



Full wwPDB EM Validation Report ⓘ

Sep 24, 2026 – 01:08 PM JST

PDB ID : 9WW7 / pdb_00009ww7
EMDB ID : EMD-66301
Title : human 80S ribosome delta eL41 rotated state
Authors : Fujino, M.; Tanaka, Y.; Iwasaki, W.; Ito, T.; Yokoyama, T.
Deposited on : 2025-09-22
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

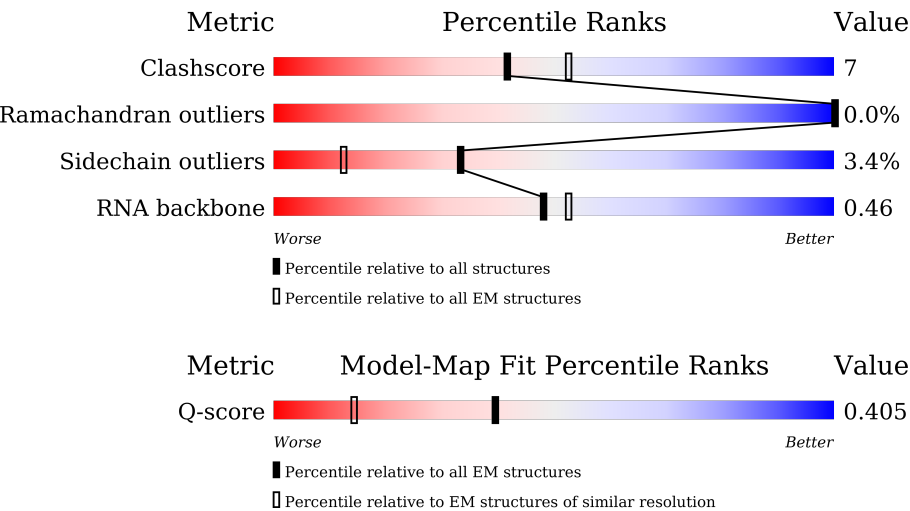
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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	AA	5069	28% 44% 26% • 26%
2	AB	120	33% 72% 27% •
3	AC	157	21% 59% 38% ••

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Mol	Chain	Length	Quality of chain
4	AD	257	
5	AE	402	
6	AF	368	
7	AG	293	
8	AH	247	
9	AI	248	
10	AJ	266	
11	AK	192	
12	AL	214	
13	AM	178	
14	AN	211	
15	AO	215	
16	AP	204	
17	AQ	203	
18	AR	184	
19	AS	188	
20	AT	196	
21	AU	176	
22	AV	160	
23	AW	128	
24	AX	140	
25	AY	157	
26	AZ	156	
27	Aa	145	
28	Ab	136	

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Mol	Chain	Length	Quality of chain
29	Ac	148	
30	Ad	159	
31	Ae	115	
32	Af	125	
33	Ag	135	
34	Ah	110	
35	Ai	117	
36	Aj	123	
37	Ak	105	
38	Al	97	
39	Am	70	
40	An	51	
41	Ao	128	
42	Aq	106	
43	Ar	92	
44	As	137	
45	BA	1869	
46	BB	263	
47	BC	295	
48	BD	264	
49	BE	243	
50	BF	204	
51	BG	194	
52	BH	208	
53	BI	165	

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Mol	Chain	Length	Quality of chain
54	BJ	158	
55	BK	145	
56	BL	146	
57	BM	152	
58	BN	145	
59	BO	119	
60	BP	83	
61	BQ	143	
62	BR	115	
63	BS	69	
64	BT	56	
65	BU	317	
66	BV	293	
67	BW	249	
68	BX	194	
69	BY	132	
70	BZ	151	
71	Ba	151	
72	Bb	130	
73	Bc	133	
74	Bd	125	
75	Be	84	
76	Bf	133	
77	Bg	156	
78	Bh	135	

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 214414 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 RNA chain called 28S rRNA (3773-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	3773	Total	C	N	O	P	0	0
			80204	35721	14588	26123	3772		

- Molecule 2 is a RNA chain called 5S rRNA (120-MER).

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

- Molecule 3 is a RNA chain called 5.8S rRNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	213	Total	C	N	O	S	0	0
			1713	1083	329	285	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	49	CYS	GLY	conflict	UNP Q96L21

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	134	Total	C	N	O	S	0	0
			1103	707	212	177	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	169	Total	C	N	O	S	0	0
			1408	873	304	222	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

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

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	99	Total	C	N	O	S	0	0
			808	502	177	125	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ae	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ah	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Aj	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ak	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	An	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ao	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Aq	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ar	88	Total	C	N	O	S	0	0
			681	430	131	113	7		

- Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	As	123	Total	C	N	O	S	0	0
			987	612	205	166	4		

- Molecule 45 is a RNA chain called 18S rRNA (1740-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BA	1737	Total	C	N	O	P	0	0
			36892	16481	6588	12086	1737		

- Molecule 46 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BB	262	Total	C	N	O	S	0	0
			2059	1312	384	356	7		

- Molecule 47 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BC	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

- Molecule 48 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BD	215	Total	C	N	O	S	0	0
			1747	1109	312	312	14		

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BE	227	Total	C	N	O	S	0	0
			1762	1122	317	315	8		

- Molecule 50 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BF	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 51 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BG	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 52 is a protein called 40S ribosomal protein S8.

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

- Molecule 53 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BI	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 54 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BJ	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

- Molecule 55 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BK	125	Total	C	N	O	S	0	0
			1027	653	193	174	7		

- Molecule 56 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BL	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 57 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BM	145	Total	C	N	O	S	0	0
			1194	748	241	203	2		

- Molecule 58 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BN	143	Total	C	N	O	S	0	0
			1110	696	214	198	2		

- Molecule 59 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BO	91	Total	C	N	O	S	0	0
			726	457	136	130	3		

- Molecule 60 is a protein called 40S ribosomal protein S21.

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

- Molecule 61 is a protein called 40S ribosomal protein S23.

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

- Molecule 62 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BR	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 63 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BS	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 64 is a protein called 40S ribosomal protein S29.

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

- Molecule 65 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 66 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BV	221	Total	C	N	O	S	1	0
			1724	1115	298	301	10		

- Molecule 67 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BW	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

- Molecule 68 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BX	182	Total	C	N	O	S	1	0
			1520	967	306	245	2		

- Molecule 69 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BY	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 70 is a protein called 40S ribosomal protein S13.

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

- Molecule 71 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ba	136	Total	C	N	O	S	0	0
			1007	617	196	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ba	138	IAS	ASP	conflict	UNP P62263

- Molecule 72 is a protein called 40S ribosomal protein S15a.

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

- Molecule 73 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bc	128	Total	C	N	O	S	1	0
			1048	661	207	175	5		

- Molecule 74 is a protein called 40S ribosomal protein S25.

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

- Molecule 75 is a protein called 40S ribosomal protein S27.

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

- Molecule 76 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bf	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bg	67	Total	C	N	O	S	0	0
			544	343	101	93	7		

- Molecule 78 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bh	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	AA	184	Total	Mg	0
			184	184	
79	AB	2	Total	Mg	0
			2	2	
79	AC	4	Total	Mg	0
			4	4	
79	AP	1	Total	Mg	0
			1	1	
79	AR	1	Total	Mg	0
			1	1	
79	AX	1	Total	Mg	0
			1	1	
79	BA	27	Total	Mg	0
			27	27	

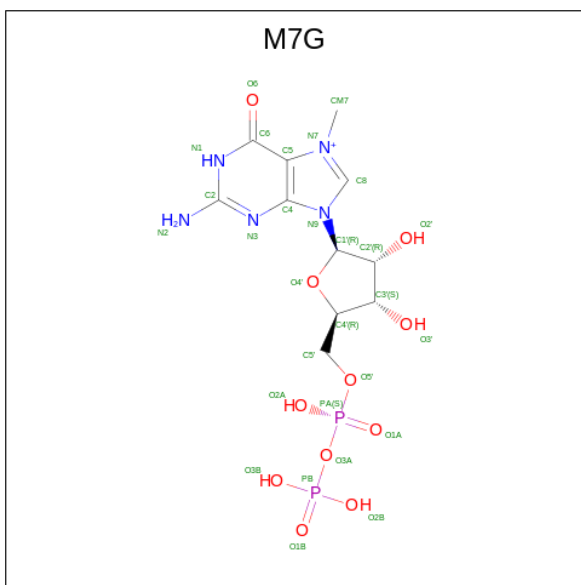
- Molecule 80 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
80	AA	51	Total 51	K 51	0
80	AB	1	Total 1	K 1	0
80	AD	1	Total 1	K 1	0
80	AL	1	Total 1	K 1	0
80	Ag	1	Total 1	K 1	0
80	Ah	1	Total 1	K 1	0
80	Aq	1	Total 1	K 1	0
80	BA	5	Total 5	K 5	0

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Ai	1	Total 1	Zn 1	0
81	Al	1	Total 1	Zn 1	0
81	Ao	1	Total 1	Zn 1	0
81	Aq	1	Total 1	Zn 1	0
81	Ar	1	Total 1	Zn 1	0
81	BR	1	Total 1	Zn 1	0
81	BT	1	Total 1	Zn 1	0
81	Bg	1	Total 1	Zn 1	0

- Molecule 82 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (CCD ID: M7G) (formula: C₁₁H₁₈N₅O₁₁P₂).

