILE:HG23	1.99	0.45
2:5:1680:C:H41	2:5:4382:A:H5''	1.82	0.45
4:9:93:U:H4'	18:EE:6:LYS:HA	1.99	0.45
4:9:220:U:H2'	4:9:221:A:H8	1.83	0.45
4:9:1578:U:O2'	15:DD:6:SER:HA	2.17	0.45
8:B:53:MET:SD	8:B:77:THR:OG1	2.64	0.45
11:C:284:MET:HG3	11:C:287:THR:HG22	1.97	0.45
24:Gg:108:VAL:HG12	24:Gg:124:SER:HB2	1.98	0.45
30:JJ:114:VAL:HG21	30:JJ:135:ILE:HD13	1.99	0.45
47:SS:22:GLY:HA2	47:SS:56:ALA:HB3	1.99	0.45
56:X:80:PRO:HA	56:X:98:PHE:HA	1.98	0.45
76:o:14:LYS:HE3	76:o:79:SER:HB3	1.99	0.45
81:t:104:GLN:NE2	81:t:110:ARG:HB3	2.31	0.45
2:5:1681:PSU:H4'	2:5:1684:G:N1	2.31	0.44
2:5:1808:A:H4'	2:5:1809:A:O5'	2.17	0.44
2:5:1881:G:O6	63:b:10:HIS:NE2	2.45	0.44
2:5:1992:G:H2'	2:5:1993:G:C8	2.52	0.44
2:5:1992:G:H2'	2:5:1993:G:H8	1.82	0.44
2:5:2900:G:H5''	44:R:134:ASN:CG	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:38:A:OP1	30:JJ:5:ARG:HB2	2.16	0.44
4:9:1183:A:H2'	4:9:1184:G:H8	1.82	0.44
4:9:1609:C:H5''	47:SS:131:VAL:HG23	1.97	0.44
6:AA:120:ARG:HH22	12:CC:267:GLN:HG2	1.82	0.44
23:GG:2:LYS:HB3	23:GG:15:LEU:HD11	1.98	0.44
44:R:67:THR:O	44:R:71:ARG:HG2	2.16	0.44
51:UU:54:VAL:HB	51:UU:88:LEU:HG	1.99	0.44
51:UU:56:MET:HB2	51:UU:86:LYS:HB3	1.99	0.44
71:j:28:HIS:HD2	71:j:31:LYS:H	1.65	0.44
81:t:32:VAL:HG13	81:t:34:LEU:HD13	1.97	0.44
82:v:590:LEU:HD23	82:v:605:LYS:HE3	1.98	0.44
2:5:739:G:H2'	2:5:740:G:C8	2.52	0.44
2:5:1331:C:H2'	2:5:1332:G:C8	2.52	0.44
2:5:1366:G:OP1	33:L:39:ARG:NH2	2.50	0.44
2:5:1687:PSU:OP1	62:a:44:ASN:ND2	2.49	0.44
2:5:1738:G:N2	2:5:1739:U:O4	2.39	0.44
2:5:2408:A:H61	2:5:2791:A:H61	1.64	0.44
2:5:4760:C:H5'	2:5:4761:C:OP1	2.17	0.44
4:9:5:U:H2'	4:9:6:G:C8	2.51	0.44
4:9:294:U:H3	34:LL:65:ASN:CB	2.30	0.44
4:9:1489:A:H62	83:w:197:SER:HA	1.83	0.44
4:9:1650:A:H5''	43:QQ:139:ALA:HB3	1.83	0.44
4:9:1791:A:O3'	23:GG:75:LEU:CD1	2.64	0.44
14:D:152:ARG:HG3	14:D:154:THR:HG23	1.98	0.44
14:D:196:ARG:NH2	14:D:237:GLU:OE2	2.41	0.44
36:N:75:VAL:HG21	36:N:80:THR:CG2	2.48	0.44
38:O:10:ASP:HB2	38:O:117:ARG:HB3	1.99	0.44
41:PP:60:LEU:HD23	41:PP:76:VAL:HG11	1.99	0.44
78:r:47:LYS:HB2	78:r:102:TYR:CZ	2.53	0.44
82:v:402:VAL:O	82:v:411:TYR:N	2.40	0.44
1:x:71:GLN:HE21	29:J:38:LYS:HZ1	1.56	0.44
2:5:1201:C:H2'	2:5:1202:G:C8	2.52	0.44
4:9:293:C:H5''	34:LL:38:LYS:HD2	1.99	0.44
4:9:1144:A:H5'	4:9:1355:C:H41	1.82	0.44
4:9:1392:U:P	51:UU:83:ARG:HH22	2.41	0.44
4:9:1650:A:P	43:QQ:138:ARG:H	2.40	0.44
10:Bb:67:THR:OG1	10:Bb:70:LYS:O	2.35	0.44
14:D:136:ASP:OD1	14:D:136:ASP:N	2.49	0.44
15:DD:163:PRO:O	15:DD:167:TYR:HB2	2.17	0.44
24:Gg:300:ALA:O	24:Gg:307:VAL:HA	2.16	0.44
25:H:24:THR:HA	25:H:37:ASP:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:II:38:ILE:HD12	28:II:94:LYS:HB3	1.99	0.44
30:JJ:149:VAL:HG11	30:JJ:157:ILE:HD11	1.99	0.44
41:PP:34:MET:HB3	41:PP:42:ARG:HG3	2.00	0.44
1:x:101:LYS:HG2	1:x:105:LYS:HE3	1.98	0.44
2:5:1336:C:H2'	2:5:1337:A:C8	2.52	0.44
2:5:4695:A:O2'	25:H:68:ALA:O	2.27	0.44
4:9:309:G:OP2	28:II:55:TYR:OH	2.14	0.44
4:9:496:C:H4'	18:EE:28:ALA:C	2.42	0.44
4:9:522:A:C2'	30:JJ:38:ARG:NH2	2.81	0.44
4:9:619:A:N1	57:XX:114:ASP:HB2	2.33	0.44
4:9:1256:G:H8	51:UU:66:ARG:CG	2.30	0.44
4:9:1580:A:C5	51:UU:57:PRO:CD	3.00	0.44
4:9:1610:G:OP1	47:SS:125:HIS:CE1	2.70	0.44
11:C:321:ASN:HD22	11:C:324:ILE:H	1.64	0.44
18:EE:60:GLU:HA	18:EE:63:LYS:HB2	2.00	0.44
35:M:121:ARG:HA	35:M:124:LYS:HG2	1.98	0.44
39:OO:34:PHE:HB3	39:OO:41:PHE:HB2	2.00	0.44
55:WW:33:VAL:O	55:WW:37:PHE:HB2	2.18	0.44
2:5:39:A:H5''	62:a:35:ALA:HB1	1.98	0.44
2:5:2643:U:O2'	68:g:26:PRO:HD3	2.17	0.44
2:5:4527:A2M:HM'3	2:5:4527:A2M:H1'	1.88	0.44
4:9:110:U:O2	4:9:351:G:N2	2.45	0.44
4:9:626:G:C2'	83:w:201:ARG:NH1	2.64	0.44
4:9:1130:G:OP2	4:9:1130:G:N2	2.50	0.44
4:9:1218:C:H1'	4:9:1683:C:H42	1.83	0.44
4:9:1522:A:C5	41:PP:131:PRO:HG3	2.52	0.44
21:FF:55:ARG:O	21:FF:62:ARG:NH1	2.51	0.44
28:II:188:TYR:OH	28:II:194:GLU:OE2	2.29	0.44
30:JJ:110:LEU:HB2	30:JJ:147:PHE:HB3	2.00	0.44
40:P:54:LYS:HA	40:P:83:TRP:CD1	2.52	0.44
65:d:23:ARG:HE	65:d:121:ASN:HD21	1.65	0.44
67:f:106:TYR:CD1	67:f:107:PRO:HD3	2.53	0.44
2:5:420:A:H61	3:8:15:G:H1'	1.83	0.44
2:5:4756:U:O4	67:f:52:LYS:NZ	2.47	0.44
4:9:331:C:P	23:GG:196:LYS:NZ	2.79	0.44
4:9:343:A:H4'	18:EE:128:LYS:NZ	2.32	0.44
4:9:358:C:OP1	57:XX:18:ARG:HG3	2.17	0.44
4:9:380:G:N1	4:9:383:G:OP2	2.47	0.44
4:9:562:U:H2'	4:9:563:G:C8	2.52	0.44
4:9:932:G:O2'	4:9:934:G:OP2	2.32	0.44
8:B:55:HIS:HB2	8:B:369:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:92:TYR:HB2	8:B:159:VAL:HB	1.99	0.44
14:D:33:ARG:HH21	48:T:27:LEU:HD12	1.81	0.44
14:D:226:TYR:OH	31:K:48:G:OP1	2.27	0.44
21:FF:39:ILE:HG13	21:FF:68:ILE:HD11	1.99	0.44
30:JJ:36:GLY:O	30:JJ:111:GLN:NE2	2.47	0.44
42:Q:119:LYS:HE2	42:Q:121:LEU:HD11	1.99	0.44
51:UU:38:ASP:OD1	51:UU:41:ARG:NH2	2.50	0.44
55:WW:42:MET:HE2	55:WW:49:GLU:HA	2.00	0.44
71:j:28:HIS:CD2	71:j:31:LYS:H	2.35	0.44
82:v:227:GLN:NE2	82:v:348:ASP:O	2.40	0.44
82:v:506:ARG:HH11	82:v:545:ILE:HG21	1.83	0.44
2:5:3941:C:H1'	36:N:125:SER:HB2	1.98	0.44
2:5:4939:C:H2'	2:5:4940:G:H8	1.82	0.44
4:9:525:A:H5'	19:Ee:105:ALA:CB	2.47	0.44
4:9:624:C:N4	57:XX:63:ASN:HD21	2.16	0.44
4:9:846:G:N7	18:EE:108:ARG:NH2	2.64	0.44
4:9:1139:C:H41	4:9:1149:A:H62	1.65	0.44
4:9:1333:U:OP1	15:DD:146:ARG:CD	2.61	0.44
4:9:1657:G:H2'	4:9:1658:G:C8	2.53	0.44
50:U:80:LYS:HZ1	50:U:109:SER:H	1.66	0.44
57:XX:9:THR:HG22	57:XX:12:LYS:HB3	1.99	0.44
67:f:4:ARG:HD2	67:f:6:TRP:O	2.18	0.44
2:5:119:G:H3'	2:5:120:A:H5''	2.00	0.44
3:8:14:OMU:HM23	3:8:14:OMU:H1'	1.57	0.44
4:9:184:G:H2'	4:9:185:G:H8	1.83	0.44
4:9:186:C:H2'	4:9:187:G:H8	1.83	0.44
4:9:346:C:H5''	18:EE:38:LEU:HB2	2.00	0.44
4:9:533:A:H2'	4:9:534:G:C8	2.53	0.44
4:9:1705:C:H2'	4:9:1706:G:C8	2.52	0.44
4:9:1791:A:O3'	23:GG:75:LEU:HD11	2.18	0.44
8:B:217:ILE:HD11	8:B:333:LEU:HD11	2.00	0.44
14:D:208:MET:HB3	14:D:233:PRO:HG3	1.99	0.44
23:GG:98:ARG:HH22	23:GG:103:ASP:HB2	1.82	0.44
31:K:24:C:H2'	31:K:25:G:O4'	2.17	0.44
42:Q:178:ARG:N	62:a:51:GLY:HA2	2.33	0.44
64:c:46:VAL:HG12	64:c:95:SER:HB3	2.00	0.44
76:o:96:ASP:OD1	76:o:96:ASP:O	2.35	0.44
81:t:18:THR:HG22	81:t:83:PRO:HA	2.00	0.44
2:5:730:G:OP2	20:F:75:ARG:NE	2.51	0.44
2:5:1448:G:H21	2:5:2114:G:H1	1.66	0.44
2:5:2033:A:H2'	2:5:2034:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2576:C:O2'	60:Z:112:ARG:NH2	2.50	0.44
2:5:2866:G:N3	2:5:3628:A:H2'	2.32	0.44
2:5:3727:A2M:HM'3	2:5:3727:A2M:H1'	1.78	0.44
2:5:5061:C:H2'	2:5:5062:A:C8	2.52	0.44
4:9:51:U:H2'	4:9:52:G:H8	1.83	0.44
4:9:1402:A:O4'	51:UU:54:VAL:HG22	2.18	0.44
4:9:1522:A:N7	41:PP:131:PRO:HD3	2.33	0.44
4:9:1618:C:H2'	4:9:1619:A:C8	2.53	0.44
24:Gg:40:ILE:HG23	24:Gg:59:LEU:HB2	2.00	0.44
27:I:87:ILE:HG12	27:I:138:ILE:HG12	1.98	0.44
35:M:90:ARG:O	35:M:94:LYS:HG2	2.18	0.44
2:5:1465:C:OP1	42:Q:144:LYS:NZ	2.50	0.43
2:5:2734:U:H2'	2:5:2735:C:C6	2.53	0.43
2:5:3871:A2M:HM'3	2:5:3884:P7G:N2	2.33	0.43
2:5:4452:G:H4'	2:5:4453:A:OP2	2.18	0.43
2:5:4595:U:H2'	2:5:4596:C:C6	2.53	0.43
4:9:30:C:O2'	4:9:596:U:OP1	2.36	0.43
4:9:483:C:C5	57:XX:44:ALA:HB1	2.53	0.43
4:9:526:A:H5'	19:Ee:104:ARG:HH12	1.79	0.43
4:9:829:C:OP1	18:EE:22:LYS:HB3	2.18	0.43
4:9:1404:U:C2	51:UU:56:MET:HE1	2.52	0.43
4:9:1489:A:N6	83:w:197:SER:CB	2.80	0.43
10:Bb:8:LEU:HD21	55:WW:62:VAL:HB	2.00	0.43
20:F:227:VAL:HA	46:S:39:VAL:HG12	1.99	0.43
32:KK:4:PRO:HD2	32:KK:7:ASN:HD22	1.82	0.43
1:x:150:GLU:O	1:x:154:THR:OG1	2.30	0.43
2:5:658:C:H2'	2:5:659:G:H8	1.83	0.43
2:5:4574:G:H2'	2:5:4575:A2M:H8	2.00	0.43
4:9:581:U:H5''	59:YY:65:GLY:H	1.83	0.43
4:9:894:G:H2'	4:9:895:G:H8	1.83	0.43
4:9:1656:G:H1	4:9:1668:U:H3	1.67	0.43
24:Gg:285:GLN:H	24:Gg:303:THR:HG22	1.81	0.43
28:II:190:LEU:HD12	28:II:195:LEU:HA	2.00	0.43
30:JJ:32:ILE:HG23	30:JJ:37:LEU:HB2	1.99	0.43
40:P:94:MET:HE1	40:P:146:ILE:HB	2.00	0.43
43:QQ:19:ALA:HB2	43:QQ:75:GLY:HA3	2.00	0.43
45:RR:72:LYS:HA	45:RR:75:GLU:HG2	2.00	0.43
55:WW:18:GLU:HB3	55:WW:65:LEU:HD13	2.00	0.43
69:h:105:LYS:HE3	69:h:105:LYS:HB2	1.89	0.43
2:5:261:G:H2'	2:5:262:G:C8	2.53	0.43
2:5:261:G:H2'	2:5:262:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1946:A:N3	2:5:4436:C:O2'	2.49	0.43
2:5:2072:C:OP1	67:f:15:LYS:NZ	2.50	0.43
2:5:4641:OMG:HM23	2:5:4641:OMG:H1'	1.80	0.43
4:9:126:G:O6	23:GG:196:LYS:CG	2.65	0.43
4:9:674:C:H2'	4:9:675:U:C6	2.53	0.43
4:9:1277:C:H2'	4:9:1278:A:H8	1.83	0.43
4:9:1417:C:C1'	49:TT:3:GLY:CA	2.87	0.43
4:9:1446:A:H5''	51:UU:58:THR:HG22	2.01	0.43
4:9:1607:A:OP1	49:TT:87:VAL:HB	2.17	0.43
14:D:53:VAL:HB	14:D:159:VAL:HG23	2.00	0.43
38:O:54:TYR:CE1	38:O:145:VAL:HG11	2.53	0.43
45:RR:27:ASP:OD1	45:RR:30:THR:OG1	2.34	0.43
50:U:35:ASP:OD1	50:U:35:ASP:N	2.50	0.43
2:5:2524:C:O2	2:5:2644:G:N2	2.52	0.43
2:5:2903:C:OP1	44:R:108:ARG:NH2	2.51	0.43
2:5:3897:C:O2'	2:5:4983:A:N1	2.50	0.43
4:9:1804:U:OP1	52:V:67:LYS:HE2	2.17	0.43
17:E:165:VAL:HG11	17:E:178:VAL:HG13	2.01	0.43
17:E:193:HIS:HB3	17:E:196:PHE:HD1	1.83	0.43
21:FF:155:CYS:HB3	21:FF:159:ARG:HH22	1.83	0.43
45:RR:66:VAL:HG11	45:RR:69:ILE:HB	1.99	0.43
82:v:27:HIS:HB3	82:v:30:HIS:CE1	2.53	0.43
82:v:394:LEU:HA	82:v:419:GLY:HA3	1.99	0.43
2:5:4480:C:O2'	2:5:4482:G:OP2	2.32	0.43
4:9:421:G:H4'	34:LL:98:LYS:HE3	2.00	0.43
4:9:527:C:H2'	4:9:528:A:H8	1.84	0.43
4:9:625:G:O6	57:XX:63:ASN:OD1	2.36	0.43
4:9:688:U:O2	26:HH:122:LEU:HG	2.19	0.43
4:9:916:A:C6	37:NN:73:ARG:CG	3.02	0.43
9:BB:46:LYS:HE2	39:OO:19:PRO:HG2	2.01	0.43
13:Cc:51:ARG:HH21	21:FF:61:PHE:HB3	1.83	0.43
20:F:28:LYS:HE2	20:F:28:LYS:HB3	1.91	0.43
22:G:85:PHE:HE1	60:Z:53:VAL:HG12	1.82	0.43
23:GG:51:ARG:HB2	23:GG:112:VAL:HG23	2.00	0.43
28:II:78:ILE:H	28:II:78:ILE:HG13	1.51	0.43
57:XX:105:PHE:HD1	57:XX:121:LYS:HD3	1.83	0.43
59:YY:25:ILE:O	59:YY:70:THR:HA	2.19	0.43
1:x:161:LYS:O	1:x:161:LYS:CG	2.55	0.43
2:5:135:G:O2'	69:h:96:ASN:HB2	2.19	0.43
2:5:405:U:OP1	58:Y:87:ARG:NH1	2.52	0.43
2:5:4346:C:O3'	76:o:37:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:857:U:H2'	4:9:858:A:C8	2.54	0.43
4:9:1358:U:H5'	12:CC:114:LYS:HD3	2.01	0.43
5:A:158:ILE:HG23	5:A:162:ASN:HD21	1.84	0.43
7:Aa:65:PRO:HB3	9:BB:108:ASP:OD2	2.17	0.43
21:FF:193:LYS:HE2	21:FF:193:LYS:HB3	1.90	0.43
22:G:234:TYR:CZ	22:G:279:TYR:HB3	2.54	0.43
27:I:202:ASN:N	27:I:202:ASN:OD1	2.50	0.43
30:JJ:45:ARG:NH2	30:JJ:146:SER:OG	2.50	0.43
46:S:3:ALA:HB1	46:S:7:LEU:HD21	2.01	0.43
78:r:105:ASP:OD1	78:r:105:ASP:N	2.51	0.43
2:5:994:U:H3	2:5:1068:G:H1	1.66	0.43
4:9:948:C:H2'	4:9:949:G:H8	1.83	0.43
4:9:1588:A:H2'	4:9:1589:A:C8	2.54	0.43
4:9:1661:A:OP2	16:Dd:19:ARG:NH2	2.52	0.43
26:HH:44:ASN:HB3	26:HH:68:GLN:HE22	1.84	0.43
26:HH:50:GLU:OE2	26:HH:90:LYS:NZ	2.37	0.43
44:R:44:LEU:HD22	44:R:49:LEU:HD12	2.00	0.43
45:RR:107:LYS:HA	45:RR:112:GLY:HA2	1.99	0.43
50:U:43:LEU:HB3	50:U:63:LEU:HD11	2.00	0.43
55:WW:102:ILE:HG22	55:WW:128:PHE:HB3	2.01	0.43
56:X:82:THR:HG21	69:h:37:THR:HG22	2.00	0.43
79:s:109:ALA:N	79:s:183:PHE:O	2.47	0.43
82:v:490:HIS:ND1	82:v:490:HIS:O	2.52	0.43
2:5:1488:G:H2'	2:5:1488:G:N3	2.33	0.43
2:5:1502:G:OP1	42:Q:150:ARG:NH1	2.52	0.43
2:5:3652:A:H1'	2:5:3789:A2M:N6	2.34	0.43
2:5:5051:C:H5''	2:5:5054:C:H5	1.82	0.43
4:9:107:A:H2'	4:9:108:G:C8	2.52	0.43
4:9:873:G:H5''	44:R:162:ARG:CB	2.48	0.43
4:9:919:A:C5'	37:NN:16:LEU:HD12	2.48	0.43
4:9:1365:G:H2'	4:9:1366:G:H8	1.83	0.43
4:9:1479:G:H4'	43:QQ:131:LYS:NZ	2.33	0.43
5:A:30:ARG:NH1	5:A:36:GLU:OE1	2.52	0.43
11:C:84:THR:HA	80:s1:88:VAL:HB	2.01	0.43
12:CC:70:VAL:HG11	12:CC:93:ILE:HG12	1.99	0.43
17:E:158:GLY:O	17:E:161:ARG:HG3	2.18	0.43
34:LL:11:GLN:HB3	34:LL:56:ILE:HG21	2.01	0.43
35:M:50:MET:HE3	35:M:55:MET:HB3	2.01	0.43
43:QQ:31:LEU:HB3	43:QQ:67:ASP:HB2	2.01	0.43
45:RR:9:VAL:HG13	45:RR:50:ILE:HG22	2.01	0.43
46:S:82:LEU:HD11	46:S:109:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:YY:76:TYR:OH	59:YY:86:GLU:OE1	2.35	0.43
82:v:642:ASP:OD1	82:v:642:ASP:N	2.50	0.43
2:5:1894:G:N2	2:5:1943:A:H61	2.16	0.43
4:9:122:G:H21	18:EE:146:THR:HG21	1.84	0.43
4:9:1479:G:H4'	43:QQ:131:LYS:HZ1	1.84	0.43
7:Aa:59:PHE:HZ	39:OO:128:ARG:HH11	1.66	0.43
10:Bb:8:LEU:HG	55:WW:62:VAL:HG11	2.00	0.43
11:C:73:VAL:HB	11:C:78:ARG:HH21	1.84	0.43
12:CC:171:GLY:O	55:WW:98:GLN:NE2	2.31	0.43
12:CC:209:VAL:HG21	12:CC:233:LEU:HD11	2.01	0.43
29:J:12:MET:HG3	29:J:137:PRO:HB2	2.01	0.43
41:PP:68:PRO:HB2	41:PP:71:GLU:HG2	2.01	0.43
48:T:7:LYS:O	48:T:55:LYS:NZ	2.52	0.43
57:XX:90:CYS:HA	57:XX:93:PHE:HD2	1.84	0.43
79:s:26:LYS:HE3	79:s:28:PHE:HE2	1.82	0.43
79:s:62:ARG:NH2	79:s:82:ILE:O	2.50	0.43
1:x:87:ILE:HA	1:x:90:LEU:HD12	2.00	0.43
2:5:1395:A:P	42:Q:181:ARG:HH12	2.41	0.43
2:5:4888:G:HO2'	2:5:4889:U:P	2.42	0.43
3:8:92:U:H2'	3:8:93:C:O4'	2.19	0.43
4:9:384:U:H4'	34:LL:135:SER:CA	2.49	0.43
4:9:857:U:H2'	4:9:858:A:H8	1.83	0.43
4:9:1298:G:C4'	41:PP:79:HIS:HD1	2.29	0.43
4:9:1468:C:H2'	4:9:1469:A:C8	2.54	0.43
9:BB:24:PRO:O	9:BB:28:LYS:NZ	2.45	0.43
15:DD:148:LYS:HB2	83:w:206:HIS:NE2	2.33	0.43
24:Gg:254:PRO:HA	24:Gg:285:GLN:HA	2.00	0.43
28:II:34:ALA:HB2	28:II:56:ARG:HH11	1.84	0.43
28:II:150:ASP:HA	28:II:153:LYS:HB2	2.01	0.43
34:LL:93:LEU:CD1	57:XX:8:ARG:HH22	2.25	0.43
35:M:11:ARG:NH2	35:M:58:THR:O	2.49	0.43
36:N:178:HIS:HA	36:N:181:HIS:NE2	2.33	0.43
45:RR:36:GLU:HG2	45:RR:47:ARG:HH11	1.84	0.43
64:c:44:LYS:HB3	64:c:105:ILE:HD13	2.01	0.43
79:s:106:LYS:HG2	79:s:186:GLY:HA3	2.01	0.43
82:v:120:ARG:HH21	82:v:497:MET:HA	1.83	0.43
82:v:227:GLN:NE2	82:v:349:ALA:HA	2.34	0.43
2:5:150:U:OP2	22:G:253:THR:OG1	2.29	0.42
2:5:691:C:H2'	2:5:692:A:C8	2.54	0.42
2:5:1808:A:H5'	2:5:1810:G:O4'	2.19	0.42
2:5:1822:G:O2'	2:5:1823:G:OP1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:2643:U:H2'	2:5:2698:G:N1	2.33	0.42
2:5:4134:C:H2'	2:5:4135:G:H8	1.84	0.42
2:5:4270:G:H2'	2:5:4270:G:N3	2.34	0.42
4:9:17:C:H2'	4:9:18:C:C6	2.54	0.42
4:9:17:C:O2'	4:9:1194:A:N1	2.52	0.42
4:9:1230:C:P	47:SS:139:THR:HB	2.59	0.42
4:9:1451:G:OP1	45:RR:32:LYS:HE3	2.18	0.42
4:9:1668:U:H5''	51:UU:77:TRP:CD1	2.54	0.42
4:9:1714:U:H2'	4:9:1715:A:H8	1.83	0.42
4:9:1852:C:OP1	75:n:1:MET:HA	2.18	0.42
8:B:220:ILE:HG12	8:B:278:THR:HG23	2.01	0.42
13:Cc:65:ALA:HB3	13:Cc:67:ARG:HE	1.83	0.42
17:E:206:ILE:O	17:E:209:VAL:HG12	2.18	0.42
24:Gg:8:ARG:NH1	24:Gg:311:GLN:H	2.17	0.42
33:L:57:PRO:HG3	33:L:75:GLY:O	2.19	0.42
44:R:13:SER:OG	44:R:38:ARG:NH1	2.46	0.42
65:d:101:LYS:HG3	65:d:102:LEU:HG	2.01	0.42
71:j:72:ARG:O	71:j:75:ARG:HG2	2.20	0.42
82:v:772:GLU:HB3	82:v:785:LYS:HZ2	1.84	0.42
1:x:121:PRO:CG	81:t:93:ILE:CD1	2.96	0.42
2:5:2398:G:O2'	2:5:2823:U:O4	2.22	0.42
2:5:4492:A:H4'	2:5:4493:G:C8	2.54	0.42
2:5:5006:U:H2'	2:5:5007:U:C6	2.54	0.42
4:9:388:U:H2'	4:9:389:A:C8	2.54	0.42
4:9:496:C:OP1	18:EE:29:PRO:HD3	2.18	0.42
4:9:1320:G:C4'	82:v:629:LYS:NZ	2.82	0.42
4:9:1401:A:O3'	51:UU:52:GLY:HA3	2.19	0.42
6:AA:21:ALA:HB1	6:AA:170:SER:HA	2.01	0.42
22:G:276:ARG:HG3	22:G:280:ASN:HB2	2.00	0.42
39:OO:29:GLY:HA3	39:OO:90:ILE:HD11	2.01	0.42
39:OO:31:CYS:HB3	39:OO:93:LEU:HD12	2.02	0.42
41:PP:18:ARG:NE	41:PP:36:LEU:O	2.45	0.42
64:c:38:ILE:HG21	64:c:63:TYR:HB3	2.00	0.42
79:s:29:ILE:HD11	79:s:78:LEU:HD11	2.00	0.42
2:5:158:A:H5''	2:5:159:C:H2'	2.02	0.42
2:5:972:C:H42	2:5:2099:A:N6	2.13	0.42
2:5:3756:C:HO2'	2:5:3780:G:H1'	1.84	0.42
2:5:3760:A:H61	2:5:3772:U:H3	1.67	0.42
4:9:120:U:C1'	18:EE:33:THR:OG1	2.67	0.42
4:9:1520:G:OP2	47:SS:137:LYS:HD2	2.19	0.42
6:AA:176:TRP:CD2	6:AA:199:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:218:VAL:O	11:C:222:ARG:HB2	2.19	0.42
18:EE:72:ILE:HG23	18:EE:90:ILE:HG22	2.01	0.42
23:GG:58:LYS:HA	23:GG:107:SER:HB3	2.01	0.42
29:J:174:ILE:H	29:J:174:ILE:HG13	1.67	0.42
33:L:182:LEU:O	33:L:186:ARG:HG2	2.19	0.42
37:NN:136:PRO:HG2	37:NN:139:TRP:HB2	2.02	0.42
41:PP:44:ARG:NH2	41:PP:53:GLN:OE1	2.52	0.42
49:TT:61:ALA:HB2	49:TT:107:LEU:HD13	2.02	0.42
79:s:130:LEU:HD12	79:s:134:LYS:HD2	2.01	0.42
1:x:36:ILE:HD11	1:x:165:LEU:HD12	2.02	0.42
2:5:1283:A:O2'	2:5:1285:G:N7	2.42	0.42
2:5:2646:A:C2	72:k:2:PRO:HD2	2.54	0.42
2:5:2670:U:O2'	2:5:2672:G:N7	2.49	0.42
2:5:4942:A:H1'	17:E:188:PRO:HG3	2.01	0.42
4:9:331:C:OP1	23:GG:192:ILE:HD13	2.19	0.42
4:9:382:C:H2'	4:9:383:G:C8	2.54	0.42
4:9:386:C:OP2	34:LL:136:LYS:HD2	2.19	0.42
4:9:730:C:H2'	4:9:731:G:H8	1.84	0.42
4:9:980:A:H2'	4:9:981:A:C8	2.54	0.42
4:9:1787:G:H2'	4:9:1788:A:H8	1.85	0.42
9:BB:85:LYS:HB3	9:BB:101:HIS:HB3	2.01	0.42
15:DD:8:LYS:HE2	51:UU:61:LEU:HD21	2.01	0.42
18:EE:166:THR:HB	18:EE:168:LYS:HE2	2.01	0.42
82:v:140:GLU:O	82:v:144:ARG:HB2	2.19	0.42
2:5:85:G:O2'	2:5:97:G:O6	2.31	0.42
2:5:93:G:H2'	2:5:94:A:C8	2.54	0.42
2:5:308:G:OP2	2:5:308:G:N2	2.37	0.42
2:5:969:A:H1'	2:5:971:C:N4	2.34	0.42
2:5:2543:C:H2'	2:5:2544:C:C6	2.55	0.42
2:5:5005:U:H2'	2:5:5006:U:O4'	2.19	0.42
3:8:141:C:H2'	3:8:142:U:C6	2.54	0.42
4:9:123:G:H1'	18:EE:146:THR:HG21	2.01	0.42
4:9:222:U:H5''	34:LL:17:PHE:CD1	2.54	0.42
4:9:730:C:H2'	4:9:731:G:C8	2.54	0.42
4:9:1030:A:H2'	4:9:1031:A2M:H8	2.00	0.42
4:9:1256:G:C8	51:UU:66:ARG:HG3	2.54	0.42
4:9:1454:A:O4'	45:RR:3:ARG:NH2	2.52	0.42
15:DD:143:ARG:HD2	83:w:216:HIS:C	2.30	0.42
15:DD:171:ALA:O	15:DD:185:LYS:HA	2.19	0.42
18:EE:159:THR:HG22	18:EE:173:ILE:HB	2.02	0.42
22:G:139:VAL:HG11	22:G:238:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Gg:57:ARG:NH1	24:Gg:94:THR:O	2.53	0.42
24:Gg:217:MET:HB3	24:Gg:229:THR:HG23	2.00	0.42
25:H:139:ALA:O	25:H:140:GLN:NE2	2.53	0.42
41:PP:86:LEU:HD12	41:PP:87:PRO:HD2	2.02	0.42
48:T:17:ARG:HH11	48:T:45:MET:HG3	1.84	0.42
59:YY:90:ARG:HG3	59:YY:93:ARG:HD2	2.01	0.42
66:e:23:HIS:HA	66:e:53:ILE:HD12	2.00	0.42
2:5:152:U:P	36:N:49:ARG:HH12	2.42	0.42
2:5:1484:C:O2'	2:5:1486:G:OP2	2.37	0.42
2:5:1492:G:OP1	33:L:183:ARG:NE	2.48	0.42
2:5:2265:G:H5''	17:E:115:MET:SD	2.60	0.42
2:5:3860:A:H5''	40:P:83:TRP:O	2.20	0.42
2:5:4326:G:N2	2:5:4329:A:OP2	2.48	0.42
4:9:290:U:O2'	4:9:292:A:N7	2.47	0.42
4:9:1232:U:H2'	4:9:1233:G:C8	2.55	0.42
4:9:1337:4AC:H2'	4:9:1338:G:H8	1.84	0.42
6:AA:184:ARG:HD3	6:AA:191:ARG:HG2	2.01	0.42
8:B:223:THR:HA	8:B:338:VAL:HG22	2.00	0.42
8:B:224:LYS:HE3	8:B:340:THR:HG22	2.01	0.42
11:C:315:LYS:HD2	20:F:167:ALA:HB1	2.02	0.42
20:F:225:HIS:ND1	20:F:227:VAL:HG22	2.35	0.42
28:II:73:THR:HA	28:II:109:TYR:HE1	1.84	0.42
32:KK:37:ASP:OD1	32:KK:37:ASP:N	2.51	0.42
59:YY:78:SER:HB3	59:YY:81:TYR:HD2	1.84	0.42
65:d:23:ARG:HE	65:d:121:ASN:ND2	2.18	0.42
82:v:265:TYR:HA	82:v:287:ARG:HA	2.01	0.42
2:5:1649:C:H2'	2:5:1650:A:C8	2.55	0.42
2:5:2643:U:O2	68:g:26:PRO:HB3	2.20	0.42
2:5:3736:A:H2'	2:5:3737:A:C8	2.55	0.42
2:5:3752:A:H5''	5:A:243:THR:HB	2.02	0.42
2:5:4340:A:H5''	2:5:4341:C:H5'	2.01	0.42
2:5:4540:OMC:HM22	2:5:4541:C:O4'	2.19	0.42
3:8:87:G:O6	58:Y:113:LYS:NZ	2.51	0.42
4:9:309:G:OP2	28:II:55:TYR:CZ	2.73	0.42
4:9:587:A:O2'	4:9:588:G:N2	2.52	0.42
4:9:1036:A:N3	4:9:1844:U:O2'	2.52	0.42
6:AA:209:GLU:HA	6:AA:212:LYS:HG2	2.02	0.42
11:C:77:PRO:O	11:C:90:GLY:HA2	2.20	0.42
44:R:114:LYS:O	44:R:146:LYS:NZ	2.43	0.42
82:v:139:THR:HA	82:v:142:VAL:HG12	2.02	0.42
2:5:1965:G:OP2	79:s:59:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1982:C:H42	2:5:1992:G:H1	1.68	0.42
2:5:2409:G:H5'	71:j:14:LYS:NZ	2.34	0.42
2:5:2849:A:H61	2:5:3847:C:H42	1.67	0.42
2:5:4749:G:H22	2:5:4959:A:H2	1.67	0.42
4:9:15:U:O2'	4:9:669:A:N6	2.52	0.42
4:9:334:C:H41	23:GG:190:ARG:NH2	2.17	0.42
4:9:941:C:H2'	4:9:942:G:C8	2.55	0.42
4:9:1051:G:H2'	4:9:1052:A:H8	1.84	0.42
4:9:1499:U:H2'	4:9:1500:G:H8	1.85	0.42
9:BB:113:MET:HB3	9:BB:142:PHE:CE2	2.55	0.42
11:C:157:LYS:HE3	11:C:157:LYS:HB2	1.85	0.42
15:DD:145:GLN:HB2	83:w:202:SER:OG	2.19	0.42
20:F:236:GLU:OE1	46:S:41:LYS:NZ	2.40	0.42
21:FF:28:VAL:HG11	21:FF:109:LEU:HD12	2.01	0.42
25:H:129:ARG:HA	25:H:129:ARG:HD3	1.85	0.42
37:NN:63:VAL:O	37:NN:67:THR:OG1	2.29	0.42
44:R:134:ASN:OD1	44:R:135:LYS:N	2.52	0.42
52:V:13:LYS:HD2	52:V:128:LEU:HD22	2.00	0.42
55:WW:52:ILE:HG12	55:WW:61:ILE:HG12	2.02	0.42
62:a:79:TRP:CZ2	62:a:122:VAL:HG12	2.55	0.42
1:x:49:PHE:CE1	1:x:159:MET:HB2	2.55	0.42
2:5:962:G:OP2	2:5:962:G:H8	2.03	0.42
2:5:1177:G:H2'	2:5:1178:G:C8	2.55	0.42
2:5:1935:C:N4	2:5:2044:A:N3	2.68	0.42
2:5:1983:A:O2'	2:5:1984:U:OP1	2.26	0.42
2:5:5006:U:OP2	8:B:385:LYS:NZ	2.48	0.42
4:9:65:C:H41	4:9:169:U:HO2'	1.62	0.42
4:9:307:G:O3'	28:II:45:THR:CG2	2.67	0.42
4:9:1016:U:OP2	10:Bb:20:LYS:NZ	2.43	0.42
4:9:1375:G:H2'	4:9:1376:A:C8	2.54	0.42
20:F:240:ASN:O	20:F:244:ARG:HG2	2.20	0.42
29:J:94:LEU:HB3	29:J:98:ASN:HD22	1.84	0.42
30:JJ:60:LEU:HD22	30:JJ:70:ARG:HA	2.02	0.42
59:YY:110:ARG:NH2	59:YY:114:MET:SD	2.93	0.42
62:a:74:ASN:HA	62:a:112:LEU:O	2.20	0.42
78:r:2:SER:O	78:r:6:GLN:HG2	2.20	0.42
79:s:20:LEU:HB3	79:s:90:PHE:CD2	2.55	0.42
82:v:609:PHE:CD2	82:v:699:GLY:HA2	2.55	0.42
82:v:839:ARG:HB3	82:v:844:LEU:HB2	2.01	0.42
1:x:160:LYS:HB3	1:x:160:LYS:HE2	1.52	0.42
2:5:658:C:H2'	2:5:659:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1394:G:N2	2:5:1397:G:OP2	2.44	0.42
2:5:2054:OMG:HM22	2:5:2055:C:O4'	2.20	0.42
2:5:3726:G:H2'	2:5:3727:A2M:H8	2.01	0.42
4:9:793:G:H2'	4:9:794:A:H8	1.85	0.42
4:9:827:A:OP1	30:JJ:10:ARG:CZ	2.68	0.42
4:9:1438:A:H2'	4:9:1439:A:C8	2.55	0.42
4:9:1647:A:OP1	43:QQ:138:ARG:NH2	2.52	0.42
6:AA:203:PHE:CZ	45:RR:91:LEU:HD21	2.50	0.42
11:C:60:HIS:HA	11:C:92:PHE:HE1	1.85	0.42
13:Cc:32:VAL:HG11	13:Cc:56:LEU:HD21	2.02	0.42
15:DD:106:ARG:HH11	15:DD:110:LEU:HD12	1.85	0.42
20:F:125:ASN:HB2	48:T:132:PRO:HB2	2.02	0.42
26:HH:105:THR:HG23	26:HH:108:SER:H	1.84	0.42
29:J:95:ARG:H	29:J:98:ASN:ND2	2.18	0.42
48:T:48:VAL:HG21	48:T:94:GLU:HG2	2.01	0.42
53:VV:34:MET:HE3	53:VV:34:MET:HB3	1.81	0.42
82:v:592:LEU:HD13	82:v:603:TYR:CZ	2.55	0.42
2:5:409:G:OP2	40:P:2:VAL:N	2.53	0.41
2:5:1374:G:H4'	2:5:1375:A:O5'	2.20	0.41
2:5:3672:C:H5'	5:A:8:GLN:O	2.20	0.41
2:5:3684:U:OP1	5:A:54:ARG:NH2	2.36	0.41
2:5:3722:A2M:H8	2:5:3722:A2M:O5'	2.19	0.41
2:5:3759:G:O2'	2:5:3760:A:H8	2.02	0.41
4:9:318:A:H3'	4:9:319:C:H5''	2.02	0.41
4:9:1610:G:C8	47:SS:132:ARG:NH2	2.80	0.41
4:9:1613:G:H3'	41:PP:39:ALA:HB1	2.01	0.41
5:A:36:GLU:OE2	5:A:163:ARG:NH1	2.53	0.41
9:BB:57:ILE:HG22	9:BB:59:SER:H	1.84	0.41
9:BB:57:ILE:HB	9:BB:60:ASP:HB2	2.02	0.41
13:Cc:49:PRO:HA	21:FF:60:ARG:HH21	1.85	0.41
17:E:165:VAL:HG12	17:E:178:VAL:HG22	2.00	0.41
18:EE:72:ILE:HB	18:EE:77:ARG:HD3	2.01	0.41
22:G:215:ASP:HB2	22:G:216:PRO:HD3	2.02	0.41
24:Gg:39:THR:HA	24:Gg:60:ARG:HH11	1.85	0.41
26:HH:133:LEU:HD23	26:HH:134:VAL:HG13	2.00	0.41
27:I:149:VAL:O	27:I:153:ARG:HB2	2.20	0.41
37:NN:45:LEU:HG	37:NN:49:GLN:HG3	2.01	0.41
39:OO:43:HIS:CD2	39:OO:55:ARG:HB2	2.55	0.41
48:T:80:VAL:O	48:T:81:LYS:C	2.62	0.41
55:WW:86:LEU:HB3	55:WW:117:ARG:HH21	1.85	0.41
2:5:25:A:N3	2:5:339:C:O2'	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:4508:C:H2'	2:5:4509:C:C6	2.55	0.41
2:5:5021:G:OP1	28:II:92:ARG:HD2	2.20	0.41
4:9:160:U:O2'	4:9:162:C:O5'	2.38	0.41
4:9:354:U:OP1	34:LL:107:LYS:HG3	2.19	0.41
4:9:455:A:O2'	4:9:1735:A:N3	2.52	0.41
4:9:641:A:O2'	4:9:645:C:OP1	2.38	0.41
4:9:931:C:OP2	9:BB:159:GLN:HG3	2.20	0.41
4:9:1253:A:OP2	4:9:1526:G:N2	2.43	0.41
4:9:1549:U:H5''	16:Dd:33:LYS:HE3	2.01	0.41
4:9:1585:U:C4	49:TT:67:ARG:NH1	2.87	0.41
9:BB:111:CYS:HA	9:BB:114:VAL:HG12	2.02	0.41
20:F:219:MET:HB3	20:F:231:ASP:OD2	2.20	0.41
45:RR:31:ASN:HA	45:RR:34:VAL:HG12	2.01	0.41
47:SS:5:ILE:HG12	61:ZZ:49:LEU:HB2	1.94	0.41
48:T:88:ARG:NH2	63:b:30:GLU:OE2	2.51	0.41
82:v:421:VAL:HB	82:v:464:VAL:HB	2.01	0.41
82:v:559:LYS:HE2	82:v:559:LYS:HB3	1.82	0.41
82:v:753:GLU:HB3	82:v:782:PHE:CE1	2.54	0.41
2:5:18:C:H4'	36:N:138:PHE:CD1	2.55	0.41
2:5:28:C:OP2	36:N:193:ARG:NH1	2.39	0.41
2:5:737:C:C2	2:5:739:G:H5'	2.56	0.41
2:5:1097:C:H2'	2:5:1098:G:C8	2.55	0.41
2:5:1242:A:HO2'	2:5:1243:C:P	2.42	0.41
2:5:1454:C:H1'	2:5:2109:A:H1'	2.02	0.41
2:5:4461:U:H1'	8:B:252:ALA:HB3	2.03	0.41
2:5:4534:UR3:H2'	2:5:4535:PSU:C6	2.56	0.41
2:5:4694:B8K:O6	2:5:4702:C:H5''	2.20	0.41
4:9:561:A:N3	30:JJ:132:GLN:NE2	2.64	0.41
4:9:1402:A:O2'	51:UU:54:VAL:HG13	2.21	0.41
4:9:1608:U:H5''	47:SS:130:ARG:HH11	1.86	0.41
6:AA:10:MET:HE2	6:AA:55:TRP:HB2	2.02	0.41
9:BB:70:SER:HA	9:BB:83:LYS:HA	2.01	0.41
10:Bb:25:VAL:HG23	55:WW:55:ASP:HB3	2.02	0.41
23:GG:5:ILE:HD11	23:GG:14:LYS:HG3	2.02	0.41
25:H:4:ILE:HG12	25:H:61:TRP:CH2	2.55	0.41
29:J:113:ILE:HG21	29:J:119:TYR:HD2	1.85	0.41
30:JJ:46:VAL:HG11	30:JJ:106:LEU:HD12	2.01	0.41
37:NN:18:TYR:CE2	55:WW:56:HIS:CE1	3.08	0.41
64:c:47:ILE:HD12	64:c:94:LEU:HD11	2.02	0.41
81:t:19:PHE:HE2	81:t:21:MET:HE3	1.85	0.41
2:5:453:G:N3	2:5:453:G:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:1484:C:O2	2:5:1486:G:N2	2.53	0.41
2:5:2478:G:C6	56:X:47:ARG:HD3	2.55	0.41
2:5:4593:A:N1	2:5:4625:C:O2'	2.49	0.41
4:9:127:C:O2	18:EE:134:LYS:CD	2.69	0.41
4:9:141:A:O3'	23:GG:188:LYS:HE3	2.19	0.41
4:9:527:C:O3'	30:JJ:121:LYS:NZ	2.53	0.41
4:9:628:A:C2	83:w:216:HIS:CD2	3.08	0.41
4:9:1213:C:H2'	4:9:1214:A:C8	2.55	0.41
4:9:1489:A:H62	83:w:197:SER:CA	2.33	0.41
4:9:1648:G:H2'	43:QQ:127:CYS:HA	2.03	0.41
7:Aa:22:ARG:NH1	39:OO:141:ARG:HE	2.16	0.41
9:BB:28:LYS:HD2	9:BB:28:LYS:H	1.85	0.41
24:Gg:41:ILE:HG13	24:Gg:58:ALA:HB2	2.01	0.41
26:HH:130:LEU:HD21	26:HH:156:VAL:HG21	2.03	0.41
29:J:144:LYS:HE3	29:J:147:ARG:O	2.20	0.41
36:N:145:ASN:HD22	36:N:148:THR:HG22	1.85	0.41
40:P:122:ALA:HB3	40:P:143:PRO:HG2	2.02	0.41
43:QQ:57:LEU:HD23	43:QQ:111:ILE:HG22	2.02	0.41
54:W:35:LYS:HE2	54:W:51:TRP:CZ2	2.54	0.41
61:ZZ:41:ARG:HB3	61:ZZ:42:ASP:H	1.71	0.41
78:r:113:ARG:O	78:r:117:ILE:HG12	2.20	0.41
82:v:689:GLU:O	82:v:730:TYR:OH	2.32	0.41
1:x:128:LEU:HD23	1:x:128:LEU:HA	1.91	0.41
2:5:1666:C:H2'	2:5:1667:C:C6	2.56	0.41
2:5:1673:A:OP1	63:b:18:ARG:NH2	2.47	0.41
2:5:4753:C:H2'	2:5:4754:G:O4'	2.20	0.41
4:9:496:C:H5'	18:EE:29:PRO:HB3	2.02	0.41
4:9:675:U:H2'	4:9:676:C:H6	1.86	0.41
4:9:694:G:H1	4:9:732:U:H3	1.69	0.41
5:A:225:ILE:HD11	5:A:233:ARG:HG3	2.02	0.41
30:JJ:136:ARG:NH2	30:JJ:158:ASP:OD2	2.54	0.41
44:R:15:LEU:O	44:R:52:ARG:NH1	2.53	0.41
48:T:64:VAL:HG13	48:T:72:VAL:HG13	2.03	0.41
64:c:65:MET:HE2	64:c:65:MET:HB2	1.99	0.41
2:5:1745:G:H3'	2:5:1746:A:C5'	2.50	0.41
2:5:2408:A:H1'	71:j:12:ARG:HH11	1.85	0.41
2:5:2463:G:H2'	2:5:2465:G:OP2	2.21	0.41
2:5:2901:G:H4'	44:R:101:ILE:HD13	2.02	0.41
2:5:4944:C:H42	17:E:223:LYS:HG2	1.86	0.41
2:5:5009:G:N2	2:5:5045:G:O2'	2.54	0.41
4:9:1018:U:H2'	4:9:1019:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:1122:A:C4'	9:BB:205:TYR:CD1	2.94	0.41
10:Bb:50:ALA:O	10:Bb:52:THR:N	2.54	0.41
25:H:43:VAL:HG12	25:H:59:LYS:HD3	2.03	0.41
27:I:184:MET:HA	27:I:187:GLU:HG2	2.02	0.41
82:v:76:SER:HA	82:v:101:ASN:HA	2.02	0.41
82:v:582:THR:HB	82:v:739:ARG:HB2	2.01	0.41
82:v:749:ILE:HD11	82:v:796:PHE:HZ	1.86	0.41
2:5:275:C:H2'	2:5:276:C:C6	2.55	0.41
2:5:1881:G:O3'	20:F:99:GLY:HA2	2.21	0.41
4:9:122:G:O2'	18:EE:146:THR:N	2.46	0.41
4:9:502:C:N3	18:EE:67:GLN:OE1	2.53	0.41
4:9:862:A:N3	55:WW:105:THR:OG1	2.42	0.41
4:9:1650:A:OP1	43:QQ:136:GLY:CA	2.69	0.41
12:CC:212:LYS:O	12:CC:216:MET:HG2	2.21	0.41
17:E:271:GLN:O	17:E:275:ARG:HG3	2.21	0.41
19:Ee:80:ALA:CB	82:v:684:GLN:NE2	2.83	0.41
24:Gg:82:SER:OG	24:Gg:83:TRP:N	2.54	0.41
43:QQ:51:LEU:HD13	43:QQ:85:ARG:HE	1.86	0.41
56:X:150:ALA:HB1	56:X:155:ILE:HG13	2.02	0.41
82:v:18:ASN:HB2	82:v:94:ASP:OD1	2.21	0.41
82:v:464:VAL:HG21	82:v:470:VAL:HG11	2.02	0.41
2:5:230:G:OP1	58:Y:15:ARG:NH1	2.48	0.41
2:5:1861:C:H2'	2:5:1862:A:C8	2.56	0.41
2:5:2656:G:N1	77:p:58:GLY:O	2.42	0.41
2:5:4684:G:H2'	2:5:4685:A:C8	2.55	0.41
4:9:146:G:O2'	4:9:147:A:O5'	2.33	0.41
4:9:496:C:OP1	18:EE:49:ARG:NH1	2.53	0.41
4:9:979:C:H2'	4:9:980:A:C8	2.56	0.41
7:Aa:59:PHE:CZ	39:OO:128:ARG:NH1	2.89	0.41
9:BB:78:GLU:HG3	9:BB:79:VAL:H	1.85	0.41
9:BB:144:LYS:HD3	9:BB:208:HIS:CG	2.56	0.41
11:C:276:ASN:ND2	11:C:276:ASN:O	2.54	0.41
15:DD:74:GLN:HA	15:DD:79:PHE:HB2	2.02	0.41
22:G:138:GLN:OE1	22:G:282:ARG:NH2	2.54	0.41
24:Gg:244:ASN:ND2	24:Gg:294:ASP:O	2.53	0.41
26:HH:144:ILE:HG23	55:WW:52:ILE:HB	2.03	0.41
28:II:86:SER:O	34:LL:8:ARG:NH2	2.43	0.41
42:Q:35:LEU:O	42:Q:39:THR:OG1	2.22	0.41
46:S:2:LYS:HE3	46:S:2:LYS:HB2	1.90	0.41
46:S:168:THR:HG22	46:S:170:LYS:H	1.85	0.41
47:SS:84:LEU:O	47:SS:87:GLN:NE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:m:68:MET:HG2	74:m:79:PRO:HA	2.03	0.41
77:p:30:GLU:HA	77:p:33:GLN:HG2	2.03	0.41
1:x:45:LYS:HE2	1:x:45:LYS:HB3	1.60	0.41
2:5:69:A:N1	2:5:324:A:O2'	2.48	0.41
2:5:223:G:H4'	2:5:225:G:N7	2.35	0.41
2:5:972:C:H4'	2:5:973:G:H5''	2.02	0.41
2:5:1664:U:H3'	62:a:13:GLY:HA2	2.03	0.41
2:5:1998:C:H2'	2:5:1999:G:C8	2.55	0.41
2:5:2339:C:H2'	2:5:2340:G:H8	1.85	0.41
2:5:2442:A:O2'	2:5:2444:U:OP2	2.38	0.41
2:5:4308:A:C2	62:a:43:ILE:HG23	2.56	0.41
2:5:4419:1MA:H4'	27:I:74:LYS:HD2	2.02	0.41
2:5:4478:A:H5'	74:m:99:LYS:HB2	2.01	0.41
2:5:4939:C:H2'	2:5:4940:G:C8	2.55	0.41
4:9:42:A:O2'	4:9:98:C:OP1	2.36	0.41
4:9:642:U:O2'	4:9:643:A:O5'	2.39	0.41
4:9:1198:G:H2'	4:9:1199:A:C8	2.56	0.41
4:9:1623:A:C5	47:SS:132:ARG:HB3	2.56	0.41
6:AA:24:HIS:O	6:AA:49:ILE:N	2.50	0.41
6:AA:74:VAL:HG22	6:AA:121:LEU:HB3	2.02	0.41
8:B:214:ASP:OD2	8:B:363:ILE:N	2.52	0.41
9:BB:139:CYS:SG	9:BB:140:VAL:N	2.94	0.41
9:BB:143:THR:OG1	9:BB:144:LYS:N	2.54	0.41
11:C:94:ASN:OD1	11:C:94:ASN:N	2.51	0.41
15:DD:146:ARG:HG2	83:w:206:HIS:CB	2.42	0.41
17:E:209:VAL:HG23	17:E:259:GLN:HB2	2.03	0.41
18:EE:72:ILE:HG12	18:EE:90:ILE:HG22	2.03	0.41
22:G:163:LYS:NZ	22:G:166:ARG:HH12	2.19	0.41
23:GG:61:PHE:HA	23:GG:62:PRO:HD3	1.89	0.41
25:H:63:ASN:O	25:H:67:LEU:HG	2.20	0.41
28:II:36:THR:O	28:II:96:LEU:N	2.50	0.41
29:J:35:ARG:NH2	29:J:122:SER:O	2.53	0.41
32:KK:32:HIS:CD2	32:KK:45:VAL:HG11	2.56	0.41
32:KK:50:GLN:HA	32:KK:53:LYS:HG2	2.02	0.41
35:M:35:ARG:HA	35:M:51:PRO:HA	2.02	0.41
43:QQ:8:GLN:OE1	43:QQ:95:TYR:OH	2.32	0.41
52:V:61:VAL:O	52:V:79:ALA:N	2.50	0.41
59:YY:26:ASP:HB2	59:YY:68:LYS:HD2	2.03	0.41
72:k:27:LYS:HE3	72:k:27:LYS:HB2	1.86	0.41
77:p:5:THR:OG1	77:p:8:VAL:O	2.31	0.41
79:s:26:LYS:HE2	79:s:98:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:t:113:LEU:HD23	81:t:113:LEU:HA	1.94	0.41
82:v:10:ARG:CZ	82:v:465:PRO:HD3	2.50	0.41
82:v:285:LEU:HA	82:v:286:PRO:HD3	1.91	0.41
82:v:714:ILE:HD13	83:w:198:GLY:HA2	2.03	0.41
2:5:35:U:H5'	2:5:36:U:OP2	2.20	0.41
2:5:1792:A:H2'	27:I:22:PHE:CZ	2.56	0.41
2:5:4276:G:OP2	2:5:4276:G:N2	2.33	0.41
4:9:581:U:OP1	59:YY:64:PHE:CD1	2.73	0.41
4:9:1256:G:C5	16:Dd:40:ARG:CD	3.04	0.41
4:9:1332:A:O2'	15:DD:145:GLN:CA	2.68	0.41
4:9:1474:A:O2'	43:QQ:124:PRO:HG3	2.20	0.41
4:9:1568:C:O2	4:9:1627:C:O2'	2.32	0.41
4:9:1613:G:P	41:PP:39:ALA:N	2.94	0.41
4:9:1746:U:C4'	23:GG:65:GLN:HG2	2.38	0.41
5:A:112:ILE:HG13	77:p:79:VAL:HG22	2.03	0.41
8:B:3:HIS:ND1	8:B:4:ARG:O	2.48	0.41
17:E:165:VAL:HG13	17:E:179:THR:C	2.45	0.41
24:Gg:165:ILE:HG12	24:Gg:177:TRP:HB2	2.01	0.41
39:OO:107:THR:HA	39:OO:108:PRO:HD3	1.97	0.41
43:QQ:13:PHE:HA	43:QQ:21:ALA:O	2.21	0.41
60:Z:47:ASP:N	60:Z:69:LYS:O	2.52	0.41
79:s:132:PRO:HB3	79:s:147:ILE:HD12	2.03	0.41
2:5:2897:U:H2'	2:5:2898:A:C8	2.56	0.40
2:5:4629:C:OP1	8:B:224:LYS:HG3	2.21	0.40
4:9:27:A2M:HM'3	57:XX:46:HIS:CD2	2.57	0.40
4:9:496:C:P	18:EE:29:PRO:HD3	2.60	0.40
4:9:533:A:H2'	4:9:534:G:H8	1.86	0.40
4:9:586:G:N7	30:JJ:172:ARG:NE	2.70	0.40
4:9:1649:U:H5''	43:QQ:137:ALA:HB3	2.03	0.40
5:A:70:LYS:HD2	5:A:72:ARG:NH1	2.36	0.40
6:AA:15:VAL:HG21	45:RR:111:PHE:CD2	2.56	0.40
6:AA:42:LYS:HG2	45:RR:99:ASP:OD2	2.21	0.40
8:B:220:ILE:HB	8:B:346:THR:HB	2.02	0.40
9:BB:137:LEU:HD22	9:BB:215:VAL:HG13	2.03	0.40
12:CC:104:ASP:HB3	12:CC:130:ILE:HG13	2.02	0.40
13:Cc:45:ASN:N	13:Cc:67:ARG:HH22	2.19	0.40
14:D:152:ARG:O	14:D:157:ASN:ND2	2.45	0.40
15:DD:175:VAL:HG13	15:DD:182:LEU:HB2	2.03	0.40
22:G:159:THR:HG22	22:G:248:HIS:NE2	2.37	0.40
22:G:219:LEU:HD21	36:N:45:PRO:HG2	2.03	0.40
29:J:146:ARG:HG2	29:J:147:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:PP:41:GLN:HG2	41:PP:84:ILE:HD13	2.04	0.40
61:ZZ:51:ASP:HB2	61:ZZ:54:THR:HG23	2.04	0.40
69:h:13:LYS:HB2	69:h:16:GLU:HG3	2.03	0.40
82:v:78:PHE:CE2	82:v:80:GLU:HB2	2.56	0.40
2:5:739:G:H2'	2:5:740:G:H8	1.87	0.40
2:5:4421:C:N4	2:5:4426:A:O2'	2.54	0.40
2:5:4429:G:OP1	74:m:74:TYR:OH	2.31	0.40
4:9:53:C:O2'	4:9:507:G:N7	2.51	0.40
4:9:163:U:H5''	23:GG:85:ARG:HG3	2.03	0.40
4:9:294:U:N3	34:LL:65:ASN:CB	2.79	0.40
4:9:532:C:H2'	4:9:533:A:C8	2.56	0.40
4:9:1101:U:H2'	4:9:1102:G:H8	1.87	0.40
4:9:1152:U:O2'	55:WW:16:ASN:OD1	2.38	0.40
4:9:1221:G:H2'	4:9:1222:G:C8	2.57	0.40
4:9:1678:A2M:HM'3	4:9:1678:A2M:H1'	1.96	0.40
4:9:1856:C:H2'	4:9:1857:G:C8	2.57	0.40
8:B:35:ASP:OD2	8:B:193:LYS:NZ	2.52	0.40
11:C:195:LYS:HB3	11:C:200:ARG:NE	2.36	0.40
14:D:64:ILE:HG13	14:D:105:LEU:HD21	2.04	0.40
21:FF:68:ILE:HG21	21:FF:116:ILE:HD11	2.01	0.40
23:GG:75:LEU:O	23:GG:94:ARG:HA	2.21	0.40
27:I:193:ASP:HB2	27:I:198:LYS:HG3	2.04	0.40
28:II:22:HIS:ND1	28:II:23:LYS:O	2.36	0.40
28:II:90:LEU:HD22	28:II:95:THR:HG21	2.03	0.40
28:II:129:LEU:HD12	28:II:131:PRO:HD2	2.02	0.40
29:J:10:ASN:HA	29:J:11:PRO:HD3	1.97	0.40
38:O:181:ALA:O	38:O:185:VAL:HG22	2.20	0.40
47:SS:114:LEU:HD13	47:SS:122:GLY:HA2	2.03	0.40
63:b:101:HIS:HD2	63:b:103:LYS:H	1.69	0.40
71:j:34:CYS:HB3	71:j:39:TYR:H	1.86	0.40
2:5:417:G:H1'	3:8:16:G:N2	2.35	0.40
2:5:425:U:H4'	40:P:6:LEU:HD21	2.04	0.40
2:5:987:U:C6	17:E:73:ARG:HD3	2.57	0.40
2:5:1434:C:H2'	2:5:1435:C:C6	2.57	0.40
2:5:1869:G:H5'	27:I:118:ALA:O	2.22	0.40
2:5:1924:C:H3'	2:5:1925:C:H5''	2.04	0.40
2:5:4525:U:H1'	8:B:253:CYS:SG	2.62	0.40
4:9:15:U:H2'	4:9:16:G:O4'	2.22	0.40
4:9:60:A:N6	4:9:61:A:N1	2.69	0.40
4:9:78:C:H1'	23:GG:175:LYS:CE	2.51	0.40
4:9:93:U:O2	18:EE:8:HIS:HE1	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:189:U:OP1	28:II:152:ARG:NH2	2.54	0.40
4:9:561:A:H1'	30:JJ:132:GLN:OE1	2.21	0.40
5:A:60:LYS:HE3	5:A:60:LYS:HB2	1.88	0.40
5:A:146:THR:N	5:A:158:ILE:O	2.50	0.40
8:B:122:TRP:CE2	8:B:127:LYS:HE3	2.56	0.40
21:FF:118:ASN:O	21:FF:193:LYS:NZ	2.49	0.40
26:HH:80:VAL:HG13	26:HH:92:VAL:HG13	2.03	0.40
38:O:19:LEU:HD12	38:O:22:ILE:HD11	2.03	0.40
39:OO:137:SER:OG	39:OO:138:ASP:N	2.53	0.40
43:QQ:57:LEU:HD21	43:QQ:115:TYR:CG	2.56	0.40
58:Y:31:SER:HA	58:Y:48:PRO:HA	2.03	0.40
2:5:1348:C:H2'	2:5:1349:A:C8	2.56	0.40
2:5:2093:G:H1'	2:5:2094:U:OP2	2.20	0.40
2:5:2372:A:N6	2:5:2831:G:O2'	2.53	0.40
2:5:4097:G:H22	2:5:4119:G:H1	1.70	0.40
2:5:4531:G:OP2	2:5:4531:G:N2	2.49	0.40
4:9:358:C:P	57:XX:18:ARG:CD	3.09	0.40
4:9:420:G:H2'	4:9:660:C:H42	1.86	0.40
4:9:671:A:H4'	4:9:672:A:H5''	2.04	0.40
4:9:693:A:H61	4:9:733:C:H42	1.67	0.40
4:9:916:A:C1'	37:NN:73:ARG:NH1	2.84	0.40
4:9:993:G:H2'	4:9:994:C:H6	1.86	0.40
4:9:1221:G:H2'	4:9:1222:G:H8	1.86	0.40
4:9:1616:U:O4	41:PP:40:ARG:NH1	2.47	0.40
18:EE:187:ALA:O	18:EE:245:ARG:NH1	2.53	0.40
21:FF:41:VAL:HG23	21:FF:42:LYS:HB2	2.03	0.40
22:G:229:LYS:HE3	22:G:229:LYS:HB3	1.89	0.40
46:S:99:ASP:OD1	46:S:100:LEU:N	2.50	0.40
52:V:43:LYS:HE2	52:V:43:LYS:HB2	1.93	0.40
57:XX:95:GLU:HB2	57:XX:140:ARG:HH22	1.86	0.40
79:s:141:LEU:HD22	79:s:174:LEU:HD13	2.03	0.40
82:v:364:ALA:HA	82:v:367:TYR:CE2	2.56	0.40
82:v:710:HIS:ND1	82:v:712:ASP:OD1	2.54	0.40
82:v:839:ARG:HE	82:v:847:GLY:H	1.68	0.40
1:x:47:LYS:O	1:x:159:MET:CG	2.69	0.40
2:5:1943:A:O2'	2:5:1944:G:OP2	2.30	0.40
2:5:3691:A:H3'	5:A:198:ARG:HH22	1.86	0.40
2:5:3817:A:N3	2:5:4542:G:O2'	2.50	0.40
2:5:3934:U:H2'	2:5:3935:C:C6	2.57	0.40
2:5:4240:G:H4'	2:5:4332:G:O2'	2.21	0.40
4:9:355:G:OP1	34:LL:105:ARG:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:386:C:H4'	28:II:9:HIS:CE1	2.57	0.40
4:9:1236:G:O3'	41:PP:133:ILE:HG22	2.21	0.40
4:9:1617:G:C4'	16:Dd:14:PHE:CE1	2.89	0.40
4:9:1648:G:H5'	43:QQ:126:ARG:O	2.22	0.40
8:B:206:PRO:HD2	8:B:209:GLN:NE2	2.37	0.40
17:E:189:LEU:N	17:E:253:GLN:HE22	2.12	0.40
18:EE:124:CYS:HB3	18:EE:141:THR:HB	2.02	0.40
23:GG:5:ILE:HA	23:GG:111:LEU:HB2	2.03	0.40
30:JJ:50:LEU:HD12	30:JJ:53:ILE:HD11	2.03	0.40
31:K:3:C:H2'	31:K:4:U:C6	2.57	0.40
37:NN:125:LEU:HD23	37:NN:125:LEU:HA	1.96	0.40
47:SS:25:LYS:O	47:SS:29:ALA:CB	2.69	0.40
57:XX:51:VAL:HG13	57:XX:70:VAL:HG13	2.03	0.40
65:d:42:ALA:HB3	65:d:43:PRO:HD3	2.04	0.40
66:e:36:ARG:HA	66:e:36:ARG:HD3	1.88	0.40
66:e:92:ASN:HD21	66:e:119:ALA:HB3	1.86	0.40
82:v:839:ARG:HG2	82:v:844:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	159/217 (73%)	151 (95%)	8 (5%)	0	100	100
5	A	245/257 (95%)	233 (95%)	12 (5%)	0	100	100
6	AA	215/295 (73%)	206 (96%)	9 (4%)	0	100	100
7	Aa	99/115 (86%)	89 (90%)	10 (10%)	0	100	100
8	B	392/403 (97%)	382 (97%)	10 (3%)	0	100	100
9	BB	211/264 (80%)	203 (96%)	8 (4%)	0	100	100
10	Bb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	C	355/413 (86%)	344 (97%)	11 (3%)	0	100	100
12	CC	219/293 (75%)	205 (94%)	14 (6%)	0	100	100
13	Cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
14	D	287/297 (97%)	281 (98%)	6 (2%)	0	100	100
15	DD	226/243 (93%)	216 (96%)	10 (4%)	0	100	100
16	Dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
17	E	205/291 (70%)	197 (96%)	8 (4%)	0	100	100
18	EE	260/263 (99%)	244 (94%)	16 (6%)	0	100	100
19	Ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
20	F	223/249 (90%)	216 (97%)	7 (3%)	0	100	100
21	FF	181/204 (89%)	162 (90%)	19 (10%)	0	100	100
22	G	211/266 (79%)	208 (99%)	3 (1%)	0	100	100
23	GG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
24	Gg	311/317 (98%)	281 (90%)	30 (10%)	0	100	100
25	H	182/192 (95%)	179 (98%)	3 (2%)	0	100	100
26	HH	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
27	I	198/214 (92%)	192 (97%)	6 (3%)	0	100	100
28	II	204/208 (98%)	185 (91%)	19 (9%)	0	100	100
29	J	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
30	JJ	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
32	KK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
33	L	203/211 (96%)	198 (98%)	4 (2%)	1 (0%)	24	31
34	LL	139/158 (88%)	131 (94%)	8 (6%)	0	100	100
35	M	133/218 (61%)	130 (98%)	3 (2%)	0	100	100
36	N	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
37	NN	147/151 (97%)	138 (94%)	9 (6%)	0	100	100
38	O	197/203 (97%)	193 (98%)	4 (2%)	0	100	100
39	OO	134/151 (89%)	123 (92%)	11 (8%)	0	100	100
40	P	150/187 (80%)	147 (98%)	3 (2%)	0	100	100
41	PP	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
42	Q	185/188 (98%)	177 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	QQ	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
44	R	164/196 (84%)	162 (99%)	2 (1%)	0	100	100
45	RR	130/135 (96%)	121 (93%)	9 (7%)	0	100	100
46	S	174/224 (78%)	168 (97%)	6 (3%)	0	100	100
47	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
48	T	156/160 (98%)	151 (97%)	5 (3%)	0	100	100
49	TT	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
50	U	96/141 (68%)	93 (97%)	3 (3%)	0	100	100
51	UU	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
52	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
53	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
54	W	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
55	WW	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
56	X	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
57	XX	139/143 (97%)	132 (95%)	4 (3%)	3 (2%)	5	4
58	Y	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
59	YY	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
60	Z	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
61	ZZ	73/124 (59%)	70 (96%)	3 (4%)	0	100	100
62	a	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
63	b	94/245 (38%)	92 (98%)	2 (2%)	0	100	100
64	c	92/115 (80%)	91 (99%)	1 (1%)	0	100	100
65	d	104/125 (83%)	101 (97%)	3 (3%)	0	100	100
66	e	126/157 (80%)	122 (97%)	4 (3%)	0	100	100
67	f	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
68	g	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
69	h	119/123 (97%)	119 (100%)	0	0	100	100
70	i	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
71	j	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
72	k	66/70 (94%)	66 (100%)	0	0	100	100
73	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	m	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
75	n	23/25 (92%)	23 (100%)	0	0	100	100
76	o	100/106 (94%)	98 (98%)	2 (2%)	0	100	100
77	p	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
78	r	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
79	s	194/318 (61%)	185 (95%)	8 (4%)	1 (0%)	24	31
80	s1	14/109 (13%)	13 (93%)	1 (7%)	0	100	100
81	t	121/154 (79%)	117 (97%)	4 (3%)	0	100	100
82	v	711/858 (83%)	684 (96%)	27 (4%)	0	100	100
83	w	30/407 (7%)	28 (93%)	2 (7%)	0	100	100
All	All	12093/14939 (81%)	11610 (96%)	478 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	XX	62	PRO
57	XX	61	GLN
57	XX	86	PRO
79	s	118	PRO
33	L	62	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	146/195 (75%)	143 (98%)	3 (2%)	47	66
5	A	189/199 (95%)	187 (99%)	2 (1%)	65	81
6	AA	180/245 (74%)	180 (100%)	0	100	100
7	Aa	88/98 (90%)	88 (100%)	0	100	100
8	B	342/348 (98%)	335 (98%)	7 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BB	194/231 (84%)	191 (98%)	3 (2%)	57	75
10	Bb	75/76 (99%)	75 (100%)	0	100	100
11	C	298/336 (89%)	294 (99%)	4 (1%)	61	77
12	CC	187/224 (84%)	187 (100%)	0	100	100
13	Cc	55/62 (89%)	55 (100%)	0	100	100
14	D	245/250 (98%)	243 (99%)	2 (1%)	73	86
15	DD	190/202 (94%)	187 (98%)	3 (2%)	55	73
16	Dd	48/49 (98%)	47 (98%)	1 (2%)	47	66
17	E	189/251 (75%)	185 (98%)	4 (2%)	47	66
18	EE	224/225 (100%)	219 (98%)	5 (2%)	45	65
19	Ee	46/106 (43%)	45 (98%)	1 (2%)	45	65
20	F	196/218 (90%)	196 (100%)	0	100	100
21	FF	158/170 (93%)	155 (98%)	3 (2%)	50	69
22	G	188/224 (84%)	187 (100%)	1 (0%)	81	90
23	GG	207/218 (95%)	205 (99%)	2 (1%)	68	82
24	Gg	272/275 (99%)	270 (99%)	2 (1%)	76	87
25	H	166/171 (97%)	166 (100%)	0	100	100
26	HH	165/360 (46%)	164 (99%)	1 (1%)	78	89
27	I	172/181 (95%)	168 (98%)	4 (2%)	44	63
28	II	178/180 (99%)	177 (99%)	1 (1%)	78	89
29	J	141/149 (95%)	139 (99%)	2 (1%)	59	76
30	JJ	161/168 (96%)	161 (100%)	0	100	100
32	KK	87/136 (64%)	86 (99%)	1 (1%)	65	81
33	L	170/176 (97%)	169 (99%)	1 (1%)	78	89
34	LL	130/142 (92%)	129 (99%)	1 (1%)	73	86
35	M	115/160 (72%)	115 (100%)	0	100	100
36	N	171/172 (99%)	169 (99%)	2 (1%)	63	79
37	NN	130/131 (99%)	129 (99%)	1 (1%)	73	86
38	O	171/174 (98%)	169 (99%)	2 (1%)	63	79
39	OO	106/119 (89%)	106 (100%)	0	100	100
40	P	133/165 (81%)	132 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	PP	111/130 (85%)	109 (98%)	2 (2%)	51	70
42	Q	164/165 (99%)	162 (99%)	2 (1%)	63	79
43	QQ	117/121 (97%)	117 (100%)	0	100	100
44	R	147/175 (84%)	145 (99%)	2 (1%)	59	76
45	RR	119/121 (98%)	118 (99%)	1 (1%)	73	86
46	S	156/192 (81%)	154 (99%)	2 (1%)	61	77
47	SS	125/132 (95%)	123 (98%)	2 (2%)	55	73
48	T	139/140 (99%)	137 (99%)	2 (1%)	59	76
49	TT	111/115 (96%)	111 (100%)	0	100	100
50	U	88/127 (69%)	87 (99%)	1 (1%)	65	81
51	UU	92/107 (86%)	92 (100%)	0	100	100
52	V	100/107 (94%)	100 (100%)	0	100	100
53	VV	67/67 (100%)	67 (100%)	0	100	100
54	W	54/126 (43%)	54 (100%)	0	100	100
55	WW	112/113 (99%)	111 (99%)	1 (1%)	70	84
56	X	106/133 (80%)	106 (100%)	0	100	100
57	XX	113/115 (98%)	111 (98%)	2 (2%)	51	70
58	Y	123/135 (91%)	120 (98%)	3 (2%)	43	62
59	YY	107/115 (93%)	107 (100%)	0	100	100
60	Z	117/118 (99%)	117 (100%)	0	100	100
61	ZZ	66/102 (65%)	65 (98%)	1 (2%)	57	75
62	a	119/120 (99%)	119 (100%)	0	100	100
63	b	80/184 (44%)	79 (99%)	1 (1%)	61	77
64	c	80/98 (82%)	79 (99%)	1 (1%)	61	77
65	d	97/110 (88%)	96 (99%)	1 (1%)	68	82
66	e	114/141 (81%)	113 (99%)	1 (1%)	70	84
67	f	88/89 (99%)	88 (100%)	0	100	100
68	g	95/100 (95%)	95 (100%)	0	100	100
69	h	109/110 (99%)	109 (100%)	0	100	100
70	i	85/89 (96%)	85 (100%)	0	100	100
71	j	73/80 (91%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	k	63/65 (97%)	62 (98%)	1 (2%)	55	73
73	l	47/48 (98%)	47 (100%)	0	100	100
74	m	46/115 (40%)	45 (98%)	1 (2%)	45	65
75	n	24/24 (100%)	24 (100%)	0	100	100
76	o	90/94 (96%)	89 (99%)	1 (1%)	65	81
77	p	74/75 (99%)	73 (99%)	1 (1%)	59	76
78	r	107/121 (88%)	106 (99%)	1 (1%)	70	84
79	s	163/258 (63%)	161 (99%)	2 (1%)	63	79
80	s1	18/97 (19%)	18 (100%)	0	100	100
81	t	105/128 (82%)	100 (95%)	5 (5%)	23	35
82	v	619/729 (85%)	606 (98%)	13 (2%)	47	66
83	w	26/327 (8%)	25 (96%)	1 (4%)	29	44
All	All	10569/12644 (84%)	10458 (99%)	111 (1%)	63	81