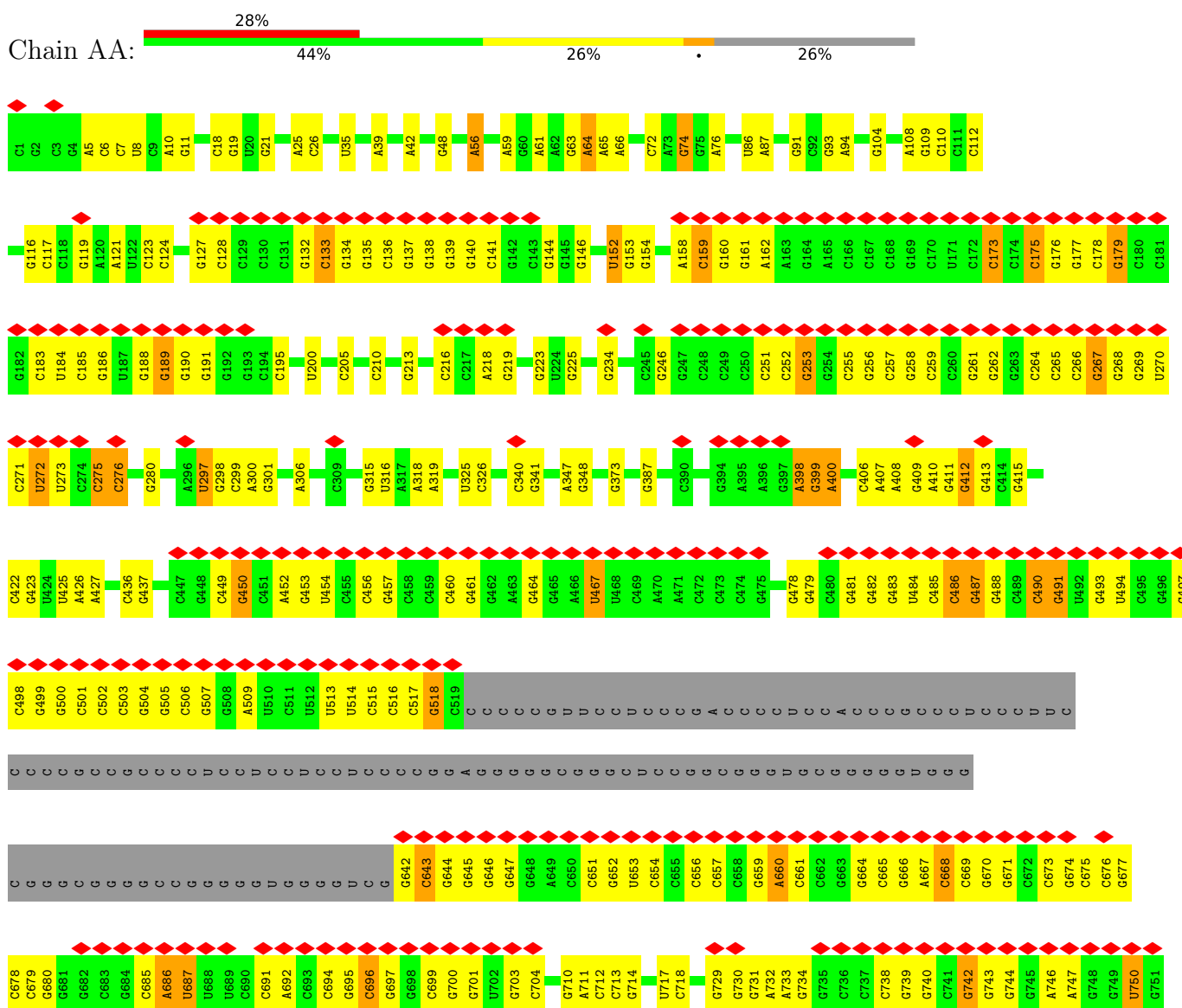


Mol	Chain	Residues	Atoms					AltConf
82	BA	1	Total	C	N	O	P	0
			24	11	5	7	1	

3 Residue-property plots

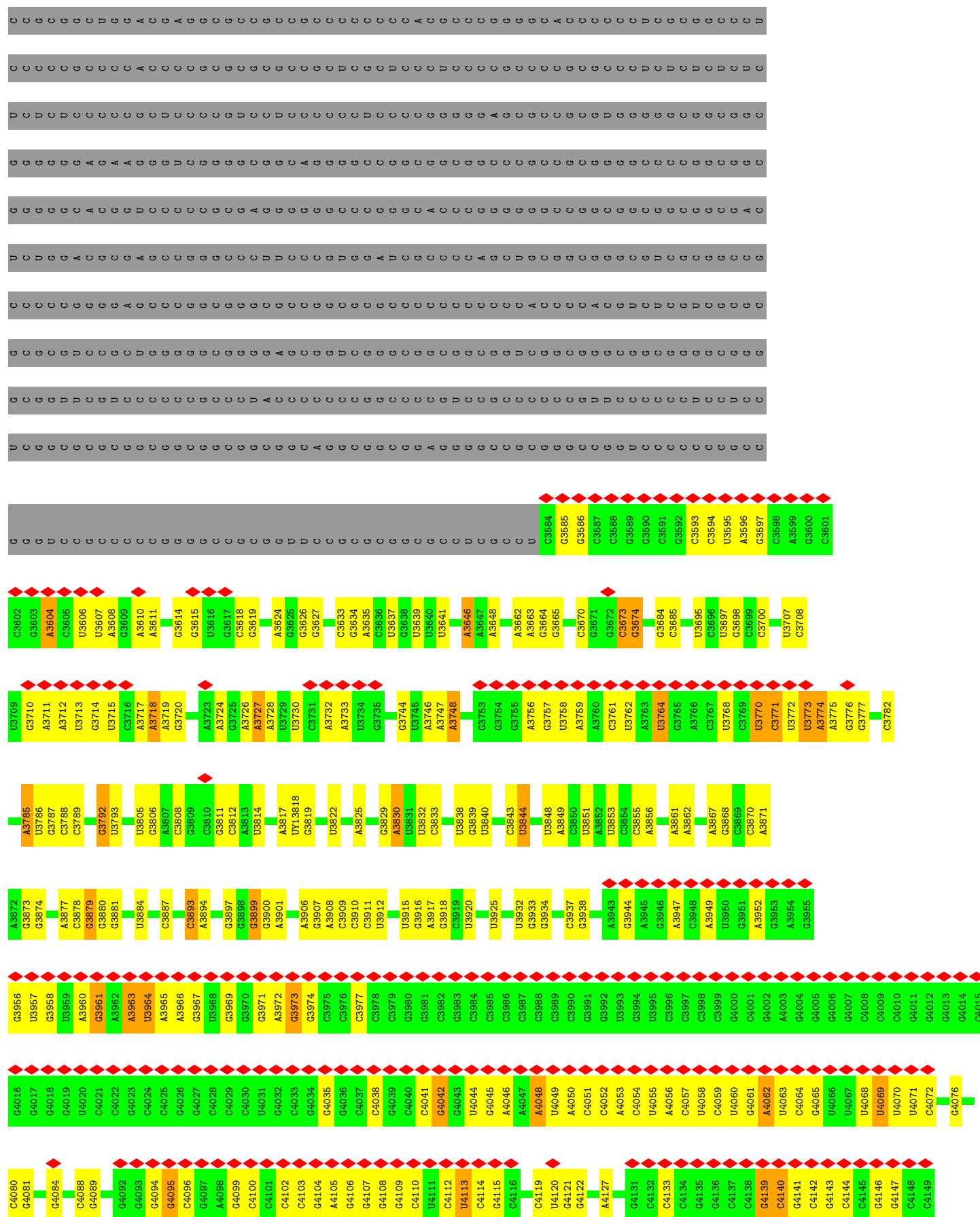
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

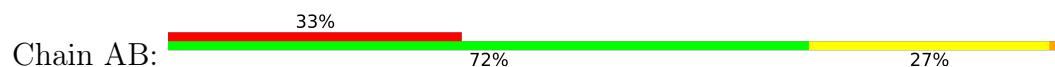
• Molecule 1: 28S rRNA (3773-MER)

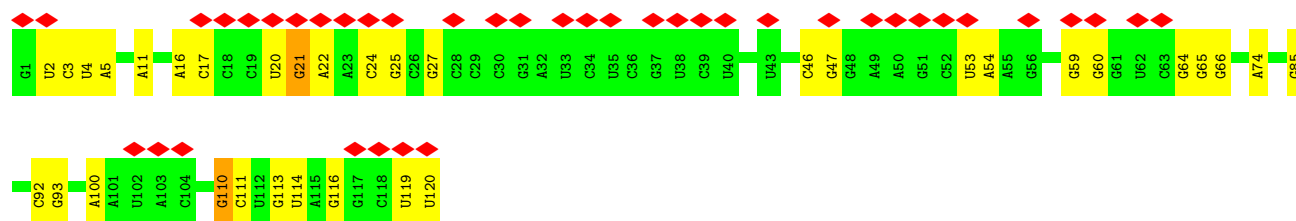




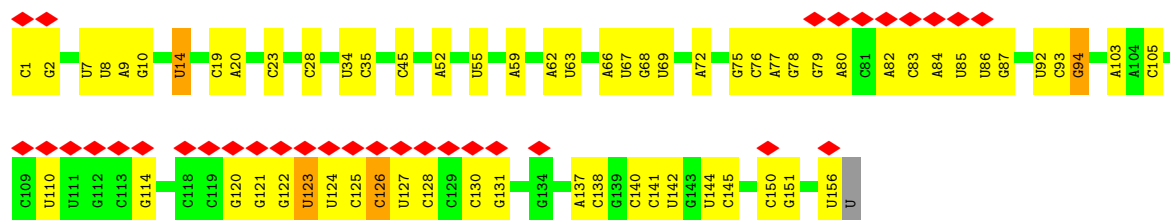
U2865	A2746	C2671	G2574	U2495	A2381	C	G	G1969	C1875	C1714
A2870	C2749	C2672	U2575	G2496	G2391	C	G	A1970	C1881	C1715
A2871	G2750	G2675	G2576	C2497	C2392	C	G	C1971	C1784	G1716
G2756	G2756	A2676	C2583	C2498	C	C	G	G1972	C1785	C1717
A2757	A2757	C2683	G2586	C2499	A2395	C	C	G1973	A1786	C1718
G2758	G2758	C2684	A2587	G2500	A2396	C	C	U1974	A1787	A1719
G2759	G2759	C2685	C2588	C2501	A2397	C	C	G1975	A1788	C1720
G2760	G2760	G2686	C2589	G2502	G2400	C	C	G1976	U1792	G1721
U2761	U2761	U2687	C2589	G2503	A2401	C	C	C1977	A1793	C1722
G2762	G2762	C2688	A2601	C2504	G2406	C	C	U1978	U1794	U1725
U2763	U2763	C2689		C2505	G2406	C	C	A1979	U1726	U1726
A2764	A2764	C2690		C2506	G2410	C	C	A1907	A1801	
A2765	A2765	G2697		C2507	C2411	C	C	A1908	A1802	C1731
A2766	A2766	A2698		U2508	A2412	C	C	G1981	G1803	C1732
U2767	U2767	G2699		A2513	A2415	C	C	G1982	A1804	G1733
C2768	C2768	C2699		G2514	G2416	C	C	A1983	A1805	
U2769	U2769	G2700		G2518	A2417	C	C	U1986	G1806	C1740
G2770	G2770	C2701		U2519	G2421	C	C	C1987	C1807	G1741
G2771	G2771	U2702		C2520	C2422	C	C	G1988	G1808	A1742
G2777	G2777	G2703		G2521	A2423	C	C	U1989	C1809	U1743
C2778	C2778	C2704		G2522	U2425	C	C	G1990	G1810	U1744
G2779	G2779	G2705		A2529	C2441	C	C	A1991	A1811	G1745
C2780	C2780	C2706		C2539	G2448	C	C	U1992	C1812	A1746
G2781	G2781	U2707		C2540	A2449	C	C	C1993	C1820	U1747
A2787	A2787	G2708		G2543	G2450	C	C	U1994	G1821	U1748
U2788	U2788	U2709		G2544		C	C	C1995	U1822	A1749
A2789	A2789	C2710		U2545		C	C	U1996	G1823	G1750
U2790	U2790	G2711		G2546		C	C	U1997	G1824	U1751
C2791	C2791	U2712		G2547		C	C	A1998	A1825	
C2804	C2804	G2713		C2548		C	C	U1999	G1830	G1752
C2805	C2805	U2714		G2549		C	C	G2000	G1831	G1753
A2806	A2806	G2715		C2550		C	C	G2001	U1834	U1754
		C2716		A2551		C	C	G2002	G1835	G1755
		G2717		G2552		C	C	G2003	G1836	G1756
		U2718		A2553		C	C	U2004	A1837	G1757
		C2719		U2554		C	C	U1947	G1842	U1757
		G2720		G2555		C	C	U1954	U1845	U1757
		U2721		C2556		C	C	G1955	G1846	G1758
		G2722		G2557		C	C	G1956	G1847	G1759
		C2723		C2558		C	C	U1957	G1848	G1760
		G2724		G2559		C	C	A1958	G1849	G1761
		A2725		C2560		C	C	U1959	A1766	A1765
		G2726		G2561		C	C	A1960	C1857	A1766
		U2727		G2562		C	C	G1961	A1767	A1767
		C2728		C2563		C	C	U1962	G1769	G1769
		U2729		G2564		C	C	U1862	A1770	A1770
		G2730		A2565		C	C	C1963	U1771	U1771
		C2731		G2566		C	C	A1964	C1772	C1772
		G2739		C2567		C	C	G1965	U1773	U1773
				C2568		C	C	C1966	C1774	C1774
				G2662		C	C	A1871	A1775	A1775
				C2669		C	C		C1776	A1776
				U2570		C	C		C1777	C1777
				C2571		C	C		C1778	C1778
				C2572		C	C		U1779	U1779
				A2573		C	C		A1780	A1780
						C	C		U1781	U1781
						C	C		U1782	U1782



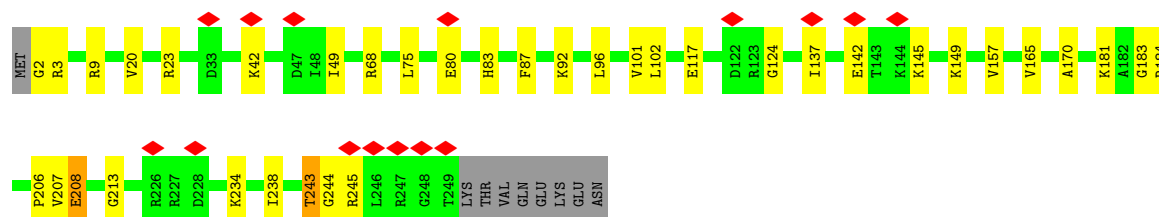
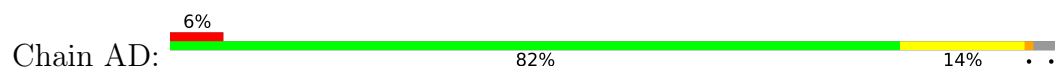




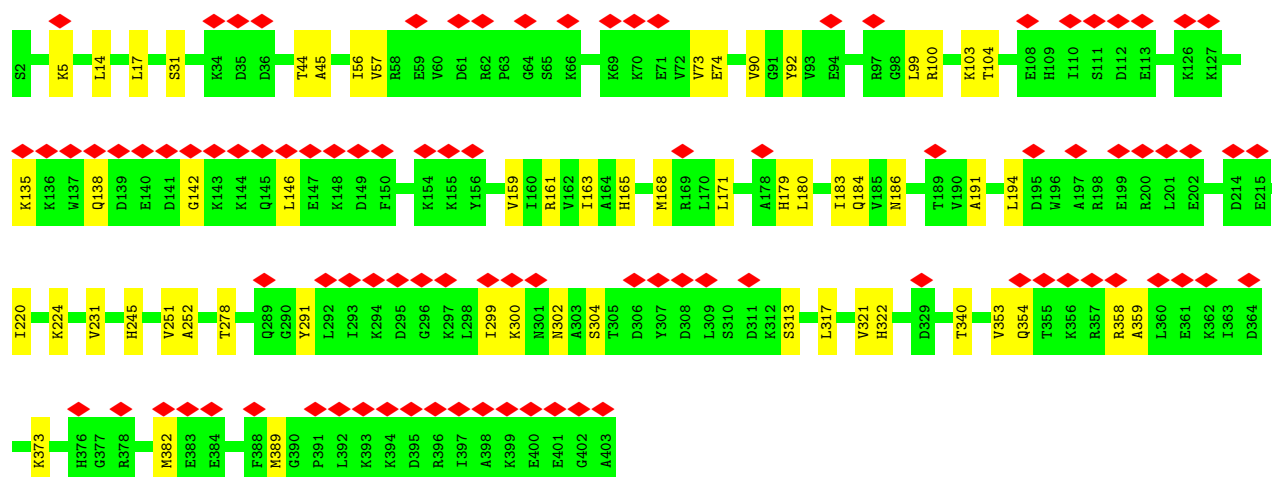
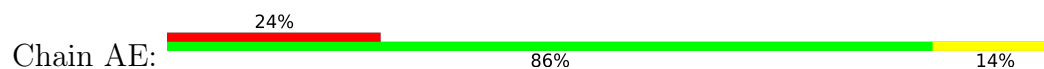
• Molecule 3: 5.8S rRNA (156-MER)



• Molecule 4: 60S ribosomal protein L8

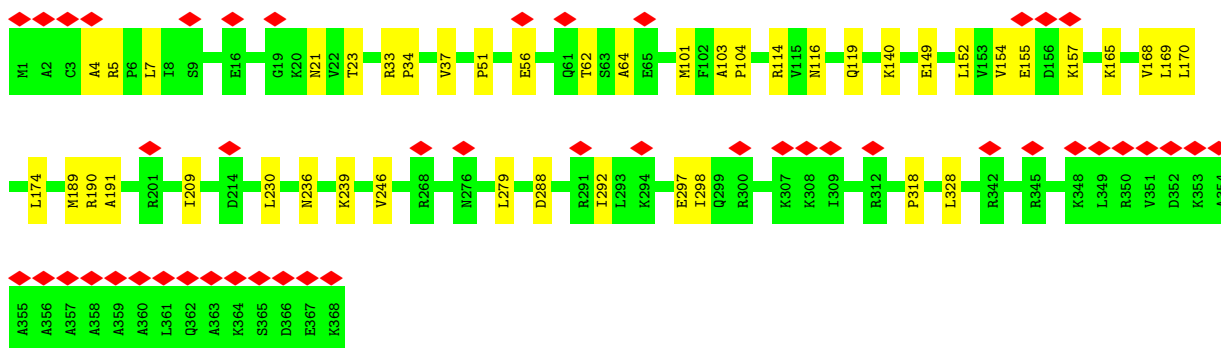


• Molecule 5: Large ribosomal subunit protein uL3



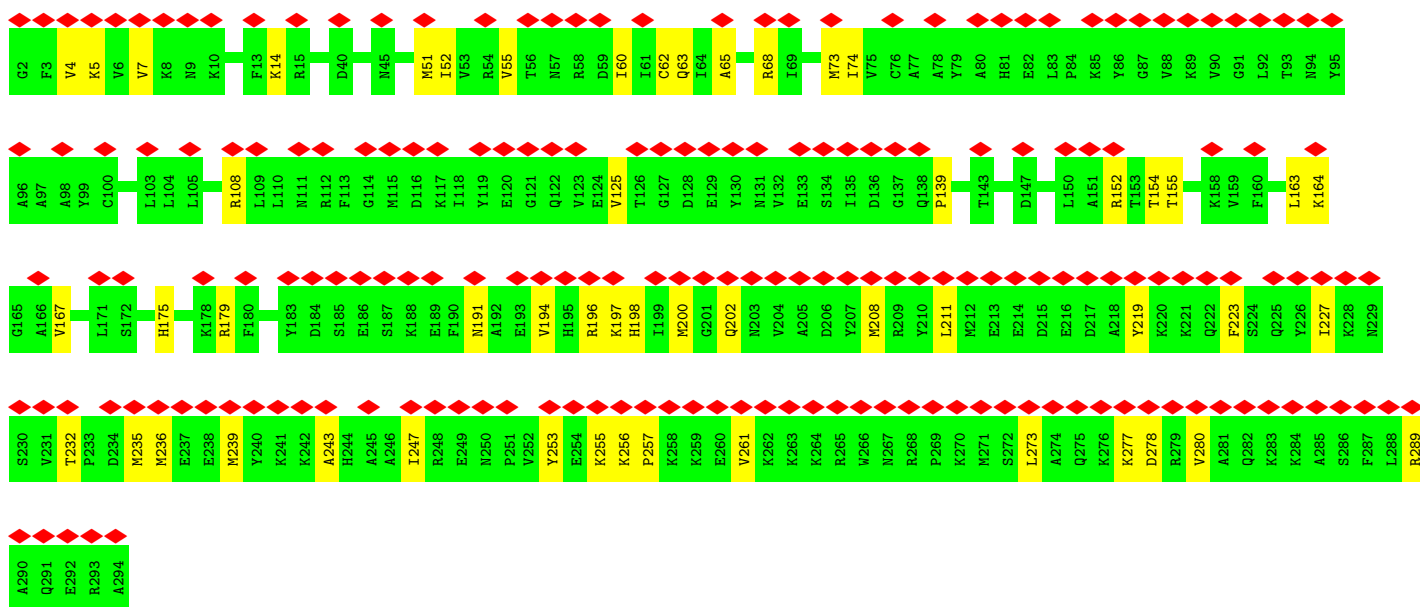
• Molecule 6: Large ribosomal subunit protein uL4

Chain AF: 



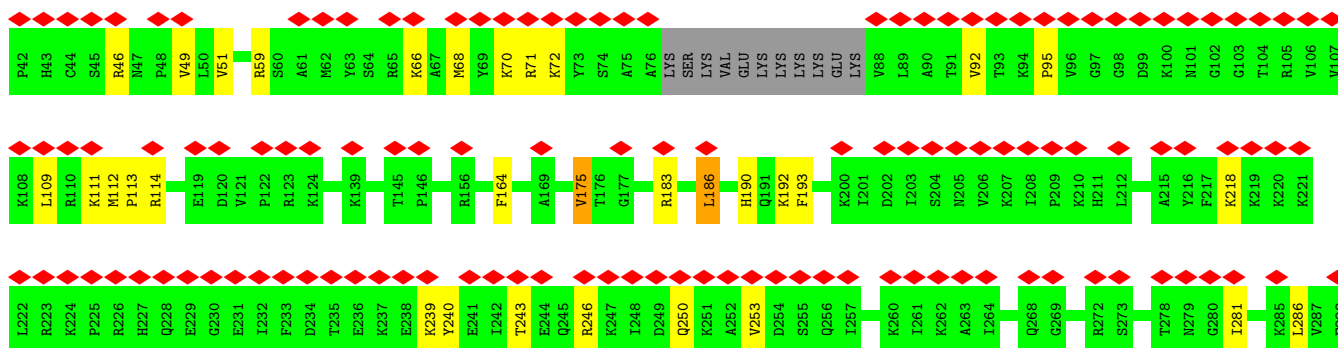
• Molecule 7: Large ribosomal subunit protein uL18

Chain AG: 

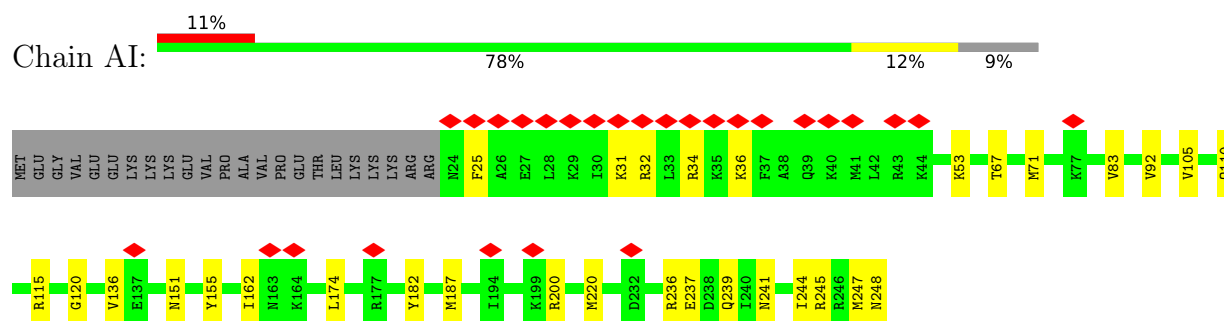


• Molecule 8: Large ribosomal subunit protein eL6

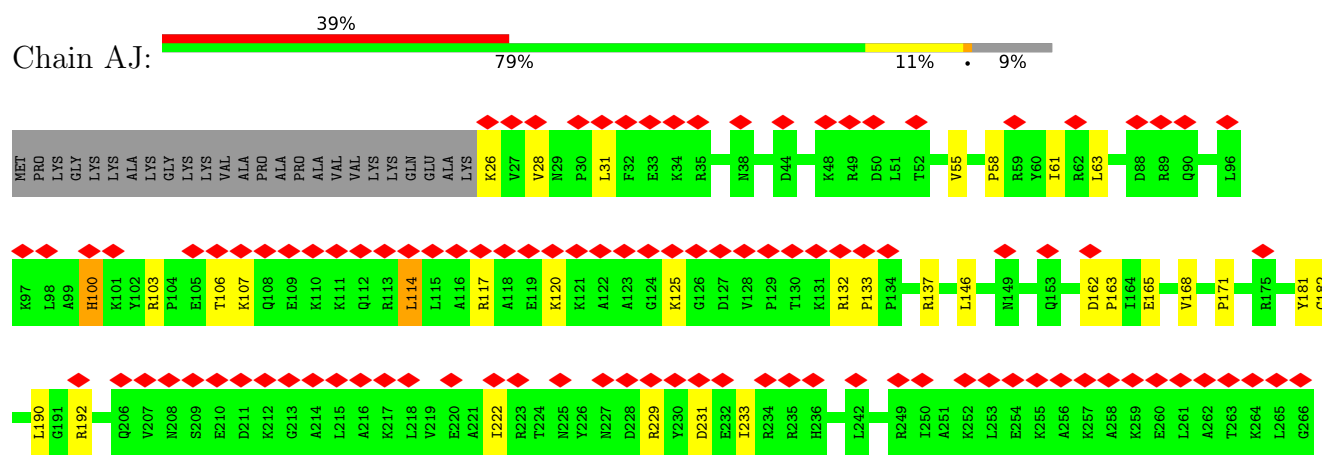
Chain AH: 



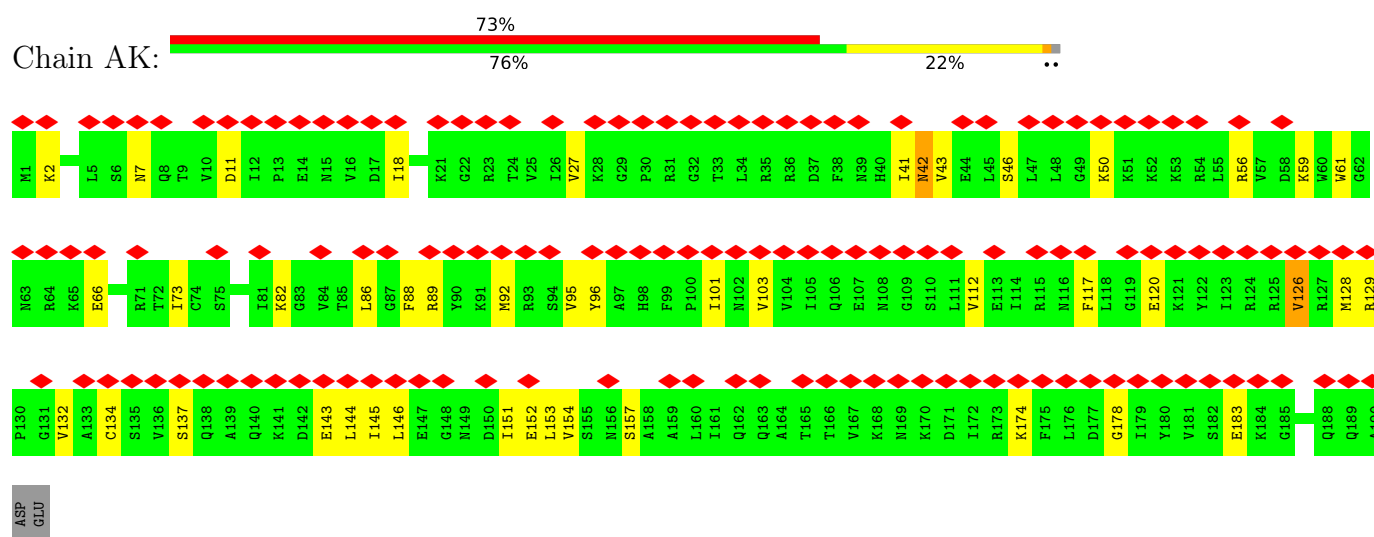
- Molecule 9: 60S ribosomal protein L7



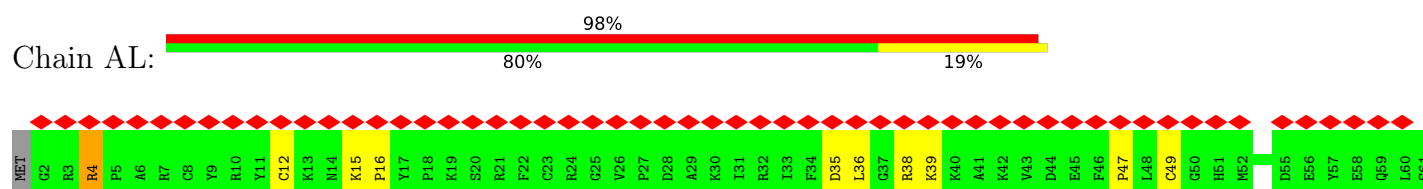
- Molecule 10: 60S ribosomal protein L7a