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	139	THR
1	x	159	MET
1	x	160	LYS
5	A	143	THR
5	A	208	GLU
8	B	56	ILE
8	B	73	VAL
8	B	90	VAL
8	B	162	VAL
8	B	207	VAL
8	B	345	LEU
8	B	371	THR
9	BB	28	LYS
9	BB	97	LEU
9	BB	189	ILE
11	C	143	ARG
11	C	150	LEU
11	C	154	VAL
11	C	321	ASN
14	D	7	VAL
14	D	56	THR

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Mol	Chain	Res	Type
15	DD	48	ILE
15	DD	113	LEU
15	DD	142	LEU
16	Dd	26	ASN
17	E	109	VAL
17	E	124	VAL
17	E	178	VAL
17	E	197	VAL
18	EE	20	LEU
18	EE	52	LEU
18	EE	114	ILE
18	EE	183	VAL
18	EE	208	VAL
19	Ee	81	ARG
21	FF	76	MET
21	FF	169	ILE
21	FF	173	LEU
22	G	162	GLU
23	GG	77	LEU
23	GG	102	VAL
24	Gg	92	LEU
24	Gg	164	ILE
26	HH	60	ILE
27	I	43	VAL
27	I	96	VAL
27	I	126	VAL
27	I	202	ASN
28	II	78	ILE
29	J	43	LEU
29	J	174	ILE
32	KK	15	LEU
33	L	4	SER
34	LL	126	VAL
36	N	142	ILE
36	N	198	LEU
37	NN	122	ILE
38	O	129	LEU
38	O	195	VAL
40	P	24	VAL
41	PP	25	LEU
41	PP	85	ILE
42	Q	13	VAL

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Mol	Chain	Res	Type
42	Q	83	VAL
44	R	10	LEU
44	R	24	LEU
45	RR	85	VAL
46	S	7	LEU
46	S	39	VAL
47	SS	33	ILE
47	SS	111	LEU
48	T	72	VAL
48	T	80	VAL
50	U	96	LEU
55	WW	103	VAL
57	XX	3	LYS
57	XX	7	LEU
58	Y	55	VAL
58	Y	79	VAL
58	Y	104	VAL
61	ZZ	97	ILE
63	b	8	THR
64	c	66	LEU
65	d	111	VAL
66	e	48	ARG
72	k	23	VAL
74	m	51	ILE
76	o	99	ARG
77	p	52	VAL
78	r	103	HIS
79	s	18	ILE
79	s	30	VAL
81	t	34	LEU
81	t	92	LEU
81	t	99	TYR
81	t	109	VAL
81	t	115	LEU
82	v	4	PHE
82	v	135	VAL
82	v	469	ILE
82	v	479	LEU
82	v	480	VAL
82	v	517	LEU
82	v	539	GLU
82	v	582	THR