- Molecule 11: 60S ribosomal protein L9

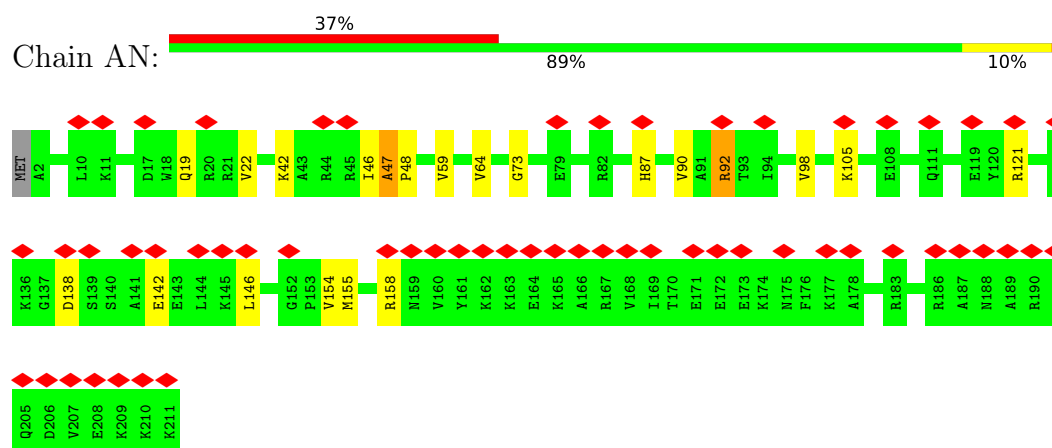


- Molecule 12: Ribosomal protein uL16-like

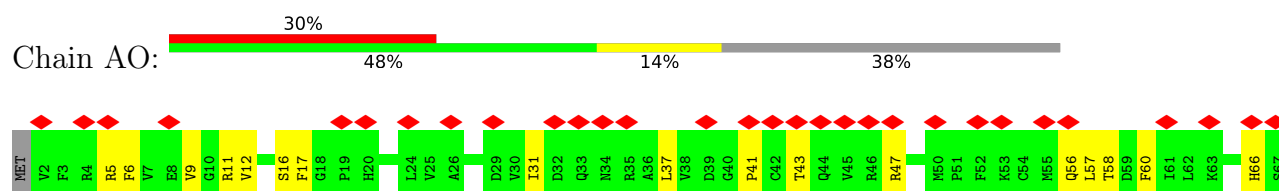


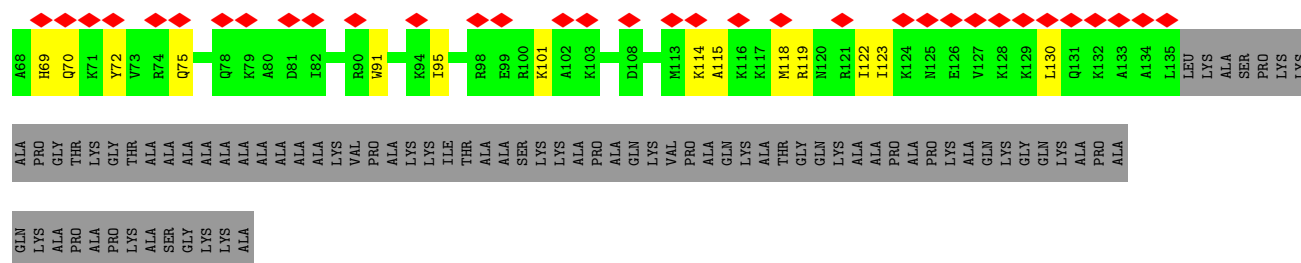


• Molecule 14: 60S ribosomal protein L13

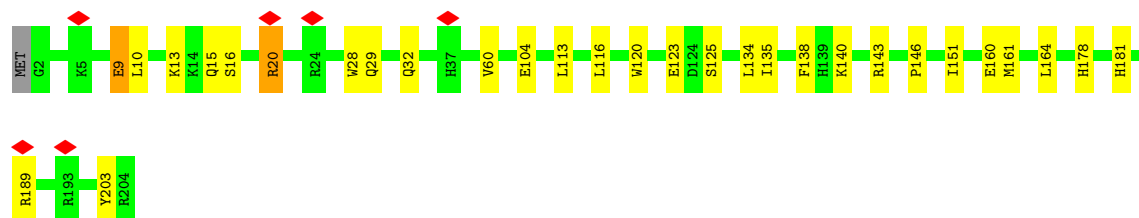
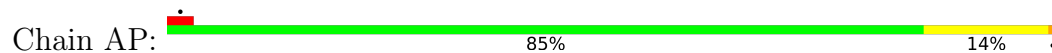


• Molecule 15: 60S ribosomal protein L14

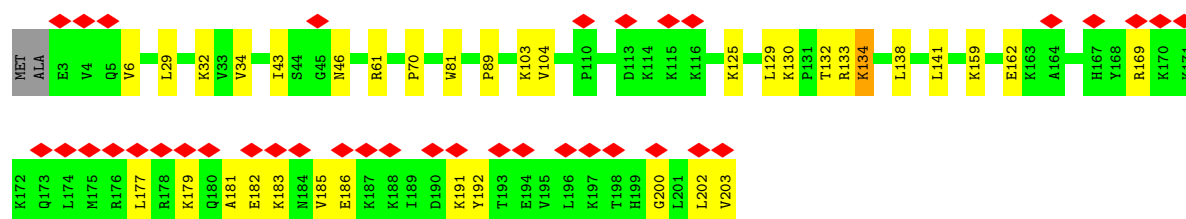
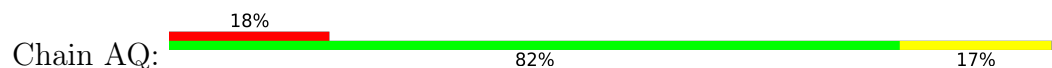




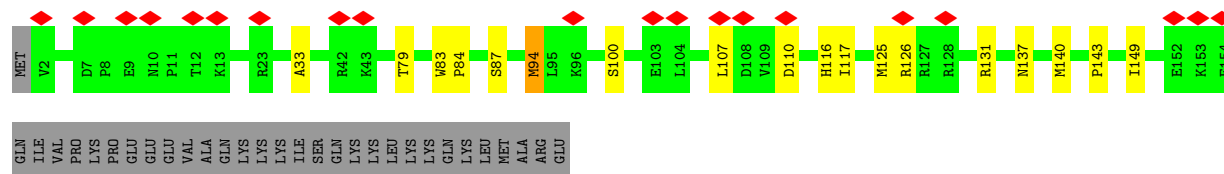
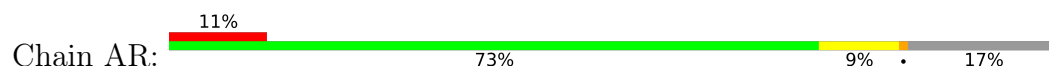
- Molecule 16: 60S ribosomal protein L15



- Molecule 17: 60S ribosomal protein L13a



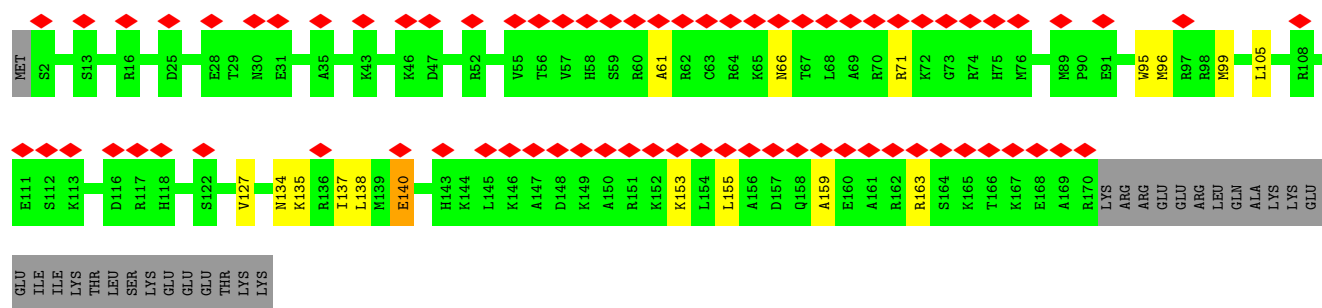
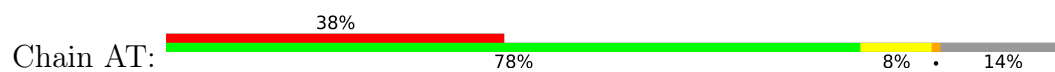
- Molecule 18: 60S ribosomal protein L17



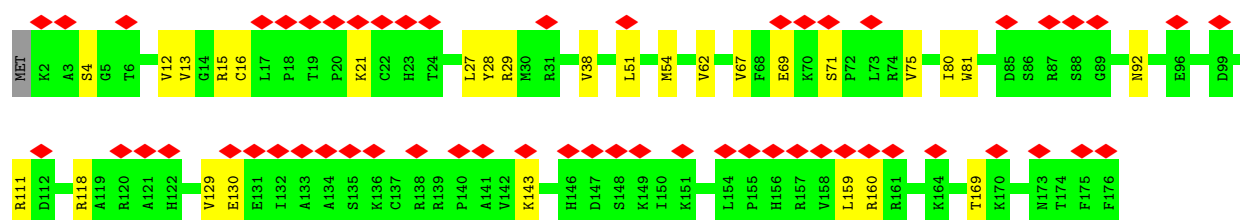
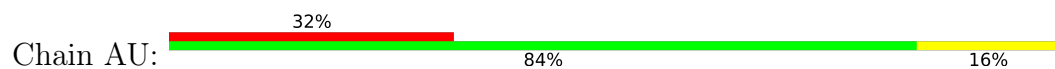
- Molecule 19: 60S ribosomal protein L18



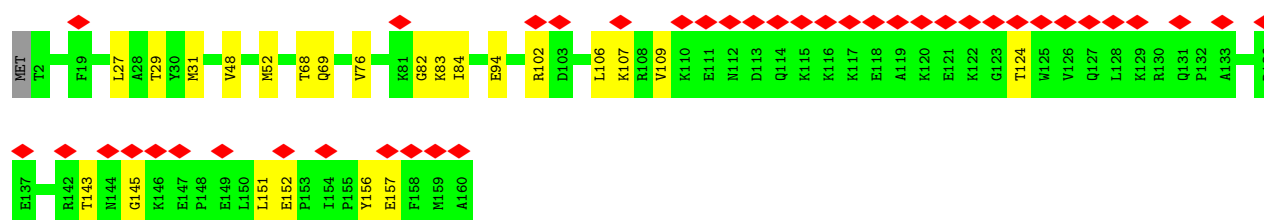
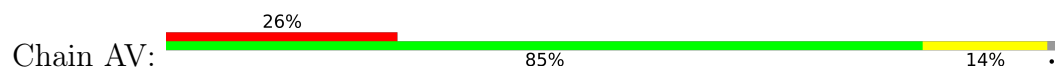
- Molecule 20: 60S ribosomal protein L19



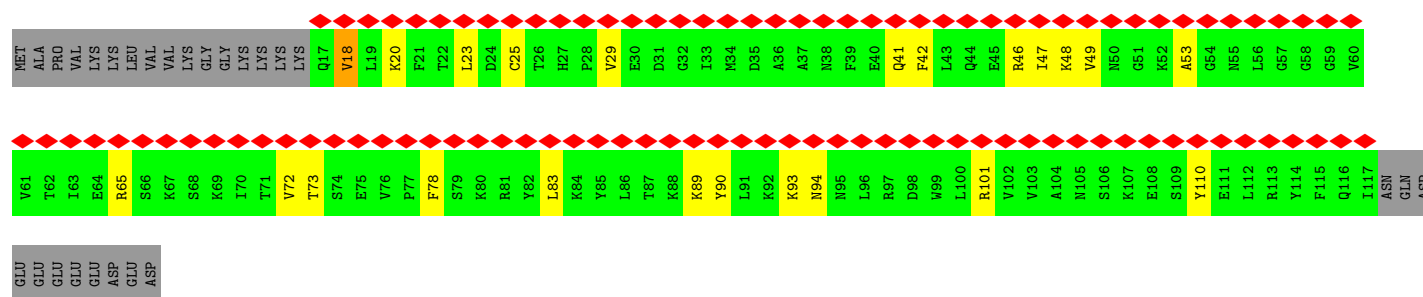
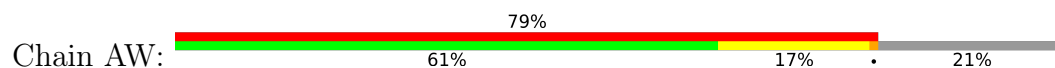
- Molecule 21: 60S ribosomal protein L18a



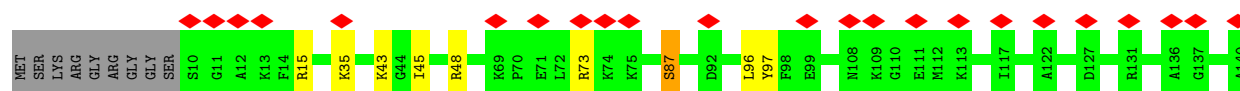
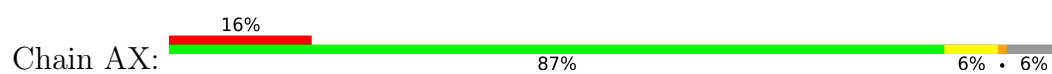
- Molecule 22: 60S ribosomal protein L21



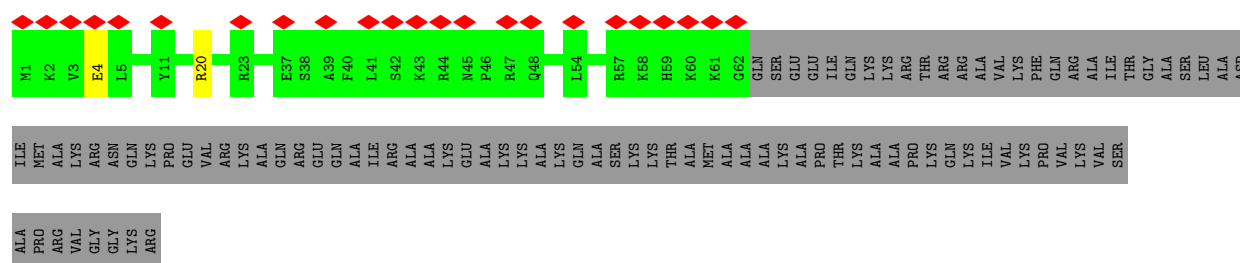
- Molecule 23: 60S ribosomal protein L22



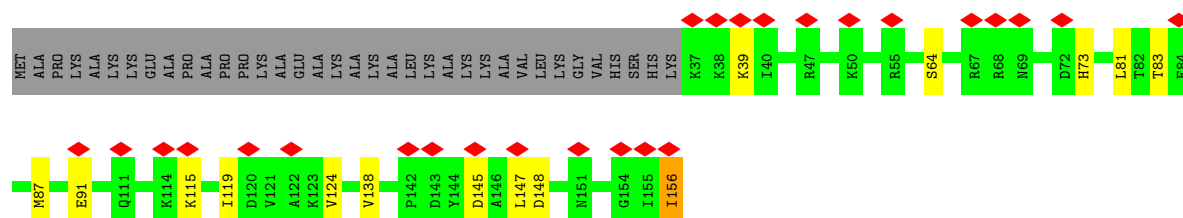
- Molecule 24: 60S ribosomal protein L23



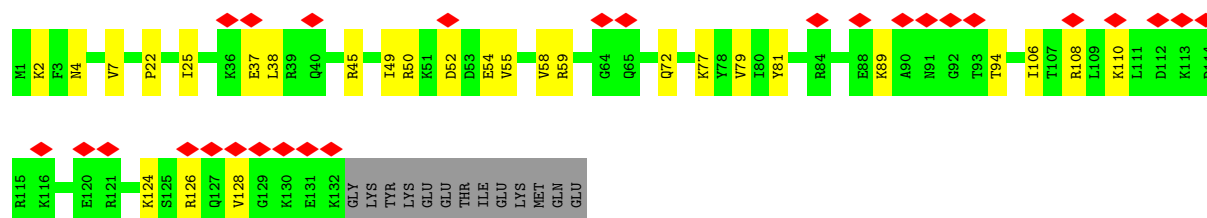
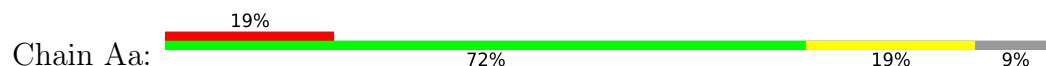
• Molecule 25: 60S ribosomal protein L24



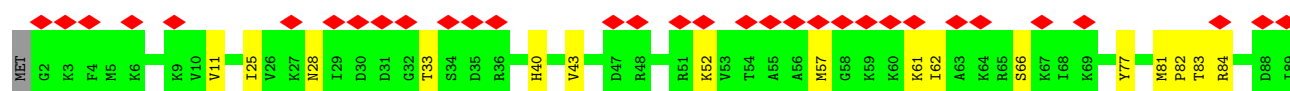
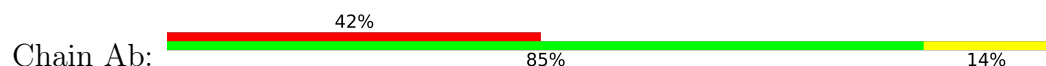
• Molecule 26: 60S ribosomal protein L23a

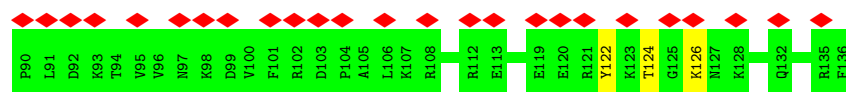


• Molecule 27: 60S ribosomal protein L26

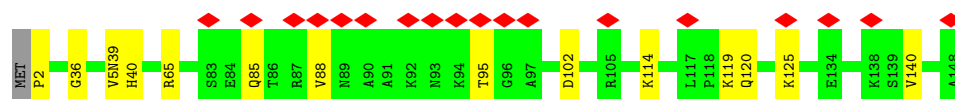


• Molecule 28: 60S ribosomal protein L27

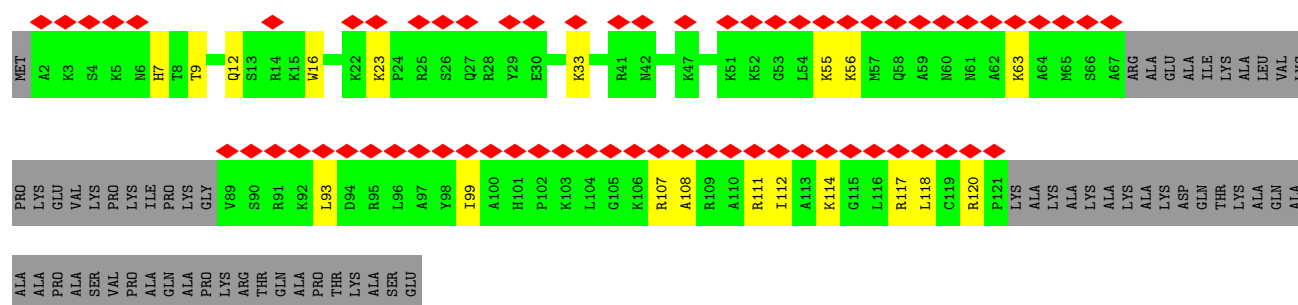
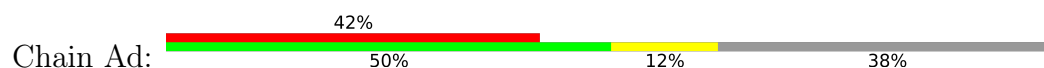




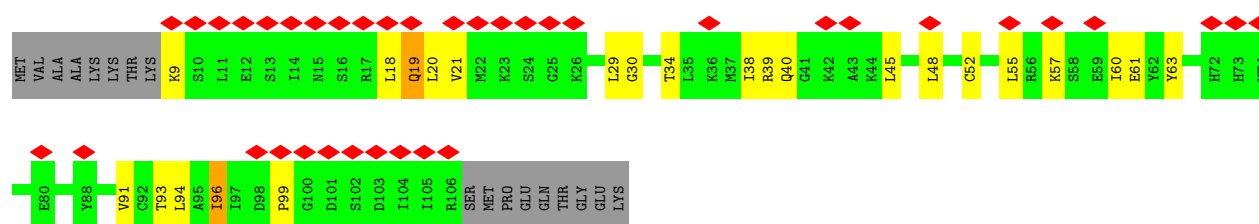
- Molecule 29: Large ribosomal subunit protein uL15



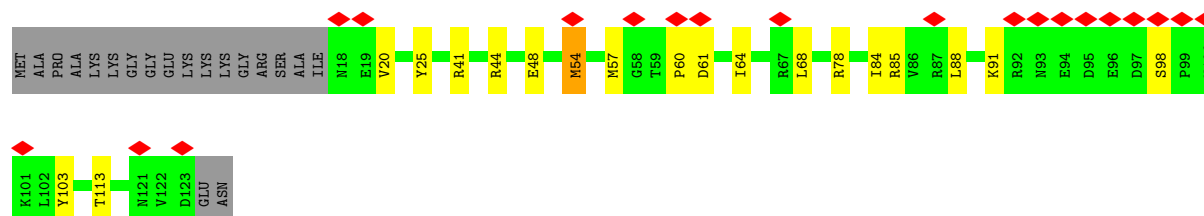
- Molecule 30: 60S ribosomal protein L29



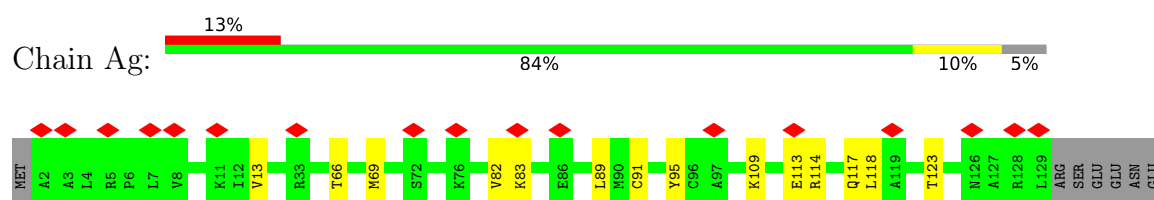
- Molecule 31: 60S ribosomal protein L30



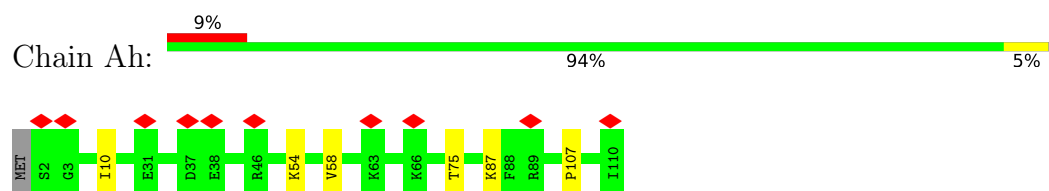
- Molecule 32: 60S ribosomal protein L31



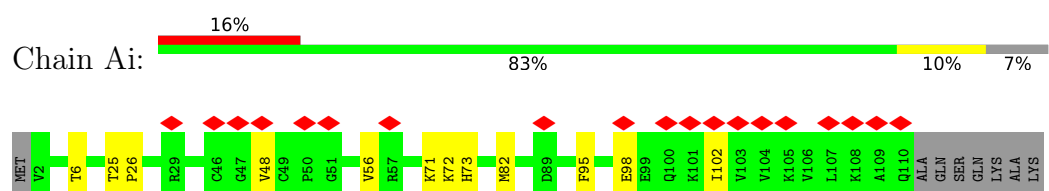
- Molecule 33: 60S ribosomal protein L32