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Mol	Chain	Res	Type
82	v	616	ASP
82	v	638	LYS
82	v	753	GLU
82	v	770	VAL
82	v	851	LEU
83	w	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (192) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	44	GLN
1	x	71	GLN
1	x	94	ASN
1	x	96	ASN
1	x	129	ASN
5	A	22	HIS
5	A	83	HIS
5	A	95	GLN
5	A	100	ASN
5	A	205	ASN
6	AA	113	GLN
8	B	138	GLN
8	B	209	GLN
8	B	213	GLN
8	B	258	HIS
8	B	354	GLN
9	BB	158	HIS
10	Bb	26	GLN
11	C	85	HIS
11	C	119	GLN
11	C	212	ASN
11	C	276	ASN
11	C	321	ASN
12	CC	113	GLN
14	D	42	ASN
14	D	122	GLN
14	D	175	HIS
14	D	275	GLN
14	D	282	GLN
14	D	291	GLN
15	DD	165	ASN
16	Dd	26	ASN

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Mol	Chain	Res	Type
17	E	170	GLN
17	E	185	ASN
17	E	193	HIS
17	E	253	GLN
18	EE	36	HIS
18	EE	50	ASN
18	EE	98	ASN
18	EE	224	ASN
20	F	23	ASN
20	F	62	GLN
20	F	205	ASN
21	FF	74	ASN
21	FF	79	HIS
21	FF	101	HIS
21	FF	110	GLN
21	FF	114	ASN
21	FF	118	ASN
22	G	91	ASN
22	G	99	GLN
22	G	134	ASN
22	G	143	GLN
22	G	206	GLN
22	G	259	GLN
23	GG	81	HIS
23	GG	227	GLN
24	Gg	76	GLN
24	Gg	162	ASN
24	Gg	222	ASN
25	H	98	HIS
25	H	102	ASN
25	H	189	GLN
26	HH	73	GLN
26	HH	186	ASN
28	II	35	ASN
28	II	99	ASN
29	J	42	GLN
29	J	46	GLN
29	J	98	ASN
29	J	110	GLN
30	JJ	124	HIS
30	JJ	156	HIS
32	KK	28	HIS

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Mol	Chain	Res	Type
32	KK	44	HIS
33	L	15	HIS
33	L	19	GLN
33	L	67	HIS
33	L	149	GLN
33	L	175	ASN
34	LL	18	GLN
34	LL	65	ASN
34	LL	83	GLN
35	M	56	GLN
35	M	70	GLN
35	M	131	GLN
36	N	87	HIS
36	N	90	ASN
36	N	109	HIS
36	N	117	ASN
36	N	149	GLN
36	N	158	HIS
36	N	199	GLN
37	NN	62	GLN
38	O	180	GLN
39	OO	83	GLN
39	OO	113	GLN
40	P	25	HIS
40	P	28	ASN
40	P	137	ASN
41	PP	98	ASN
42	Q	7	HIS
42	Q	21	GLN
42	Q	162	HIS
43	QQ	11	GLN
43	QQ	80	GLN
43	QQ	142	GLN
44	R	39	GLN
44	R	66	ASN
44	R	75	HIS
44	R	141	HIS
45	RR	93	GLN
45	RR	116	ASN
46	S	91	HIS
48	T	77	ASN
48	T	127	GLN

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Mol	Chain	Res	Type
49	TT	12	GLN
50	U	41	GLN
50	U	44	GLN
51	UU	81	GLN
51	UU	92	HIS
52	V	84	GLN
52	V	108	ASN
53	VV	29	HIS
53	VV	47	ASN
53	VV	82	ASN
55	WW	56	HIS
55	WW	91	ASN
55	WW	113	HIS
55	WW	120	HIS
56	X	93	ASN
56	X	108	GLN
56	X	111	GLN
57	XX	16	HIS
57	XX	46	HIS
57	XX	92	ASN
58	Y	14	ASN
58	Y	18	HIS
58	Y	61	HIS
58	Y	72	GLN
58	Y	96	HIS
59	YY	19	GLN
62	a	40	HIS
62	a	66	ASN
63	b	6	ASN
63	b	27	GLN
63	b	60	ASN
63	b	61	ASN
63	b	101	HIS
64	c	33	GLN
64	c	40	GLN
65	d	116	ASN
65	d	121	ASN
66	e	23	HIS
66	e	57	ASN
66	e	68	HIS
67	f	65	ASN
68	g	110	GLN

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Mol	Chain	Res	Type
69	h	107	GLN
70	i	36	HIS
70	i	80	HIS
71	j	13	ASN
71	j	28	HIS
71	j	57	ASN
71	j	66	HIS
72	k	28	ASN
72	k	58	GLN
73	l	17	GLN
73	l	25	GLN
74	m	58	GLN
77	p	33	GLN
77	p	56	HIS
78	r	45	HIS
78	r	95	HIS
79	s	39	GLN
79	s	105	ASN
79	s	127	ASN
79	s	191	GLN
81	t	22	GLN
81	t	96	GLN
81	t	104	GLN
82	v	87	ASN
82	v	138	GLN
82	v	168	GLN
82	v	306	ASN
82	v	544	HIS
82	v	626	GLN
82	v	684	GLN
82	v	720	GLN
82	v	803	ASN
82	v	807	GLN
83	w	206	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	3321/3740 (88%)	486 (14%)	38 (1%)
3	8	140/156 (89%)	14 (10%)	0
31	K	118/120 (98%)	7 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	9	1682/1786 (94%)	389 (23%)	18 (1%)
All	All	5261/5802 (90%)	896 (17%)	56 (1%)

All (896) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	5	17	A
2	5	25	A
2	5	39	A
2	5	42	A
2	5	56	A
2	5	58	G
2	5	59	A
2	5	64	A
2	5	65	A
2	5	73	A
2	5	91	G
2	5	98	A
2	5	104	G
2	5	108	A
2	5	109	G
2	5	110	C
2	5	119	G
2	5	120	A
2	5	126	C
2	5	134	G
2	5	135	G
2	5	136	C
2	5	157	U
2	5	159	C
2	5	166	C
2	5	168	C
2	5	180	C
2	5	182	G
2	5	200	U
2	5	209	U
2	5	224	U
2	5	233	U
2	5	234	G
2	5	246	G
2	5	258	G
2	5	266	C

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Mol	Chain	Res	Type
2	5	276	C
2	5	280	G
2	5	297	U
2	5	306	A
2	5	309	C
2	5	315	G
2	5	316	U
2	5	326	C
2	5	334	A
2	5	340	C
2	5	350	C
2	5	386	A
2	5	387	G
2	5	407	A
2	5	410	A
2	5	412	G
2	5	450	G
2	5	452	A
2	5	453	G
2	5	454	U
2	5	455	C
2	5	463	A
2	5	464	G
2	5	486	C
2	5	492	U
2	5	493	G
2	5	505	G
2	5	666	G
2	5	669	C
2	5	685	C
2	5	686	A
2	5	704	C
2	5	730	G
2	5	731	G
2	5	738	C
2	5	742	G
2	5	747	A
2	5	749	G
2	5	914	U
2	5	917	A
2	5	923	C
2	5	927	C

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Mol	Chain	Res	Type
2	5	928	G
2	5	933	C
2	5	934	A
2	5	935	G
2	5	937	G
2	5	939	C
2	5	947	A
2	5	948	U
2	5	959	A
2	5	962	G
2	5	963	A
2	5	964	G
2	5	967	A
2	5	969	A
2	5	970	C
2	5	972	C
2	5	973	G
2	5	976	C
2	5	982	C
2	5	987	U
2	5	993	C
2	5	1074	G
2	5	1076	C
2	5	1077	G
2	5	1083	C
2	5	1102	G
2	5	1174	G
2	5	1179	A
2	5	1184	C
2	5	1199	G
2	5	1214	C
2	5	1215	G
2	5	1216	G
2	5	1218	C
2	5	1219	C
2	5	1238	G
2	5	1239	G
2	5	1241	C
2	5	1243	C
2	5	1248	G
2	5	1277	G
2	5	1279	G

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Mol	Chain	Res	Type
2	5	1284	C
2	5	1288	G
2	5	1291	G
2	5	1296	C
2	5	1297	G
2	5	1300	G
2	5	1305	C
2	5	1308	C
2	5	1330	A2M
2	5	1334	A
2	5	1341	A
2	5	1352	P4U
2	5	1358	A
2	5	1362	G
2	5	1363	G
2	5	1375	A
2	5	1381	G
2	5	1383	C
2	5	1391	A
2	5	1398	G
2	5	1401	A
2	5	1402	A
2	5	1425	G
2	5	1440	C
2	5	1441	C
2	5	1443	C
2	5	1444	U
2	5	1449	U
2	5	1450	C
2	5	1460	B8Q
2	5	1461	G
2	5	1486	G
2	5	1487	C
2	5	1501	A
2	5	1502	G
2	5	1506	G
2	5	1518	U
2	5	1527	A
2	5	1538	A2M
2	5	1539	C
2	5	1551	A
2	5	1570	C

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Mol	Chain	Res	Type
2	5	1582	U
2	5	1595	U
2	5	1600	U
2	5	1606	U
2	5	1616	G
2	5	1617	A
2	5	1628	G
2	5	1629	OMG
2	5	1635	A
2	5	1637	G
2	5	1638	A
2	5	1642	A
2	5	1644	C
2	5	1646	A
2	5	1658	G
2	5	1665	C
2	5	1680	C
2	5	1681	PSU
2	5	1683	A
2	5	1733	A
2	5	1738	G
2	5	1745	G
2	5	1746	A
2	5	1754	G
2	5	1785	U
2	5	1791	A
2	5	1808	A
2	5	1809	A
2	5	1823	G
2	5	1838	U
2	5	1839	G
2	5	1840	G
2	5	1841	A
2	5	1846	G
2	5	1859	G
2	5	1873	G
2	5	1901	A
2	5	1903	G
2	5	1922	U
2	5	1924	C
2	5	1925	C
2	5	1926	G

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Mol	Chain	Res	Type
2	5	1935	C
2	5	1944	G
2	5	1945	A
2	5	1952	G
2	5	1955	G
2	5	1962	A
2	5	1965	G
2	5	1968	A
2	5	1978	U
2	5	1979	G
2	5	1982	C
2	5	1984	U
2	5	1988	A
2	5	1989	G
2	5	1991	C
2	5	1994	A
2	5	1995	A
2	5	2001	U
2	5	2005	G
2	5	2006	A
2	5	2007	G
2	5	2008	U
2	5	2012	U
2	5	2030	A
2	5	2050	G
2	5	2051	A
2	5	2052	U
2	5	2056	G
2	5	2059	G
2	5	2060	G
2	5	2073	A
2	5	2088	U
2	5	2094	U
2	5	2097	G
2	5	2101	A
2	5	2102	G
2	5	2104	G
2	5	2106	G
2	5	2110	G
2	5	2112	G
2	5	2264	C
2	5	2271	U

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Mol	Chain	Res	Type
2	5	2279	G
2	5	2293	C
2	5	2304	A
2	5	2305	G
2	5	2317	A
2	5	2320	G
2	5	2337	G
2	5	2352	G
2	5	2355	C
2	5	2368	OMG
2	5	2384	B8W
2	5	2399	A
2	5	2400	A
2	5	2425	G
2	5	2426	OMC
2	5	2428	OMG
2	5	2429	U
2	5	2437	G
2	5	2445	C
2	5	2454	G
2	5	2475	G
2	5	2479	G
2	5	2506	A
2	5	2507	G
2	5	2508	C
2	5	2509	C
2	5	2510	G
2	5	2517	A
2	5	2533	A
2	5	2541	A
2	5	2557	A
2	5	2579	U
2	5	2587	C
2	5	2591	A
2	5	2605	A
2	5	2642	G
2	5	2644	G
2	5	2657	C
2	5	2666	G
2	5	2673	C
2	5	2691	U
2	5	2699	A

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Mol	Chain	Res	Type
2	5	2700	A
2	5	2719	G
2	5	2720	C
2	5	2725	G
2	5	2729	A
2	5	2730	G
2	5	2744	U
2	5	2747	A
2	5	2748	A
2	5	2758	B9B
2	5	2768	A
2	5	2773	U
2	5	2791	A
2	5	2792	U
2	5	2794	U
2	5	2802	A
2	5	2818	C
2	5	2830	U
2	5	2831	G
2	5	2833	U
2	5	2846	G
2	5	2859	G
2	5	3620	U
2	5	3622	C
2	5	3629	G
2	5	3630	G
2	5	3639	A
2	5	3652	A
2	5	3666	A
2	5	3677	C
2	5	3700	C
2	5	3715	A
2	5	3733	PSU
2	5	3752	A
2	5	3758	G
2	5	3760	A
2	5	3762	U
2	5	3771	C
2	5	3777	U
2	5	3781	G
2	5	3788	A
2	5	3790	U

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Mol	Chain	Res	Type
2	5	3796	OMG
2	5	3814	C
2	5	3816	C
2	5	3818	U
2	5	3821	A
2	5	3823	G
2	5	3842	U
2	5	3843	G
2	5	3844	U
2	5	3871	A2M
2	5	3881	A
2	5	3882	C
2	5	3883	G
2	5	3893	G
2	5	3901	B8K
2	5	3905	A
2	5	3909	A
2	5	3910	A
2	5	3911	G
2	5	3919	U
2	5	3920	G
2	5	3921	A
2	5	3943	G
2	5	3945	G
2	5	4080	G
2	5	4089	A
2	5	4090	G
2	5	4092	C
2	5	4120	C
2	5	4122	U
2	5	4131	A
2	5	4162	C
2	5	4166	C
2	5	4167	U
2	5	4174	A
2	5	4187	G
2	5	4188	G
2	5	4195	G
2	5	4197	C
2	5	4207	A
2	5	4233	U
2	5	4237	A

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Mol	Chain	Res	Type
2	5	4255	A
2	5	4258	G
2	5	4262	C
2	5	4270	G
2	5	4272	A
2	5	4275	A
2	5	4277	A
2	5	4285	A
2	5	4295	G
2	5	4297	PSU
2	5	4309	G
2	5	4310	OMU
2	5	4318	C
2	5	4323	C
2	5	4334	G
2	5	4336	C
2	5	4353	C
2	5	4375	MHG
2	5	4377	G
2	5	4380	A
2	5	4381	G
2	5	4382	A
2	5	4384	A
2	5	4391	C
2	5	4395	G
2	5	4398	A
2	5	4399	U
2	5	4402	C
2	5	4423	U
2	5	4426	A
2	5	4452	G
2	5	4453	A
2	5	4454	PSU
2	5	4468	A
2	5	4470	C
2	5	4479	G
2	5	4504	PSU
2	5	4514	A
2	5	4515	A
2	5	4516	U
2	5	4517	A
2	5	4523	C

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Mol	Chain	Res	Type
2	5	4524	G
2	5	4526	G
2	5	4527	A2M
2	5	4528	G
2	5	4532	G
2	5	4534	UR3
2	5	4552	A
2	5	4553	G
2	5	4564	C
2	5	4571	G
2	5	4577	G
2	5	4578	U
2	5	4579	G
2	5	4588	A
2	5	4593	A
2	5	4594	A
2	5	4640	PSU
2	5	4641	OMG
2	5	4660	A
2	5	4674	C
2	5	4676	A
2	5	4681	U
2	5	4699	C
2	5	4704	A
2	5	4713	U
2	5	4723	G
2	5	4724	C
2	5	4740	C
2	5	4749	G
2	5	4755	G
2	5	4756	U
2	5	4758	G
2	5	4760	C
2	5	4761	C
2	5	4763	C
2	5	4765	G
2	5	4769	G
2	5	4872	G
2	5	4874	OMG
2	5	4875	C
2	5	4879	G
2	5	4886	U

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Mol	Chain	Res	Type
2	5	4887	C
2	5	4889	U
2	5	4899	C
2	5	4900	G
2	5	4914	A
2	5	4917	G
2	5	4920	G
2	5	4922	C
2	5	4941	C
2	5	4942	A
2	5	4947	A
2	5	4948	C
2	5	4953	G
2	5	4954	U
2	5	4955	G
2	5	4962	C
2	5	4964	G
2	5	4971	A
2	5	4980	U
2	5	4992	U
2	5	4997	G
2	5	5018	A
2	5	5021	G
2	5	5045	G
2	5	5051	C
2	5	5054	C
2	5	5057	U
2	5	5058	C
2	5	5065	A
2	5	5066	G
3	8	23	C
3	8	34	U
3	8	35	C
3	8	59	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	87	G
3	8	94	G
3	8	103	A
3	8	105	C
3	8	110	U

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Mol	Chain	Res	Type
3	8	114	G
3	8	156	U
4	9	3	C
4	9	4	C
4	9	14	C
4	9	23	G
4	9	25	A
4	9	26	U
4	9	33	G
4	9	41	G
4	9	44	U
4	9	45	A
4	9	46	A
4	9	47	G
4	9	56	G
4	9	58	C
4	9	64	A
4	9	67	C
4	9	68	A
4	9	69	C
4	9	72	C
4	9	73	C
4	9	74	G
4	9	75	G
4	9	77	A
4	9	79	A
4	9	81	U
4	9	103	A
4	9	110	U
4	9	111	A
4	9	113	G
4	9	115	U
4	9	116	OMU
4	9	120	U
4	9	121	OMU
4	9	124	U
4	9	126	G
4	9	127	C
4	9	130	G
4	9	141	A
4	9	143	U
4	9	146	G

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Mol	Chain	Res	Type
4	9	147	A
4	9	155	G
4	9	159	A2M
4	9	160	U
4	9	162	C
4	9	163	U
4	9	166	A2M
4	9	167	G
4	9	170	A
4	9	171	A
4	9	175	A
4	9	180	G
4	9	182	C
4	9	183	G
4	9	184	G
4	9	188	C
4	9	189	U
4	9	190	G
4	9	191	A
4	9	192	C
4	9	202	G
4	9	206	G
4	9	215	G
4	9	294	U
4	9	297	A
4	9	304	C
4	9	306	C
4	9	307	G
4	9	308	G
4	9	309	G
4	9	312	G
4	9	313	A
4	9	318	A
4	9	319	C
4	9	332	G
4	9	347	G
4	9	350	C
4	9	351	G
4	9	360	A
4	9	362	C
4	9	364	A
4	9	368	U

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Mol	Chain	Res	Type
4	9	369	C
4	9	370	G
4	9	381	C
4	9	385	G
4	9	398	A
4	9	400	C
4	9	407	G
4	9	408	A
4	9	409	C
4	9	417	C
4	9	418	A
4	9	420	G
4	9	429	C
4	9	435	A
4	9	441	C
4	9	448	A
4	9	449	A
4	9	450	C
4	9	455	A
4	9	465	A
4	9	466	G
4	9	471	G
4	9	472	C
4	9	473	A
4	9	474	G
4	9	480	G
4	9	482	G
4	9	487	U
4	9	492	C
4	9	516	A
4	9	517	OMC
4	9	518	G
4	9	525	A
4	9	530	U
4	9	531	A
4	9	532	C
4	9	533	A
4	9	536	A
4	9	537	C
4	9	544	G
4	9	546	G
4	9	547	G

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Mol	Chain	Res	Type
4	9	548	C
4	9	549	C
4	9	550	C
4	9	551	U
4	9	554	A
4	9	555	A
4	9	556	U
4	9	559	G
4	9	560	A
4	9	563	G
4	9	564	A
4	9	568	E3C
4	9	576	A
4	9	583	A
4	9	587	A
4	9	588	G
4	9	589	G
4	9	590	A
4	9	591	U
4	9	603	C
4	9	606	G
4	9	607	U
4	9	608	C
4	9	614	C
4	9	617	G
4	9	621	C
4	9	627	U
4	9	631	U
4	9	643	A
4	9	655	A
4	9	660	C
4	9	662	G
4	9	664	A
4	9	666	U
4	9	668	A2M
4	9	669	A
4	9	671	A
4	9	672	A
4	9	673	G
4	9	678	U
4	9	684	G
4	9	688	U

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Mol	Chain	Res	Type
4	9	689	U
4	9	690	G
4	9	752	G
4	9	753	C
4	9	754	G
4	9	798	G
4	9	811	A
4	9	821	G
4	9	822	PSU
4	9	830	A
4	9	833	C
4	9	834	C
4	9	847	A
4	9	868	G
4	9	870	A
4	9	871	U
4	9	872	A
4	9	873	G
4	9	875	A
4	9	876	C
4	9	877	C
4	9	878	G
4	9	879	C
4	9	885	U
4	9	887	U
4	9	888	U
4	9	890	U
4	9	891	G
4	9	893	U
4	9	894	G
4	9	898	U
4	9	901	G
4	9	902	G
4	9	904	A
4	9	907	G
4	9	913	A
4	9	914	U
4	9	920	A
4	9	922	A
4	9	933	G
4	9	934	G
4	9	943	U

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Mol	Chain	Res	Type
4	9	971	G
4	9	985	G
4	9	989	C
4	9	990	A
4	9	992	A
4	9	999	G
4	9	1017	U
4	9	1022	U
4	9	1023	A
4	9	1030	A
4	9	1040	G
4	9	1041	G
4	9	1060	A
4	9	1081	PSU
4	9	1083	A
4	9	1085	C
4	9	1086	G
4	9	1087	A
4	9	1088	U
4	9	1097	G
4	9	1100	A
4	9	1109	C
4	9	1110	G
4	9	1114	U
4	9	1115	U
4	9	1116	C
4	9	1117	C
4	9	1118	C
4	9	1121	G
4	9	1123	C
4	9	1131	G
4	9	1133	A
4	9	1138	C
4	9	1150	A
4	9	1153	C
4	9	1154	U
4	9	1170	A
4	9	1195	A
4	9	1207	G
4	9	1208	A
4	9	1215	C
4	9	1216	C

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Mol	Chain	Res	Type
4	9	1221	G
4	9	1224	G
4	9	1242	U
4	9	1243	PSU
4	9	1250	A
4	9	1251	A
4	9	1253	A
4	9	1256	G
4	9	1257	G
4	9	1259	A
4	9	1265	A
4	9	1273	C
4	9	1274	G
4	9	1275	G
4	9	1282	A
4	9	1284	A
4	9	1285	G
4	9	1293	A
4	9	1298	G
4	9	1300	U
4	9	1301	A
4	9	1302	G
4	9	1304	U
4	9	1307	U
4	9	1308	U
4	9	1309	C
4	9	1312	G
4	9	1314	U
4	9	1315	U
4	9	1322	G
4	9	1327	G
4	9	1333	U
4	9	1341	C
4	9	1342	U
4	9	1348	G
4	9	1358	U
4	9	1371	U
4	9	1372	U
4	9	1376	A
4	9	1378	A
4	9	1395	C
4	9	1396	A

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Mol	Chain	Res	Type
4	9	1397	U
4	9	1398	G
4	9	1399	C
4	9	1401	A
4	9	1402	A
4	9	1404	U
4	9	1428	G
4	9	1454	A
4	9	1455	A
4	9	1462	U
4	9	1463	U
4	9	1464	C
4	9	1465	A
4	9	1466	G
4	9	1473	G
4	9	1475	G
4	9	1476	A
4	9	1477	U
4	9	1480	A
4	9	1486	A
4	9	1489	A
4	9	1490	G
4	9	1494	U
4	9	1497	G
4	9	1498	A
4	9	1506	A
4	9	1510	G
4	9	1521	C
4	9	1522	A
4	9	1533	A
4	9	1544	C
4	9	1548	G
4	9	1552	G
4	9	1553	C
4	9	1554	C
4	9	1556	A
4	9	1557	C
4	9	1560	U
4	9	1570	G
4	9	1574	C
4	9	1575	G
4	9	1580	A

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Mol	Chain	Res	Type
4	9	1585	U
4	9	1586	U
4	9	1587	G
4	9	1588	A
4	9	1597	C
4	9	1601	A
4	9	1602	U
4	9	1603	G
4	9	1604	G
4	9	1606	G
4	9	1621	U
4	9	1623	A
4	9	1625	U
4	9	1637	A
4	9	1638	G
4	9	1648	G
4	9	1649	U
4	9	1663	A
4	9	1664	A
4	9	1665	G
4	9	1683	C
4	9	1695	A
4	9	1698	C
4	9	1699	A
4	9	1702	G
4	9	1721	U
4	9	1722	G
4	9	1725	U
4	9	1726	G
4	9	1742	C
4	9	1744	G
4	9	1748	G
4	9	1757	G
4	9	1779	G
4	9	1783	C
4	9	1784	G
4	9	1785	C
4	9	1800	A
4	9	1824	A
4	9	1825	A
4	9	1826	G
4	9	1831	A

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Mol	Chain	Res	Type
4	9	1835	A
4	9	1836	G
4	9	1838	U
4	9	1849	G
4	9	1851	MA6
4	9	1861	G
4	9	1862	G
4	9	1863	A
4	9	1864	U
4	9	1865	C
4	9	1866	A
4	9	1867	U
4	9	1869	A
31	K	7	G
31	K	33	U
31	K	53	U
31	K	54	A
31	K	64	G
31	K	100	A
31	K	110	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	125	C
2	5	134	G
2	5	245	C
2	5	275	C
2	5	385	A
2	5	406	C
2	5	504	G
2	5	932	G
2	5	938	A
2	5	975	G
2	5	1076	C
2	5	1178	G
2	5	1215	G
2	5	1240	C
2	5	1242	A
2	5	1295	G
2	5	1333	G
2	5	1374	G

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Mol	Chain	Res	Type
2	5	1443	C
2	5	1449	U
2	5	1637	G
2	5	1808	A
2	5	1822	G
2	5	1943	A
2	5	1983	A
2	5	2050	G
2	5	2093	G
2	5	2270	C
2	5	2506	A
2	5	2643	U
2	5	2699	A
2	5	3892	G
2	5	4236	U
2	5	4452	G
2	5	4703	U
2	5	4888	G
2	5	4940	G
2	5	4953	G
4	9	110	U
4	9	434	G
4	9	465	A
4	9	479	C
4	9	532	C
4	9	553	U
4	9	642	U
4	9	688	U
4	9	752	G
4	9	870	A
4	9	874	G
4	9	1137	U
4	9	1394	G
4	9	1395	C
4	9	1489	A
4	9	1520	G
4	9	1637	A
4	9	1664	A

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

138 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$
2	B9B	5	1578	2	25,28,29	1.72	5 (20%)	35,40,43	2.14	12 (34%)
2	I4U	5	1663	2	21,24,25	3.63	9 (42%)	27,34,37	0.95	1 (3%)
2	PSU	5	4297	2	18,21,22	4.91	7 (38%)	22,30,33	1.86	5 (22%)
2	E6G	5	4359	2	24,27,28	1.75	5 (20%)	34,39,42	2.19	13 (38%)
4	UR3	9	1830	4	19,22,23	2.69	6 (31%)	26,32,35	1.57	4 (15%)
2	2MG	5	4876	2	23,26,27	2.98	8 (34%)	32,38,41	2.22	10 (31%)
2	OMG	5	1320	2	23,26,27	2.43	9 (39%)	33,38,41	2.24	11 (33%)
4	4AC	9	1337	4	21,24,25	3.19	9 (42%)	29,34,37	1.23	3 (10%)
2	B8H	5	4300	2	19,22,23	6.53	6 (31%)	22,32,35	2.34	5 (22%)
2	PSU	5	1586	2	18,21,22	4.95	7 (38%)	22,30,33	1.85	5 (22%)
2	PSU	5	4640	2	18,21,22	4.96	7 (38%)	22,30,33	1.89	5 (22%)
2	OMG	5	4641	2	23,26,27	2.42	9 (39%)	33,38,41	2.27	11 (33%)
2	2MG	5	729	2	23,26,27	3.05	8 (34%)	32,38,41	2.16	9 (28%)
4	5MC	9	1374	4	18,22,23	3.69	7 (38%)	26,32,35	1.34	4 (15%)
3	OMU	8	14	2,3	19,22,23	3.00	8 (42%)	26,31,34	1.69	4 (15%)
2	A2M	5	2367	84,2	22,25,26	3.59	9 (40%)	31,36,39	2.45	10 (32%)
2	OMC	5	3705	84,2	19,22,23	3.31	8 (42%)	26,31,34	0.75	0
4	PSU	9	119	4	18,21,22	0.94	1 (5%)	22,30,33	1.60	5 (22%)
2	OMG	5	1629	2	23,26,27	2.43	8 (34%)	33,38,41	2.36	10 (30%)
2	OMC	5	2426	84,2	19,22,23	3.35	8 (42%)	26,31,34	0.76	0
4	B8Q	9	1219	4	17,22,23	2.92	4 (23%)	22,32,35	2.34	7 (31%)
2	PSU	5	3719	2	18,21,22	4.94	7 (38%)	22,30,33	1.86	5 (22%)
4	OMU	9	116	4	19,22,23	2.88	7 (36%)	26,31,34	1.75	5 (19%)
2	A2M	5	1528	2	22,25,26	3.57	9 (40%)	31,36,39	2.50	10 (32%)
4	OMC	9	174	4	19,22,23	2.95	7 (36%)	26,31,34	0.81	1 (3%)
4	OMG	9	644	4	23,26,27	2.39	9 (39%)	33,38,41	1.83	8 (24%)
2	A2M	5	4527	84,2	22,25,26	3.55	9 (40%)	31,36,39	2.45	12 (38%)
4	OMC	9	1710	4	19,22,23	2.94	7 (36%)	26,31,34	0.92	1 (3%)
2	B8W	5	4476	2	23,26,27	2.01	3 (13%)	33,38,41	2.70	14 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UR3	5	4601	2	19,22,23	3.21	7 (36%)	26,32,35	1.29	2 (7%)
2	OMG	5	2428	2	23,26,27	2.43	8 (34%)	33,38,41	2.32	10 (30%)
2	A2M	5	398	2	22,25,26	3.57	9 (40%)	31,36,39	2.45	10 (32%)
2	OMG	5	373	2	23,26,27	2.40	9 (39%)	33,38,41	2.24	11 (33%)
2	OMG	5	2054	2	23,26,27	2.41	9 (39%)	33,38,41	2.26	10 (30%)
2	A2M	5	3789	2	22,25,26	3.54	11 (50%)	31,36,39	2.55	11 (35%)
4	A2M	9	1031	4	22,25,26	3.83	10 (45%)	31,36,39	2.51	13 (41%)
2	B9B	5	2758	84,2	25,28,29	1.71	5 (20%)	35,40,43	2.18	10 (28%)
4	OMU	9	121	4	19,22,23	2.96	8 (42%)	26,31,34	1.77	5 (19%)
4	MA6	9	1851	4	23,26,27	1.42	4 (17%)	34,38,41	2.76	12 (35%)
4	PSU	9	822	4	18,21,22	1.03	2 (11%)	22,30,33	1.93	5 (22%)
2	OMG	5	2368	2	23,26,27	2.41	9 (39%)	33,38,41	2.26	11 (33%)
2	UR3	5	4534	2	19,22,23	3.20	7 (36%)	26,32,35	1.31	3 (11%)
2	OMC	5	4540	2	19,22,23	3.34	8 (42%)	26,31,34	0.74	0
2	2MG	5	1521	2	23,26,27	3.00	8 (34%)	32,38,41	2.29	10 (31%)
2	7MG	5	2526	2	22,26,27	3.92	10 (45%)	29,39,42	2.04	9 (31%)
2	OMC	5	2808	2	19,22,23	3.33	8 (42%)	26,31,34	0.71	0
2	PSU	5	4454	84,2	18,21,22	4.95	7 (38%)	22,30,33	1.84	5 (22%)
4	A2M	9	166	4	22,25,26	3.81	11 (50%)	31,36,39	2.51	10 (32%)
2	B8T	5	4487	2	19,22,23	3.25	8 (42%)	26,31,34	0.85	1 (3%)
2	OMG	5	1526	2	23,26,27	2.42	9 (39%)	33,38,41	2.24	10 (30%)
2	5MU	5	4087	2	19,22,23	4.98	7 (36%)	28,32,35	3.62	9 (32%)
2	M7A	5	4568	2	20,25,26	2.02	3 (15%)	28,37,40	3.67	8 (28%)
2	7MG	5	4554	2	22,26,27	3.95	10 (45%)	29,39,42	1.99	9 (31%)
4	OMG	9	683	4	23,26,27	2.37	9 (39%)	33,38,41	1.80	9 (27%)
4	PSU	9	823	4	18,21,22	1.09	1 (5%)	22,30,33	1.83	4 (18%)
2	OMC	5	3913	2	19,22,23	3.34	8 (42%)	26,31,34	0.71	0
2	A2M	5	1330	2	22,25,26	3.57	10 (45%)	31,36,39	2.40	10 (32%)
4	A2M	9	1678	4	22,25,26	3.83	11 (50%)	31,36,39	2.41	11 (35%)
2	OMC	5	3873	2	19,22,23	3.34	8 (42%)	26,31,34	0.74	0
74	MLZ	m	72	74	8,9,10	0.76	0	4,9,11	0.64	0
2	A2M	5	3722	2	22,25,26	3.57	9 (40%)	31,36,39	2.44	11 (35%)
4	6MZ	9	1832	4	22,25,26	3.13	5 (22%)	30,36,39	4.04	12 (40%)
2	PSU	5	4504	2	18,21,22	4.95	7 (38%)	22,30,33	1.88	5 (22%)
2	A2M	5	1875	84,2	22,25,26	3.60	9 (40%)	31,36,39	2.47	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	5	1887	2	23,26,27	2.42	9 (39%)	33,38,41	2.29	11 (33%)
2	OMG	5	2777	2	23,26,27	2.43	9 (39%)	33,38,41	2.26	11 (33%)
4	MA6	9	1850	4	23,26,27	1.44	5 (21%)	34,38,41	2.85	13 (38%)
2	A2M	5	3829	2	22,25,26	3.58	10 (45%)	31,36,39	2.42	10 (32%)
2	PSU	5	3768	2	18,21,22	4.97	7 (38%)	22,30,33	1.71	6 (27%)
4	OMC	9	1703	4	19,22,23	2.94	7 (36%)	26,31,34	0.83	1 (3%)
2	P7G	5	3884	2	24,28,29	4.14	11 (45%)	27,41,44	1.60	3 (11%)
2	5MC	5	4339	2	18,22,23	3.92	7 (38%)	26,32,35	1.04	2 (7%)
2	7MG	5	1609	2	22,26,27	3.92	10 (45%)	29,39,42	2.03	9 (31%)
2	1MA	5	1326	84,2	21,25,26	2.86	5 (23%)	31,37,40	1.91	8 (25%)
2	E7G	5	1801	2	24,27,28	3.87	11 (45%)	30,40,43	2.22	10 (33%)
2	B8H	5	1864	2	19,22,23	6.50	6 (31%)	22,32,35	2.35	5 (22%)
2	B8K	5	3901	2	24,28,29	3.30	11 (45%)	30,42,45	2.28	11 (36%)
2	PSU	5	1681	2	18,21,22	4.95	8 (44%)	22,30,33	1.88	5 (22%)
2	BGH	5	3903	84,2	25,29,30	4.62	18 (72%)	31,43,46	2.35	12 (38%)
11	MLZ	C	333	11	8,9,10	0.77	0	4,9,11	0.67	0
2	B8W	5	2384	2	23,26,27	2.02	3 (13%)	33,38,41	2.40	12 (36%)
2	A2M	5	2405	84,2	22,25,26	3.56	9 (40%)	31,36,39	2.44	10 (32%)
2	PSU	5	3733	2	18,21,22	4.95	7 (38%)	22,30,33	1.82	5 (22%)
2	B9H	5	2790	2	20,25,26	2.95	5 (25%)	22,35,38	1.47	3 (13%)
2	MHG	5	4375	2	29,32,33	3.95	11 (37%)	34,46,49	2.29	10 (29%)
2	B9B	5	237	2	25,28,29	1.71	5 (20%)	35,40,43	2.20	13 (37%)
2	B8W	5	4133	2	23,26,27	2.04	3 (13%)	33,38,41	2.40	12 (36%)
4	M7A	9	1806	4	20,25,26	2.04	3 (15%)	28,37,40	3.72	8 (28%)
2	A2M	5	3727	2	22,25,26	3.58	9 (40%)	31,36,39	2.46	10 (32%)
2	B8W	5	4533	84,2	23,26,27	1.99	3 (13%)	33,38,41	2.55	13 (39%)
2	OMC	5	2865	2	19,22,23	3.33	8 (42%)	26,31,34	0.69	0
2	OMC	5	2369	2	19,22,23	3.34	8 (42%)	26,31,34	0.75	0
2	I4U	5	4198	2	21,24,25	3.61	8 (38%)	27,34,37	1.00	1 (3%)
2	PSU	5	4535	2	18,21,22	4.93	7 (38%)	22,30,33	1.81	5 (22%)
2	B8W	5	4189	2	23,26,27	2.02	3 (13%)	33,38,41	2.47	13 (39%)
2	OMG	5	4874	2	23,26,27	2.42	9 (39%)	33,38,41	2.29	11 (33%)
2	B8Q	5	1460	2	17,22,23	2.93	5 (29%)	22,32,35	2.08	4 (18%)
2	A2M	5	3871	2	22,25,26	3.58	9 (40%)	31,36,39	2.40	11 (35%)
4	OMC	9	517	4	19,22,23	2.84	7 (36%)	26,31,34	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	9	612	4	18,21,22	0.99	1 (5%)	22,30,33	1.74	4 (18%)
4	E3C	9	568	4	18,23,24	3.37	6 (33%)	21,33,36	2.23	5 (23%)
82	DDE	v	715	82	17,20,21	1.06	1 (5%)	20,28,30	0.88	1 (5%)
4	A2M	9	27	4	22,25,26	3.83	11 (50%)	31,36,39	2.49	13 (41%)
4	OMG	9	509	4	23,26,27	2.37	9 (39%)	33,38,41	1.84	8 (24%)
4	A2M	9	159	4	22,25,26	3.88	11 (50%)	31,36,39	2.51	12 (38%)
81	5CT	t	51	81	13,14,15	0.66	0	9,15,17	1.20	1 (11%)
4	4AC	9	1842	4	21,24,25	3.13	10 (47%)	29,34,37	1.18	4 (13%)
4	PSU	9	1081	4	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)
2	A2M	5	4575	2	22,25,26	3.60	9 (40%)	31,36,39	2.42	10 (32%)
4	5MU	9	814	4	19,22,23	4.87	7 (36%)	28,32,35	3.59	12 (42%)
2	P7G	5	1913	2	24,28,29	4.23	11 (45%)	27,41,44	1.56	3 (11%)
2	OMC	5	3891	2	19,22,23	3.34	8 (42%)	26,31,34	0.72	0
2	OMG	5	4374	2	23,26,27	2.42	9 (39%)	33,38,41	2.27	11 (33%)
4	PSU	9	1243	4	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
2	UR3	5	1870	2	19,22,23	3.20	7 (36%)	26,32,35	1.27	3 (11%)
2	PSU	5	2512	2	18,21,22	4.95	7 (38%)	22,30,33	1.88	5 (22%)
2	5MC	5	3786	2	18,22,23	3.91	7 (38%)	26,32,35	1.03	2 (7%)
2	E7G	5	2301	2	24,27,28	3.86	11 (45%)	30,40,43	2.24	10 (33%)
2	B8K	5	4694	2	24,28,29	3.38	11 (45%)	30,42,45	2.33	11 (36%)
2	OMG	5	3796	2	23,26,27	2.42	9 (39%)	33,38,41	2.29	10 (30%)
2	OMG	5	4627	2	23,26,27	2.41	9 (39%)	33,38,41	2.23	10 (30%)
4	A2M	9	484	4	22,25,26	3.81	11 (50%)	31,36,39	2.31	10 (32%)
2	PSU	5	1687	2	18,21,22	4.91	7 (38%)	22,30,33	1.84	5 (22%)
2	OMU	5	4624	2	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
2	P4U	5	1352	2	21,24,25	4.09	7 (33%)	27,33,36	0.98	1 (3%)
2	OMU	5	4310	2	19,22,23	3.03	8 (42%)	26,31,34	1.71	5 (19%)
2	PSU	5	4446	2	18,21,22	4.95	7 (38%)	22,30,33	1.86	5 (22%)
2	OMG	5	4200	2	23,26,27	2.42	9 (39%)	33,38,41	2.29	11 (33%)
4	A2M	9	668	4	22,25,26	3.87	11 (50%)	31,36,39	2.45	14 (45%)
2	A2M	5	1538	84,2	22,25,26	3.60	9 (40%)	31,36,39	2.45	10 (32%)
2	OMG	5	4498	2	23,26,27	2.41	9 (39%)	33,38,41	2.27	10 (30%)
2	6MZ	5	4224	2	22,25,26	3.00	3 (13%)	30,36,39	2.29	11 (36%)
2	5MC	5	4451	2	18,22,23	3.93	7 (38%)	26,32,35	1.05	1 (3%)
2	PSU	5	4632	2	18,21,22	4.90	7 (38%)	22,30,33	1.93	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	B8N	9	1248	4	24,29,30	2.79	6 (25%)	29,42,45	1.75	5 (17%)
2	PSU	5	4407	2	18,21,22	4.92	7 (38%)	22,30,33	1.76	5 (22%)
2	B8T	5	4675	2	19,22,23	3.25	8 (42%)	26,31,34	0.91	1 (3%)
2	1MA	5	4419	2	21,25,26	2.85	5 (23%)	31,37,40	1.86	8 (25%)