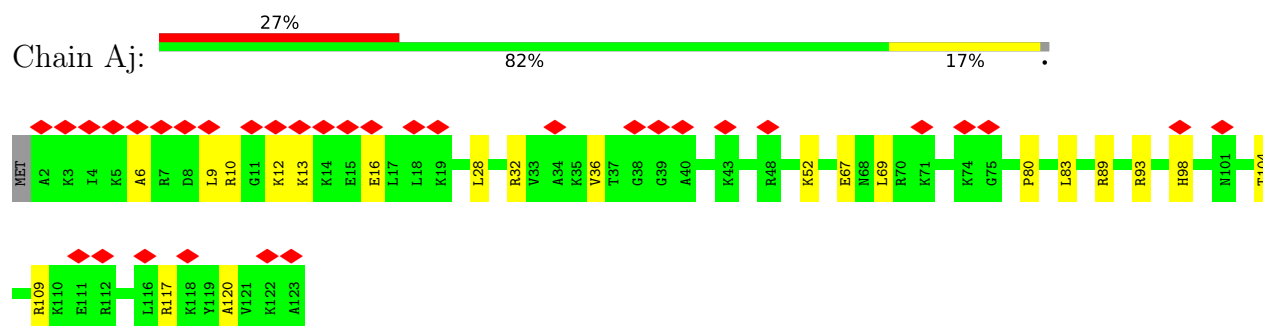
- Molecule 34: 60S ribosomal protein L35a



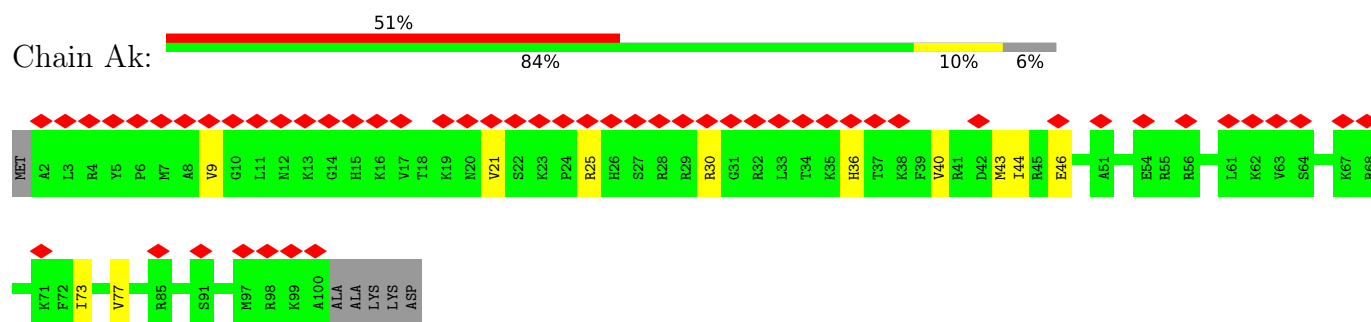
- Molecule 35: 60S ribosomal protein L34



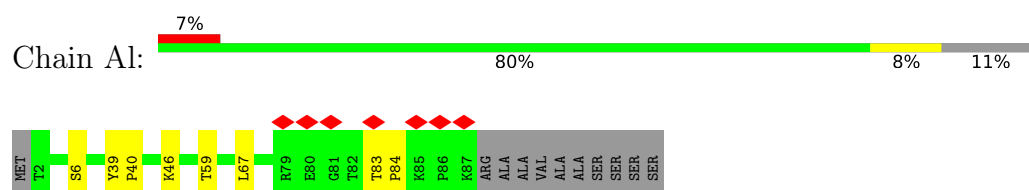
- Molecule 36: 60S ribosomal protein L35



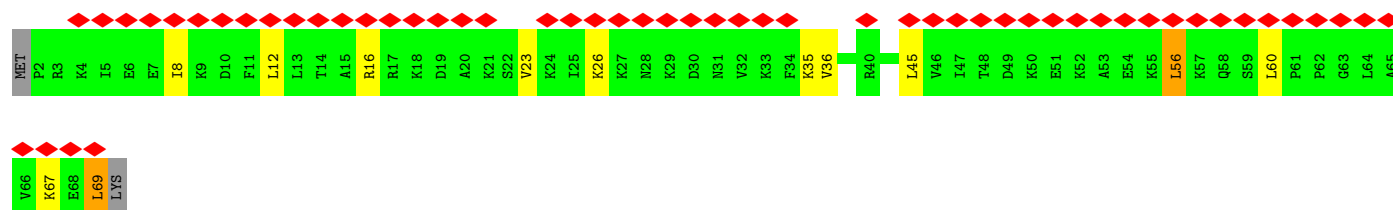
- Molecule 37: 60S ribosomal protein L36



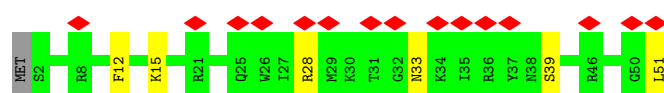
- Molecule 38: 60S ribosomal protein L37



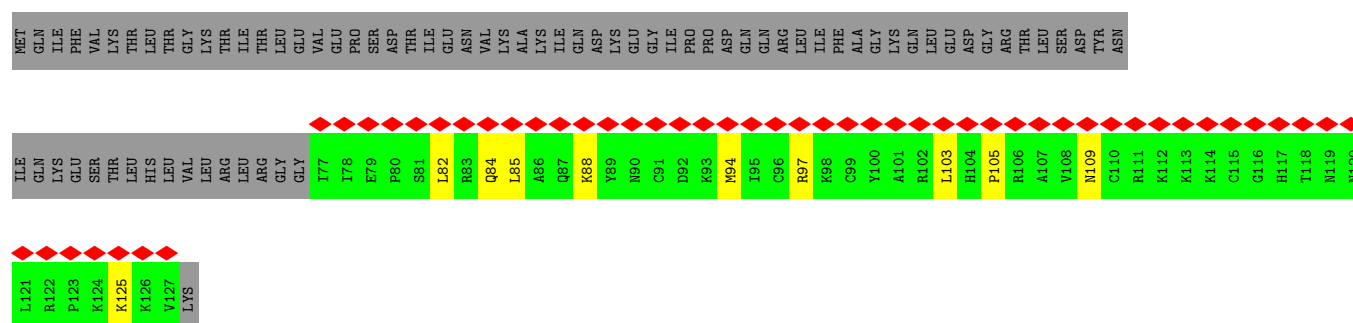
Chain Am: 79% 80% 14%



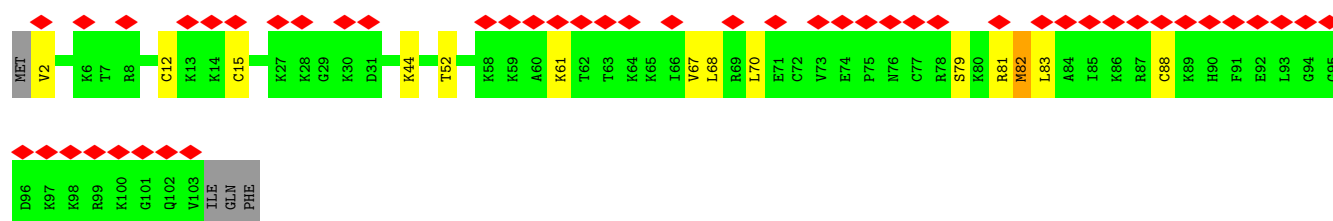
Chain An:



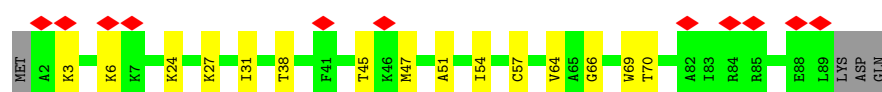
Chain Ao:



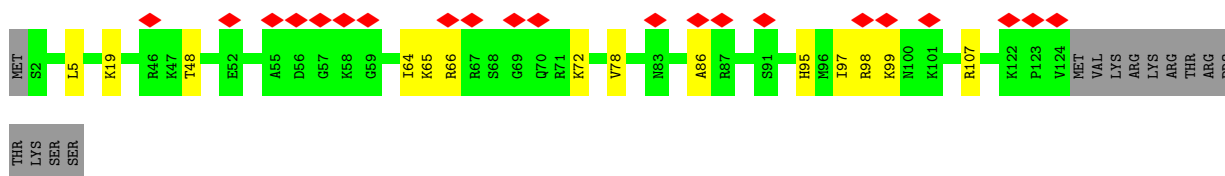
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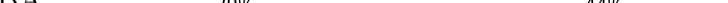


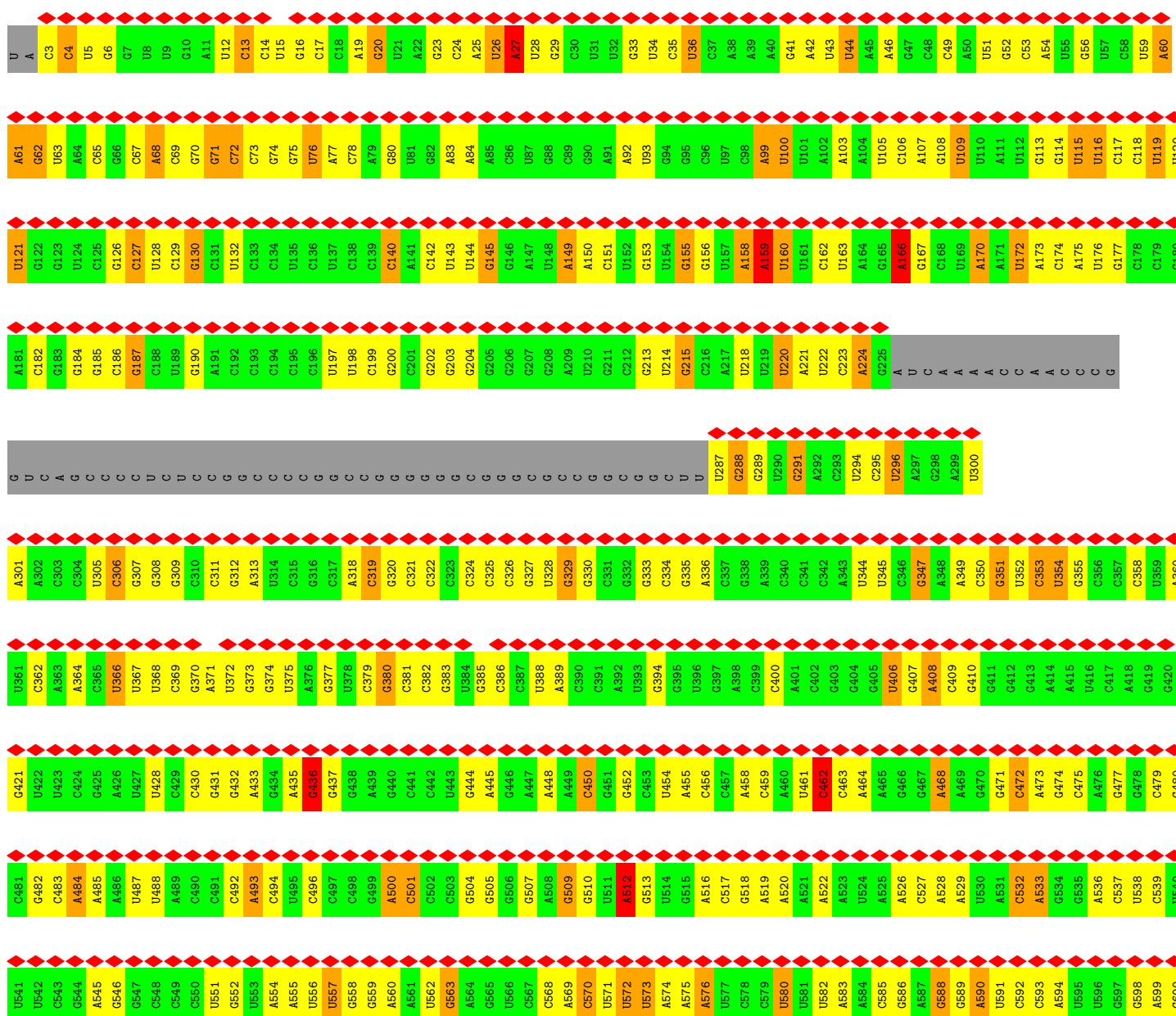
Chain Ar:



- Chain As: 