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
2	B9B	5	1578	2	-	2/11/29/30	0/3/3/3
2	I4U	5	1663	2	-	1/9/29/30	0/2/2/2
2	PSU	5	4297	2	-	2/7/25/26	0/2/2/2
2	E6G	5	4359	2	-	2/10/28/29	0/3/3/3
4	UR3	9	1830	4	-	4/7/25/26	0/2/2/2
2	2MG	5	4876	2	-	0/9/27/28	0/3/3/3
2	OMG	5	1320	2	-	0/9/27/28	0/3/3/3
4	4AC	9	1337	4	-	0/11/29/30	0/2/2/2
2	B8H	5	4300	2	-	0/7/25/26	0/2/2/2
2	PSU	5	1586	2	-	0/7/25/26	0/2/2/2
2	PSU	5	4640	2	-	3/7/25/26	0/2/2/2
2	OMG	5	4641	2	-	3/9/27/28	0/3/3/3
2	2MG	5	729	2	-	1/9/27/28	0/3/3/3
4	5MC	9	1374	4	-	0/7/25/26	0/2/2/2
3	OMU	8	14	2,3	-	1/9/27/28	0/2/2/2
2	A2M	5	2367	84,2	-	1/9/27/28	0/3/3/3
2	OMC	5	3705	84,2	-	4/9/27/28	0/2/2/2
4	PSU	9	119	4	-	2/7/25/26	0/2/2/2
2	OMG	5	1629	2	-	0/9/27/28	0/3/3/3
2	OMC	5	2426	84,2	-	1/9/27/28	0/2/2/2
4	B8Q	9	1219	4	-	0/7/42/43	0/2/2/2
2	PSU	5	3719	2	-	0/7/25/26	0/2/2/2
4	OMU	9	116	4	-	3/9/27/28	0/2/2/2
2	A2M	5	1528	2	-	1/9/27/28	0/3/3/3
4	OMC	9	174	4	-	0/9/27/28	0/2/2/2
4	OMG	9	644	4	-	1/9/27/28	0/3/3/3
2	A2M	5	4527	84,2	-	3/9/27/28	0/3/3/3
4	OMC	9	1710	4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8W	5	4476	2	-	2/9/27/28	0/3/3/3
2	UR3	5	4601	2	-	0/7/25/26	0/2/2/2
2	OMG	5	2428	2	-	2/9/27/28	0/3/3/3
2	A2M	5	398	2	-	2/9/27/28	0/3/3/3
2	OMG	5	373	2	-	1/9/27/28	0/3/3/3
2	OMG	5	2054	2	-	0/9/27/28	0/3/3/3
2	A2M	5	3789	2	-	3/9/27/28	0/3/3/3
4	A2M	9	1031	4	-	0/9/27/28	0/3/3/3
2	B9B	5	2758	84,2	-	2/11/29/30	0/3/3/3
4	OMU	9	121	4	-	2/9/27/28	0/2/2/2
4	MA6	9	1851	4	-	3/11/29/30	0/3/3/3
4	PSU	9	822	4	-	2/7/25/26	0/2/2/2
2	OMG	5	2368	2	-	2/9/27/28	0/3/3/3
2	UR3	5	4534	2	-	2/7/25/26	0/2/2/2
2	OMC	5	4540	2	-	0/9/27/28	0/2/2/2
2	2MG	5	1521	2	-	0/9/27/28	0/3/3/3
2	7MG	5	2526	2	-	0/7/37/38	0/3/3/3
2	OMC	5	2808	2	-	0/9/27/28	0/2/2/2
2	PSU	5	4454	84,2	-	3/7/25/26	0/2/2/2
4	A2M	9	166	4	-	2/9/27/28	0/3/3/3
2	B8T	5	4487	2	-	0/7/27/28	0/2/2/2
2	OMG	5	1526	2	-	0/9/27/28	0/3/3/3
2	5MU	5	4087	2	-	0/7/25/26	0/2/2/2
2	M7A	5	4568	2	-	0/7/37/38	0/3/3/3
2	7MG	5	4554	2	-	0/7/37/38	0/3/3/3
4	OMG	9	683	4	-	2/9/27/28	0/3/3/3
4	PSU	9	823	4	-	0/7/25/26	0/2/2/2
2	OMC	5	3913	2	-	0/9/27/28	0/2/2/2
2	A2M	5	1330	2	-	1/9/27/28	0/3/3/3
4	A2M	9	1678	4	-	0/9/27/28	0/3/3/3
2	OMC	5	3873	2	-	0/9/27/28	0/2/2/2
74	MLZ	m	72	74	-	0/7/8/10	-
2	A2M	5	3722	2	-	0/9/27/28	0/3/3/3
4	6MZ	9	1832	4	-	2/9/27/28	0/3/3/3
2	PSU	5	4504	2	-	3/7/25/26	0/2/2/2
2	A2M	5	1875	84,2	-	0/9/27/28	0/3/3/3
2	OMG	5	1887	2	-	0/9/27/28	0/3/3/3
2	OMG	5	2777	2	-	1/9/27/28	0/3/3/3
4	MA6	9	1850	4	-	1/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	5	3829	2	-	0/9/27/28	0/3/3/3
2	PSU	5	3768	2	-	4/7/25/26	0/2/2/2
4	OMC	9	1703	4	-	2/9/27/28	0/2/2/2
2	P7G	5	3884	2	-	2/10/40/41	0/3/3/3
2	5MC	5	4339	2	-	0/7/25/26	0/2/2/2
2	7MG	5	1609	2	-	0/7/37/38	0/3/3/3
2	1MA	5	1326	84,2	-	2/7/25/26	0/3/3/3
2	E7G	5	1801	2	-	2/9/39/40	0/3/3/3
2	B8H	5	1864	2	-	0/7/25/26	0/2/2/2
2	B8K	5	3901	2	-	3/11/41/42	0/3/3/3
2	PSU	5	1681	2	-	2/7/25/26	0/2/2/2
2	BGH	5	3903	84,2	-	2/13/43/44	0/3/3/3
11	MLZ	C	333	11	-	0/7/8/10	-
2	B8W	5	2384	2	-	4/9/27/28	0/3/3/3
2	A2M	5	2405	84,2	-	2/9/27/28	0/3/3/3
2	PSU	5	3733	2	-	2/7/25/26	0/2/2/2
2	B9H	5	2790	2	-	1/12/47/48	0/2/2/2
2	MHG	5	4375	2	-	7/16/46/47	0/3/3/3
2	B9B	5	237	2	-	2/11/29/30	0/3/3/3
2	B8W	5	4133	2	-	2/9/27/28	0/3/3/3
4	M7A	9	1806	4	-	0/7/37/38	0/3/3/3
2	A2M	5	3727	2	-	1/9/27/28	0/3/3/3
2	B8W	5	4533	84,2	-	2/9/27/28	0/3/3/3
2	OMC	5	2865	2	-	0/9/27/28	0/2/2/2
2	OMC	5	2369	2	-	0/9/27/28	0/2/2/2
2	I4U	5	4198	2	-	2/9/29/30	0/2/2/2
2	PSU	5	4535	2	-	2/7/25/26	0/2/2/2
2	B8W	5	4189	2	-	2/9/27/28	0/3/3/3
2	OMG	5	4874	2	-	4/9/27/28	0/3/3/3
2	B8Q	5	1460	2	-	0/7/42/43	0/2/2/2
2	A2M	5	3871	2	-	3/9/27/28	0/3/3/3
4	OMC	9	517	4	-	2/9/27/28	0/2/2/2
4	PSU	9	612	4	-	0/7/25/26	0/2/2/2
4	E3C	9	568	4	-	4/9/44/45	0/2/2/2
82	DDE	v	715	82	-	14/20/21/23	0/1/1/1
4	A2M	9	27	4	-	0/9/27/28	0/3/3/3
4	OMG	9	509	4	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	9	159	4	-	3/9/27/28	0/3/3/3
81	5CT	t	51	81	-	5/13/14/16	-
4	4AC	9	1842	4	-	0/11/29/30	0/2/2/2
4	PSU	9	1081	4	-	3/7/25/26	0/2/2/2
2	A2M	5	4575	2	-	0/9/27/28	0/3/3/3
4	5MU	9	814	4	-	0/7/25/26	0/2/2/2
2	P7G	5	1913	2	-	2/10/40/41	0/3/3/3
2	OMC	5	3891	2	-	0/9/27/28	0/2/2/2
2	OMG	5	4374	2	-	0/9/27/28	0/3/3/3
4	PSU	9	1243	4	-	2/7/25/26	0/2/2/2
2	UR3	5	1870	2	-	0/7/25/26	0/2/2/2
2	PSU	5	2512	2	-	0/7/25/26	0/2/2/2
2	5MC	5	3786	2	-	0/7/25/26	0/2/2/2
2	E7G	5	2301	2	-	1/9/39/40	0/3/3/3
2	B8K	5	4694	2	-	0/11/41/42	0/3/3/3
2	OMG	5	3796	2	-	2/9/27/28	0/3/3/3
2	OMG	5	4627	2	-	0/9/27/28	0/3/3/3
4	A2M	9	484	4	-	0/9/27/28	0/3/3/3
2	PSU	5	1687	2	-	0/7/25/26	0/2/2/2
2	OMU	5	4624	2	-	1/9/27/28	0/2/2/2
2	P4U	5	1352	2	-	3/10/29/30	0/2/2/2
2	OMU	5	4310	2	-	0/9/27/28	0/2/2/2
2	PSU	5	4446	2	-	0/7/25/26	0/2/2/2
2	OMG	5	4200	2	-	0/9/27/28	0/3/3/3
4	A2M	9	668	4	-	5/9/27/28	0/3/3/3
2	A2M	5	1538	84,2	-	2/9/27/28	0/3/3/3
2	OMG	5	4498	2	-	0/9/27/28	0/3/3/3
2	6MZ	5	4224	2	-	0/9/27/28	0/3/3/3
2	5MC	5	4451	2	-	4/7/25/26	0/2/2/2
2	PSU	5	4632	2	-	0/7/25/26	0/2/2/2
4	B8N	9	1248	4	-	3/16/34/35	0/2/2/2
2	PSU	5	4407	2	-	2/7/25/26	0/2/2/2
2	B8T	5	4675	2	-	1/7/27/28	0/2/2/2
2	1MA	5	4419	2	-	2/7/25/26	0/3/3/3

All (1011) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4300	B8H	C4-N3	-14.95	1.11	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1864	B8H	C4-N3	-14.87	1.11	1.38
2	5	4300	B8H	C4-C5	13.89	1.83	1.44
2	5	1864	B8H	C4-C5	13.85	1.83	1.44
2	5	4300	B8H	C6-C5	-13.49	1.16	1.34
2	5	1864	B8H	C6-C5	-13.39	1.16	1.34
4	9	1832	6MZ	C6-N6	13.07	1.48	1.34
2	5	4224	6MZ	C6-N6	12.92	1.48	1.34
2	5	4300	B8H	C6-N1	12.78	1.68	1.36
2	5	1864	B8H	C6-N1	12.72	1.67	1.36
2	5	3768	PSU	C6-C5	11.99	1.49	1.35
2	5	4087	5MU	C2-N1	11.95	1.57	1.38
2	5	4640	PSU	C2-N1	11.87	1.52	1.36
2	5	4407	PSU	C6-C5	11.85	1.49	1.35
2	5	2512	PSU	C6-C5	11.80	1.49	1.35
2	5	4454	PSU	C6-C5	11.79	1.49	1.35
2	5	1681	PSU	C2-N1	11.79	1.52	1.36
2	5	2512	PSU	C2-N1	11.78	1.52	1.36
2	5	3733	PSU	C6-C5	11.77	1.49	1.35
2	5	4640	PSU	C6-C5	11.76	1.49	1.35
2	5	4446	PSU	C6-C5	11.76	1.49	1.35
2	5	4504	PSU	C2-N1	11.75	1.52	1.36
2	5	3719	PSU	C2-N1	11.75	1.52	1.36
2	5	4504	PSU	C6-C5	11.75	1.49	1.35
2	5	1687	PSU	C6-C5	11.73	1.49	1.35
2	5	4535	PSU	C2-N1	11.73	1.52	1.36
2	5	1586	PSU	C2-N1	11.72	1.52	1.36
2	5	4407	PSU	C2-N1	11.72	1.52	1.36
2	5	4454	PSU	C2-N1	11.72	1.52	1.36
2	5	3768	PSU	C2-N1	11.72	1.52	1.36
2	5	1913	P7G	C8-N9	11.72	1.52	1.46
2	5	4446	PSU	C2-N1	11.70	1.52	1.36
2	5	4632	PSU	C6-C5	11.69	1.48	1.35
2	5	1586	PSU	C6-C5	11.69	1.48	1.35
2	5	3719	PSU	C6-C5	11.68	1.48	1.35
2	5	3733	PSU	C2-N1	11.65	1.52	1.36
2	5	4297	PSU	C6-C5	11.61	1.48	1.35
2	5	1687	PSU	C2-N1	11.59	1.52	1.36
2	5	4297	PSU	C2-N1	11.58	1.52	1.36
2	5	4535	PSU	C6-C5	11.55	1.48	1.35
2	5	4632	PSU	C2-N1	11.52	1.52	1.36
2	5	1681	PSU	C6-C5	11.50	1.48	1.35
4	9	814	5MU	C2-N1	11.44	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1663	I4U	C4-N3	11.27	1.45	1.31
2	5	4198	I4U	C4-N3	11.23	1.45	1.31
2	5	3884	P7G	C8-N9	10.97	1.52	1.46
2	5	1352	P4U	C4-N3	10.78	1.45	1.31
2	5	4087	5MU	C6-N1	10.70	1.56	1.38
2	5	4087	5MU	C4-C5	10.33	1.61	1.44
4	9	814	5MU	C6-N1	10.28	1.55	1.38
2	5	3903	BGH	O4'-C4'	10.19	1.67	1.45
2	5	4375	MHG	C8-N9	10.16	1.51	1.46
2	5	4451	5MC	C6-C5	10.15	1.51	1.34
2	5	3786	5MC	C6-C5	10.06	1.51	1.34
2	5	4339	5MC	C6-C5	10.01	1.51	1.34
2	5	3903	BGH	C3'-C4'	-9.70	1.28	1.53
2	5	4554	7MG	C8-N9	9.68	1.51	1.46
2	5	2301	E7G	C8-N9	9.62	1.51	1.46
4	9	814	5MU	C4-C5	9.50	1.60	1.44
4	9	1374	5MC	C6-C5	9.37	1.50	1.34
2	5	1801	E7G	C8-N9	9.34	1.51	1.46
4	9	166	A2M	O4'-C1'	9.28	1.64	1.42
2	5	2526	7MG	C8-N9	9.27	1.51	1.46
4	9	159	A2M	O4'-C1'	9.27	1.64	1.42
4	9	1678	A2M	O4'-C1'	9.24	1.63	1.42
2	5	1609	7MG	C8-N9	9.21	1.51	1.46
2	5	1875	A2M	O4'-C1'	9.17	1.63	1.42
2	5	4527	A2M	O4'-C1'	9.17	1.63	1.42
2	5	3727	A2M	O4'-C1'	9.15	1.63	1.42
2	5	3722	A2M	O4'-C1'	9.13	1.63	1.42
2	5	4575	A2M	O4'-C1'	9.12	1.63	1.42
2	5	2367	A2M	O4'-C1'	9.12	1.63	1.42
2	5	2405	A2M	O4'-C1'	9.11	1.63	1.42
2	5	398	A2M	O4'-C1'	9.11	1.63	1.42
2	5	3829	A2M	O4'-C1'	9.11	1.63	1.42
2	5	1538	A2M	O4'-C1'	9.10	1.63	1.42
4	9	1031	A2M	O4'-C1'	9.09	1.63	1.42
2	5	1528	A2M	O4'-C1'	9.01	1.63	1.42
2	5	1330	A2M	O4'-C1'	8.99	1.63	1.42
2	5	3871	A2M	O4'-C1'	8.99	1.63	1.42
4	9	484	A2M	O4'-C1'	8.97	1.63	1.42
4	9	27	A2M	O4'-C1'	8.85	1.63	1.42
2	5	4694	B8K	C8-N9	8.79	1.50	1.46
2	5	1870	UR3	C2-N1	8.76	1.51	1.38
2	5	1326	1MA	C2-N3	8.75	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3789	A2M	O4'-C1'	8.75	1.62	1.42
2	5	4601	UR3	C2-N1	8.70	1.51	1.38
4	9	668	A2M	O4'-C1'	8.68	1.62	1.42
2	5	4419	1MA	C2-N3	8.67	1.46	1.30
2	5	4534	UR3	C2-N1	8.64	1.50	1.38
2	5	2790	B9H	C2-N3	8.52	1.48	1.37
4	9	568	E3C	C2-N3	8.49	1.48	1.37
2	5	3733	PSU	C2-N3	8.48	1.52	1.37
2	5	1913	P7G	C5-N7	8.45	1.45	1.35
4	9	814	5MU	C4-N3	-8.45	1.23	1.38
2	5	4535	PSU	C2-N3	8.44	1.52	1.37
2	5	4454	PSU	C2-N3	8.42	1.51	1.37
2	5	4446	PSU	C2-N3	8.42	1.51	1.37
2	5	3719	PSU	C2-N3	8.38	1.51	1.37
2	5	4504	PSU	C2-N3	8.38	1.51	1.37
2	5	4297	PSU	C2-N3	8.38	1.51	1.37
4	9	1219	B8Q	C6-C5	8.37	1.52	1.33
2	5	1586	PSU	C2-N3	8.37	1.51	1.37
2	5	4632	PSU	C2-N3	8.36	1.51	1.37
2	5	1681	PSU	C2-N3	8.36	1.51	1.37
2	5	1687	PSU	C2-N3	8.33	1.51	1.37
2	5	3768	PSU	C2-N3	8.33	1.51	1.37
2	5	729	2MG	C2-N3	8.27	1.47	1.31
2	5	4640	PSU	C2-N3	8.27	1.51	1.37
2	5	3884	P7G	C5-N7	8.26	1.44	1.35
2	5	2512	PSU	C2-N3	8.23	1.51	1.37
2	5	3901	B8K	C8-N9	8.22	1.50	1.46
2	5	4375	MHG	C5-N7	8.22	1.44	1.35
2	5	3903	BGH	C8-N9	8.20	1.50	1.46
2	5	4407	PSU	C2-N3	8.14	1.51	1.37
2	5	1801	E7G	C5-N7	8.11	1.44	1.35
2	5	2301	E7G	C5-N7	7.97	1.44	1.35
4	9	668	A2M	O4'-C4'	-7.96	1.27	1.45
4	9	568	E3C	C2-N1	7.95	1.50	1.38
4	9	1248	B8N	C4-N3	-7.93	1.25	1.40
2	5	4876	2MG	C2-N3	7.91	1.47	1.31
2	5	1521	2MG	C2-N3	7.91	1.47	1.31
2	5	2526	7MG	C5-N7	7.90	1.44	1.35
2	5	4554	7MG	C5-N7	7.90	1.44	1.35
2	5	4375	MHG	C2-N3	7.88	1.47	1.31
2	5	4133	B8W	C2-N2	7.88	1.49	1.33
2	5	1609	7MG	C5-N7	7.87	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3789	A2M	C2'-C1'	-7.83	1.32	1.53
4	9	27	A2M	C2'-C1'	-7.83	1.32	1.53
2	5	1460	B8Q	C6-C5	7.81	1.50	1.33
2	5	1330	A2M	C2'-C1'	-7.80	1.33	1.53
2	5	4575	A2M	C2'-C1'	-7.79	1.33	1.53
2	5	2367	A2M	C2'-C1'	-7.77	1.33	1.53
2	5	2384	B8W	C2-N2	7.77	1.49	1.33
2	5	1875	A2M	C2'-C1'	-7.77	1.33	1.53
2	5	4476	B8W	C2-N2	7.75	1.49	1.33
2	5	4189	B8W	C2-N2	7.75	1.49	1.33
2	5	1538	A2M	C2'-C1'	-7.73	1.33	1.53
2	5	4533	B8W	C2-N2	7.70	1.49	1.33
2	5	2405	A2M	C2'-C1'	-7.70	1.33	1.53
2	5	398	A2M	C2'-C1'	-7.69	1.33	1.53
2	5	3829	A2M	C2'-C1'	-7.67	1.33	1.53
2	5	3722	A2M	C2'-C1'	-7.67	1.33	1.53
2	5	3871	A2M	C2'-C1'	-7.66	1.33	1.53
2	5	3727	A2M	C2'-C1'	-7.64	1.33	1.53
4	9	159	A2M	C2'-C1'	-7.63	1.33	1.53
4	9	166	A2M	C2'-C1'	-7.63	1.33	1.53
4	9	484	A2M	O4'-C4'	-7.59	1.28	1.45
4	9	484	A2M	C2'-C1'	-7.56	1.33	1.53
4	9	159	A2M	O4'-C4'	-7.54	1.28	1.45
2	5	1528	A2M	C2'-C1'	-7.53	1.33	1.53
4	9	1031	A2M	C2'-C1'	-7.52	1.33	1.53
4	9	668	A2M	C2'-C1'	-7.51	1.33	1.53
2	5	4527	A2M	C2'-C1'	-7.50	1.33	1.53
4	9	1678	A2M	O4'-C4'	-7.47	1.28	1.45
4	9	1678	A2M	C2'-C1'	-7.44	1.33	1.53
4	9	1031	A2M	O4'-C4'	-7.42	1.28	1.45
4	9	27	A2M	O4'-C4'	-7.35	1.28	1.45
2	5	1352	P4U	C2-N3	7.31	1.51	1.36
2	5	1870	UR3	C6-C5	7.31	1.52	1.35
2	5	4601	UR3	C6-C5	7.31	1.52	1.35
2	5	4534	UR3	C6-C5	7.29	1.52	1.35
4	9	1248	B8N	C6-N1	7.22	1.54	1.36
4	9	166	A2M	O4'-C4'	-7.22	1.28	1.45
2	5	1352	P4U	C6-C5	7.06	1.51	1.35
2	5	4339	5MC	C4-N3	7.04	1.46	1.34
4	9	1830	UR3	C2-N1	7.04	1.48	1.38
2	5	1352	P4U	O4-C4	7.00	1.43	1.35
2	5	1528	A2M	O4'-C4'	-7.00	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3871	A2M	O4'-C4'	-6.97	1.29	1.45
2	5	3786	5MC	C4-N3	6.97	1.45	1.34
3	8	14	OMU	C2-N1	6.95	1.49	1.38
2	5	4087	5MU	C4-N3	-6.95	1.25	1.38
2	5	729	2MG	C4-N3	6.94	1.50	1.34
2	5	4375	MHG	C8-N7	6.92	1.52	1.45
2	5	4310	OMU	C2-N1	6.91	1.49	1.38
2	5	4451	5MC	C4-N3	6.91	1.45	1.34
2	5	4675	B8T	C4-N3	6.90	1.44	1.32
2	5	1538	A2M	O4'-C4'	-6.89	1.29	1.45
2	5	4487	B8T	C4-N3	6.88	1.44	1.32
2	5	4310	OMU	C2-N3	6.87	1.50	1.38
2	5	4624	OMU	C2-N1	6.86	1.49	1.38
2	5	4575	A2M	O4'-C4'	-6.85	1.29	1.45
2	5	1521	2MG	C4-N3	6.81	1.50	1.34
2	5	4624	OMU	C2-N3	6.80	1.50	1.38
2	5	2790	B9H	C6-C5	6.80	1.48	1.33
4	9	121	OMU	C2-N1	6.80	1.49	1.38
2	5	3727	A2M	O4'-C4'	-6.78	1.29	1.45
2	5	1875	A2M	O4'-C4'	-6.77	1.29	1.45
2	5	2367	A2M	O4'-C4'	-6.76	1.29	1.45
4	9	1842	4AC	C4-N3	6.75	1.44	1.32
2	5	4375	MHG	C2-N1	6.72	1.47	1.36
2	5	4527	A2M	O4'-C4'	-6.72	1.30	1.45
2	5	3829	A2M	O4'-C4'	-6.71	1.30	1.45
2	5	4087	5MU	C6-C5	6.71	1.45	1.34
2	5	1330	A2M	O4'-C4'	-6.70	1.30	1.45
3	8	14	OMU	C2-N3	6.68	1.49	1.38
2	5	3789	A2M	O4'-C4'	-6.68	1.30	1.45
2	5	2405	A2M	O4'-C4'	-6.68	1.30	1.45
2	5	3722	A2M	O4'-C4'	-6.67	1.30	1.45
2	5	398	A2M	O4'-C4'	-6.66	1.30	1.45
4	9	116	OMU	C2-N3	6.64	1.49	1.38
2	5	1460	B8Q	C2-N3	6.63	1.46	1.35
4	9	568	E3C	C6-C5	6.62	1.48	1.33
4	9	1678	A2M	C6-N6	6.61	1.50	1.34
2	5	3786	5MC	C2-N3	6.60	1.49	1.36
2	5	4876	2MG	C4-N3	6.60	1.49	1.34
2	5	1352	P4U	C5-C4	6.60	1.51	1.43
2	5	4339	5MC	C2-N3	6.59	1.49	1.36
4	9	166	A2M	C6-N6	6.59	1.50	1.34
4	9	116	OMU	C2-N1	6.59	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	1337	4AC	C4-N3	6.58	1.44	1.32
2	5	4451	5MC	C2-N3	6.57	1.49	1.36
4	9	668	A2M	C6-N6	6.57	1.50	1.34
4	9	27	A2M	C6-N6	6.56	1.50	1.34
4	9	1031	A2M	C6-N6	6.56	1.50	1.34
2	5	3903	BGH	C2-N3	6.55	1.49	1.33
4	9	159	A2M	C6-N6	6.55	1.50	1.34
2	5	1586	PSU	C6-N1	6.55	1.47	1.36
2	5	4640	PSU	C6-N1	6.54	1.47	1.36
2	5	4504	PSU	C6-N1	6.53	1.47	1.36
2	5	3719	PSU	C6-N1	6.52	1.47	1.36
2	5	2512	PSU	C6-N1	6.51	1.47	1.36
4	9	1374	5MC	C4-N3	6.51	1.45	1.34
4	9	121	OMU	C2-N3	6.50	1.49	1.38
2	5	3733	PSU	C6-N1	6.50	1.47	1.36
2	5	3768	PSU	C6-N1	6.49	1.47	1.36
2	5	1681	PSU	C6-N1	6.48	1.47	1.36
4	9	484	A2M	C6-N6	6.47	1.50	1.34
2	5	4446	PSU	C6-N1	6.46	1.47	1.36
2	5	4198	I4U	C6-C5	6.44	1.50	1.35
2	5	4297	PSU	C6-N1	6.44	1.46	1.36
2	5	1629	OMG	C4-N3	6.43	1.49	1.34
2	5	4540	OMC	C6-C5	6.43	1.50	1.35
2	5	1663	I4U	C6-C5	6.43	1.50	1.35
2	5	4535	PSU	C6-N1	6.43	1.46	1.36
2	5	3705	OMC	C6-C5	6.42	1.50	1.35
2	5	2428	OMG	C4-N3	6.42	1.49	1.34
2	5	3891	OMC	C2-N3	6.41	1.49	1.36
2	5	2369	OMC	C6-C5	6.38	1.49	1.35
2	5	2426	OMC	C6-C5	6.38	1.49	1.35
2	5	4454	PSU	C6-N1	6.38	1.46	1.36
2	5	4407	PSU	C6-N1	6.37	1.46	1.36
2	5	3873	OMC	C2-N3	6.37	1.49	1.36
2	5	3913	OMC	C6-C5	6.36	1.49	1.35
2	5	1887	OMG	C4-N3	6.36	1.49	1.34
2	5	2369	OMC	C2-N3	6.36	1.49	1.36
2	5	2865	OMC	C6-C5	6.36	1.49	1.35
4	9	1703	OMC	C6-C5	6.34	1.49	1.35
2	5	2426	OMC	C2-N3	6.34	1.49	1.36
2	5	2865	OMC	C2-N3	6.34	1.49	1.36
2	5	3873	OMC	C6-C5	6.34	1.49	1.35
2	5	2777	OMG	C4-N3	6.34	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2368	OMG	C4-N3	6.34	1.49	1.34
2	5	4374	OMG	C4-N3	6.33	1.49	1.34
2	5	4632	PSU	C6-N1	6.33	1.46	1.36
4	9	1219	B8Q	C2-N3	6.32	1.46	1.35
2	5	2808	OMC	C2-N3	6.32	1.49	1.36
2	5	4200	OMG	C4-N3	6.32	1.49	1.34
2	5	4641	OMG	C4-N3	6.32	1.49	1.34
2	5	4540	OMC	C2-N3	6.32	1.49	1.36
2	5	4498	OMG	C4-N3	6.31	1.49	1.34
2	5	4874	OMG	C4-N3	6.31	1.49	1.34
2	5	3796	OMG	C4-N3	6.31	1.49	1.34
2	5	1526	OMG	C4-N3	6.31	1.49	1.34
2	5	3891	OMC	C6-C5	6.31	1.49	1.35
2	5	4487	B8T	C2-N3	6.31	1.49	1.36
2	5	2054	OMG	C4-N3	6.30	1.49	1.34
2	5	3913	OMC	C2-N3	6.30	1.49	1.36
2	5	1687	PSU	C6-N1	6.30	1.46	1.36
2	5	2808	OMC	C6-C5	6.29	1.49	1.35
2	5	1320	OMG	C4-N3	6.29	1.49	1.34
4	9	174	OMC	C6-C5	6.28	1.49	1.35
2	5	4675	B8T	C2-N3	6.28	1.49	1.36
2	5	373	OMG	C4-N3	6.28	1.49	1.34
2	5	3705	OMC	C2-N3	6.27	1.49	1.36
2	5	4627	OMG	C4-N3	6.27	1.49	1.34
2	5	3884	P7G	C4-N3	6.26	1.48	1.37
2	5	1326	1MA	C4-N3	6.26	1.48	1.35
2	5	4419	1MA	C4-N3	6.25	1.48	1.35
2	5	1913	P7G	C4-N3	6.25	1.48	1.37
4	9	1710	OMC	C6-C5	6.23	1.49	1.35
4	9	1710	OMC	C2-N3	6.21	1.48	1.36
2	5	4300	B8H	C2-N3	6.20	1.49	1.38
4	9	174	OMC	C2-N3	6.20	1.48	1.36
2	5	1864	B8H	C2-N3	6.19	1.49	1.38
2	5	2790	B9H	C2-N1	6.18	1.47	1.38
2	5	4675	B8T	C6-C5	6.18	1.49	1.35
2	5	4487	B8T	C6-C5	6.17	1.49	1.35
2	5	3873	OMC	C4-N3	6.16	1.46	1.34
2	5	2369	OMC	C4-N3	6.16	1.46	1.34
2	5	3891	OMC	C4-N3	6.16	1.46	1.34
2	5	2808	OMC	C4-N3	6.16	1.46	1.34
4	9	509	OMG	C4-N3	6.15	1.48	1.34
4	9	1337	4AC	C6-C5	6.13	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1801	E7G	C8-N7	6.09	1.51	1.45
2	5	3913	OMC	C4-N3	6.08	1.46	1.34
2	5	2426	OMC	C4-N3	6.08	1.46	1.34
2	5	3884	P7G	C4-N9	6.07	1.44	1.35
2	5	4540	OMC	C4-N3	6.06	1.46	1.34
4	9	517	OMC	C2-N3	6.06	1.48	1.36
2	5	4554	7MG	C4-N3	6.05	1.48	1.34
4	9	1703	OMC	C2-N3	6.04	1.48	1.36
4	9	683	OMG	C4-N3	6.04	1.48	1.34
2	5	3705	OMC	C4-N3	6.03	1.46	1.34
2	5	2865	OMC	C4-N3	6.01	1.46	1.34
2	5	1913	P7G	C8-N7	5.99	1.51	1.45
4	9	1830	UR3	C6-C5	5.98	1.48	1.35
4	9	517	OMC	C6-C5	5.97	1.48	1.35
2	5	2526	7MG	C4-N3	5.96	1.48	1.34
4	9	814	5MU	C6-C5	5.96	1.44	1.34
4	9	644	OMG	C4-N3	5.95	1.48	1.34
2	5	1609	7MG	C4-N3	5.94	1.48	1.34
2	5	1609	7MG	C2-N3	5.92	1.47	1.33
4	9	1374	5MC	C2-N3	5.92	1.48	1.36
2	5	1913	P7G	C2-N1	5.91	1.47	1.33
2	5	2301	E7G	C8-N7	5.91	1.51	1.45
2	5	2426	OMC	C4-N4	5.91	1.47	1.33
2	5	1609	7MG	C4-N9	5.90	1.44	1.37
2	5	2865	OMC	C4-N4	5.90	1.47	1.33
4	9	1337	4AC	C2-N3	5.89	1.48	1.36
2	5	3884	P7G	C8-N7	5.89	1.51	1.45
2	5	2808	OMC	C4-N4	5.89	1.47	1.33
2	5	2369	OMC	C4-N4	5.88	1.47	1.33
2	5	2526	7MG	C2-N3	5.88	1.47	1.33
2	5	3913	OMC	C4-N4	5.88	1.47	1.33
2	5	4554	7MG	C2-N3	5.87	1.47	1.33
4	9	1842	4AC	C2-N3	5.86	1.48	1.36
2	5	4601	UR3	C2-N3	5.86	1.50	1.39
2	5	2301	E7G	C2-N3	5.86	1.47	1.33
2	5	3884	P7G	C2-N1	5.85	1.47	1.33
2	5	4540	OMC	C4-N4	5.85	1.47	1.33
2	5	1801	E7G	C2-N3	5.85	1.47	1.33
4	9	1806	M7A	C4-N9	5.83	1.49	1.38
2	5	3727	A2M	C6-N6	5.83	1.48	1.34
2	5	3891	OMC	C4-N4	5.82	1.47	1.33
2	5	3873	OMC	C4-N4	5.82	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4876	2MG	C2-N1	5.82	1.46	1.36
2	5	1913	P7G	C4-N9	5.81	1.43	1.35
2	5	2526	7MG	C4-N9	5.81	1.44	1.37
2	5	4534	UR3	C2-N3	5.81	1.50	1.39
4	9	1703	OMC	C4-N3	5.80	1.46	1.34
2	5	3705	OMC	C4-N4	5.79	1.47	1.33
2	5	4575	A2M	C6-N6	5.78	1.48	1.34
4	9	1842	4AC	C6-C5	5.78	1.48	1.35
2	5	3722	A2M	C6-N6	5.78	1.48	1.34
2	5	398	A2M	C6-N6	5.77	1.48	1.34
2	5	1538	A2M	C6-N6	5.77	1.48	1.34
2	5	2405	A2M	C6-N6	5.77	1.48	1.34
2	5	3903	BGH	C4-N3	5.76	1.48	1.34
2	5	729	2MG	C2-N1	5.76	1.45	1.36
2	5	237	B9B	C2-N2	5.75	1.45	1.33
2	5	3871	A2M	C6-N6	5.75	1.48	1.34
2	5	2367	A2M	C6-N6	5.74	1.48	1.34
2	5	3901	B8K	C2-N3	5.74	1.47	1.33
2	5	1578	B9B	C2-N2	5.74	1.45	1.33
2	5	1528	A2M	C6-N6	5.73	1.48	1.34
2	5	4694	B8K	C2-N3	5.73	1.47	1.33
2	5	1875	A2M	C6-N6	5.72	1.48	1.34
2	5	1521	2MG	C2-N1	5.72	1.45	1.36
2	5	3829	A2M	C6-N6	5.72	1.48	1.34
2	5	4375	MHG	C2-N2	5.72	1.46	1.33
2	5	4568	M7A	C4-N9	5.72	1.48	1.38
2	5	4694	B8K	C4-N3	5.71	1.47	1.34
4	9	1710	OMC	C4-N3	5.71	1.46	1.34
2	5	4310	OMU	C6-C5	5.71	1.48	1.35
2	5	4359	E6G	C2-N2	5.71	1.45	1.33
2	5	4554	7MG	C4-N9	5.70	1.44	1.37
2	5	4527	A2M	C6-N6	5.70	1.48	1.34
2	5	3901	B8K	C4-N3	5.70	1.47	1.34
2	5	1870	UR3	C2-N3	5.70	1.50	1.39
2	5	2758	B9B	C2-N2	5.70	1.45	1.33
4	9	121	OMU	C6-C5	5.69	1.48	1.35
4	9	174	OMC	C4-N3	5.69	1.45	1.34
2	5	1663	I4U	C2-N3	5.68	1.47	1.36
2	5	1801	E7G	C4-N9	5.67	1.44	1.37
2	5	4624	OMU	C6-C5	5.67	1.48	1.35
2	5	3903	BGH	C4-N9	5.65	1.44	1.37
3	8	14	OMU	C6-C5	5.65	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4198	I4U	C2-N3	5.65	1.47	1.36
2	5	1330	A2M	C6-N6	5.64	1.48	1.34
4	9	517	OMC	C4-N3	5.61	1.45	1.34
2	5	1801	E7G	C4-N3	5.59	1.47	1.34
2	5	2301	E7G	C4-N3	5.57	1.47	1.34
2	5	3789	A2M	C6-N6	5.54	1.48	1.34
2	5	1629	OMG	C2-N3	5.50	1.46	1.33
2	5	1521	2MG	C2-N2	5.49	1.45	1.33
2	5	2301	E7G	C4-N9	5.48	1.44	1.37
2	5	4375	MHG	C4-N3	5.48	1.47	1.34
2	5	2428	OMG	C2-N3	5.47	1.46	1.33
2	5	729	2MG	C2-N2	5.45	1.45	1.33
2	5	4374	OMG	C2-N3	5.43	1.46	1.33
2	5	4874	OMG	C2-N3	5.43	1.46	1.33
2	5	3796	OMG	C2-N3	5.40	1.46	1.33
2	5	4627	OMG	C2-N3	5.40	1.46	1.33
2	5	4200	OMG	C2-N3	5.40	1.46	1.33
2	5	2777	OMG	C2-N3	5.39	1.46	1.33
4	9	644	OMG	C2-N3	5.37	1.46	1.33
2	5	1526	OMG	C2-N3	5.35	1.46	1.33
2	5	4498	OMG	C2-N3	5.34	1.46	1.33
2	5	4641	OMG	C2-N3	5.33	1.46	1.33
2	5	2054	OMG	C2-N3	5.32	1.46	1.33
4	9	116	OMU	C6-C5	5.31	1.47	1.35
2	5	1887	OMG	C2-N3	5.31	1.46	1.33
4	9	1248	B8N	C2-N1	5.29	1.55	1.39
2	5	1320	OMG	C2-N3	5.28	1.45	1.33
2	5	373	OMG	C2-N3	5.27	1.45	1.33
4	9	509	OMG	C2-N3	5.26	1.45	1.33
2	5	2368	OMG	C2-N3	5.25	1.45	1.33
2	5	4876	2MG	C2-N2	5.23	1.45	1.33
2	5	4375	MHG	C4-N9	5.23	1.43	1.37
2	5	4694	B8K	C4-N9	5.20	1.43	1.37
2	5	4451	5MC	C6-N1	5.16	1.46	1.38
2	5	2426	OMC	C2-N1	5.13	1.51	1.40
2	5	4339	5MC	C4-N4	5.09	1.47	1.34
2	5	3901	B8K	C4-N9	5.08	1.43	1.37
2	5	3786	5MC	C4-N4	5.06	1.47	1.34
2	5	4451	5MC	C4-N4	5.06	1.47	1.34
2	5	3913	OMC	C2-N1	5.05	1.50	1.40
2	5	3873	OMC	C2-N1	5.05	1.50	1.40
2	5	3891	OMC	C2-N1	5.04	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3786	5MC	C6-N1	5.04	1.46	1.38
2	5	4339	5MC	C6-N1	5.02	1.46	1.38
2	5	4540	OMC	C2-N1	5.01	1.50	1.40
2	5	2865	OMC	C2-N1	4.98	1.50	1.40
2	5	2808	OMC	C2-N1	4.96	1.50	1.40
2	5	3903	BGH	O4'-C1'	-4.94	1.30	1.42
2	5	3705	OMC	C2-N1	4.94	1.50	1.40
4	9	683	OMG	C2-N3	4.92	1.45	1.33
4	9	1830	UR3	C2-N3	4.92	1.48	1.39
2	5	3884	P7G	C2-N2	4.92	1.45	1.34
2	5	2526	7MG	C2-N2	4.91	1.45	1.34
2	5	1352	P4U	C2-N1	4.91	1.50	1.40
2	5	2369	OMC	C2-N1	4.90	1.50	1.40
2	5	1913	P7G	C2-N2	4.90	1.45	1.34
2	5	4694	B8K	C2-N2	4.88	1.45	1.34
2	5	4554	7MG	C2-N2	4.87	1.45	1.34
4	9	1374	5MC	C2-N1	4.86	1.50	1.40
4	9	1337	4AC	C7-N4	4.85	1.46	1.37
2	5	1609	7MG	C2-N2	4.85	1.45	1.34
2	5	3901	B8K	C2-N2	4.83	1.45	1.34
2	5	1326	1MA	C2-N1	4.80	1.44	1.35
4	9	1374	5MC	C4-N4	4.77	1.46	1.34
2	5	4874	OMG	C2-N2	4.77	1.45	1.34
2	5	2428	OMG	C2-N2	4.75	1.45	1.34
2	5	2777	OMG	C2-N2	4.74	1.45	1.34
4	9	1248	B8N	C6-C5	4.73	1.41	1.34
2	5	4568	M7A	C6-N6	4.72	1.46	1.34
2	5	1887	OMG	C2-N2	4.72	1.45	1.34
2	5	4419	1MA	C2-N1	4.71	1.44	1.35
2	5	1801	E7G	C2-N2	4.71	1.45	1.34
2	5	4200	OMG	C2-N2	4.71	1.45	1.34
2	5	1320	OMG	C2-N2	4.70	1.45	1.34
4	9	683	OMG	C2-N2	4.70	1.45	1.34
2	5	4487	B8T	C4-N4	4.70	1.45	1.35
4	9	1842	4AC	C7-N4	4.69	1.45	1.37
2	5	1629	OMG	C2-N2	4.69	1.45	1.34
2	5	4374	OMG	C2-N2	4.68	1.45	1.34
2	5	2368	OMG	C2-N2	4.66	1.45	1.34
2	5	2301	E7G	C2-N2	4.66	1.45	1.34
2	5	4498	OMG	C2-N2	4.65	1.45	1.34
2	5	2054	OMG	C2-N2	4.65	1.45	1.34
2	5	3796	OMG	C2-N2	4.65	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3903	BGH	C5-C6	4.65	1.55	1.43
4	9	1031	A2M	O3'-C3'	-4.64	1.32	1.43
2	5	4297	PSU	C4-N3	4.64	1.47	1.38
2	5	1526	OMG	C2-N2	4.63	1.45	1.34
4	9	166	A2M	O3'-C3'	-4.63	1.32	1.43
2	5	4675	B8T	C4-N4	4.63	1.45	1.35
2	5	4627	OMG	C2-N2	4.61	1.45	1.34
2	5	3768	PSU	C4-N3	4.61	1.47	1.38
2	5	4641	OMG	C2-N2	4.61	1.45	1.34
4	9	27	A2M	O3'-C3'	-4.60	1.32	1.43
2	5	373	OMG	C2-N2	4.60	1.45	1.34
4	9	159	A2M	O3'-C3'	-4.60	1.32	1.43
2	5	4535	PSU	C4-N3	4.57	1.47	1.38
2	5	4675	B8T	C2-N1	4.56	1.49	1.40
2	5	1586	PSU	C4-N3	4.55	1.47	1.38
2	5	4446	PSU	C4-N3	4.55	1.47	1.38
2	5	4504	PSU	C4-N3	4.55	1.47	1.38
4	9	1219	B8Q	C2-N1	4.54	1.45	1.38
2	5	3733	PSU	C4-N3	4.54	1.47	1.38
2	5	1681	PSU	C4-N3	4.52	1.47	1.38
4	9	1337	4AC	C4-N4	4.52	1.46	1.39
2	5	3786	5MC	C2-N1	4.50	1.49	1.40
2	5	4487	B8T	C2-N1	4.50	1.49	1.40
2	5	4339	5MC	C2-N1	4.50	1.49	1.40
2	5	2512	PSU	C4-N3	4.49	1.47	1.38
2	5	3719	PSU	C4-N3	4.49	1.47	1.38
4	9	1806	M7A	C6-N6	4.48	1.45	1.34
2	5	4407	PSU	C4-N3	4.48	1.47	1.38
4	9	668	A2M	O3'-C3'	-4.48	1.32	1.43
2	5	4454	PSU	C4-N3	4.48	1.47	1.38
2	5	1663	I4U	C2-N1	4.48	1.49	1.40
2	5	1687	PSU	C4-N3	4.48	1.47	1.38
4	9	1374	5MC	C6-N1	4.46	1.45	1.38
4	9	1678	A2M	O3'-C3'	-4.46	1.32	1.43
2	5	4451	5MC	C2-N1	4.45	1.49	1.40
2	5	4632	PSU	C4-N3	4.44	1.47	1.38
4	9	644	OMG	C2-N2	4.44	1.44	1.34
4	9	509	OMG	C2-N2	4.42	1.44	1.34
2	5	4640	PSU	C4-N3	4.42	1.47	1.38
2	5	1460	B8Q	C2-N1	4.36	1.44	1.38
2	5	3903	BGH	C6-N1	4.34	1.46	1.38
2	5	4198	I4U	C2-N1	4.29	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4198	I4U	O4-C4	4.24	1.43	1.35
2	5	1663	I4U	O4-C4	4.23	1.43	1.35
4	9	484	A2M	O3'-C3'	-4.19	1.33	1.43
2	5	1609	7MG	C2-N1	4.18	1.48	1.37
2	5	4554	7MG	C2-N1	4.15	1.47	1.37
4	9	1842	4AC	C4-N4	4.14	1.45	1.39
2	5	2526	7MG	C2-N1	4.14	1.47	1.37
2	5	4310	OMU	C4-N3	4.12	1.45	1.38
2	5	4624	OMU	C4-N3	4.06	1.45	1.38
2	5	4632	PSU	C1'-C5	-4.04	1.41	1.50
4	9	1806	M7A	C5-N7	4.01	1.49	1.39
2	5	4454	PSU	C1'-C5	-4.01	1.41	1.50
2	5	3901	B8K	C5-N7	4.00	1.46	1.39
2	5	1586	PSU	C1'-C5	-3.99	1.41	1.50
2	5	3733	PSU	C1'-C5	-3.99	1.41	1.50
2	5	4535	PSU	C1'-C5	-3.98	1.41	1.50
2	5	2512	PSU	C1'-C5	-3.97	1.41	1.50
2	5	4640	PSU	C1'-C5	-3.97	1.41	1.50
2	5	4504	PSU	C1'-C5	-3.97	1.41	1.50
3	8	14	OMU	C4-N3	3.96	1.45	1.38
2	5	3884	P7G	C2-N3	3.96	1.47	1.37
2	5	4694	B8K	C5-N7	3.96	1.46	1.39
2	5	2865	OMC	C6-N1	3.95	1.47	1.38
2	5	1681	PSU	C1'-C5	-3.95	1.41	1.50
4	9	174	OMC	C4-N4	3.95	1.43	1.33
2	5	1687	PSU	C1'-C5	-3.94	1.41	1.50
2	5	4297	PSU	C1'-C5	-3.94	1.41	1.50
2	5	2369	OMC	C6-N1	3.93	1.47	1.38
2	5	2808	OMC	C6-N1	3.93	1.47	1.38
2	5	3719	PSU	C1'-C5	-3.92	1.41	1.50
2	5	4540	OMC	C6-N1	3.91	1.47	1.38
2	5	4446	PSU	C1'-C5	-3.91	1.41	1.50
2	5	4694	B8K	C5-C6	3.90	1.53	1.43
2	5	3891	OMC	C6-N1	3.90	1.47	1.38
2	5	1609	7MG	C5-C6	3.90	1.53	1.43
2	5	3913	OMC	C6-N1	3.90	1.47	1.38
2	5	3903	BGH	C2-N1	3.90	1.47	1.37
4	9	1710	OMC	C4-N4	3.88	1.43	1.33
2	5	3903	BGH	O2'-C2'	-3.88	1.32	1.42
4	9	1703	OMC	C4-N4	3.88	1.43	1.33
2	5	2426	OMC	C6-N1	3.87	1.47	1.38
2	5	1913	P7G	C2-N3	3.87	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3901	B8K	C5-C6	3.87	1.53	1.43
2	5	3873	OMC	C6-N1	3.86	1.47	1.38
4	9	1337	4AC	C2-N1	3.85	1.48	1.40
4	9	1710	OMC	C2-N1	3.84	1.48	1.40
2	5	3705	OMC	C6-N1	3.84	1.47	1.38
2	5	4554	7MG	C5-C6	3.83	1.53	1.43
2	5	2526	7MG	C5-C6	3.82	1.53	1.43
2	5	4568	M7A	C5-N7	3.81	1.48	1.39
2	5	4198	I4U	C5-C4	3.80	1.48	1.43
4	9	116	OMU	C4-N3	3.79	1.45	1.38
4	9	1703	OMC	C2-N1	3.77	1.48	1.40
4	9	1842	4AC	C2-N1	3.77	1.48	1.40
4	9	517	OMC	C4-N4	3.77	1.42	1.33
4	9	1337	4AC	C5-C4	3.77	1.48	1.40
2	5	4675	B8T	C5-C4	3.77	1.48	1.40
4	9	174	OMC	C2-N1	3.76	1.48	1.40
2	5	4487	B8T	C5-C4	3.74	1.48	1.40
4	9	121	OMU	C4-N3	3.73	1.45	1.38
2	5	2301	E7G	C2-N1	3.73	1.46	1.37
2	5	1663	I4U	C5-C4	3.73	1.48	1.43
2	5	1801	E7G	C2-N1	3.72	1.46	1.37
2	5	3884	P7G	C5-C4	3.65	1.44	1.37
2	5	4419	1MA	C5-C6	3.65	1.53	1.43
2	5	3901	B8K	C2-N1	3.63	1.46	1.37
2	5	1326	1MA	C5-C6	3.63	1.53	1.43
2	5	3903	BGH	C5-N7	3.63	1.45	1.39
2	5	4407	PSU	C1'-C5	-3.62	1.41	1.50
4	9	174	OMC	C6-N1	3.61	1.46	1.38
2	5	1913	P7G	C6-N1	3.60	1.44	1.38
2	5	4694	B8K	C2-N1	3.58	1.46	1.37
4	9	1842	4AC	C5-C4	3.57	1.48	1.40
2	5	3768	PSU	C1'-C5	-3.57	1.42	1.50
4	9	668	A2M	C5-C4	-3.55	1.32	1.39
2	5	2526	7MG	C6-N1	3.52	1.45	1.38
2	5	4375	MHG	C6-N1	3.51	1.45	1.38
2	5	3884	P7G	C6-N1	3.51	1.44	1.38
2	5	1801	E7G	C5-C6	3.51	1.52	1.43
2	5	1609	7MG	O6-C6	-3.49	1.16	1.23
4	9	1850	MA6	C6-N6	3.49	1.47	1.36
2	5	4375	MHG	C5-C6	3.48	1.52	1.43
4	9	517	OMC	C6-N1	3.48	1.46	1.38
4	9	1710	OMC	C6-N1	3.47	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1913	P7G	C5-C4	3.46	1.44	1.37
2	5	4554	7MG	O6-C6	-3.45	1.17	1.23
2	5	2301	E7G	C5-C6	3.45	1.52	1.43
2	5	1609	7MG	C6-N1	3.44	1.45	1.38
4	9	1851	MA6	C6-N6	3.44	1.47	1.36
2	5	2526	7MG	O6-C6	-3.44	1.17	1.23
4	9	1678	A2M	O2'-C2'	3.43	1.51	1.42
4	9	484	A2M	O2'-C2'	3.43	1.51	1.42
4	9	644	OMG	C5-N7	-3.41	1.32	1.39
4	9	517	OMC	C2-N1	3.41	1.47	1.40
2	5	4359	E6G	O6-C6	3.40	1.40	1.35
2	5	3871	A2M	C5-N7	-3.40	1.32	1.39
4	9	509	OMG	C5-N7	-3.39	1.32	1.39
2	5	237	B9B	O6-C6	3.38	1.40	1.35
2	5	3829	A2M	C5-N7	-3.38	1.32	1.39
2	5	2758	B9B	O6-C6	3.36	1.40	1.35
2	5	1875	A2M	C5-N7	-3.36	1.32	1.39
4	9	166	A2M	O2'-C2'	3.36	1.51	1.42
2	5	1330	A2M	C5-N7	-3.35	1.32	1.39
2	5	1538	A2M	C5-N7	-3.35	1.32	1.39
4	9	668	A2M	O2'-C2'	3.34	1.51	1.42
2	5	4554	7MG	C6-N1	3.34	1.45	1.38
4	9	1243	PSU	C6-C5	3.33	1.39	1.35
2	5	1528	A2M	C5-N7	-3.33	1.32	1.39
2	5	398	A2M	C5-N7	-3.33	1.32	1.39
2	5	4527	A2M	C5-N7	-3.33	1.32	1.39
2	5	2367	A2M	C5-N7	-3.31	1.32	1.39
2	5	4487	B8T	C6-N1	3.31	1.46	1.38
2	5	1578	B9B	O6-C6	3.31	1.40	1.35
2	5	2301	E7G	C6-N1	3.31	1.45	1.38
2	5	3789	A2M	C5-C4	-3.30	1.32	1.39
4	9	159	A2M	O2'-C2'	3.29	1.51	1.42
2	5	2405	A2M	C5-N7	-3.29	1.32	1.39
4	9	1703	OMC	C6-N1	3.29	1.45	1.38
2	5	3722	A2M	C5-N7	-3.28	1.32	1.39
2	5	4575	A2M	C5-N7	-3.28	1.32	1.39
2	5	4533	B8W	O6-C6	3.27	1.40	1.35
2	5	3789	A2M	C5-N7	-3.27	1.32	1.39
2	5	4419	1MA	C5-N7	-3.27	1.32	1.39
2	5	1801	E7G	C6-N1	3.26	1.44	1.38
2	5	3901	B8K	C6-N1	3.25	1.44	1.38
2	5	1326	1MA	C5-N7	-3.25	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1875	A2M	C5-C4	-3.24	1.32	1.39
2	5	4675	B8T	C6-N1	3.23	1.45	1.38
2	5	3727	A2M	C5-N7	-3.22	1.32	1.39
2	5	4694	B8K	C71-N7	3.21	1.46	1.39
2	5	1330	A2M	C5-C4	-3.21	1.33	1.39
2	5	3829	A2M	C5-C4	-3.21	1.33	1.39
2	5	4694	B8K	C6-N1	3.21	1.44	1.38
2	5	2367	A2M	C5-C4	-3.20	1.33	1.39
2	5	3913	OMC	O2-C2	-3.20	1.17	1.23
2	5	4407	PSU	C4-C5	3.19	1.53	1.44
2	5	1352	P4U	C6-N1	3.19	1.45	1.38
4	9	159	A2M	C5-C4	-3.19	1.33	1.39
2	5	3705	OMC	O2-C2	-3.18	1.17	1.23
4	9	1031	A2M	O2'-C2'	3.18	1.50	1.42
2	5	1538	A2M	C5-C4	-3.17	1.33	1.39
4	9	484	A2M	C5-N7	-3.17	1.33	1.39
2	5	3768	PSU	C4-C5	3.17	1.53	1.44
4	9	1081	PSU	C6-C5	3.16	1.39	1.35
4	9	1031	A2M	C5-N7	-3.16	1.33	1.39
2	5	3871	A2M	C5-C4	-3.16	1.33	1.39
4	9	1703	OMC	O2-C2	-3.15	1.17	1.23
2	5	1528	A2M	C5-C4	-3.15	1.33	1.39
2	5	2426	OMC	O2-C2	-3.15	1.17	1.23
4	9	1031	A2M	C5-C4	-3.15	1.33	1.39
2	5	4575	A2M	C5-C4	-3.15	1.33	1.39
4	9	823	PSU	C6-C5	3.14	1.39	1.35
4	9	1832	6MZ	C8-N9	-3.14	1.31	1.37
4	9	27	A2M	C5-N7	-3.14	1.33	1.39
2	5	4198	I4U	C6-N1	3.14	1.45	1.38
4	9	568	E3C	C4-N3	3.13	1.53	1.48
2	5	2865	OMC	O2-C2	-3.13	1.17	1.23
4	9	1678	A2M	C5-N7	-3.13	1.33	1.39
4	9	27	A2M	C5-C4	-3.13	1.33	1.39
2	5	3722	A2M	C5-C4	-3.12	1.33	1.39
2	5	4476	B8W	O6-C6	3.12	1.40	1.35
2	5	2369	OMC	O2-C2	-3.12	1.17	1.23
2	5	3871	A2M	C8-N9	-3.11	1.31	1.37
2	5	3727	A2M	C5-C4	-3.11	1.33	1.39
2	5	4540	OMC	O2-C2	-3.11	1.17	1.23
2	5	3873	OMC	O2-C2	-3.11	1.18	1.23
2	5	2405	A2M	C5-C4	-3.11	1.33	1.39
2	5	2808	OMC	O2-C2	-3.10	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	159	A2M	C5-N7	-3.10	1.33	1.39
2	5	398	A2M	C5-C4	-3.10	1.33	1.39
2	5	1663	I4U	C6-N1	3.09	1.45	1.38
4	9	683	OMG	C5-N7	-3.09	1.33	1.39
2	5	3891	OMC	O2-C2	-3.08	1.18	1.23
2	5	1913	P7G	O6-C6	-3.08	1.18	1.23
2	5	3903	BGH	C2-N2	3.08	1.41	1.34
2	5	3901	B8K	C71-N7	3.08	1.46	1.39
2	5	1538	A2M	C8-N9	-3.07	1.32	1.37
4	9	1374	5MC	O2-C2	-3.07	1.18	1.23
2	5	4527	A2M	C5-C4	-3.07	1.33	1.39
4	9	668	A2M	C5-N7	-3.07	1.33	1.39
4	9	1337	4AC	C6-N1	3.06	1.45	1.38
4	9	1842	4AC	C6-N1	3.05	1.45	1.38
2	5	4601	UR3	O4-C4	-3.05	1.17	1.23
2	5	1870	UR3	O4-C4	-3.05	1.17	1.23
2	5	4534	UR3	O4-C4	-3.04	1.17	1.23
2	5	1687	PSU	C4-C5	3.03	1.52	1.44
4	9	568	E3C	C6-N1	3.03	1.45	1.38
4	9	1851	MA6	C5-N7	-3.03	1.33	1.39
4	9	119	PSU	C6-C5	3.01	1.38	1.35
2	5	1528	A2M	C8-N9	-3.01	1.32	1.37
4	9	116	OMU	O4-C4	-3.01	1.18	1.24
2	5	4133	B8W	O6-C6	3.01	1.39	1.35
4	9	121	OMU	O4-C4	-3.00	1.18	1.24
2	5	4535	PSU	C4-C5	3.00	1.52	1.44
3	8	14	OMU	O4-C4	-3.00	1.18	1.24
2	5	3884	P7G	O6-C6	-3.00	1.19	1.23
2	5	4446	PSU	C4-C5	3.00	1.52	1.44
2	5	1681	PSU	C4-C5	2.99	1.52	1.44
2	5	4575	A2M	C8-N9	-2.98	1.32	1.37
2	5	4694	B8K	O6-C6	-2.98	1.17	1.23
2	5	2512	PSU	C4-C5	2.97	1.52	1.44
2	5	3722	A2M	C8-N9	-2.97	1.32	1.37
2	5	4876	2MG	C5-C6	2.97	1.55	1.44
2	5	3789	A2M	C8-N9	-2.97	1.32	1.37
4	9	1710	OMC	O2-C2	-2.96	1.18	1.23
2	5	4504	PSU	C4-C5	2.95	1.52	1.44
2	5	2367	A2M	C8-N9	-2.95	1.32	1.37
2	5	1875	A2M	C8-N9	-2.95	1.32	1.37
2	5	1586	PSU	C4-C5	2.95	1.52	1.44
2	5	2405	A2M	C8-N9	-2.94	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	517	OMC	O2-C2	-2.94	1.18	1.23
2	5	3727	A2M	C8-N9	-2.94	1.32	1.37
4	9	27	A2M	O2'-C2'	2.94	1.50	1.42
2	5	4310	OMU	O4-C4	-2.93	1.18	1.24
2	5	4624	OMU	O4-C4	-2.93	1.18	1.24
2	5	3719	PSU	C4-C5	2.93	1.52	1.44
2	5	1521	2MG	C5-C6	2.93	1.55	1.44
2	5	4632	PSU	C4-C5	2.93	1.52	1.44
2	5	4454	PSU	C4-C5	2.93	1.52	1.44
2	5	3829	A2M	C8-N9	-2.93	1.32	1.37
3	8	14	OMU	C6-N1	2.92	1.45	1.38
2	5	4189	B8W	C5-C4	-2.92	1.33	1.39
4	9	166	A2M	C5-N7	-2.92	1.33	1.39
2	5	4297	PSU	C4-C5	2.92	1.52	1.44
4	9	1850	MA6	C8-N9	-2.91	1.32	1.37
4	9	484	A2M	C5-C4	-2.91	1.33	1.39
2	5	1330	A2M	C8-N9	-2.91	1.32	1.37
4	9	1832	6MZ	C5-C4	-2.91	1.33	1.39
2	5	2428	OMG	C5-N7	-2.90	1.33	1.39
2	5	3733	PSU	C4-C5	2.90	1.52	1.44
2	5	3901	B8K	O6-C6	-2.89	1.18	1.23
2	5	4640	PSU	C4-C5	2.89	1.52	1.44
2	5	4359	E6G	C5-C4	-2.89	1.33	1.39
2	5	398	A2M	C8-N9	-2.88	1.32	1.37
2	5	729	2MG	C5-C6	2.88	1.55	1.44
4	9	822	PSU	C6-C5	2.87	1.38	1.35
2	5	1629	OMG	C5-N7	-2.87	1.33	1.39
2	5	2054	OMG	C5-N7	-2.87	1.33	1.39
2	5	3903	BGH	O3'-C3'	2.87	1.49	1.43
4	9	1842	4AC	O2-C2	-2.87	1.18	1.23
2	5	3705	OMC	C5-C4	2.86	1.49	1.42
2	5	1578	B9B	C5-C4	-2.86	1.33	1.39
2	5	4498	OMG	C5-N7	-2.86	1.33	1.39
4	9	174	OMC	O2-C2	-2.85	1.18	1.23
4	9	166	A2M	C5-C4	-2.84	1.33	1.39
2	5	4310	OMU	C6-N1	2.84	1.44	1.38
2	5	237	B9B	C5-C4	-2.84	1.33	1.39
2	5	4374	OMG	C5-N7	-2.83	1.33	1.39
4	9	1337	4AC	O2-C2	-2.83	1.18	1.23
2	5	3913	OMC	C5-C4	2.83	1.49	1.42
2	5	4624	OMU	C6-N1	2.82	1.44	1.38
2	5	4641	OMG	C5-N7	-2.82	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1330	A2M	O2'-C2'	2.81	1.49	1.42
2	5	3727	A2M	O2'-C2'	2.81	1.49	1.42
2	5	4200	OMG	C5-N7	-2.81	1.33	1.39
2	5	4527	A2M	O2'-C2'	2.81	1.49	1.42
4	9	668	A2M	C8-N9	-2.81	1.32	1.37
2	5	4575	A2M	O2'-C2'	2.81	1.49	1.42
2	5	398	A2M	O2'-C2'	2.81	1.49	1.42
2	5	4527	A2M	C8-N9	-2.81	1.32	1.37
2	5	1538	A2M	O2'-C2'	2.80	1.49	1.42
2	5	1320	OMG	C5-N7	-2.80	1.33	1.39
2	5	1526	OMG	C5-N7	-2.80	1.33	1.39
2	5	3722	A2M	O2'-C2'	2.79	1.49	1.42
2	5	4498	OMG	C2-N1	2.79	1.44	1.37
2	5	2368	OMG	C2-N1	2.79	1.44	1.37
2	5	3829	A2M	O2'-C2'	2.79	1.49	1.42
2	5	1528	A2M	O2'-C2'	2.79	1.49	1.42
4	9	121	OMU	O2-C2	-2.79	1.18	1.23
2	5	1320	OMG	C2-N1	2.79	1.44	1.37
2	5	3891	OMC	C5-C4	2.78	1.49	1.42
2	5	373	OMG	C5-N7	-2.78	1.33	1.39
2	5	1875	A2M	O2'-C2'	2.78	1.49	1.42
2	5	3796	OMG	C5-N7	-2.78	1.33	1.39
2	5	2865	OMC	C5-C4	2.78	1.49	1.42
2	5	2369	OMC	C5-C4	2.78	1.49	1.42
2	5	2405	A2M	O2'-C2'	2.78	1.49	1.42
2	5	1521	2MG	C6-N1	2.78	1.44	1.38
4	9	1830	UR3	C6-N1	2.78	1.44	1.38
2	5	2758	B9B	C5-C4	-2.78	1.33	1.39
2	5	2808	OMC	C5-C4	2.77	1.49	1.42
2	5	2777	OMG	C2-N1	2.77	1.44	1.37
2	5	3796	OMG	C2-N1	2.77	1.44	1.37
2	5	4874	OMG	C2-N1	2.77	1.44	1.37
2	5	2367	A2M	O2'-C2'	2.77	1.49	1.42
2	5	1460	B8Q	O2-C2	-2.77	1.17	1.22
2	5	2384	B8W	O6-C6	2.77	1.39	1.35
2	5	4200	OMG	C2-N1	2.77	1.44	1.37
2	5	3786	5MC	O2-C2	-2.77	1.18	1.23
4	9	27	A2M	C8-N9	-2.77	1.32	1.37
2	5	1887	OMG	C5-N7	-2.76	1.33	1.39
4	9	814	5MU	O4-C4	-2.76	1.18	1.23
2	5	3873	OMC	C5-C4	2.76	1.49	1.42
2	5	3789	A2M	O2'-C2'	2.75	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4451	5MC	O2-C2	-2.74	1.18	1.23
4	9	1219	B8Q	O2-C2	-2.74	1.17	1.22
2	5	2777	OMG	C5-N7	-2.74	1.33	1.39
2	5	2426	OMC	C5-C4	2.74	1.49	1.42
2	5	4874	OMG	C5-N7	-2.74	1.33	1.39
2	5	729	2MG	C5-N7	-2.74	1.33	1.39
2	5	4627	OMG	C2-N1	2.73	1.44	1.37
2	5	4189	B8W	O6-C6	2.73	1.39	1.35
2	5	1681	PSU	O4'-C1'	-2.73	1.40	1.43
2	5	4339	5MC	O2-C2	-2.73	1.18	1.23
2	5	1887	OMG	C2-N1	2.73	1.44	1.37
2	5	2054	OMG	C2-N1	2.73	1.44	1.37
4	9	159	A2M	C8-N9	-2.72	1.32	1.37
4	9	1850	MA6	C5-N7	-2.72	1.33	1.39
2	5	1629	OMG	C2-N1	2.72	1.44	1.37
2	5	4133	B8W	C5-C4	-2.72	1.33	1.39
2	5	4476	B8W	C5-C4	-2.72	1.33	1.39
2	5	2368	OMG	C5-N7	-2.71	1.33	1.39
2	5	2384	B8W	C5-C4	-2.71	1.33	1.39
2	5	373	OMG	C2-N1	2.71	1.44	1.37
4	9	644	OMG	O6-C6	-2.71	1.18	1.23
2	5	1526	OMG	C2-N1	2.71	1.44	1.37
4	9	1031	A2M	C8-N9	-2.71	1.32	1.37
2	5	3727	A2M	O3'-C3'	-2.71	1.36	1.43
2	5	3871	A2M	O2'-C2'	2.71	1.49	1.42
2	5	4641	OMG	C2-N1	2.71	1.44	1.37
2	5	4540	OMC	C5-C4	2.71	1.49	1.42
4	9	1851	MA6	C8-N9	-2.70	1.32	1.37
2	5	1875	A2M	O3'-C3'	-2.69	1.36	1.43
2	5	3903	BGH	O6-C6	-2.69	1.18	1.23
4	9	1678	A2M	C5-C4	-2.69	1.34	1.39
2	5	2428	OMG	C2-N1	2.69	1.44	1.37
4	9	509	OMG	O6-C6	-2.69	1.18	1.23
4	9	1678	A2M	C8-N9	-2.69	1.32	1.37
2	5	4374	OMG	C2-N1	2.69	1.44	1.37
2	5	4627	OMG	C5-N7	-2.69	1.33	1.39
2	5	1330	A2M	O3'-C3'	-2.69	1.36	1.43
2	5	3829	A2M	O3'-C3'	-2.67	1.36	1.43
2	5	1887	OMG	O6-C6	-2.67	1.18	1.23
2	5	1320	OMG	O6-C6	-2.66	1.18	1.23
2	5	1521	2MG	C5-N7	-2.66	1.33	1.39
4	9	121	OMU	C6-N1	2.65	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	398	A2M	O3'-C3'	-2.65	1.36	1.43
2	5	2405	A2M	O3'-C3'	-2.65	1.36	1.43
2	5	1870	UR3	C6-N1	2.65	1.44	1.38
2	5	4575	A2M	O3'-C3'	-2.64	1.36	1.43
4	9	683	OMG	O6-C6	-2.64	1.18	1.23
2	5	4601	UR3	C6-N1	2.63	1.44	1.38
2	5	1538	A2M	O3'-C3'	-2.63	1.36	1.43
2	5	4675	B8T	O2-C2	-2.61	1.18	1.23
2	5	4374	OMG	O6-C6	-2.61	1.18	1.23
2	5	4876	2MG	C6-N1	2.61	1.43	1.38
2	5	1460	B8Q	C4-N3	-2.60	1.44	1.48
2	5	1801	E7G	O6-C6	-2.60	1.18	1.23
2	5	1526	OMG	O6-C6	-2.60	1.18	1.23
2	5	3871	A2M	O3'-C3'	-2.60	1.36	1.43
2	5	4487	B8T	O2-C2	-2.60	1.18	1.23
2	5	1526	OMG	C5-C6	2.59	1.54	1.44
2	5	3722	A2M	O3'-C3'	-2.59	1.36	1.43
2	5	2367	A2M	O3'-C3'	-2.59	1.36	1.43
2	5	1320	OMG	C6-N1	2.58	1.43	1.38
4	9	484	A2M	C8-N9	-2.58	1.32	1.37
4	9	1850	MA6	C5-C4	-2.58	1.34	1.39
2	5	373	OMG	O6-C6	-2.58	1.18	1.23
2	5	4527	A2M	O3'-C3'	-2.58	1.36	1.43
2	5	1528	A2M	O3'-C3'	-2.57	1.36	1.43
2	5	1629	OMG	O6-C6	-2.56	1.18	1.23
2	5	4876	2MG	C5-N7	-2.56	1.34	1.39
2	5	4200	OMG	O6-C6	-2.56	1.18	1.23
82	v	715	DDE	CD2-CG	2.56	1.41	1.36
2	5	4198	I4U	O4-C41	-2.56	1.41	1.47
2	5	2301	E7G	O6-C6	-2.56	1.18	1.23
2	5	4641	OMG	O6-C6	-2.56	1.18	1.23
2	5	4534	UR3	C6-N1	2.55	1.44	1.38
2	5	4641	OMG	C5-C6	2.55	1.53	1.44
2	5	2777	OMG	C5-C6	2.55	1.53	1.44
2	5	2777	OMG	C6-N1	2.55	1.43	1.38
4	9	814	5MU	O2-C2	-2.54	1.18	1.23
2	5	4533	B8W	C5-C4	-2.54	1.34	1.39
2	5	1663	I4U	O4-C41	-2.54	1.41	1.47
2	5	2368	OMG	C5-C6	2.54	1.53	1.44
2	5	4627	OMG	C5-C6	2.54	1.53	1.44
2	5	2758	B9B	C5-N7	-2.54	1.34	1.39
2	5	4498	OMG	C5-C6	2.54	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2054	OMG	O6-C6	-2.54	1.18	1.23
2	5	4627	OMG	O6-C6	-2.54	1.18	1.23
2	5	1578	B9B	C5-N7	-2.53	1.34	1.39
2	5	2368	OMG	C6-N1	2.52	1.43	1.38
2	5	2368	OMG	O6-C6	-2.52	1.18	1.23
2	5	4627	OMG	C6-N1	2.52	1.43	1.38
2	5	2777	OMG	O6-C6	-2.52	1.18	1.23
2	5	3903	BGH	C71-N7	2.52	1.45	1.39
2	5	4874	OMG	C6-N1	2.52	1.43	1.38
2	5	3796	OMG	C5-C6	2.51	1.53	1.44
2	5	3796	OMG	O6-C6	-2.51	1.18	1.23
2	5	4200	OMG	C5-C6	2.51	1.53	1.44
2	5	729	2MG	CM2-N2	-2.51	1.41	1.45
4	9	1851	MA6	C5-C4	-2.51	1.34	1.39
2	5	1320	OMG	C5-C6	2.51	1.53	1.44
2	5	2428	OMG	O6-C6	-2.51	1.18	1.23
2	5	729	2MG	C6-N1	2.50	1.43	1.38
2	5	4874	OMG	C5-C6	2.50	1.53	1.44
2	5	3903	BGH	C5-C4	2.50	1.46	1.38
2	5	373	OMG	C5-C6	2.50	1.53	1.44
2	5	4498	OMG	O6-C6	-2.50	1.18	1.23
2	5	1526	OMG	C6-N1	2.50	1.43	1.38
2	5	3796	OMG	C6-N1	2.50	1.43	1.38
2	5	4641	OMG	C6-N1	2.50	1.43	1.38
4	9	116	OMU	O2-C2	-2.49	1.18	1.23
2	5	1887	OMG	C6-N1	2.49	1.43	1.38
4	9	612	PSU	C6-C5	2.49	1.38	1.35
2	5	4874	OMG	O6-C6	-2.49	1.18	1.23
2	5	4374	OMG	C5-C6	2.49	1.53	1.44
2	5	1870	UR3	C5-C4	2.49	1.50	1.43
2	5	2054	OMG	C5-C6	2.49	1.53	1.44
4	9	509	OMG	C2-N1	2.49	1.43	1.37
2	5	4601	UR3	C5-C4	2.48	1.50	1.43
2	5	1629	OMG	C5-C6	2.48	1.53	1.44
2	5	2428	OMG	C5-C6	2.47	1.53	1.44
3	8	14	OMU	O2-C2	-2.47	1.18	1.23
4	9	683	OMG	C2-N1	2.47	1.43	1.37
2	5	2790	B9H	C6-N1	2.46	1.43	1.38
4	9	1832	6MZ	C4-N9	-2.46	1.32	1.37
2	5	4534	UR3	C5-C4	2.46	1.50	1.43
2	5	4876	2MG	CM2-N2	-2.46	1.41	1.45
2	5	4374	OMG	C6-N1	2.46	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	2428	OMG	C6-N1	2.46	1.43	1.38
4	9	683	OMG	C4-N9	-2.45	1.31	1.38
2	5	4200	OMG	C6-N1	2.45	1.43	1.38
2	5	2054	OMG	C6-N1	2.45	1.43	1.38
2	5	4498	OMG	C6-N1	2.45	1.43	1.38
2	5	1629	OMG	C6-N1	2.44	1.43	1.38
2	5	4359	E6G	C5-N7	-2.43	1.34	1.39
4	9	644	OMG	C4-N9	-2.42	1.31	1.38
2	5	1887	OMG	C5-C6	2.42	1.53	1.44
2	5	4224	6MZ	C5-N7	-2.42	1.34	1.39
2	5	4375	MHG	O6-C6	-2.42	1.19	1.23
2	5	237	B9B	C5-N7	-2.42	1.34	1.39
2	5	4601	UR3	C4-N3	2.42	1.46	1.40
2	5	3789	A2M	O3'-C3'	-2.41	1.37	1.43
4	9	116	OMU	C6-N1	2.41	1.43	1.38
2	5	373	OMG	C6-N1	2.40	1.43	1.38
2	5	4310	OMU	O2-C2	-2.40	1.18	1.23
2	5	4534	UR3	C4-N3	2.40	1.46	1.40
2	5	1870	UR3	C4-N3	2.39	1.46	1.40
4	9	644	OMG	C2-N1	2.39	1.43	1.37
4	9	1832	6MZ	C6-N1	-2.38	1.31	1.35
2	5	4224	6MZ	C5-C4	-2.36	1.34	1.39
2	5	4310	OMU	C5-C4	2.36	1.48	1.43
2	5	4624	OMU	O2-C2	-2.36	1.18	1.23
3	8	14	OMU	C5-C4	2.35	1.48	1.43
4	9	159	A2M	C5'-C4'	2.33	1.58	1.51
4	9	166	A2M	C8-N9	-2.33	1.33	1.37
2	5	373	OMG	C4-N9	-2.32	1.32	1.38
4	9	668	A2M	C4-N9	-2.32	1.32	1.37
4	9	1830	UR3	O2-C2	-2.31	1.18	1.22
4	9	683	OMG	C5-C6	2.31	1.53	1.44
4	9	1830	UR3	O4-C4	-2.30	1.18	1.23
2	5	4087	5MU	O4-C4	-2.29	1.19	1.23
4	9	484	A2M	C3'-C4'	2.28	1.58	1.53
4	9	509	OMG	C5-C6	2.28	1.52	1.44
4	9	644	OMG	C5-C6	2.27	1.52	1.44
2	5	4087	5MU	O2-C2	-2.25	1.18	1.23
4	9	1678	A2M	C3'-C4'	2.25	1.58	1.53
4	9	1678	A2M	C5'-C4'	2.25	1.58	1.51
2	5	4624	OMU	C5-C4	2.25	1.48	1.43
4	9	121	OMU	C5-C4	2.24	1.48	1.43
4	9	683	OMG	C6-N1	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	1248	B8N	O4-C4	-2.24	1.18	1.23
2	5	3789	A2M	C3'-C4'	2.22	1.58	1.53
2	5	1320	OMG	C4-N9	-2.22	1.32	1.38
4	9	1850	MA6	C8-N7	2.21	1.35	1.31
2	5	1521	2MG	CM2-N2	-2.20	1.41	1.45
2	5	1887	OMG	C4-N9	-2.19	1.32	1.38
2	5	2054	OMG	C4-N9	-2.18	1.32	1.38
4	9	644	OMG	C6-N1	2.18	1.42	1.38
2	5	4874	OMG	C4-N9	-2.18	1.32	1.38
2	5	2368	OMG	C4-N9	-2.16	1.32	1.38
2	5	1578	B9B	C8-N9	-2.16	1.33	1.37
2	5	1864	B8H	O2-C2	-2.16	1.19	1.23
2	5	4300	B8H	O2-C2	-2.15	1.19	1.23
4	9	1842	4AC	O7-C7	-2.15	1.18	1.23
2	5	4641	OMG	C4-N9	-2.15	1.32	1.38
4	9	27	A2M	O5'-C5'	-2.15	1.39	1.44
4	9	668	A2M	O5'-C5'	-2.15	1.39	1.44
2	5	2777	OMG	C4-N9	-2.14	1.32	1.38
2	5	4200	OMG	C4-N9	-2.13	1.32	1.38
4	9	509	OMG	C6-N1	2.13	1.42	1.38
4	9	568	E3C	O2-C2	-2.12	1.18	1.22
2	5	4627	OMG	C4-N9	-2.12	1.32	1.38
2	5	1526	OMG	C4-N9	-2.12	1.32	1.38
2	5	3789	A2M	C4-N9	-2.12	1.33	1.37
2	5	4374	OMG	C4-N9	-2.11	1.32	1.38
4	9	166	A2M	C3'-C4'	2.10	1.58	1.53
2	5	4359	E6G	C8-N9	-2.10	1.33	1.37
4	9	484	A2M	C5'-C4'	2.09	1.58	1.51
2	5	2758	B9B	C8-N9	-2.09	1.33	1.37
2	5	237	B9B	C8-N9	-2.09	1.33	1.37
2	5	3796	OMG	C4-N9	-2.07	1.32	1.38
4	9	1248	B8N	O2-C2	-2.06	1.18	1.22
2	5	1663	I4U	O2-C2	-2.06	1.19	1.23
4	9	822	PSU	O4'-C1'	-2.05	1.41	1.43
4	9	27	A2M	C5'-C4'	2.05	1.58	1.51
2	5	2790	B9H	O2-C2	-2.05	1.18	1.22
4	9	166	A2M	C5'-C4'	2.05	1.58	1.51
2	5	4498	OMG	C4-N9	-2.04	1.32	1.38
4	9	1031	A2M	O5'-C5'	-2.03	1.39	1.44
2	5	3903	BGH	C3'-C2'	2.02	1.57	1.52
4	9	509	OMG	C4-N9	-2.02	1.32	1.38
2	5	3829	A2M	C4-N9	-2.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	9	159	A2M	C3'-C4'	2.01	1.58	1.53
2	5	1330	A2M	C4-N9	-2.00	1.33	1.37