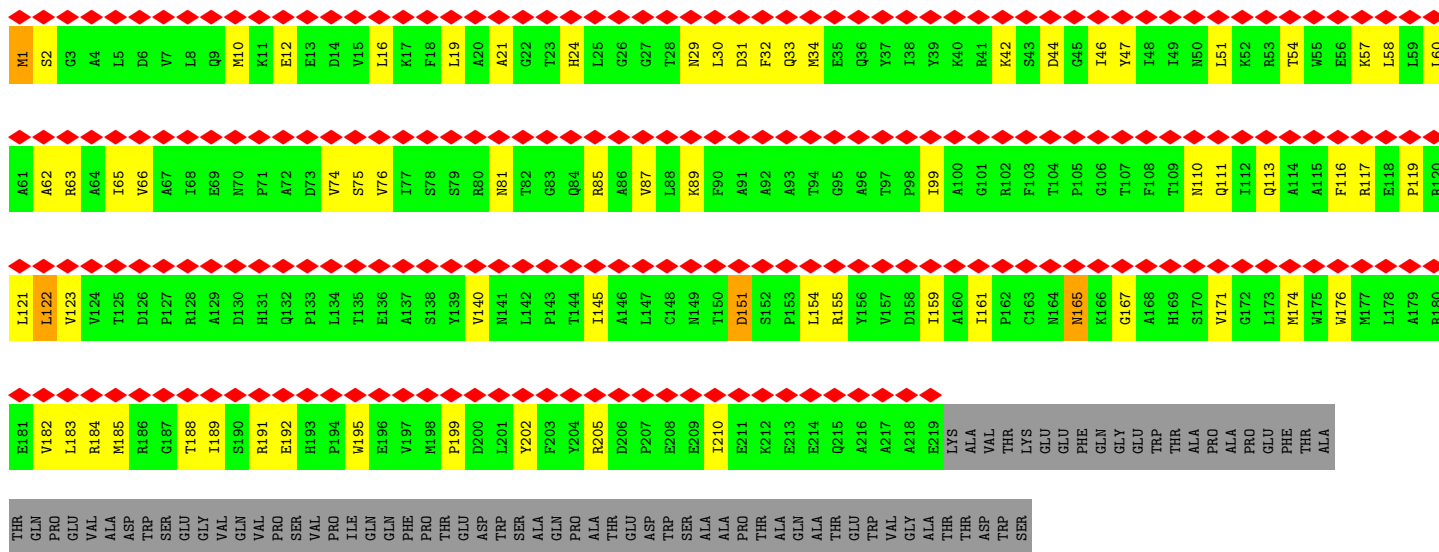
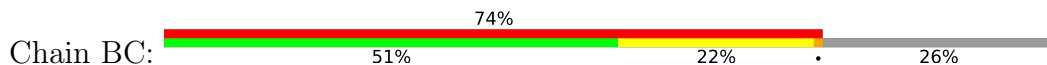
- Chain BA: 



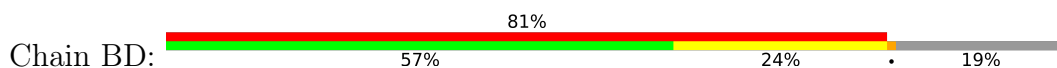
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G1328	G1268	A1208	A1148	A1024	A964	A904	U944	A	G602
U1329	G1269	A1209	G1089		U965	C905	G845	C	C603
G1330	G1270	G1210	A1149	A1027	U966	U906	G846	C	A604
C1331	G1271	G1211	G1091	A1028	C967	G907	A947	C	A605
A1332	G1272	G1212	G1092	G1029	U968	A908	U948		G606
U1333	C1273	C1213	A1093	A1030	U969	G909	A949		U607
G1334	G1274	A1214	C1094	A1031	G970	G910	C790		C608
G1335	G1275	C1215	G1095	C1032	G971	G911	C791		U609
G1336	A1276	C1216	G1096	A1033	A972	C912	C792		G610
U1337	C1277	A1217	G1097		C973	A913	G793		G611
G1338	A1278	C1218	C1098	U1038	C974	U914	A794		U612
U1339	G1279	C1219	G1099	C1039	G975	G915	A795		G613
U1340	G1280	A1220	A1100	G1040	U976	A916	G796		U614
C1341	G1281	G1221	U1101	G1041	C977	U917	C797		C615
U1342	A1282	C1222	G1102	A1042	U978	U918	G798		A616
U1343	G1283	A1223	C1103	G1043	C979	A919	U799		C617
A1344	A1284	G1224	G1104	G1044	A980	A920	U800		A618
G1345	G1285	U1225	G1105	U1045	A981	G921	U801		A619
U1346	G1286	G1226	G1106	U1046	G982	A922	A802		G620
U1347	A1287	G1227	G1107	C1047	A983	G923	A803		C621
G1348	U1288	A1228	G1108	G1048	C984	G924	U804		C622
G1349	U1289	G1229	G1109	A1049	G985	G925	U805		G623
U1350	G1290	C1230	A1170	A1050	U986	A926	U806		C624
G1351	A1291	C1231	G1171	G1051	A987	G927	G807		G625
G1352	G1292	U1232	U1112	A1052	C988	G928	U808		G626
A1353	A1293	G1233	A1113	C1053	C989	G929	A809		U627
G1354	G1294	C1234	U1174	G1054	A990	C930	A810		A628
A1295	A1295	G1235	G1175	A1055	G991	C931	A811		A629
G1356	U1296	G1236	G1176	U1056	A992	G932	A812		U630
U1297	U1297	C1237	U1177	C1057	G993	G933	A813		U631
G1298	U1298	U1238	U1178	G1058	C994	G934	U814		C632
U1359	G1299	U1239	G1179	G1059	G995	G935	U815		C633
U1360	U1300	U1240	A1119	A1060	A996	G936	A816		A634
G1361	A1301	A1241	U1120	U1061	A997	C937	G817		G635
U1362	G1302	A1242	G1121	A1062	A998	A938	A818		C636
C1363	C1303	U1243	A1182	C1063	G999	U939	G819		U637
U1364	U1304	U1244	C1123	C1064	C1000	U940	G820		C638
G1365	C1305	G1245	C1124	G1065	A1001	C941	G821		C639
G1366	U1306	U1246	C1125	U1066	U1002	G942	U822		A641
U1367	U1307	C1247	G1126	U1067	U1003	U943	U823		U642
U1368	U1308	B8N1248	C1127	G1068	U1004	A944	C824		A643
A1369	C1309	A1190	C1128	U1069	G1005	U945	A825		G644
U1370	U1310	C1249	G1129	A1070	C1006	U946	A826		C645
U1371	C1311	U1251	U1130	G1071	C1007	G947	A827		G646
U1372	U1312	G1252	G1131	U1072	A1008	C948	G828		U647
C1373	A1313	A1253	C1132		A1009	G949	C829		A648
C1374	U1314	G1254	A1133	C1075	A1010	C950	A830		U649
G1375	U1315	G1255	G1134	A1076	A1011	C951	G831		A650
A1376	C1316	G1256	C1135	A1077	A1012	G952	G832		U651
U1377	U1317	G1257	U1136	C1078	U1013	C953	C833		A653
A1378	G1318	A1258	U1137	C1079	U1014	U954	C834		U652
A1379	U1319	A1259	C1138	U1081	A955	G894	C835		A654
C1380	G1320	U1260	U1016	A1082	G956	U957	G836		G656
G1381	G1321	C1261	U1017	A1083	A957	U958	A837		U657
A1382	G1322	G1262	A1084	C1085	G958	U959	G838		G658
A1383	U1323	U1263	G1142	G1086	C1019	U960	C840		G659
C1384	G1324	C1264	A1143		A1020	G961	G841		C660
G1385	G1325	A1265	A1144		U1021				
A1386	UY11326	C1266	A1145		U1022				
			C1146						



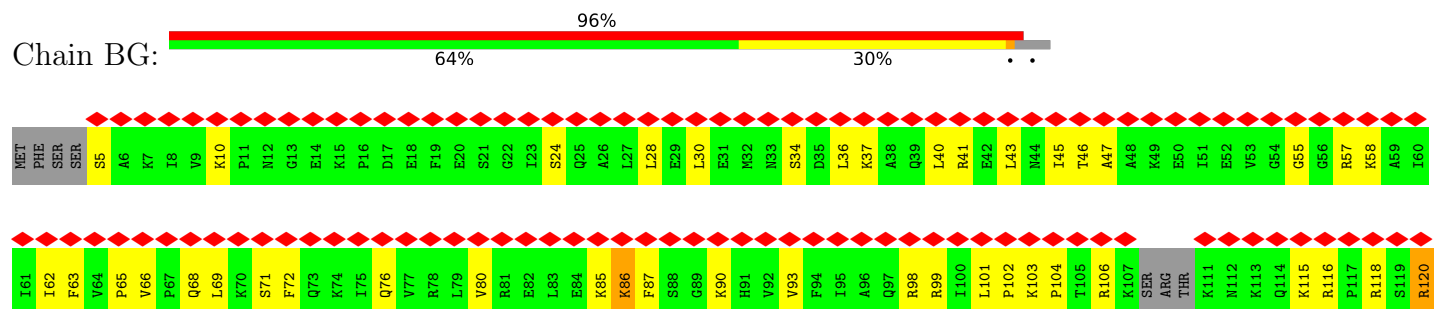
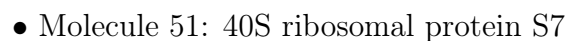
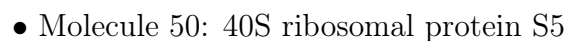
- Molecule 47: Small ribosomal subunit protein uS2



- Molecule 48: 40S ribosomal protein S3a

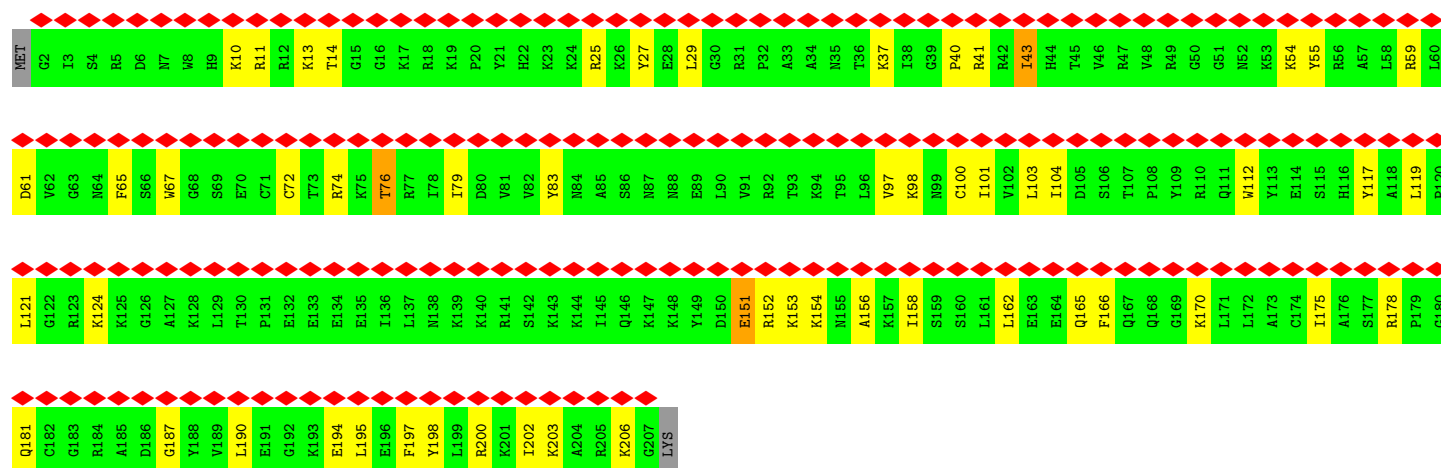
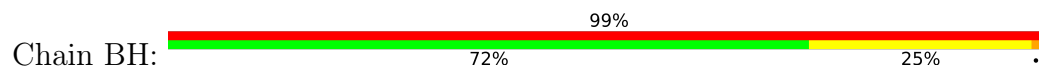