All (960) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9	1806	M7A	C5-C6-N6	12.77	145.55	123.74
4	9	1832	6MZ	C4-N9-C8	12.53	119.31	105.73
2	5	4568	M7A	C5-C6-N6	12.30	144.75	123.74
2	5	4087	5MU	C5-C4-N3	12.06	125.61	115.31
4	9	814	5MU	C5-C4-N3	11.64	125.25	115.31
4	9	1806	M7A	N6-C6-N1	-10.95	94.37	118.35
2	5	4568	M7A	N6-C6-N1	-10.58	95.18	118.35
4	9	1832	6MZ	N9-C8-N7	-10.11	100.08	113.91
2	5	4087	5MU	C5-C6-N1	-9.99	113.06	123.34
4	9	814	5MU	C5-C6-N1	-9.81	113.24	123.34
4	9	1850	MA6	N1-C6-N6	-9.78	106.39	117.08
4	9	1851	MA6	N1-C6-N6	-9.28	106.93	117.08
4	9	1832	6MZ	C5-C6-N1	7.57	126.26	118.20
2	5	1521	2MG	C2-N3-C4	7.18	120.94	112.04
2	5	4476	B8W	O6-C6-C5	7.13	125.91	116.97
2	5	1864	B8H	C4-N3-C2	-6.70	118.67	127.35
2	5	4300	B8H	C4-N3-C2	-6.70	118.67	127.35
2	5	1629	OMG	C1'-N9-C8	-6.63	107.81	126.70
2	5	4375	MHG	C2-N3-C4	6.56	120.17	112.04
2	5	2384	B8W	C5-C4-N3	-6.52	119.85	127.19
2	5	3884	P7G	C4-C5-N7	6.48	110.09	106.67
2	5	1913	P7G	C4-C5-N7	6.47	110.08	106.67
2	5	4533	B8W	O6-C6-C5	6.46	125.07	116.97
2	5	729	2MG	C2-N3-C4	6.45	120.04	112.04
2	5	2758	B9B	C5-C4-N3	-6.45	119.94	127.19
2	5	2428	OMG	C1'-N9-C8	-6.44	108.37	126.70
2	5	4533	B8W	C5-C4-N3	-6.44	119.95	127.19
2	5	4876	2MG	C2-N3-C4	6.36	119.92	112.04
2	5	237	B9B	C5-C4-N3	-6.34	120.06	127.19
2	5	4874	OMG	C1'-N9-C8	-6.33	108.67	126.70
2	5	4133	B8W	C5-C4-N3	-6.32	120.09	127.19
2	5	3796	OMG	C1'-N9-C8	-6.29	108.78	126.70
2	5	4359	E6G	C5-C4-N3	-6.26	120.14	127.19
2	5	1887	OMG	C1'-N9-C8	-6.20	109.06	126.70
2	5	4200	OMG	C1'-N9-C8	-6.20	109.06	126.70
2	5	1578	B9B	C5-C4-N3	-6.19	120.22	127.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9	1832	6MZ	N3-C4-N9	6.19	137.28	127.08
2	5	4374	OMG	C1'-N9-C8	-6.14	109.21	126.70
2	5	4189	B8W	C5-C4-N3	-6.14	120.28	127.19
4	9	166	A2M	N3-C2-N1	-6.08	119.09	128.60
4	9	568	E3C	C1'-N1-C2	6.04	127.19	116.99
2	5	4498	OMG	C1'-N9-C8	-6.04	109.50	126.70
2	5	1864	B8H	N3-C2-N1	5.95	121.57	115.14
2	5	2054	OMG	C1'-N9-C8	-5.93	109.83	126.70
2	5	1526	OMG	C1'-N9-C8	-5.92	109.84	126.70
2	5	1460	B8Q	N3-C2-N1	5.91	124.08	117.13
2	5	4641	OMG	C1'-N9-C8	-5.90	109.91	126.70
2	5	2301	E7G	C4-C5-N7	5.90	110.16	104.91
2	5	2368	OMG	C1'-N9-C8	-5.89	109.92	126.70
2	5	2777	OMG	C1'-N9-C8	-5.88	109.95	126.70
2	5	4476	B8W	C5-C4-N3	-5.88	120.58	127.19
4	9	1806	M7A	N3-C2-N1	-5.87	119.42	128.60
4	9	1031	A2M	N3-C2-N1	-5.79	119.54	128.60
2	5	4300	B8H	N3-C2-N1	5.79	121.39	115.14
4	9	1678	A2M	C5-C4-N3	-5.76	119.24	126.75
2	5	373	OMG	C1'-N9-C8	-5.71	110.44	126.70
2	5	4627	OMG	C1'-N9-C8	-5.71	110.45	126.70
2	5	4189	B8W	N2-C2-N3	5.70	126.12	117.25
2	5	1521	2MG	C5-C4-N3	-5.70	119.22	128.46
4	9	27	A2M	C5-C4-N3	-5.69	119.33	126.75
2	5	4476	B8W	N2-C2-N3	5.66	126.06	117.25
4	9	1850	MA6	N1-C2-N3	-5.64	119.78	128.60
4	9	1851	MA6	N1-C2-N3	-5.63	119.80	128.60
4	9	484	A2M	N3-C2-N1	-5.61	119.83	128.60
4	9	1678	A2M	N3-C2-N1	-5.61	119.83	128.60
2	5	2384	B8W	N2-C2-N3	5.61	125.97	117.25
4	9	27	A2M	N3-C2-N1	-5.60	119.84	128.60
2	5	1320	OMG	C1'-N9-C8	-5.59	110.78	126.70
2	5	4568	M7A	N3-C2-N1	-5.59	119.86	128.60
2	5	729	2MG	C5-C4-N3	-5.59	119.40	128.46
2	5	1801	E7G	C4-C5-N7	5.57	109.87	104.91
2	5	4694	B8K	C5-C6-N1	5.57	120.81	110.99
2	5	1875	A2M	N3-C2-N1	-5.56	119.90	128.60
4	9	166	A2M	C5-C4-N3	-5.55	119.51	126.75
2	5	4533	B8W	N2-C2-N3	5.53	125.85	117.25
2	5	4133	B8W	N2-C2-N3	5.51	125.83	117.25
4	9	1832	6MZ	N1-C2-N3	-5.51	119.98	128.60
4	9	159	A2M	N3-C2-N1	-5.51	119.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	398	A2M	N6-C6-N1	-5.50	106.31	118.35
2	5	2367	A2M	N6-C6-N1	-5.50	106.32	118.35
4	9	1031	A2M	C5-C4-N3	-5.49	119.58	126.75
2	5	1538	A2M	N6-C6-N1	-5.49	106.32	118.35
2	5	4375	MHG	C4-C5-N7	5.48	109.79	104.91
2	5	4224	6MZ	N1-C2-N3	-5.47	120.04	128.60
2	5	3727	A2M	N3-C2-N1	-5.46	120.06	128.60
2	5	3789	A2M	N3-C2-N1	-5.46	120.07	128.60
4	9	668	A2M	N3-C2-N1	-5.45	120.07	128.60
2	5	1528	A2M	N3-C2-N1	-5.45	120.08	128.60
2	5	1538	A2M	N3-C2-N1	-5.45	120.08	128.60
2	5	1460	B8Q	C31-N3-C4	5.44	122.45	114.25
2	5	2367	A2M	N3-C2-N1	-5.44	120.09	128.60
2	5	3722	A2M	N6-C6-N1	-5.44	106.44	118.35
2	5	2405	A2M	N6-C6-N1	-5.44	106.44	118.35
2	5	3789	A2M	N6-C6-N1	-5.44	106.44	118.35
2	5	1629	OMG	C1'-N9-C4	5.43	142.64	126.50
2	5	3903	BGH	C5-C6-N1	5.43	120.56	110.99
2	5	1528	A2M	N6-C6-N1	-5.43	106.47	118.35
2	5	4575	A2M	N6-C6-N1	-5.42	106.47	118.35
2	5	398	A2M	N3-C2-N1	-5.41	120.14	128.60
2	5	3727	A2M	N6-C6-N1	-5.40	106.52	118.35
2	5	1875	A2M	N6-C6-N1	-5.39	106.54	118.35
2	5	2405	A2M	N3-C2-N1	-5.39	120.18	128.60
2	5	3829	A2M	N3-C2-N1	-5.38	120.18	128.60
2	5	4575	A2M	N3-C2-N1	-5.38	120.18	128.60
2	5	1330	A2M	N6-C6-N1	-5.37	106.59	118.35
2	5	4527	A2M	N3-C2-N1	-5.36	120.21	128.60
2	5	3901	B8K	C5-C6-N1	5.35	120.42	110.99
2	5	2790	B9H	C31-N3-C2	5.35	123.89	117.21
4	9	1219	B8Q	N3-C2-N1	5.34	123.41	117.13
2	5	3829	A2M	N6-C6-N1	-5.34	106.67	118.35
3	8	14	OMU	C4-N3-C2	-5.32	119.57	126.58
2	5	3722	A2M	N3-C2-N1	-5.31	120.29	128.60
2	5	1330	A2M	N3-C2-N1	-5.30	120.32	128.60
2	5	2428	OMG	C1'-N9-C4	5.29	142.23	126.50
2	5	3871	A2M	N3-C2-N1	-5.28	120.33	128.60
4	9	509	OMG	C5-C4-N3	-5.28	119.89	128.46
2	5	3871	A2M	N6-C6-N1	-5.28	106.78	118.35
4	9	121	OMU	C4-N3-C2	-5.27	119.63	126.58
2	5	4527	A2M	N6-C6-N1	-5.26	106.84	118.35
2	5	3871	A2M	C5-C4-N3	-5.25	119.90	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4310	OMU	C4-N3-C2	-5.25	119.65	126.58
2	5	2405	A2M	C5-C4-N3	-5.25	119.90	126.75
4	9	159	A2M	C5-C4-N3	-5.25	119.90	126.75
2	5	4224	6MZ	C5-C4-N3	-5.23	119.92	126.75
2	5	4876	2MG	C5-C4-N3	-5.23	119.98	128.46
2	5	1528	A2M	C5-C4-N3	-5.23	119.93	126.75
2	5	2367	A2M	C5-C4-N3	-5.21	119.95	126.75
2	5	1330	A2M	C5-C4-N3	-5.21	119.95	126.75
2	5	398	A2M	C5-C4-N3	-5.21	119.96	126.75
2	5	3727	A2M	C5-C4-N3	-5.19	119.97	126.75
2	5	1326	1MA	N1-C2-N3	-5.19	119.83	126.00
4	9	1850	MA6	C5-C6-N6	5.19	134.33	125.30
2	5	4527	A2M	C5-C4-N3	-5.18	120.00	126.75
2	5	3722	A2M	C5-C4-N3	-5.15	120.03	126.75
2	5	4575	A2M	C5-C4-N3	-5.13	120.06	126.75
2	5	3829	A2M	C5-C4-N3	-5.13	120.06	126.75
4	9	116	OMU	C4-N3-C2	-5.09	119.86	126.58
2	5	4624	OMU	C4-N3-C2	-5.09	119.87	126.58
4	9	1248	B8N	C5-C4-N3	5.09	125.59	116.17
4	9	1219	B8Q	C31-N3-C4	5.07	121.89	114.25
2	5	237	B9B	O6-C6-C5	5.07	122.98	116.57
2	5	1875	A2M	C5-C4-N3	-5.06	120.15	126.75
2	5	3789	A2M	C5-C4-N3	-5.04	120.17	126.75
2	5	4189	B8W	O6-C6-C5	5.04	123.29	116.97
4	9	484	A2M	C5-C4-N3	-5.03	120.18	126.75
2	5	4419	1MA	N1-C2-N3	-5.03	120.02	126.00
4	9	159	A2M	N6-C6-N1	-5.02	107.36	118.35
2	5	1538	A2M	C5-C4-N3	-5.02	120.20	126.75
2	5	3796	OMG	C1'-N9-C4	5.01	141.39	126.50
2	5	1801	E7G	C5-C6-N1	5.01	119.82	110.99
4	9	644	OMG	C5-C4-N3	-5.01	120.34	128.46
4	9	814	5MU	N3-C2-N1	5.00	121.53	114.89
4	9	668	A2M	C5-C4-N3	-5.00	120.22	126.75
4	9	1031	A2M	N6-C6-N1	-4.99	107.42	118.35
2	5	1629	OMG	C5-C4-N3	-4.98	120.38	128.46
2	5	2301	E7G	C5-C6-N1	4.98	119.77	110.99
2	5	1326	1MA	C5-C4-N3	-4.97	119.85	127.26
2	5	2428	OMG	C5-C4-N3	-4.97	120.40	128.46
4	9	1243	PSU	N1-C2-N3	4.96	120.75	115.13
2	5	2526	7MG	C5-C6-N1	4.96	119.73	110.99
2	5	4133	B8W	O6-C6-C5	4.96	123.19	116.97
2	5	4375	MHG	C5-C6-N1	4.96	119.72	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4087	5MU	C4-N3-C2	-4.95	120.94	127.35
2	5	1609	7MG	C5-C6-N1	4.95	119.71	110.99
2	5	4874	OMG	C1'-N9-C4	4.94	141.18	126.50
4	9	1851	MA6	C5-C6-N6	4.91	133.86	125.30
4	9	1850	MA6	C5-C4-N3	-4.91	120.35	126.75
2	5	4568	M7A	C4-N9-C1'	-4.89	114.98	126.60
4	9	484	A2M	N6-C6-N1	-4.89	107.63	118.35
2	5	4087	5MU	O4-C4-C5	-4.89	119.24	124.90
4	9	822	PSU	C4-N3-C2	-4.89	119.30	126.34
2	5	4419	1MA	C5-C4-N3	-4.88	119.97	127.26
2	5	4554	7MG	C5-C6-N1	4.88	119.59	110.99
2	5	4200	OMG	C1'-N9-C4	4.88	141.00	126.50
4	9	822	PSU	N1-C2-N3	4.88	120.65	115.13
2	5	4498	OMG	C1'-N9-C4	4.86	140.95	126.50
2	5	4694	B8K	C4-C5-N7	4.86	109.23	104.91
2	5	4374	OMG	C1'-N9-C4	4.86	140.93	126.50
4	9	166	A2M	N6-C6-N1	-4.86	107.72	118.35
4	9	814	5MU	O4-C4-C5	-4.81	119.32	124.90
4	9	1851	MA6	C5-C4-N3	-4.81	120.48	126.75
2	5	1887	OMG	C1'-N9-C4	4.80	140.76	126.50
4	9	668	A2M	N6-C6-N1	-4.79	107.85	118.35
2	5	4568	M7A	N3-C4-N9	4.79	132.92	126.87
4	9	1219	B8Q	O2-C2-N3	-4.77	115.94	122.95
2	5	4476	B8W	N9-C8-N7	-4.75	107.41	113.91
2	5	4601	UR3	C4-N3-C2	-4.75	120.09	124.56
2	5	3901	B8K	C4-C5-N7	4.75	109.13	104.91
2	5	4454	PSU	C4-N3-C2	-4.74	119.50	126.34
2	5	4876	2MG	C2-N1-C6	-4.73	119.04	124.48
2	5	3903	BGH	C2-N3-C4	4.72	120.72	112.30
4	9	1806	M7A	N3-C4-N9	4.71	132.82	126.87
2	5	4640	PSU	C4-N3-C2	-4.71	119.56	126.34
2	5	4498	OMG	C5-C4-N3	-4.70	120.84	128.46
2	5	1526	OMG	C1'-N9-C4	4.70	140.46	126.50
2	5	2054	OMG	C1'-N9-C4	4.70	140.45	126.50
4	9	814	5MU	C4-N3-C2	-4.69	121.28	127.35
4	9	1832	6MZ	C5-N7-C8	4.68	110.17	103.51
2	5	3722	A2M	C5-C6-N6	4.68	133.62	123.43
2	5	4200	OMG	C5-C4-N3	-4.68	120.87	128.46
2	5	1681	PSU	C4-N3-C2	-4.68	119.60	126.34
2	5	1538	A2M	C5-C6-N6	4.67	133.60	123.43
2	5	4189	B8W	N9-C8-N7	-4.67	107.52	113.91
2	5	398	A2M	C5-C6-N6	4.67	133.59	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4641	OMG	C5-C4-N3	-4.66	120.90	128.46
2	5	4534	UR3	C4-N3-C2	-4.66	120.18	124.56
4	9	27	A2M	N6-C6-N1	-4.65	108.16	118.35
2	5	2512	PSU	C4-N3-C2	-4.65	119.64	126.34
4	9	823	PSU	C4-N3-C2	-4.65	119.64	126.34
2	5	2367	A2M	C5-C6-N6	4.64	133.53	123.43
2	5	4374	OMG	C5-C4-N3	-4.64	120.94	128.46
4	9	668	A2M	N9-C8-N7	-4.64	107.57	113.91
2	5	2758	B9B	O6-C6-C5	4.63	122.44	116.57
2	5	3796	OMG	C5-C4-N3	-4.63	120.95	128.46
2	5	2054	OMG	C5-C4-N3	-4.62	120.96	128.46
2	5	4632	PSU	C4-N3-C2	-4.62	119.68	126.34
4	9	1081	PSU	N1-C2-N3	4.62	120.36	115.13
4	9	1678	A2M	N6-C6-N1	-4.62	108.24	118.35
2	5	3719	PSU	C4-N3-C2	-4.62	119.69	126.34
4	9	823	PSU	N1-C2-N3	4.61	120.36	115.13
2	5	4694	B8K	C2-N3-C4	4.61	120.52	112.30
2	5	1578	B9B	O6-C6-C5	4.61	122.41	116.57
2	5	1687	PSU	C4-N3-C2	-4.61	119.70	126.34
2	5	4446	PSU	C4-N3-C2	-4.61	119.70	126.34
2	5	1526	OMG	C5-C4-N3	-4.60	120.99	128.46
2	5	2368	OMG	C1'-N9-C4	4.60	140.18	126.50
2	5	4641	OMG	C1'-N9-C4	4.60	140.18	126.50
2	5	1586	PSU	C4-N3-C2	-4.60	119.71	126.34
2	5	4297	PSU	C4-N3-C2	-4.58	119.73	126.34
4	9	568	E3C	O2-C2-N3	-4.58	116.27	122.07
2	5	2405	A2M	C5-C6-N6	4.58	133.39	123.43
2	5	1875	A2M	C5-C6-N6	4.58	133.39	123.43
2	5	3789	A2M	N9-C8-N7	-4.57	107.66	113.91
2	5	1528	A2M	C5-C6-N6	4.57	133.38	123.43
2	5	4575	A2M	C5-C6-N6	4.57	133.37	123.43
2	5	1330	A2M	C5-C6-N6	4.57	133.37	123.43
2	5	2368	OMG	C5-C4-N3	-4.56	121.07	128.46
2	5	3901	B8K	C2-N3-C4	4.55	120.41	112.30
2	5	3903	BGH	C4-C5-N7	4.55	108.96	104.91
2	5	2777	OMG	C1'-N9-C4	4.55	140.02	126.50
2	5	4504	PSU	C4-N3-C2	-4.55	119.79	126.34
2	5	4407	PSU	C4-N3-C2	-4.55	119.79	126.34
4	9	1219	B8Q	C1'-N1-C2	4.55	124.66	116.99
2	5	1521	2MG	C2-N1-C6	-4.54	119.26	124.48
2	5	3727	A2M	C5-C6-N6	4.54	133.30	123.43
2	5	4535	PSU	C4-N3-C2	-4.54	119.80	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1887	OMG	C5-C4-N3	-4.53	121.11	128.46
2	5	1538	A2M	N9-C8-N7	-4.53	107.72	113.91
2	5	2777	OMG	C5-C4-N3	-4.53	121.12	128.46
2	5	4874	OMG	C5-C4-N3	-4.53	121.12	128.46
2	5	3871	A2M	C5-C6-N6	4.51	133.25	123.43
2	5	1320	OMG	C5-C4-N3	-4.51	121.14	128.46
4	9	1850	MA6	N9-C8-N7	-4.51	107.75	113.91
4	9	1248	B8N	C4-N3-C2	-4.51	119.76	125.46
2	5	4627	OMG	C5-C4-N3	-4.50	121.16	128.46
2	5	1801	E7G	C2-N3-C4	4.49	120.30	112.30
2	5	1870	UR3	C4-N3-C2	-4.49	120.33	124.56
2	5	4087	5MU	N3-C2-N1	4.49	120.85	114.89
2	5	3727	A2M	N9-C8-N7	-4.49	107.77	113.91
2	5	4627	OMG	C1'-N9-C4	4.48	139.80	126.50
2	5	3829	A2M	C5-C6-N6	4.47	133.16	123.43
4	9	612	PSU	C4-N3-C2	-4.47	119.90	126.34
2	5	4527	A2M	C5-C6-N6	4.47	133.15	123.43
2	5	2367	A2M	N9-C8-N7	-4.46	107.81	113.91
2	5	3733	PSU	C4-N3-C2	-4.46	119.92	126.34
2	5	2526	7MG	C2-N3-C4	4.46	120.24	112.30
2	5	4359	E6G	N9-C8-N7	-4.45	107.83	113.91
2	5	2301	E7G	C2-N3-C4	4.45	120.22	112.30
2	5	4632	PSU	N1-C2-N3	4.44	120.16	115.13
4	9	683	OMG	C5-C4-N3	-4.44	121.27	128.46
4	9	1243	PSU	C4-N3-C2	-4.43	119.95	126.34
2	5	1875	A2M	N9-C8-N7	-4.43	107.85	113.91
4	9	1832	6MZ	C1'-N9-C8	-4.43	117.13	127.14
2	5	373	OMG	C5-C4-N3	-4.42	121.29	128.46
2	5	1528	A2M	N9-C8-N7	-4.42	107.87	113.91
2	5	3829	A2M	N9-C8-N7	-4.41	107.89	113.91
2	5	1609	7MG	C2-N3-C4	4.41	120.15	112.30
2	5	237	B9B	N9-C8-N7	-4.40	107.89	113.91
4	9	159	A2M	N9-C8-N7	-4.40	107.90	113.91
2	5	4575	A2M	N9-C8-N7	-4.39	107.91	113.91
4	9	1832	6MZ	C5-C4-N9	-4.39	100.68	105.78
2	5	2405	A2M	N9-C8-N7	-4.39	107.91	113.91
2	5	1578	B9B	N9-C8-N7	-4.38	107.92	113.91
2	5	4133	B8W	N9-C8-N7	-4.38	107.92	113.91
2	5	1320	OMG	C1'-N9-C4	4.38	139.50	126.50
4	9	1081	PSU	C4-N3-C2	-4.37	120.04	126.34
2	5	3789	A2M	C5-C6-N6	4.36	132.93	123.43
2	5	4554	7MG	C2-N3-C4	4.36	120.07	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3871	A2M	N9-C8-N7	-4.36	107.95	113.91
4	9	683	OMG	C2-N3-C4	4.35	120.05	112.30
2	5	1330	A2M	N9-C8-N7	-4.34	107.97	113.91
2	5	1320	OMG	C2-N3-C4	4.34	120.04	112.30
2	5	729	2MG	C2-N1-C6	-4.34	119.48	124.48
2	5	398	A2M	N9-C8-N7	-4.34	107.98	113.91
4	9	612	PSU	N1-C2-N3	4.33	120.03	115.13
2	5	2758	B9B	N9-C8-N7	-4.32	108.01	113.91
2	5	4224	6MZ	N9-C8-N7	-4.31	108.01	113.91
2	5	373	OMG	C1'-N9-C4	4.30	139.28	126.50
2	5	2512	PSU	N1-C2-N3	4.29	119.99	115.13
2	5	4498	OMG	C2-N3-C4	4.28	119.92	112.30
2	5	3768	PSU	C4-N3-C2	-4.27	120.18	126.34
2	5	4641	OMG	C2-N3-C4	4.27	119.90	112.30
4	9	1851	MA6	N9-C8-N7	-4.26	108.08	113.91
2	5	4527	A2M	N9-C8-N7	-4.26	108.09	113.91
2	5	2368	OMG	C2-N3-C4	4.26	119.89	112.30
2	5	1629	OMG	C2-N3-C4	4.25	119.87	112.30
4	9	1031	A2M	N9-C8-N7	-4.25	108.11	113.91
2	5	2384	B8W	N9-C8-N7	-4.24	108.11	113.91
2	5	2428	OMG	C2-N3-C4	4.24	119.85	112.30
2	5	4200	OMG	C2-N3-C4	4.24	119.85	112.30
2	5	2777	OMG	C2-N3-C4	4.23	119.84	112.30
2	5	4627	OMG	C2-N3-C4	4.23	119.83	112.30
2	5	1526	OMG	C2-N3-C4	4.23	119.83	112.30
2	5	3722	A2M	N9-C8-N7	-4.22	108.14	113.91
2	5	4446	PSU	N1-C2-N3	4.22	119.91	115.13
4	9	1031	A2M	C5-C6-N6	4.21	132.60	123.43
2	5	4504	PSU	N1-C2-N3	4.21	119.90	115.13
4	9	1830	UR3	C4-N3-C2	-4.21	120.60	124.56
4	9	1830	UR3	C1'-N1-C2	4.20	124.08	116.99
2	5	2054	OMG	C2-N3-C4	4.20	119.78	112.30
2	5	4454	PSU	N1-C2-N3	4.19	119.88	115.13
2	5	4374	OMG	C2-N3-C4	4.19	119.77	112.30
2	5	4640	PSU	N1-C2-N3	4.19	119.87	115.13
2	5	1687	PSU	N1-C2-N3	4.18	119.86	115.13
2	5	2384	B8W	O6-C6-C5	4.17	122.20	116.97
2	5	1887	OMG	C2-N3-C4	4.17	119.73	112.30
2	5	4297	PSU	N1-C2-N3	4.17	119.85	115.13
2	5	1586	PSU	N1-C2-N3	4.17	119.85	115.13
4	9	509	OMG	C2-N3-C4	4.16	119.71	112.30
2	5	3796	OMG	C2-N3-C4	4.16	119.71	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4533	B8W	N9-C8-N7	-4.16	108.23	113.91
4	9	484	A2M	C5-C6-N6	4.15	132.47	123.43
2	5	4694	B8K	C72-C71-N7	4.15	125.11	118.86
2	5	4874	OMG	C2-N3-C4	4.14	119.68	112.30
2	5	1681	PSU	N1-C2-N3	4.14	119.82	115.13
2	5	3719	PSU	N1-C2-N3	4.14	119.82	115.13
2	5	373	OMG	C2-N3-C4	4.14	119.67	112.30
4	9	644	OMG	C2-N3-C4	4.14	119.67	112.30
2	5	4535	PSU	N1-C2-N3	4.13	119.81	115.13
2	5	4476	B8W	O6-C6-N1	-4.13	113.32	119.01
2	5	2301	E7G	C5-C4-N3	-4.09	120.33	128.13
2	5	4407	PSU	N1-C2-N3	4.09	119.76	115.13
4	9	166	A2M	N9-C8-N7	-4.08	108.33	113.91
4	9	159	A2M	C5-C6-N6	4.08	132.32	123.43
2	5	1801	E7G	C5-C4-N3	-4.07	120.37	128.13
4	9	121	OMU	N3-C2-N1	4.07	120.29	114.89
2	5	3733	PSU	N1-C2-N3	4.07	119.74	115.13
4	9	27	A2M	N9-C8-N7	-4.06	108.35	113.91
2	5	1326	1MA	C2-N3-C4	4.03	120.33	112.41
2	5	2526	7MG	C5-C4-N3	-4.02	120.47	128.13
2	5	1609	7MG	C5-C4-N3	-4.01	120.49	128.13
2	5	4087	5MU	C5M-C5-C6	-3.99	117.52	122.85
4	9	568	E3C	C31-N3-C2	3.98	122.55	117.44
2	5	4419	1MA	C2-N3-C4	3.97	120.21	112.41
2	5	2758	B9B	N3-C4-N9	3.96	132.49	126.99
2	5	3901	B8K	C72-C71-N7	3.94	124.78	118.86
2	5	4224	6MZ	C4-C5-C6	3.94	119.86	116.81
4	9	484	A2M	N9-C8-N7	-3.93	108.54	113.91
2	5	3768	PSU	N1-C2-N3	3.92	119.57	115.13
4	9	166	A2M	C5-C6-N6	3.92	131.96	123.43
2	5	2384	B8W	N3-C4-N9	3.91	132.42	126.99
2	5	4554	7MG	C5-C4-N3	-3.85	120.79	128.13
2	5	373	OMG	N9-C8-N7	-3.85	106.14	113.39
4	9	1851	MA6	C2-N1-C6	3.85	120.84	111.75
4	9	119	PSU	N1-C2-N3	3.85	119.49	115.13
4	9	668	A2M	C5-C6-N6	3.84	131.79	123.43
4	9	1850	MA6	C2-N1-C6	3.84	120.83	111.75
4	9	166	A2M	C2-N3-C4	3.83	120.81	111.75
3	8	14	OMU	N3-C2-N1	3.82	119.96	114.89
2	5	4087	5MU	C5M-C5-C4	3.82	122.97	118.77
2	5	4310	OMU	N3-C2-N1	3.81	119.95	114.89
2	5	4476	B8W	C5-N7-C8	3.80	108.92	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4375	MHG	C5-C4-N3	-3.80	120.88	128.13
2	5	4375	MHG	C2-N1-C6	-3.80	120.11	124.48
2	5	2368	OMG	N9-C8-N7	-3.77	106.30	113.39
4	9	1678	A2M	C2-N3-C4	3.76	120.62	111.75
2	5	2777	OMG	N9-C8-N7	-3.73	106.36	113.39
2	5	4641	OMG	N9-C8-N7	-3.73	106.36	113.39
4	9	568	E3C	C6-N1-C2	-3.73	118.45	121.79
4	9	1031	A2M	C2-N3-C4	3.72	120.54	111.75
4	9	27	A2M	C2-N3-C4	3.71	120.52	111.75
2	5	1887	OMG	N9-C8-N7	-3.71	106.40	113.39
2	5	4624	OMU	N3-C2-N1	3.70	119.81	114.89
2	5	4874	OMG	N9-C8-N7	-3.70	106.42	113.39
2	5	729	2MG	N9-C4-N3	3.70	133.37	125.94
4	9	27	A2M	C5-C6-N6	3.70	131.48	123.43
4	9	1678	A2M	C5-C6-N6	3.69	131.45	123.43
4	9	119	PSU	C4-N3-C2	-3.67	121.06	126.34
2	5	1528	A2M	C2-N3-C4	3.67	120.41	111.75
2	5	1460	B8Q	O2-C2-N3	-3.65	117.58	122.95
2	5	2367	A2M	C2-N3-C4	3.65	120.37	111.75
2	5	3903	BGH	C72-C71-N7	3.65	124.35	118.86
2	5	1578	B9B	N3-C4-N9	3.65	132.05	126.99
2	5	237	B9B	N3-C4-N9	3.65	132.05	126.99
2	5	4451	5MC	C5-C6-N1	-3.64	119.59	123.34
2	5	2405	A2M	C2-N3-C4	3.64	120.36	111.75
2	5	4200	OMG	N9-C8-N7	-3.64	106.54	113.39
2	5	2054	OMG	N9-C8-N7	-3.63	106.55	113.39
2	5	1320	OMG	N9-C8-N7	-3.63	106.55	113.39
2	5	3727	A2M	C2-N3-C4	3.63	120.32	111.75
4	9	1832	6MZ	C5-C4-N3	-3.62	122.03	126.75
2	5	398	A2M	C2-N3-C4	3.62	120.30	111.75
2	5	1526	OMG	N9-C8-N7	-3.61	106.58	113.39
2	5	1875	A2M	C2-N3-C4	3.60	120.27	111.75
2	5	1538	A2M	C2-N3-C4	3.60	120.26	111.75
2	5	4374	OMG	N9-C8-N7	-3.60	106.61	113.39
4	9	1678	A2M	N3-C4-N9	3.60	133.01	127.08
2	5	4198	I4U	C5-C4-N3	-3.59	119.45	124.91
2	5	4575	A2M	C2-N3-C4	3.59	120.23	111.75
2	5	3796	OMG	N9-C8-N7	-3.59	106.64	113.39
2	5	3789	A2M	C2-N3-C4	3.58	120.22	111.75
2	5	1330	A2M	C2-N3-C4	3.58	120.21	111.75
2	5	4627	OMG	N9-C8-N7	-3.58	106.65	113.39
2	5	3829	A2M	C2-N3-C4	3.58	120.20	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3871	A2M	C2-N3-C4	3.57	120.18	111.75
2	5	4533	B8W	N3-C4-N9	3.56	131.93	126.99
4	9	1374	5MC	O2-C2-N3	-3.56	116.54	122.33
4	9	116	OMU	N3-C2-N1	3.55	119.60	114.89
2	5	1521	2MG	N9-C4-N3	3.55	133.07	125.94
2	5	4694	B8K	C5-C4-N3	-3.55	121.37	128.13
2	5	4527	A2M	C2-N3-C4	3.55	120.14	111.75
4	9	159	A2M	C2-N3-C4	3.55	120.13	111.75
2	5	4133	B8W	N3-C4-N9	3.54	131.91	126.99
2	5	1352	P4U	C5-C4-N3	-3.54	119.52	124.91
2	5	4694	B8K	C5-C4-N9	3.54	110.94	106.35
2	5	3722	A2M	C2-N3-C4	3.54	120.11	111.75
2	5	3903	BGH	C2'-C1'-N9	-3.54	106.94	114.14
2	5	3903	BGH	C5-C4-N9	3.53	110.94	106.35
4	9	1850	MA6	C4-C5-C6	3.53	119.83	115.88
4	9	1851	MA6	C4-C5-C6	3.53	119.83	115.88
4	9	484	A2M	C2-N3-C4	3.53	120.08	111.75
4	9	1832	6MZ	C2-N3-C4	3.52	120.07	111.75
2	5	4476	B8W	N1-C2-N3	-3.51	119.91	125.42
2	5	4224	6MZ	C2-N3-C4	3.51	120.05	111.75
2	5	4498	OMG	N9-C8-N7	-3.51	106.79	113.39
2	5	4300	B8H	C5-C4-N3	3.49	124.48	116.58
2	5	4359	E6G	N3-C4-N9	3.49	131.84	126.99
2	5	4189	B8W	N3-C4-N9	3.49	131.83	126.99
4	9	166	A2M	N3-C4-N9	3.48	132.82	127.08
2	5	4359	E6G	N3-C2-N1	-3.48	119.95	125.42
4	9	1678	A2M	N9-C8-N7	-3.48	109.15	113.91
2	5	4533	B8W	O6-C6-N1	-3.47	114.22	119.01
2	5	4359	E6G	N2-C2-N3	3.47	122.65	117.25
4	9	1850	MA6	C2-N3-C4	3.47	119.94	111.75
2	5	3901	B8K	C5-C4-N3	-3.46	121.54	128.13
4	9	1850	MA6	C5-N7-C8	3.45	108.41	103.51
3	8	14	OMU	C5-C4-N3	3.45	120.00	114.84
2	5	1864	B8H	C5-C4-N3	3.45	124.38	116.58
4	9	1806	M7A	C4-N9-C1'	-3.44	118.43	126.60
4	9	814	5MU	C5M-C5-C6	-3.44	118.26	122.85
2	5	4533	B8W	C5-N7-C8	3.43	108.39	103.51
4	9	1851	MA6	C2-N3-C4	3.43	119.86	111.75
4	9	668	A2M	C2-N3-C4	3.43	119.86	111.75
2	5	3901	B8K	C5-C4-N9	3.43	110.80	106.35
2	5	2758	B9B	N3-C2-N1	-3.42	120.05	125.42
4	9	116	OMU	C5-C4-N3	3.42	119.95	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4876	2MG	CM2-N2-C2	-3.41	116.32	123.86
2	5	4339	5MC	C5-C6-N1	-3.41	119.83	123.34
2	5	1578	B9B	N3-C2-N1	-3.40	120.08	125.42
2	5	1629	OMG	N9-C4-N3	3.40	132.77	125.94
2	5	4640	PSU	C6-C5-C4	3.40	120.58	118.20
2	5	4568	M7A	C2-N3-C4	3.40	119.78	111.75
4	9	121	OMU	C5-C4-N3	3.39	119.91	114.84
2	5	237	B9B	N3-C2-N1	-3.39	120.10	125.42
2	5	1663	I4U	C5-C4-N3	-3.39	119.76	124.91
4	9	509	OMG	N9-C4-N3	3.39	132.74	125.94
2	5	4189	B8W	C5-N7-C8	3.37	108.30	103.51
2	5	1629	OMG	N9-C8-N7	-3.37	107.04	113.39
2	5	4454	PSU	C6-C5-C4	3.37	120.55	118.20
2	5	3903	BGH	C5-C4-N3	-3.36	121.72	128.13
4	9	1806	M7A	C2-N3-C4	3.36	119.68	111.75
2	5	2428	OMG	N9-C4-N3	3.35	132.66	125.94
2	5	4632	PSU	C6-C5-C4	3.35	120.54	118.20
4	9	683	OMG	N9-C8-N7	-3.33	107.12	113.39
2	5	4504	PSU	C6-C5-C4	3.32	120.52	118.20
2	5	2384	B8W	C61-O6-C6	-3.32	113.92	117.21
2	5	4189	B8W	N1-C2-N3	-3.32	120.21	125.42
4	9	27	A2M	N3-C4-N9	3.31	132.54	127.08
2	5	4310	OMU	C5-C4-N3	3.30	119.78	114.84
2	5	2428	OMG	N9-C8-N7	-3.30	107.18	113.39
2	5	3786	5MC	C5-C6-N1	-3.29	119.95	123.34
2	5	4375	MHG	C5-C4-N9	3.27	110.60	106.35
4	9	644	OMG	C2-N1-C6	-3.27	119.13	125.10
2	5	4624	OMU	C5-C4-N3	3.26	119.72	114.84
2	5	3871	A2M	N3-C4-N9	3.26	132.46	127.08
4	9	1851	MA6	C5-N7-C8	3.25	108.12	103.51
4	9	116	OMU	O4-C4-C5	-3.24	119.46	125.16
2	5	4133	B8W	C5-N7-C8	3.24	108.12	103.51
4	9	1374	5MC	C5-C6-N1	-3.24	120.00	123.34
2	5	237	B9B	C5-N7-C8	3.23	108.10	103.51
2	5	3719	PSU	C6-C5-C4	3.23	120.45	118.20
2	5	4359	E6G	C5-N7-C8	3.23	108.09	103.51
2	5	4535	PSU	C6-C5-C4	3.22	120.45	118.20
4	9	509	OMG	C2-N1-C6	-3.22	119.23	125.10
2	5	4694	B8K	N9-C8-N7	3.21	107.64	103.33
2	5	4133	B8W	N1-C2-N3	-3.21	120.38	125.42
4	9	644	OMG	N9-C8-N7	-3.21	107.34	113.39
4	9	644	OMG	N9-C4-N3	3.21	132.38	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4224	6MZ	C5-N7-C8	3.21	108.06	103.51
2	5	3901	B8K	N9-C8-N7	3.19	107.61	103.33
2	5	1538	A2M	C5-N7-C8	3.19	108.04	103.51
2	5	1326	1MA	C1'-N9-C4	-3.19	117.04	126.50
2	5	1681	PSU	C6-C5-C4	3.18	120.42	118.20
2	5	3727	A2M	C5-N7-C8	3.18	108.03	103.51
2	5	4224	6MZ	N3-C4-N9	3.18	132.32	127.08
2	5	398	A2M	C5-N7-C8	3.17	108.02	103.51
2	5	1864	B8H	O2-C2-N1	-3.17	119.30	122.87
2	5	1528	A2M	N3-C4-N9	3.17	132.31	127.08
2	5	4632	PSU	C6-N1-C2	-3.17	119.44	122.68
2	5	1609	7MG	C4-C5-N7	3.16	109.92	105.53
2	5	2384	B8W	N1-C2-N3	-3.16	120.46	125.42
2	5	2526	7MG	C4-C5-N7	3.16	109.92	105.53
2	5	3789	A2M	N3-C4-N9	3.16	132.28	127.08
2	5	1528	A2M	C5-N7-C8	3.15	107.98	103.51
4	9	1248	B8N	N3-C2-N1	3.14	121.20	116.76
2	5	1578	B9B	C5-N7-C8	3.14	107.97	103.51
2	5	2405	A2M	C5-N7-C8	3.14	107.97	103.51
2	5	4554	7MG	C4-C5-N7	3.13	109.88	105.53
2	5	1586	PSU	C6-C5-C4	3.13	120.39	118.20
2	5	2405	A2M	N3-C4-N9	3.13	132.24	127.08
4	9	1830	UR3	C6-N1-C2	-3.13	118.99	121.79
2	5	2367	A2M	C5-N7-C8	3.12	107.95	103.51
4	9	822	PSU	O2-C2-N1	-3.12	119.35	122.79
2	5	1330	A2M	N3-C4-N9	3.11	132.21	127.08
2	5	4300	B8H	O2-C2-N1	-3.11	119.37	122.87
2	5	4554	7MG	C5-C4-N9	3.11	110.38	106.35
2	5	3829	A2M	N3-C4-N9	3.11	132.20	127.08
2	5	1875	A2M	N3-C4-N9	3.10	132.19	127.08
2	5	4533	B8W	N1-C2-N3	-3.09	120.56	125.42
2	5	2512	PSU	C6-C5-C4	3.09	120.36	118.20
2	5	4200	OMG	N9-C4-N3	3.09	132.15	125.94
2	5	4527	A2M	N3-C4-N9	3.09	132.17	127.08
2	5	4446	PSU	C6-C5-C4	3.09	120.36	118.20
2	5	2758	B9B	C5-N7-C8	3.08	107.89	103.51
2	5	3871	A2M	C5-N7-C8	3.08	107.89	103.51
2	5	2367	A2M	N3-C4-N9	3.08	132.16	127.08
2	5	4374	OMG	N9-C4-N3	3.08	132.12	125.94
2	5	3727	A2M	N3-C4-N9	3.08	132.15	127.08
2	5	2526	7MG	C5-C4-N9	3.08	110.34	106.35
2	5	1887	OMG	N9-C4-N3	3.07	132.11	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1330	A2M	C5-N7-C8	3.07	107.88	103.51
2	5	3829	A2M	C5-N7-C8	3.07	107.87	103.51
2	5	4575	A2M	N3-C4-N9	3.07	132.14	127.08
2	5	4476	B8W	C4-C5-N7	-3.06	106.89	110.62
4	9	1031	A2M	N3-C4-N9	3.06	132.12	127.08
4	9	159	A2M	N3-C4-N9	3.06	132.12	127.08
2	5	1875	A2M	C5-N7-C8	3.05	107.84	103.51
4	9	1031	A2M	C5-N7-C8	3.05	107.84	103.51
2	5	4419	1MA	C1'-N9-C4	-3.05	117.45	126.50
2	5	1609	7MG	C5-C4-N9	3.05	110.30	106.35
2	5	4527	A2M	C5-N7-C8	3.04	107.82	103.51
2	5	3796	OMG	N9-C4-N3	3.03	132.03	125.94
2	5	3722	A2M	C5-N7-C8	3.03	107.81	103.51
2	5	3789	A2M	C5-N7-C8	3.03	107.81	103.51
2	5	398	A2M	N3-C4-N9	3.03	132.07	127.08
4	9	159	A2M	C5-N7-C8	3.03	107.81	103.51
2	5	3733	PSU	C6-C5-C4	3.02	120.31	118.20
2	5	2384	B8W	C5-N7-C8	3.02	107.81	103.51
2	5	4874	OMG	N9-C4-N3	3.02	132.01	125.94
2	5	4575	A2M	C5-N7-C8	3.02	107.80	103.51
2	5	4297	PSU	C6-C5-C4	3.01	120.30	118.20
2	5	3733	PSU	C6-N1-C2	-3.01	119.61	122.68
2	5	4498	OMG	N9-C4-N3	3.00	131.97	125.94
2	5	3903	BGH	N9-C8-N7	3.00	107.35	103.33
2	5	1801	E7G	C5-C4-N9	3.00	110.24	106.35
2	5	1687	PSU	C6-C5-C4	2.99	120.29	118.20
2	5	1538	A2M	N3-C4-N9	2.99	132.01	127.08
4	9	568	E3C	C1'-N1-C6	-2.98	114.35	120.84
2	5	2428	OMG	C2-N1-C6	-2.98	119.67	125.10
2	5	1629	OMG	C2-N1-C6	-2.97	119.68	125.10
2	5	3722	A2M	N3-C4-N9	2.97	131.98	127.08
2	5	4504	PSU	C6-N1-C2	-2.97	119.65	122.68
2	5	4297	PSU	C6-N1-C2	-2.96	119.65	122.68
2	5	2054	OMG	C2-N1-C6	-2.96	119.69	125.10
4	9	612	PSU	O2-C2-N1	-2.96	119.53	122.79
2	5	4535	PSU	C6-N1-C2	-2.95	119.67	122.68
2	5	4641	OMG	N9-C4-N3	2.95	131.85	125.94
4	9	159	A2M	C2'-C1'-N9	-2.94	108.58	113.53
2	5	4359	E6G	C61-O6-C6	-2.94	114.73	117.59
2	5	3796	OMG	C2-N1-C6	-2.94	119.74	125.10
2	5	4641	OMG	C2-N1-C6	-2.94	119.74	125.10
2	5	4446	PSU	C6-N1-C2	-2.93	119.68	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9	1337	4AC	C5-C4-N3	-2.93	117.87	122.59
2	5	1326	1MA	C1'-N9-C8	2.93	135.04	126.70
2	5	2512	PSU	C6-N1-C2	-2.93	119.69	122.68
2	5	3768	PSU	C6-N1-C2	-2.93	119.69	122.68
4	9	1806	M7A	C71-N7-C5	-2.93	112.77	124.01
4	9	668	A2M	C5-N7-C8	2.92	107.65	103.51
4	9	27	A2M	C5-N7-C8	2.92	107.65	103.51
2	5	2777	OMG	N9-C4-N3	2.91	131.79	125.94
4	9	814	5MU	C1'-N1-C2	2.91	122.84	117.57
2	5	2054	OMG	N9-C4-N3	2.91	131.78	125.94
2	5	4200	OMG	C2-N1-C6	-2.91	119.80	125.10
2	5	2368	OMG	C2-N1-C6	-2.90	119.80	125.10
2	5	2301	E7G	C5-C4-N9	2.90	110.11	106.35
2	5	1526	OMG	N9-C4-N3	2.90	131.76	125.94
2	5	4224	6MZ	C9-N6-C6	-2.90	120.38	122.87
2	5	1586	PSU	C6-N1-C2	-2.90	119.72	122.68
4	9	509	OMG	N9-C8-N7	-2.89	107.95	113.39
2	5	4876	2MG	N9-C4-N3	2.89	131.74	125.94
2	5	1526	OMG	C2-N1-C6	-2.88	119.85	125.10
2	5	4627	OMG	C2-N1-C6	-2.88	119.85	125.10
2	5	1887	OMG	C2-N1-C6	-2.87	119.86	125.10
2	5	2777	OMG	C2-N1-C6	-2.87	119.86	125.10
4	9	166	A2M	C5-N7-C8	2.87	107.59	103.51
4	9	1219	B8Q	C6-N1-C2	-2.87	119.22	121.79
4	9	1842	4AC	C6-C5-C4	2.86	120.47	116.96
2	5	3789	A2M	C2'-C1'-N9	-2.86	108.72	113.53
2	5	373	OMG	C2-N1-C6	-2.86	119.89	125.10
2	5	2526	7MG	O6-C6-C5	-2.85	120.55	127.54
2	5	4476	B8W	N3-C4-N9	2.85	130.94	126.99
4	9	1851	MA6	N3-C4-N9	2.85	131.78	127.08
2	5	4498	OMG	C2-N1-C6	-2.85	119.90	125.10
4	9	683	OMG	C2-N1-C6	-2.85	119.91	125.10
2	5	3789	A2M	O4'-C1'-N9	2.85	113.67	108.06
2	5	373	OMG	N9-C4-N3	2.84	131.63	125.94
2	5	1801	E7G	O6-C6-C5	-2.84	120.58	127.54
2	5	4874	OMG	C2-N1-C6	-2.84	119.93	125.10
2	5	4374	OMG	C2-N1-C6	-2.83	119.93	125.10
2	5	1609	7MG	O6-C6-C5	-2.83	120.59	127.54
4	9	1248	B8N	C31-N3-C4	2.83	121.48	117.31
2	5	4310	OMU	O4-C4-C5	-2.83	120.18	125.16
2	5	3719	PSU	C6-N1-C2	-2.83	119.79	122.68
2	5	4554	7MG	O6-C6-C5	-2.83	120.61	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4876	2MG	N9-C8-N7	-2.82	108.08	113.39
2	5	4627	OMG	N9-C4-N3	2.81	131.59	125.94
2	5	4375	MHG	O6-C6-C5	-2.81	120.65	127.54
2	5	2368	OMG	N9-C4-N3	2.81	131.57	125.94
2	5	2301	E7G	O6-C6-C5	-2.80	120.67	127.54
4	9	814	5MU	O2-C2-N3	-2.80	116.28	121.50
2	5	4407	PSU	C6-N1-C2	-2.80	119.82	122.68
2	5	4419	1MA	N9-C8-N7	-2.79	108.13	113.39
4	9	484	A2M	C5-N7-C8	2.78	107.46	103.51
2	5	4624	OMU	O4-C4-C5	-2.78	120.27	125.16
4	9	116	OMU	C1'-N1-C2	2.78	122.61	117.57
2	5	1681	PSU	C6-N1-C2	-2.78	119.84	122.68
2	5	2301	E7G	C2-N1-C6	-2.78	120.03	125.10
2	5	1687	PSU	C6-N1-C2	-2.78	119.84	122.68
2	5	1320	OMG	N9-C4-N3	2.77	131.51	125.94
2	5	4359	E6G	O6-C6-N1	2.77	123.86	120.00
2	5	1521	2MG	C5-C6-N1	2.76	120.19	113.19
4	9	814	5MU	C5M-C5-C4	2.75	121.79	118.77
2	5	1320	OMG	C2-N1-C6	-2.75	120.09	125.10
2	5	1609	7MG	C2-N1-C6	-2.75	120.09	125.10
2	5	1521	2MG	N9-C8-N7	-2.74	108.23	113.39
3	8	14	OMU	O4-C4-C5	-2.74	120.34	125.16
2	5	4568	M7A	C71-N7-C5	-2.74	113.50	124.01
2	5	2526	7MG	C2-N1-C6	-2.74	120.11	125.10
2	5	4419	1MA	C1'-N9-C8	2.74	134.48	126.70
2	5	2301	E7G	N9-C4-N3	2.73	129.55	125.47
4	9	683	OMG	C5-C6-N1	2.73	120.12	113.19
4	9	1842	4AC	C5-C4-N3	-2.73	118.21	122.59
2	5	3789	A2M	C4-N9-C8	2.72	108.68	105.73
4	9	119	PSU	O2-C2-N1	-2.72	119.79	122.79
2	5	4640	PSU	C6-N1-C2	-2.72	119.90	122.68
2	5	1326	1MA	N9-C8-N7	-2.72	108.27	113.39
2	5	1801	E7G	C2-N1-C6	-2.71	120.15	125.10
2	5	729	2MG	N9-C8-N7	-2.71	108.28	113.39
2	5	1887	OMG	C5-C6-N1	2.71	120.07	113.19
2	5	4627	OMG	C5-C6-N1	2.71	120.07	113.19
4	9	119	PSU	C6-N1-C2	-2.71	119.91	122.68
2	5	2054	OMG	C5-C6-N1	2.71	120.07	113.19
4	9	644	OMG	C5-C6-N1	2.70	120.06	113.19
2	5	4641	OMG	C5-C6-N1	2.70	120.05	113.19
4	9	121	OMU	O4-C4-C5	-2.70	120.41	125.16
4	9	1850	MA6	C4-C5-N7	-2.70	107.33	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2777	OMG	C5-C6-N1	2.69	120.03	113.19
2	5	3903	BGH	C6-C5-C4	-2.69	117.07	122.62
4	9	668	A2M	N3-C4-N9	2.69	131.52	127.08
2	5	2368	OMG	C5-C6-N1	2.69	120.02	113.19
4	9	1243	PSU	C6-N1-C2	-2.68	119.94	122.68
2	5	4200	OMG	C5-C6-N1	2.68	120.00	113.19
4	9	1832	6MZ	C6-C5-N7	2.68	135.29	132.39
2	5	373	OMG	C5-C6-N1	2.68	120.00	113.19
2	5	1629	OMG	C5-C6-N1	2.68	120.00	113.19
4	9	823	PSU	O2-C2-N1	-2.68	119.84	122.79
2	5	4876	2MG	C5-C6-N1	2.68	119.99	113.19
4	9	644	OMG	O6-C6-C5	-2.68	119.50	126.60
2	5	2428	OMG	C5-C6-N1	2.68	119.98	113.19
2	5	3796	OMG	C5-C6-N1	2.67	119.96	113.19
2	5	4454	PSU	C6-N1-C2	-2.67	119.96	122.68
4	9	1243	PSU	O2-C2-N1	-2.66	119.86	122.79
2	5	4374	OMG	C5-C6-N1	2.66	119.95	113.19
4	9	1337	4AC	C6-C5-C4	2.66	120.21	116.96
2	5	4874	OMG	C5-C6-N1	2.65	119.92	113.19
2	5	4300	B8H	O4-C4-N3	-2.65	115.04	120.12
4	9	484	A2M	N3-C4-N9	2.65	131.44	127.08
2	5	1526	OMG	C5-C6-N1	2.65	119.91	113.19
2	5	4189	B8W	O6-C6-N1	-2.65	115.36	119.01
2	5	4632	PSU	O2-C2-N1	-2.65	119.88	122.79
2	5	4498	OMG	C5-C6-N1	2.64	119.91	113.19
2	5	4675	B8T	C6-C5-C4	2.64	120.19	116.96
2	5	4087	5MU	O2-C2-N1	-2.64	119.28	122.79
2	5	4297	PSU	O2-C2-N1	-2.64	119.89	122.79
2	5	729	2MG	C5-C6-N1	2.63	119.88	113.19
2	5	1320	OMG	C5-C6-N1	2.63	119.88	113.19
2	5	4568	M7A	C5-C4-N3	-2.63	120.45	126.62
2	5	1801	E7G	N9-C4-N3	2.63	129.40	125.47
4	9	27	A2M	C3'-C2'-C1'	2.63	107.83	102.89
4	9	509	OMG	C5-C6-N1	2.62	119.85	113.19
2	5	1887	OMG	O6-C6-C5	-2.62	119.66	126.60
2	5	4533	B8W	C4-C5-N7	-2.61	107.43	110.62
2	5	4535	PSU	O2-C2-N1	-2.61	119.92	122.79
2	5	4359	E6G	C2-N1-C6	2.60	120.06	115.93
2	5	1521	2MG	O6-C6-C5	-2.59	119.73	126.60
4	9	1850	MA6	N3-C4-N9	2.59	131.35	127.08
2	5	4087	5MU	O4-C4-N3	-2.59	115.16	120.12
2	5	4189	B8W	C4-N9-C8	2.59	108.53	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1460	B8Q	C31-N3-C2	2.58	121.54	117.79
2	5	4375	MHG	N1-C2-N3	-2.58	119.96	123.95
2	5	4694	B8K	C2-N1-C6	-2.57	120.41	125.10
2	5	1864	B8H	O4-C4-N3	-2.56	115.20	120.12
2	5	1320	OMG	O6-C6-C5	-2.54	119.85	126.60
2	5	4694	B8K	C6-C5-C4	-2.54	117.38	122.62
2	5	4504	PSU	O2-C2-N1	-2.54	119.99	122.79
4	9	814	5MU	C6-N1-C2	-2.54	118.73	121.30
2	5	1538	A2M	C4-N9-C8	2.54	108.48	105.73
2	5	1521	2MG	N1-C2-N3	-2.54	120.03	123.95
2	5	2368	OMG	C8-N7-C5	2.53	108.82	104.24
2	5	1687	PSU	O2-C2-N1	-2.53	120.01	122.79
4	9	683	OMG	N9-C4-N3	2.52	131.00	125.94
4	9	683	OMG	O6-C6-C5	-2.52	119.92	126.60
4	9	1081	PSU	O2-C2-N1	-2.52	120.02	122.79
2	5	4476	B8W	C2-N1-C6	2.51	119.92	115.93
4	9	668	A2M	C4-N9-C8	2.51	108.45	105.73
2	5	2758	B9B	C2-N1-C6	2.51	119.92	115.93
2	5	3796	OMG	O6-C6-C5	-2.51	119.94	126.60
2	5	237	B9B	C2-N1-C6	2.51	119.92	115.93
4	9	1081	PSU	C6-N1-C2	-2.50	120.12	122.68
2	5	1609	7MG	N9-C8-N7	2.50	106.96	103.38
4	9	1031	A2M	C2'-C1'-N9	-2.50	109.32	113.53
2	5	1609	7MG	N9-C4-N3	2.50	129.21	125.47
4	9	1678	A2M	C5-N7-C8	2.50	107.06	103.51
2	5	2777	OMG	O6-C6-C5	-2.50	119.98	126.60
4	9	509	OMG	O6-C6-C5	-2.49	119.99	126.60
2	5	2526	7MG	N9-C4-N3	2.49	129.19	125.47
2	5	3903	BGH	C2-N1-C6	-2.49	120.55	125.10
2	5	4641	OMG	C8-N7-C5	2.48	108.74	104.24
2	5	4200	OMG	O6-C6-C5	-2.48	120.01	126.60
2	5	2054	OMG	O6-C6-C5	-2.48	120.02	126.60
2	5	729	2MG	O6-C6-C5	-2.48	120.03	126.60
2	5	3901	B8K	C6-C5-C4	-2.48	117.52	122.62
2	5	4554	7MG	C2-N1-C6	-2.47	120.59	125.10
4	9	1219	B8Q	C31-N3-C2	2.47	121.38	117.79
2	5	2301	E7G	C8-N7-C71	2.47	126.39	120.50
2	5	4133	B8W	O6-C6-N1	-2.47	115.60	119.01
2	5	3727	A2M	C4-N9-C8	2.47	108.40	105.73
2	5	1578	B9B	C2-N1-C6	2.47	119.85	115.93
2	5	1629	OMG	O6-C6-C5	-2.47	120.06	126.60
2	5	3884	P7G	N9-C8-N7	2.46	106.90	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	4374	OMG	O6-C6-C5	-2.46	120.07	126.60
4	9	1710	OMC	O2-C2-N3	-2.46	118.33	122.33
2	5	4627	OMG	O6-C6-C5	-2.46	120.08	126.60
4	9	814	5MU	O4-C4-N3	-2.45	115.41	120.12
2	5	4487	B8T	C6-C5-C4	2.45	119.96	116.96
2	5	373	OMG	O6-C6-C5	-2.45	120.10	126.60
2	5	3733	PSU	O2-C2-N1	-2.45	120.09	122.79
2	5	4446	PSU	O2-C2-N1	-2.45	120.09	122.79
2	5	373	OMG	C8-N7-C5	2.45	108.67	104.24
2	5	2428	OMG	O6-C6-C5	-2.45	120.11	126.60
2	5	4498	OMG	O6-C6-C5	-2.45	120.11	126.60
2	5	1875	A2M	C4-N9-C8	2.45	108.38	105.73
2	5	4876	2MG	O6-C6-C5	-2.44	120.13	126.60
2	5	1586	PSU	O2-C2-N1	-2.43	120.11	122.79
2	5	3871	A2M	C4-N9-C8	2.43	108.36	105.73
2	5	4575	A2M	C4-N9-C8	2.43	108.36	105.73
4	9	822	PSU	O4'-C1'-C2'	2.43	108.57	105.14
2	5	4359	E6G	C5-C6-N1	-2.43	120.09	123.46
2	5	1526	OMG	C8-N7-C5	2.41	108.61	104.24
2	5	4874	OMG	O6-C6-C5	-2.41	120.20	126.60
2	5	1681	PSU	O2-C2-N1	-2.39	120.16	122.79
4	9	1832	6MZ	C4-C5-C6	-2.39	114.95	116.81
2	5	1528	A2M	C4-N9-C8	2.39	108.32	105.73
2	5	2367	A2M	C4-N9-C8	2.39	108.32	105.73
2	5	1578	B9B	C4-N9-C8	2.39	108.32	105.73
2	5	1320	OMG	C8-N7-C5	2.39	108.56	104.24
4	9	668	A2M	C3'-C2'-C1'	2.39	107.38	102.89
2	5	2368	OMG	O6-C6-C5	-2.39	120.27	126.60
2	5	3829	A2M	C4-N9-C8	2.38	108.31	105.73
2	5	2301	E7G	N9-C8-N7	2.38	106.79	103.38
2	5	2054	OMG	C8-N7-C5	2.38	108.55	104.24
2	5	2777	OMG	C8-N7-C5	2.38	108.55	104.24
2	5	4476	B8W	C4-N9-C8	2.38	108.31	105.73
2	5	2526	7MG	N9-C8-N7	2.38	106.78	103.38
2	5	1913	P7G	N9-C8-N7	2.38	106.78	103.38
2	5	4498	OMG	C8-N7-C5	2.37	108.54	104.24
4	9	1806	M7A	C5-C4-N3	-2.37	121.06	126.62
4	9	166	A2M	C5'-C4'-C3'	-2.37	106.30	115.18
2	5	4641	OMG	O6-C6-C5	-2.37	120.32	126.60
2	5	4407	PSU	O2-C2-N1	-2.37	120.19	122.79
2	5	2384	B8W	N2-C2-N1	-2.37	113.57	117.25
2	5	4527	A2M	C2'-C1'-N9	-2.37	109.55	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	237	B9B	C5-C6-N1	-2.37	120.17	123.46
2	5	1526	OMG	O6-C6-C5	-2.37	120.33	126.60
4	9	121	OMU	C1'-N1-C2	2.36	121.84	117.57
2	5	3901	B8K	C2-N1-C6	-2.36	120.80	125.10
2	5	4874	OMG	C8-N7-C5	2.36	108.51	104.24
2	5	2758	B9B	C4-N9-C8	2.36	108.28	105.73
2	5	4419	1MA	N9-C4-N3	2.36	132.44	126.94
2	5	4533	B8W	N2-C2-N1	-2.36	113.59	117.25
2	5	4189	B8W	C4-C5-N7	-2.36	107.75	110.62
2	5	4133	B8W	C4-C5-N7	-2.35	107.75	110.62
2	5	3719	PSU	O2-C2-N1	-2.35	120.20	122.79
2	5	4200	OMG	C8-N7-C5	2.35	108.48	104.24
2	5	1801	E7G	N9-C8-N7	2.34	106.73	103.38
2	5	4454	PSU	O2-C2-N1	-2.33	120.22	122.79
2	5	3796	OMG	C8-N7-C5	2.33	108.46	104.24
2	5	4627	OMG	C8-N7-C5	2.33	108.46	104.24
2	5	4374	OMG	C8-N7-C5	2.33	108.45	104.24
4	9	1842	4AC	O7-C7-CM7	-2.33	117.73	122.06
2	5	1887	OMG	C8-N7-C5	2.32	108.44	104.24
2	5	2405	A2M	C4-N9-C8	2.32	108.25	105.73
2	5	4476	B8W	C2-N3-C4	2.32	120.30	113.89
2	5	4476	B8W	C5-C4-N9	2.31	108.47	105.78
2	5	1326	1MA	N9-C4-N3	2.31	132.33	126.94
2	5	4189	B8W	N2-C2-N1	-2.31	113.66	117.25
2	5	4534	UR3	C6-N1-C2	-2.31	119.72	121.79
2	5	4359	E6G	C4-N9-C8	2.30	108.22	105.73
2	5	237	B9B	C4-N9-C8	2.30	108.22	105.73
4	9	668	A2M	C4'-O4'-C1'	-2.30	104.41	109.47
2	5	2758	B9B	C5-C6-N1	-2.29	120.27	123.46
4	9	814	5MU	C6-C5-C4	2.29	119.95	118.03
2	5	2512	PSU	O2-C2-N1	-2.29	120.27	122.79
4	9	159	A2M	O4'-C4'-C3'	-2.29	100.59	105.11
2	5	4359	E6G	C4-C5-N7	-2.29	107.83	110.62
2	5	4189	B8W	C2-N3-C4	2.29	120.21	113.89
4	9	1850	MA6	C4-N9-C8	2.28	108.20	105.73
2	5	4133	B8W	C4-N9-C8	2.28	108.20	105.73
2	5	1578	B9B	C5-C6-N1	-2.28	120.29	123.46
2	5	1330	A2M	C4-N9-C8	2.28	108.20	105.73
4	9	823	PSU	C6-N1-C2	-2.28	120.36	122.68
2	5	4133	B8W	C2-N3-C4	2.27	120.17	113.89
2	5	1875	A2M	C2'-C1'-N9	-2.27	109.72	113.53
2	5	1578	B9B	N2-C2-N1	2.27	120.78	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2384	B8W	C4-N9-C8	2.26	108.18	105.73
2	5	1801	E7G	C8-N7-C71	2.26	125.88	120.50
2	5	237	B9B	O6-C6-N1	-2.26	116.85	120.00
2	5	2384	B8W	C2-N3-C4	2.26	120.13	113.89
2	5	729	2MG	N1-C2-N3	-2.26	120.46	123.95
2	5	1629	OMG	C8-N7-C5	2.26	108.32	104.24
2	5	237	B9B	C2-N3-C4	2.25	120.12	113.89
2	5	2758	B9B	C2-N3-C4	2.25	120.11	113.89
2	5	4554	7MG	N9-C4-N3	2.25	128.83	125.47
4	9	159	A2M	C4-N9-C8	2.25	108.16	105.73
2	5	4359	E6G	C2-N3-C4	2.25	120.10	113.89
2	5	2428	OMG	C8-N7-C5	2.24	108.30	104.24
2	5	4533	B8W	C2-N3-C4	2.24	120.08	113.89
4	9	1337	4AC	O7-C7-CM7	-2.24	117.90	122.06
2	5	237	B9B	C4-C5-N7	-2.24	107.89	110.62
2	5	3786	5MC	CM5-C5-C6	-2.24	119.86	122.85
4	9	484	A2M	C5-C4-N9	2.23	108.37	105.78
2	5	4224	6MZ	C4-N9-C8	2.22	108.14	105.73
2	5	4133	B8W	N2-C2-N1	-2.22	113.80	117.25
2	5	3884	P7G	C5-C4-N3	-2.22	120.09	124.00
2	5	3727	A2M	C4-C5-N7	-2.22	107.92	110.62
2	5	373	OMG	C8-N9-C4	2.21	110.25	106.05
2	5	1578	B9B	C2-N3-C4	2.21	119.99	113.89
4	9	1830	UR3	O2-C2-N3	-2.20	118.23	121.34
2	5	4527	A2M	C4-N9-C8	2.20	108.11	105.73
2	5	4310	OMU	O2-C2-N1	-2.20	119.86	122.79
2	5	398	A2M	C4-C5-N7	-2.20	107.94	110.62
4	9	822	PSU	C6-N1-C2	-2.18	120.45	122.68
2	5	4534	UR3	C1'-N1-C2	2.18	120.67	116.99
2	5	3901	B8K	O6-C6-C5	-2.18	122.19	127.54
2	5	4694	B8K	O6-C6-C5	-2.18	122.19	127.54
2	5	398	A2M	C4-N9-C8	2.18	108.09	105.73
2	5	3768	PSU	C6-C5-C4	2.18	119.72	118.20
2	5	3722	A2M	C4-N9-C8	2.17	108.08	105.73
4	9	1031	A2M	C4-C5-N7	-2.17	107.97	110.62
4	9	1374	5MC	O2-C2-N1	2.17	123.38	118.89
2	5	1538	A2M	C4-C5-N7	-2.17	107.97	110.62
2	5	1887	OMG	C8-N9-C4	2.17	110.18	106.05
4	9	1219	B8Q	C1'-N1-C6	-2.17	116.11	120.84
2	5	3722	A2M	C4-C5-N7	-2.17	107.98	110.62
4	9	1031	A2M	C5-C4-N9	2.16	108.30	105.78
4	9	1850	MA6	C5-C4-N9	2.16	108.30	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	v	715	DDE	CBW-CBI-NAD	2.16	118.03	115.28
2	5	4874	OMG	C8-N9-C4	2.15	110.15	106.05
2	5	1521	2MG	CM2-N2-C2	-2.15	119.10	123.86
4	9	166	A2M	C2'-C1'-N9	-2.15	109.91	113.53
2	5	3901	B8K	N1-C2-N3	-2.15	119.31	123.32
4	9	1851	MA6	C4-C5-N7	-2.15	108.00	110.62
2	5	4533	B8W	C2-N1-C6	2.15	119.34	115.93
2	5	4554	7MG	N9-C8-N7	2.15	106.45	103.38
4	9	1678	A2M	C6-C5-C4	2.15	120.07	117.18
4	9	27	A2M	C6-C5-C4	2.14	120.06	117.18
4	9	1851	MA6	C4-N9-C8	2.14	108.05	105.73
2	5	4601	UR3	C6-N1-C2	-2.14	119.87	121.79
2	5	2405	A2M	C4-C5-N7	-2.14	108.01	110.62
4	9	27	A2M	C2'-C1'-N9	-2.14	109.93	113.53
2	5	3768	PSU	O2-C2-N1	-2.14	120.44	122.79
2	5	3722	A2M	C2'-C1'-N9	-2.13	109.94	113.53
2	5	4224	6MZ	C4-C5-N7	-2.13	108.03	110.62
2	5	2367	A2M	C4-C5-N7	-2.12	108.03	110.62
4	9	1248	B8N	O4'-C1'-C2'	2.12	108.14	105.14
2	5	4375	MHG	N9-C8-N7	2.12	106.41	103.38
2	5	3903	BGH	N1-C2-N3	-2.11	119.38	123.32
4	9	668	A2M	C5-C4-N9	2.11	108.24	105.78
2	5	4339	5MC	CM5-C5-C6	-2.11	120.03	122.85
2	5	4876	2MG	C8-N7-C5	2.11	108.06	104.24
4	9	612	PSU	O4'-C1'-C2'	2.11	108.12	105.14
2	5	3903	BGH	O6-C6-C5	-2.11	122.37	127.54
2	5	237	B9B	N2-C2-N1	2.11	120.53	117.25
2	5	1870	UR3	C1'-N1-C2	2.10	120.54	116.99
4	9	668	A2M	C5'-C4'-C3'	-2.10	107.30	115.18
4	9	484	A2M	C4-C5-N7	-2.10	108.06	110.62
2	5	1528	A2M	C4-C5-N7	-2.10	108.06	110.62
4	9	668	A2M	C4-C5-N7	-2.10	108.06	110.62
4	9	1842	4AC	N4-C4-N3	2.09	117.37	113.85
4	9	1703	OMC	O2-C2-N3	-2.09	118.92	122.33
2	5	1578	B9B	C4-C5-N7	-2.09	108.07	110.62
2	5	2777	OMG	C8-N9-C4	2.09	110.02	106.05
2	5	2790	B9H	O2-C2-N1	-2.08	117.84	122.72
2	5	4624	OMU	O2-C2-N1	-2.08	120.02	122.79
2	5	1521	2MG	C8-N7-C5	2.08	108.00	104.24
2	5	3768	PSU	O4'-C1'-C2'	2.08	108.08	105.14
2	5	1870	UR3	C6-N1-C2	-2.07	119.93	121.79
2	5	4476	B8W	N2-C2-N1	-2.07	114.03	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2790	B9H	C6-N1-C2	-2.07	119.94	121.79
4	9	1678	A2M	C4'-O4'-C1'	-2.06	104.92	109.47
2	5	1330	A2M	C4-C5-N7	-2.05	108.12	110.62
2	5	4189	B8W	C61-O6-C6	-2.05	115.18	117.21
2	5	4224	6MZ	C4-N9-C1'	-2.05	121.72	126.59
2	5	4419	1MA	C8-N7-C5	2.05	107.94	104.24
2	5	4200	OMG	C8-N9-C4	2.05	109.94	106.05
2	5	4407	PSU	C6-C5-C4	2.05	119.63	118.20
4	9	644	OMG	C8-N7-C5	2.04	107.94	104.24
2	5	4375	MHG	N9-C4-N3	2.04	128.52	125.47
4	9	1081	PSU	O4'-C1'-C2'	2.04	108.02	105.14
2	5	4575	A2M	C4-C5-N7	-2.04	108.13	110.62
4	9	27	A2M	C4-C5-N7	-2.04	108.13	110.62
4	9	683	OMG	C8-N7-C5	2.04	107.93	104.24
2	5	3871	A2M	C6-C5-C4	2.04	119.92	117.18
2	5	4694	B8K	N1-C2-N3	-2.04	119.52	123.32
4	9	509	OMG	C8-N7-C5	2.04	107.93	104.24
2	5	1326	1MA	C8-N7-C5	2.03	107.92	104.24
2	5	4641	OMG	C8-N9-C4	2.03	109.91	106.05
2	5	4527	A2M	C4-C5-N7	-2.03	108.15	110.62
4	9	1678	A2M	C2'-C1'-N9	2.03	116.95	113.53
4	9	1031	A2M	C5'-C4'-C3'	-2.03	107.58	115.18
2	5	2368	OMG	C8-N9-C4	2.03	109.91	106.05
4	9	159	A2M	C4-C5-N7	-2.03	108.15	110.62
4	9	1374	5MC	CM5-C5-C6	-2.02	120.15	122.85
2	5	3871	A2M	C4-C5-N7	-2.02	108.16	110.62
2	5	1320	OMG	N1-C2-N3	-2.02	119.56	123.32
4	9	174	OMC	O2-C2-N3	-2.02	119.05	122.33
2	5	729	2MG	C8-N7-C5	2.02	107.89	104.24
4	9	27	A2M	C5-C4-N9	2.01	108.13	105.78
2	5	4876	2MG	N1-C2-N3	-2.01	120.84	123.95
2	5	1913	P7G	C5-C4-N3	-2.01	120.45	124.00
4	9	1031	A2M	C6-C5-C4	2.01	119.89	117.18
2	5	4640	PSU	O2-C2-N1	-2.01	120.58	122.79
2	5	2384	B8W	C4-C5-N7	-2.00	108.18	110.62
2	5	3829	A2M	C2'-C1'-N9	-2.00	110.16	113.53
2	5	4374	OMG	C8-N9-C4	2.00	109.86	106.05
2	5	4533	B8W	C5-C4-N9	2.00	108.11	105.78
81	t	51	5CT	C4-C3-C2	-2.00	109.25	113.47
4	9	683	OMG	N1-C2-N3	-2.00	119.58	123.32
4	9	119	PSU	O4-C4-N3	-2.00	116.28	120.12
2	5	4527	A2M	C6-C5-C4	2.00	119.87	117.18

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	8	14	OMU	C1'-C2'-O2'-CM2
81	t	51	5CT	NZ-C1-C2-C3
2	5	237	B9B	C5-C6-O6-C61
2	5	237	B9B	N1-C6-O6-C61
2	5	1352	P4U	N3-C4-O4-C41
2	5	1352	P4U	C3'-C4'-C5'-O5'
2	5	1352	P4U	O4'-C4'-C5'-O5'
2	5	1578	B9B	C5-C6-O6-C61
2	5	1578	B9B	N1-C6-O6-C61
2	5	2368	OMG	O4'-C4'-C5'-O5'
2	5	2384	B8W	C5-C6-O6-C61
2	5	2384	B8W	C3'-C4'-C5'-O5'
2	5	2384	B8W	O4'-C4'-C5'-O5'
2	5	2428	OMG	O4'-C4'-C5'-O5'
2	5	2428	OMG	C3'-C4'-C5'-O5'
2	5	2758	B9B	C5-C6-O6-C61
2	5	2758	B9B	N1-C6-O6-C61
2	5	3705	OMC	C2'-C1'-N1-C6
2	5	3727	A2M	C1'-C2'-O2'-CM'
2	5	3768	PSU	O4'-C1'-C5-C4
2	5	3768	PSU	O4'-C1'-C5-C6
2	5	3789	A2M	O4'-C4'-C5'-O5'
2	5	3796	OMG	O4'-C4'-C5'-O5'
2	5	3796	OMG	C3'-C4'-C5'-O5'
2	5	3871	A2M	O4'-C4'-C5'-O5'
2	5	3871	A2M	C3'-C4'-C5'-O5'
2	5	3901	B8K	O4'-C4'-C5'-O5'
2	5	3903	BGH	C3'-C4'-C5'-O5'
2	5	4133	B8W	C5-C6-O6-C61
2	5	4133	B8W	N1-C6-O6-C61
2	5	4189	B8W	C5-C6-O6-C61
2	5	4189	B8W	N1-C6-O6-C61
2	5	4359	E6G	C5-C6-O6-C61
2	5	4359	E6G	N1-C6-O6-C61
2	5	4375	MHG	O4'-C4'-C5'-O5'
2	5	4407	PSU	O4'-C1'-C5-C4
2	5	4407	PSU	O4'-C1'-C5-C6
2	5	4476	B8W	C5-C6-O6-C61
2	5	4476	B8W	N1-C6-O6-C61
2	5	4527	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	5	4533	B8W	C5-C6-O6-C61
2	5	4533	B8W	N1-C6-O6-C61
2	5	4534	UR3	O4'-C4'-C5'-O5'
2	5	4534	UR3	C3'-C4'-C5'-O5'
2	5	4624	OMU	C1'-C2'-O2'-CM2
2	5	4640	PSU	C3'-C4'-C5'-O5'
2	5	4641	OMG	O4'-C4'-C5'-O5'
2	5	4874	OMG	O4'-C4'-C5'-O5'
2	5	4874	OMG	C3'-C4'-C5'-O5'
4	9	116	OMU	C1'-C2'-O2'-CM2
4	9	116	OMU	C3'-C4'-C5'-O5'
4	9	116	OMU	O4'-C4'-C5'-O5'
4	9	121	OMU	C3'-C4'-C5'-O5'
4	9	121	OMU	O4'-C4'-C5'-O5'
4	9	159	A2M	C3'-C4'-C5'-O5'
4	9	166	A2M	C3'-C4'-C5'-O5'
4	9	568	E3C	O4'-C1'-N1-C2
4	9	568	E3C	O4'-C1'-N1-C6
4	9	1248	B8N	N3-C31-C32-C33
4	9	1830	UR3	O4'-C1'-N1-C2
4	9	1832	6MZ	C5-C6-N6-C9
4	9	1832	6MZ	N1-C6-N6-C9
4	9	1851	MA6	O4'-C4'-C5'-O5'
4	9	1851	MA6	C3'-C4'-C5'-O5'
82	v	715	DDE	O-C-CA-CB
2	5	2368	OMG	C3'-C4'-C5'-O5'
2	5	2405	A2M	C3'-C4'-C5'-O5'
2	5	3733	PSU	O4'-C4'-C5'-O5'
2	5	3768	PSU	C3'-C4'-C5'-O5'
2	5	3768	PSU	O4'-C4'-C5'-O5'
2	5	3789	A2M	C3'-C4'-C5'-O5'
2	5	3884	P7G	O4'-C4'-C5'-O5'
2	5	3901	B8K	C3'-C4'-C5'-O5'
2	5	3903	BGH	O4'-C4'-C5'-O5'
2	5	4454	PSU	C3'-C4'-C5'-O5'
2	5	4454	PSU	O4'-C4'-C5'-O5'
2	5	4504	PSU	C3'-C4'-C5'-O5'
2	5	4504	PSU	O4'-C4'-C5'-O5'
2	5	4527	A2M	C3'-C4'-C5'-O5'
2	5	4641	OMG	C3'-C4'-C5'-O5'
4	9	159	A2M	O4'-C4'-C5'-O5'
4	9	668	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	9	668	A2M	C3'-C4'-C5'-O5'
4	9	1081	PSU	O4'-C4'-C5'-O5'
2	5	2384	B8W	N1-C6-O6-C61
4	9	1830	UR3	O4'-C1'-N1-C6
2	5	1801	E7G	O4'-C4'-C5'-O5'
2	5	2405	A2M	O4'-C4'-C5'-O5'
2	5	3733	PSU	C3'-C4'-C5'-O5'
2	5	3884	P7G	C3'-C4'-C5'-O5'
2	5	4297	PSU	C3'-C4'-C5'-O5'
2	5	4640	PSU	O4'-C4'-C5'-O5'
4	9	119	PSU	O4'-C4'-C5'-O5'
4	9	166	A2M	O4'-C4'-C5'-O5'
4	9	568	E3C	C3'-C4'-C5'-O5'
4	9	568	E3C	O4'-C4'-C5'-O5'
4	9	683	OMG	O4'-C4'-C5'-O5'
4	9	1081	PSU	C3'-C4'-C5'-O5'
4	9	1703	OMC	O4'-C4'-C5'-O5'
4	9	1830	UR3	O4'-C4'-C5'-O5'
4	9	1830	UR3	C3'-C4'-C5'-O5'
2	5	4874	OMG	C3'-C2'-O2'-CM2
2	5	4451	5MC	C2'-C1'-N1-C6
2	5	3705	OMC	C2'-C1'-N1-C2
81	t	51	5CT	NZ-C1-C2-O1
4	9	517	OMC	C3'-C4'-C5'-O5'
2	5	1801	E7G	C3'-C4'-C5'-O5'
2	5	4297	PSU	O4'-C4'-C5'-O5'
2	5	4419	1MA	C3'-C4'-C5'-O5'
4	9	1243	PSU	O4'-C4'-C5'-O5'
2	5	4375	MHG	C72-C73-C74-C76
2	5	398	A2M	O4'-C4'-C5'-O5'
4	9	517	OMC	O4'-C4'-C5'-O5'
4	9	683	OMG	C3'-C4'-C5'-O5'
2	5	1913	P7G	C72-C71-N7-C8
4	9	1851	MA6	C5-C6-N6-C9
2	5	4375	MHG	C2'-C1'-N9-C8
2	5	4451	5MC	C2'-C1'-N1-C2
2	5	2790	B9H	C32-C31-N3-C2
2	5	4375	MHG	C75-C73-C74-C76
82	v	715	DDE	NAD-CBI-CBW-NCB
82	v	715	DDE	OAG-CBI-CBW-NCB
2	5	4527	A2M	C1'-C2'-O2'-CM'
2	5	4641	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
4	9	668	A2M	C1'-C2'-O2'-CM'
81	t	51	5CT	C2-C1-NZ-CE
82	v	715	DDE	CA-CB-CG-ND1
2	5	4451	5MC	O4'-C1'-N1-C6
2	5	4504	PSU	C4'-C5'-O5'-P
4	9	644	OMG	C4'-C5'-O5'-P
82	v	715	DDE	N-CA-CB-CG
2	5	4198	I4U	O4'-C4'-C5'-O5'
82	v	715	DDE	CAU-CBW-NCB-CAB
82	v	715	DDE	CAU-CBW-NCB-CAC
82	v	715	DDE	CAU-CBW-NCB-CAA
4	9	668	A2M	C2'-C1'-N9-C8
2	5	3705	OMC	O4'-C1'-N1-C6
2	5	373	OMG	C4'-C5'-O5'-P
4	9	159	A2M	C4'-C5'-O5'-P
4	9	119	PSU	C3'-C4'-C5'-O5'
4	9	822	PSU	C3'-C4'-C5'-O5'
2	5	4451	5MC	O4'-C1'-N1-C2
82	v	715	DDE	CAT-CAU-CBW-CBI
2	5	4375	MHG	C72-C71-N7-C5
2	5	1538	A2M	C4'-C5'-O5'-P
2	5	4419	1MA	O4'-C4'-C5'-O5'
4	9	1703	OMC	C3'-C4'-C5'-O5'
4	9	1850	MA6	C5-C6-N6-C9
82	v	715	DDE	CA-CB-CG-CD2
2	5	3705	OMC	O4'-C1'-N1-C2
2	5	1330	A2M	C4'-C5'-O5'-P
2	5	3901	B8K	C4'-C5'-O5'-P
4	9	1081	PSU	C4'-C5'-O5'-P
2	5	1528	A2M	C3'-C2'-O2'-CM'
2	5	2367	A2M	C3'-C2'-O2'-CM'
2	5	1326	1MA	C2'-C1'-N9-C8
2	5	2301	E7G	C72-C71-N7-C8
2	5	729	2MG	O4'-C4'-C5'-O5'
2	5	4375	MHG	C72-C71-N7-C8
2	5	1681	PSU	O4'-C1'-C5-C4
2	5	4454	PSU	O4'-C1'-C5-C4
2	5	4535	PSU	O4'-C1'-C5-C4
4	9	1248	B8N	O4'-C1'-C5-C4
4	9	668	A2M	C3'-C2'-O2'-CM'
4	9	1243	PSU	C3'-C4'-C5'-O5'
82	v	715	DDE	CBI-CBW-NCB-CAB

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Mol	Chain	Res	Type	Atoms
82	v	715	DDE	CBI-CBW-NCB-CAC
82	v	715	DDE	CBI-CBW-NCB-CAA
2	5	1326	1MA	C2'-C1'-N9-C4
82	v	715	DDE	CE1-CAT-CAU-CBW
81	t	51	5CT	C-CA-CB-CG
2	5	1913	P7G	C72-C71-N7-C5
2	5	4375	MHG	O4'-C1'-N9-C8
2	5	4198	I4U	C3'-C4'-C5'-O5'
4	9	822	PSU	O4'-C4'-C5'-O5'
2	5	1681	PSU	O4'-C1'-C5-C6
2	5	4535	PSU	O4'-C1'-C5-C6
2	5	4640	PSU	O4'-C1'-C5-C6
4	9	1248	B8N	C31-C32-C33-N34
2	5	3871	A2M	C4'-C5'-O5'-P
2	5	398	A2M	C3'-C4'-C5'-O5'
2	5	1538	A2M	O4'-C4'-C5'-O5'
2	5	2426	OMC	O4'-C4'-C5'-O5'
2	5	2777	OMG	O4'-C4'-C5'-O5'
2	5	3789	A2M	C2'-C1'-N9-C8
2	5	1663	I4U	C42-C41-O4-C4
81	t	51	5CT	CD-CE-NZ-C1
2	5	4675	B8T	C4'-C5'-O5'-P
2	5	4874	OMG	C4'-C5'-O5'-P

There are no ring outliers.

54 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	4876	2MG	2	0
4	9	1337	4AC	1	0
2	5	4300	B8H	6	0
2	5	4641	OMG	1	0
3	8	14	OMU	1	0
2	5	2367	A2M	2	0
2	5	1629	OMG	1	0
4	9	116	OMU	1	0
2	5	4527	A2M	3	0
2	5	4476	B8W	1	0
2	5	398	A2M	2	0
2	5	2054	OMG	1	0
2	5	3789	A2M	1	0
4	9	1031	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	9	121	OMU	3	0
2	5	4534	UR3	1	0
2	5	4540	OMC	1	0
2	5	2526	7MG	1	0
2	5	4454	PSU	1	0
4	9	166	A2M	1	0
2	5	4087	5MU	1	0
2	5	4568	M7A	1	0
2	5	4554	7MG	1	0
4	9	683	OMG	1	0
2	5	1330	A2M	1	0
4	9	1678	A2M	3	0
2	5	3722	A2M	3	0
4	9	1832	6MZ	1	0
2	5	1875	A2M	2	0
2	5	1887	OMG	1	0
2	5	2777	OMG	1	0
2	5	3829	A2M	1	0
2	5	3884	P7G	1	0
2	5	1609	7MG	1	0
2	5	1864	B8H	5	0
2	5	1681	PSU	1	0
2	5	3903	BGH	1	0
11	C	333	MLZ	1	0
2	5	2405	A2M	1	0
2	5	3727	A2M	3	0
2	5	4535	PSU	1	0
2	5	1460	B8Q	1	0
2	5	3871	A2M	2	0
4	9	27	A2M	3	0
4	9	509	OMG	3	0
4	9	159	A2M	1	0
2	5	4575	A2M	2	0
2	5	1870	UR3	1	0
2	5	4694	B8K	1	0
2	5	1687	PSU	1	0
2	5	4624	OMU	1	0
2	5	1538	A2M	2	0
2	5	4451	5MC	1	0
2	5	4419	1MA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 208 ligands modelled in this entry, 208 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	9	12
2	5	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1223:G	O3'	1237:G	P	24.58
1	9	834:C	O3'	841:G	P	17.65
1	9	697:G	O3'	729:C	P	17.13
1	9	756:C	O3'	788:G	P	17.02
1	5	994:U	O3'	1068:G	P	16.68
1	5	182:G	O3'	189:G	P	16.36
1	5	1368:U	O3'	1372:A	P	14.19
1	5	4733:A	O3'	4739:G	P	11.77
1	5	1184:C	O3'	1187:C	P	10.43
1	9	745:C	O3'	749:U	P	9.60
1	5	4744:G	O3'	4747:G	P	6.60

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	500:G	O3'	504:G	P	5.76
1	9	798:G	O3'	799:U	P	5.40
1	9	322:C	O3'	323:C	P	4.79
1	9	304:C	O3'	305:U	P	4.65
1	9	736:C	O3'	743:U	P	4.64
1	9	309:G	O3'	310:C	P	3.69
1	5	1243:C	O3'	1248:G	P	3.40
1	5	751:G	O3'	752:G	P	3.29
1	9	902:G	O3'	903:A	P	3.24
1	9	903:A	O3'	904:A	P	3.22
1	9	1295:A	O3'	1296:U	P	3.17
1	5	267:G	O3'	268:G	P	3.07

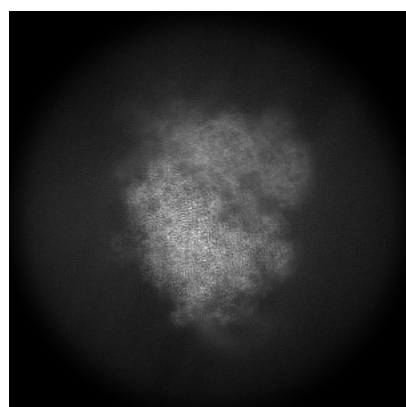
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13114. These allow visual inspection of the internal detail of the map and identification of artifacts.

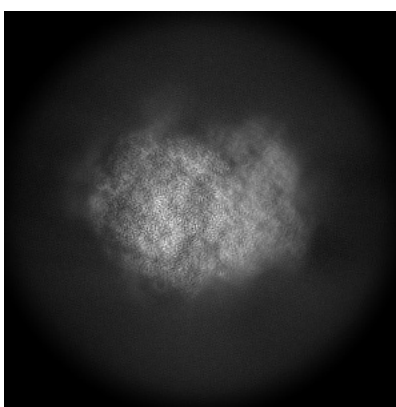
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

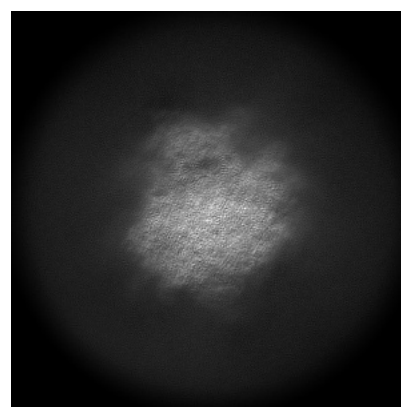
6.1.1 Primary map



X



Y

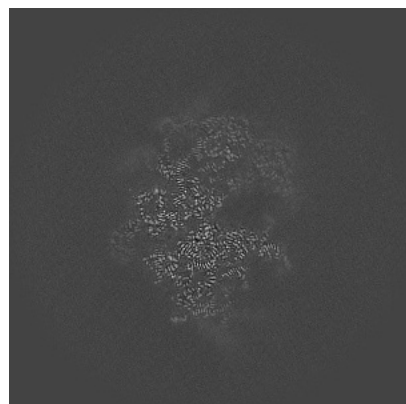


Z

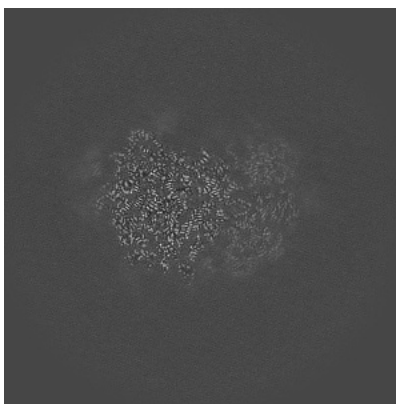
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

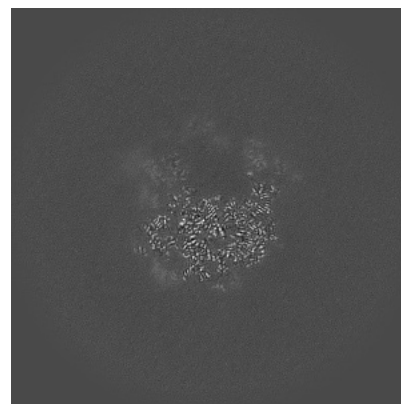
6.2.1 Primary map



X Index: 240



Y Index: 240

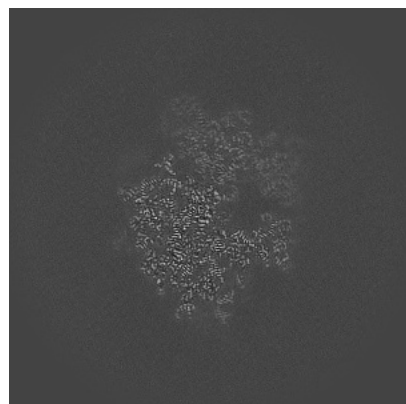


Z Index: 240

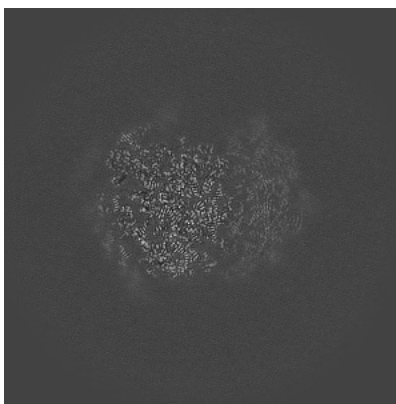
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

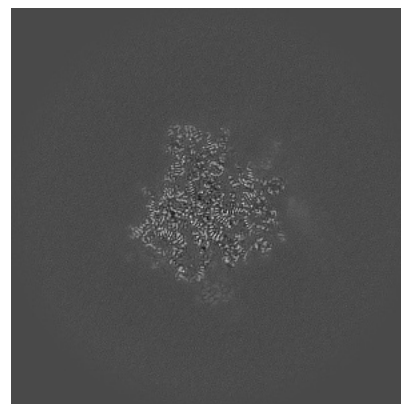
6.3.1 Primary map



X Index: 225



Y Index: 228

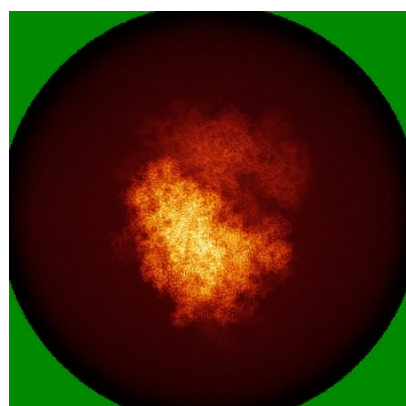


Z Index: 194

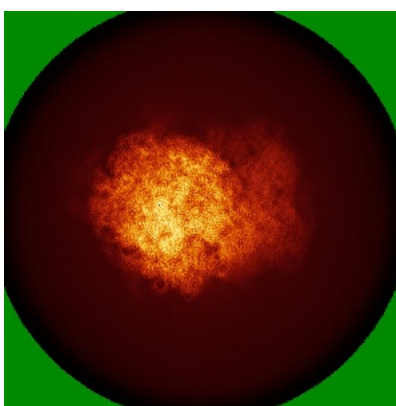
The images above show the largest variance slices of the map in three orthogonal directions.

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

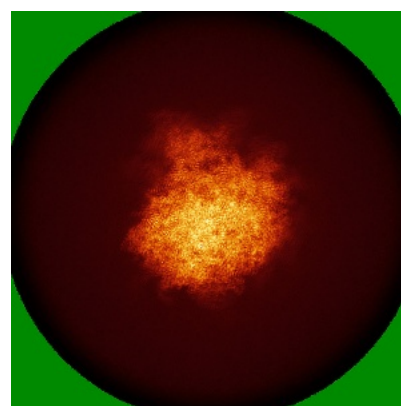
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

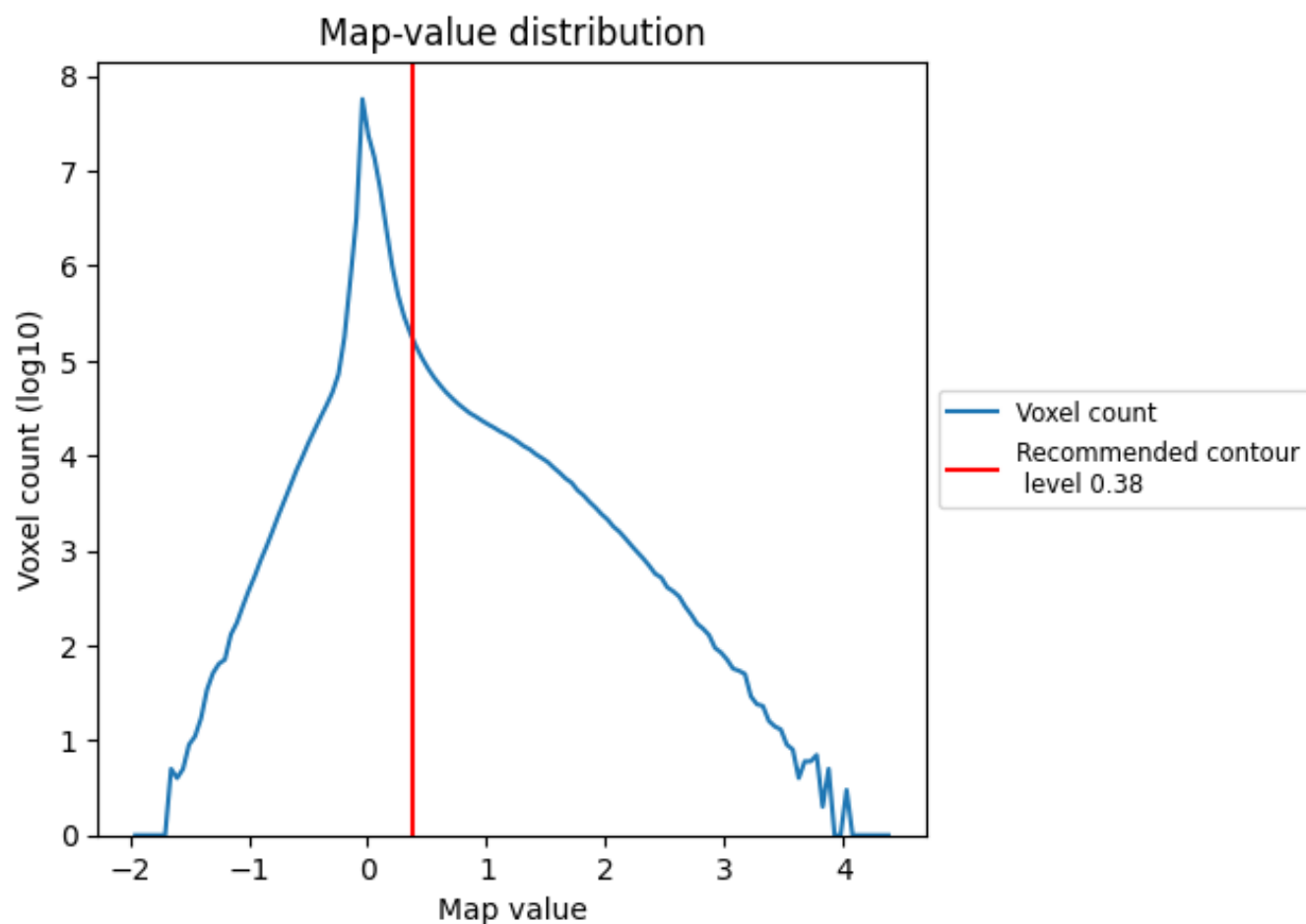
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

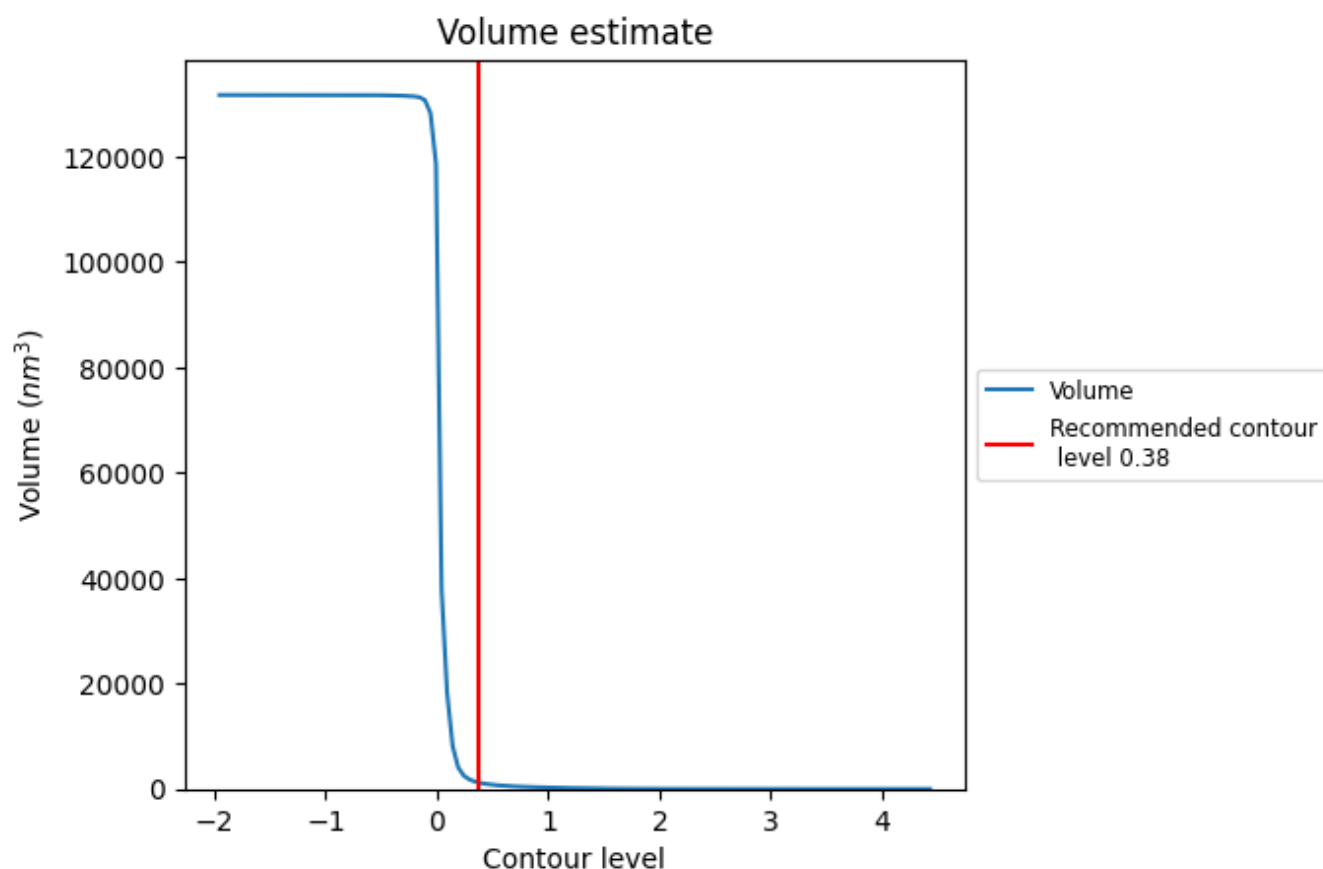
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

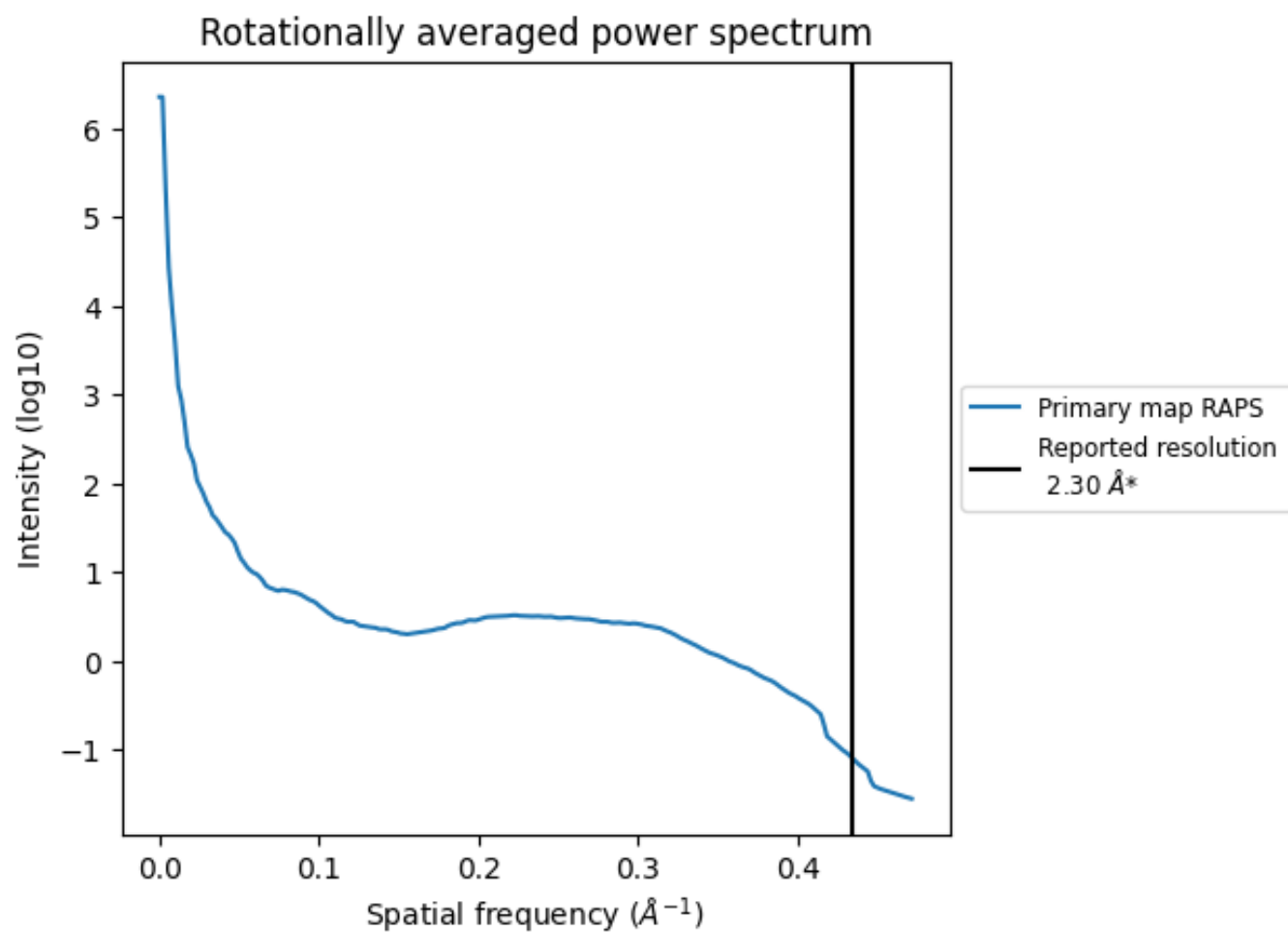
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1197 nm^3 ; this corresponds to an approximate mass of 1081 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 0.435 Å⁻¹

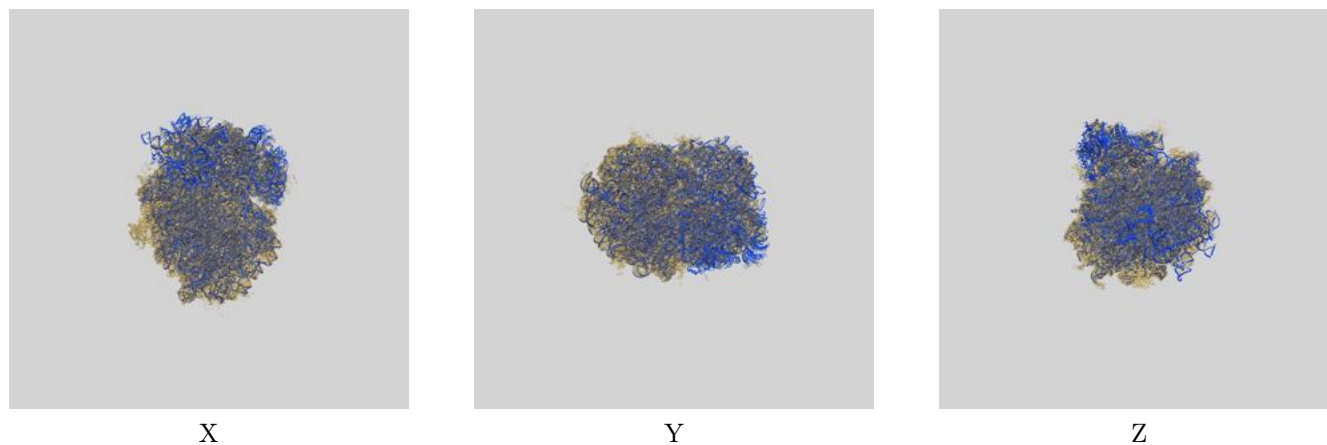
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

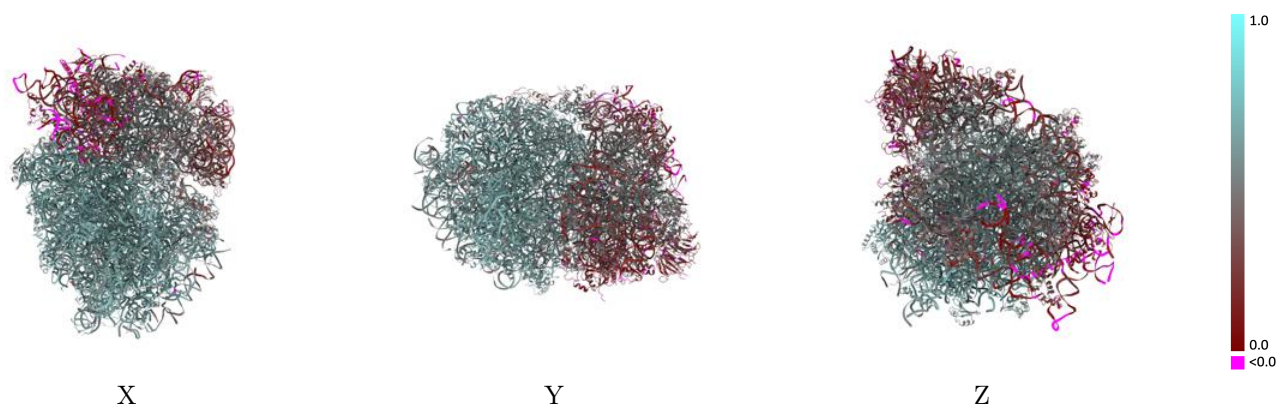
This section contains information regarding the fit between EMDB map EMD-13114 and PDB model 7OYD. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



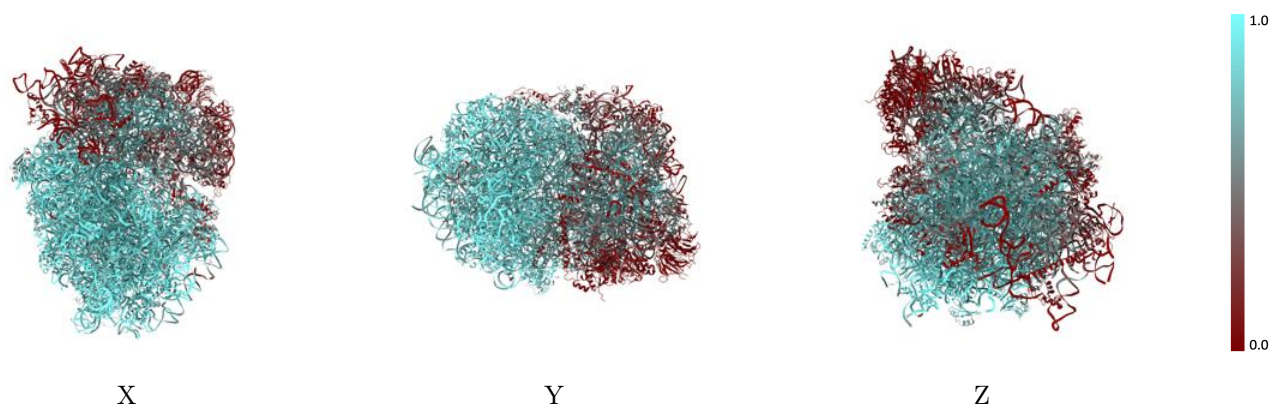
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



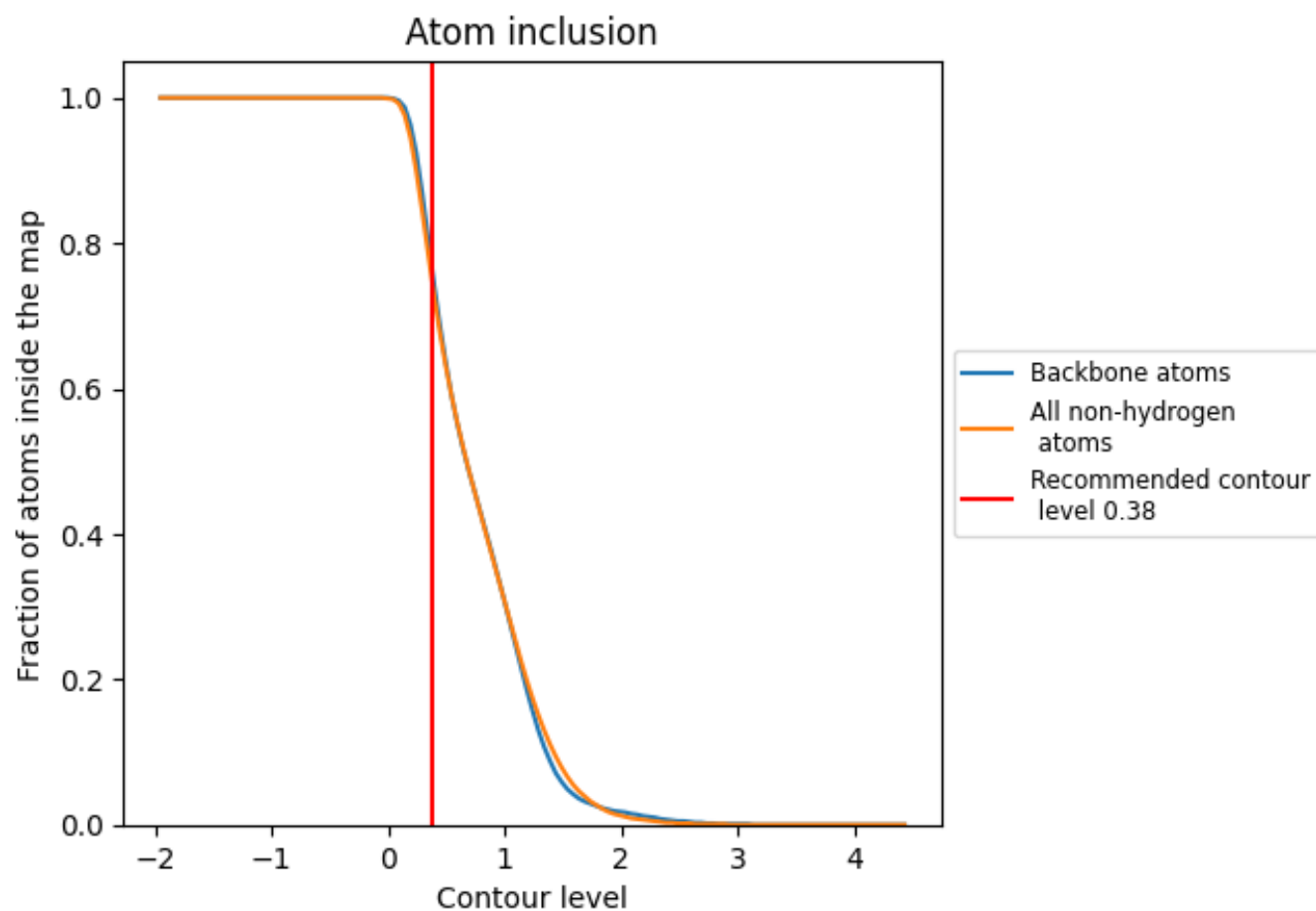
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7420	 0.5250
5	 0.9500	 0.6290
8	 0.9840	 0.6500
9	 0.5560	 0.3500
A	 0.9660	 0.6530
AA	 0.4330	 0.4270
Aa	 0.5340	 0.4140
B	 0.9410	 0.6480
BB	 0.3140	 0.3110
Bb	 0.3410	 0.3420
C	 0.9530	 0.6510
CC	 0.6390	 0.4890
Cc	 0.0740	 0.2010
D	 0.8910	 0.6200
DD	 0.3260	 0.3520
Dd	 0.5210	 0.4110
E	 0.9120	 0.6260
EE	 0.4050	 0.3880
Ee	 0.3850	 0.3670
F	 0.9520	 0.6610
FF	 0.1050	 0.2460
G	 0.8990	 0.6170
GG	 0.0690	 0.1010
Gg	 0.0400	 0.2340
H	 0.9250	 0.6330
HH	 0.2050	 0.3230
I	 0.9250	 0.6380
II	 0.3040	 0.3150
J	 0.7770	 0.5860
JJ	 0.5450	 0.4140
K	 0.9920	 0.6510
KK	 0.1950	 0.3110
L	 0.8940	 0.6290
LL	 0.4600	 0.3860
M	 0.9300	 0.6300



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Chain	Atom inclusion	Q-score
N	 0.9830	 0.6660
NN	 0.4570	 0.4280
O	 0.9470	 0.6500
OO	 0.3880	 0.3330
P	 0.9540	 0.6570
PP	 0.1980	 0.2770
Q	 0.9550	 0.6510
QQ	 0.1880	 0.3030
R	 0.8870	 0.6170
RR	 0.2250	 0.3080
S	 0.9400	 0.6450
SS	 0.1540	 0.2830
T	 0.8890	 0.6310
TT	 0.1520	 0.2890
U	 0.7760	 0.5680
UU	 0.2350	 0.3070
V	 0.9360	 0.6450
VV	 0.4740	 0.4530
W	 0.9200	 0.6380
WW	 0.6750	 0.5040
X	 0.9150	 0.6350
XX	 0.6550	 0.4950
Y	 0.9200	 0.6380
YY	 0.1260	 0.1680
Z	 0.9110	 0.6160
ZZ	 0.0430	 0.1860
a	 0.9540	 0.6530
b	 0.8600	 0.6100
c	 0.9090	 0.6200
d	 0.8990	 0.6230
e	 0.9660	 0.6580
f	 0.9640	 0.6590
g	 0.9290	 0.6400
h	 0.9080	 0.6260
i	 0.9000	 0.6210
j	 0.9640	 0.6540
k	 0.8120	 0.5810
l	 0.9320	 0.6170
m	 0.9360	 0.6480
n	 0.8030	 0.5850
o	 0.9260	 0.6460
p	 0.9190	 0.6350

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Chain	Atom inclusion	Q-score
r	 0.9580	 0.6520
s	 0.2950	 0.4130
s1	 0.6640	 0.5360
t	 0.6530	 0.5960
v	 0.4350	 0.4840
w	 0.5640	 0.5190
x	 0.3850	 0.5130