- Molecule 49: 40S ribosomal protein S3

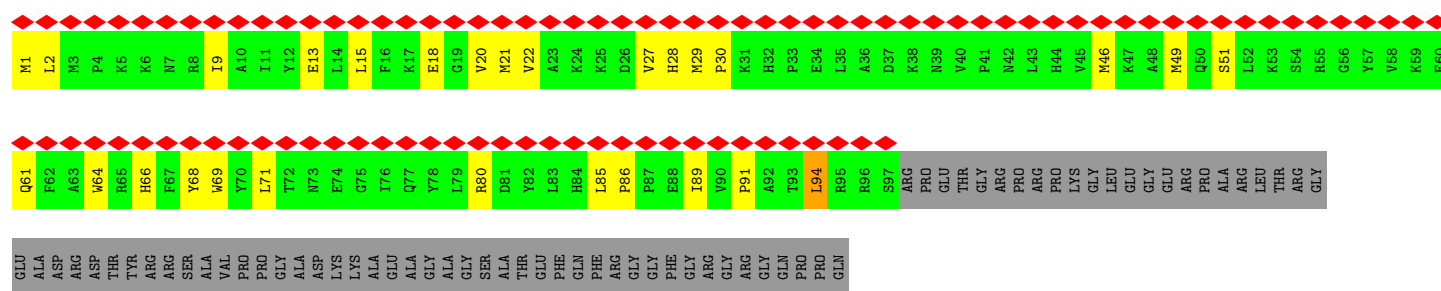




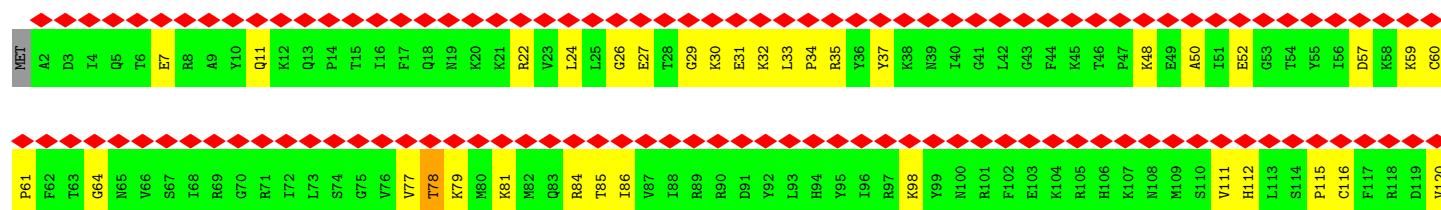
• Molecule 52: 40S ribosomal protein S8

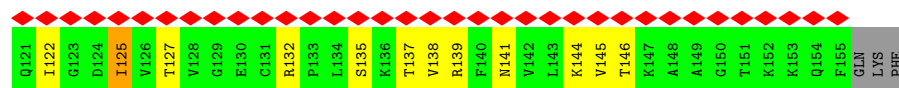


• Molecule 53: 40S ribosomal protein S10

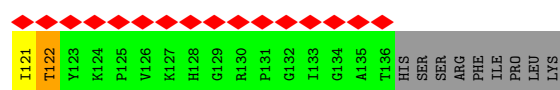
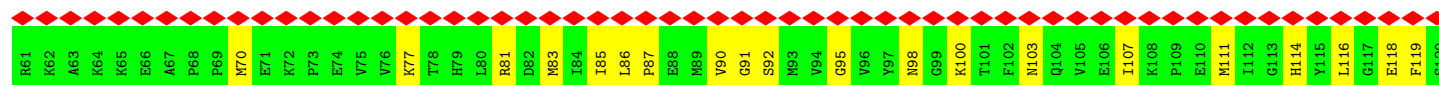
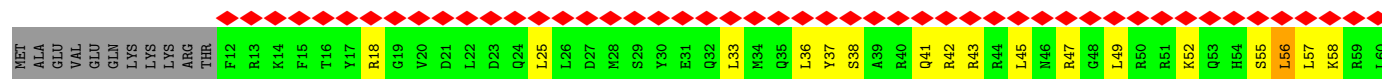
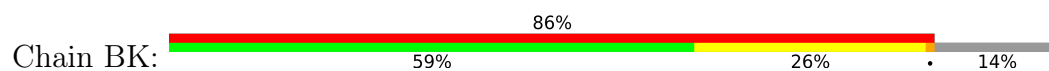


• Molecule 54: 40S ribosomal protein S11

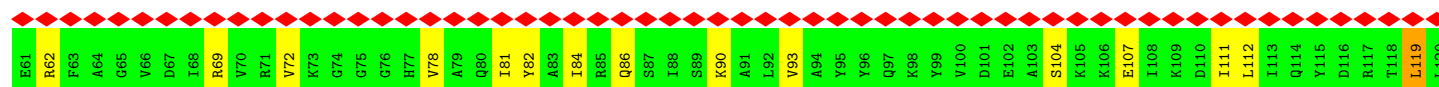
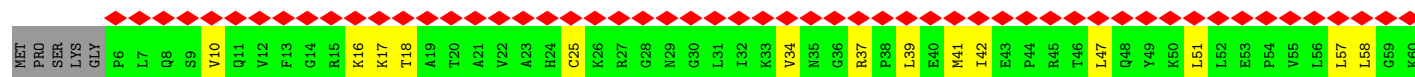
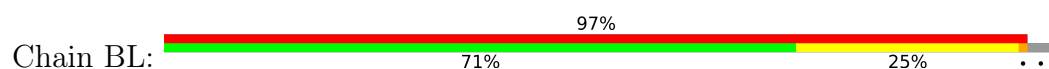




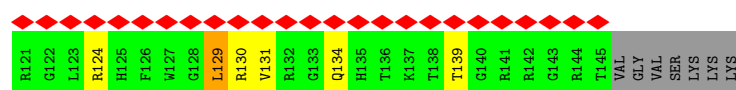
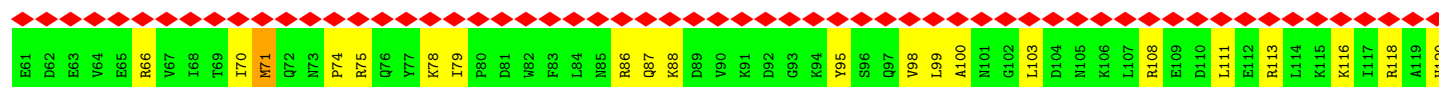
- Molecule 55: 40S ribosomal protein S15



- Molecule 56: 40S ribosomal protein S16

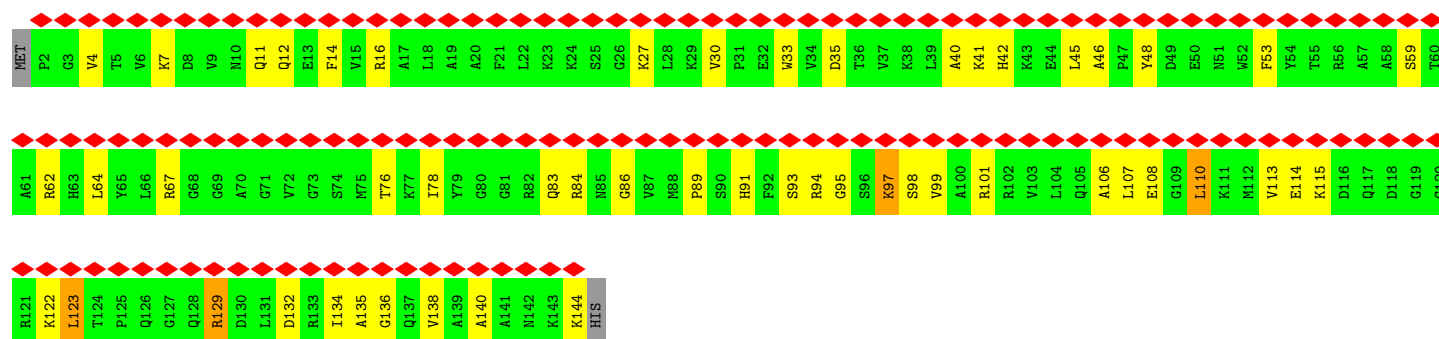


- Molecule 57: 40S ribosomal protein S18

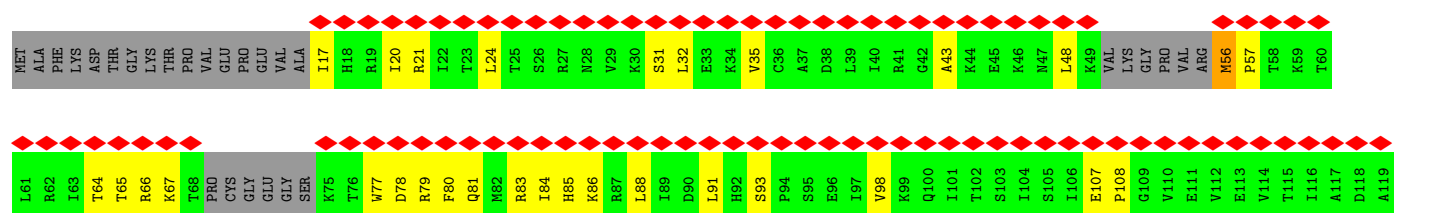
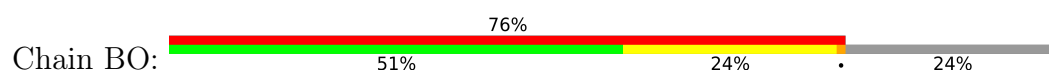


- Molecule 58: Small ribosomal subunit protein eS19

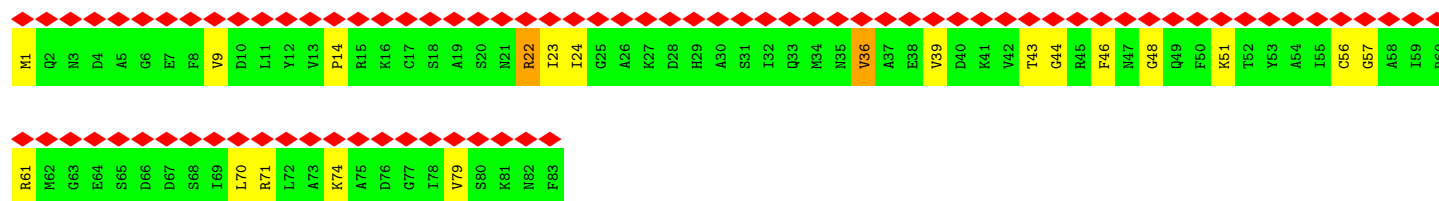
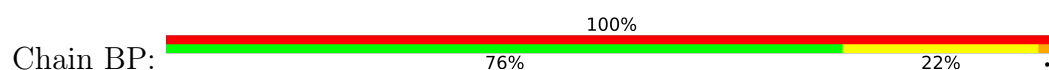




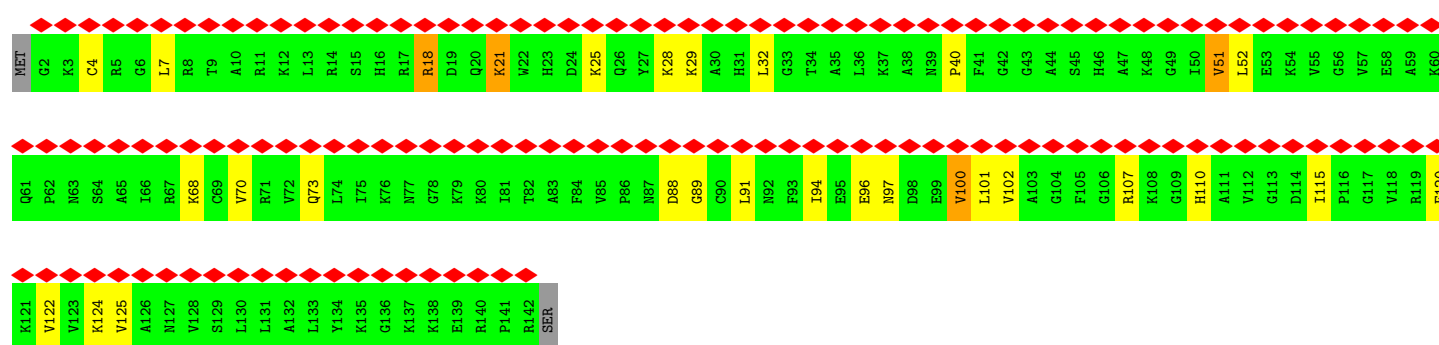
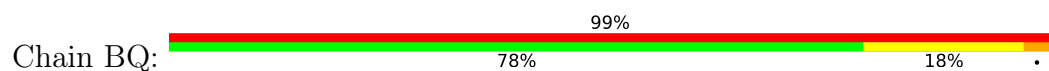
• Molecule 59: 40S ribosomal protein S20



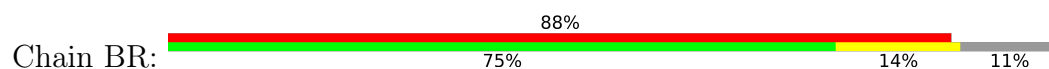
• Molecule 60: 40S ribosomal protein S21



• Molecule 61: 40S ribosomal protein S23

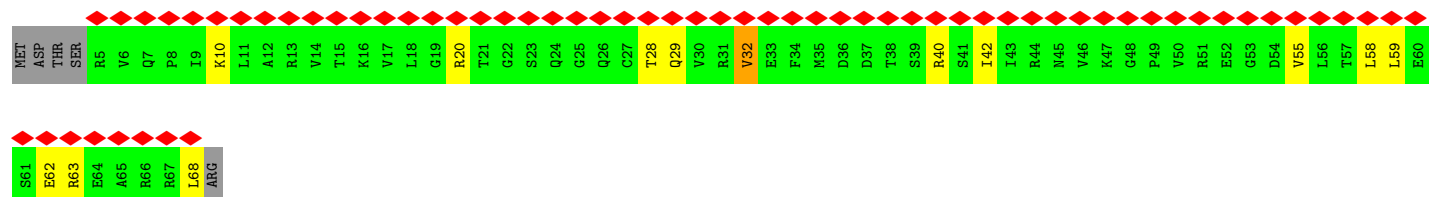
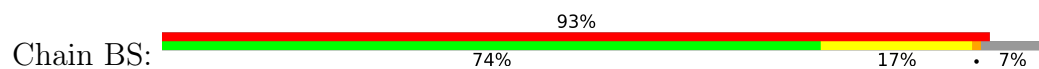


• Molecule 62: 40S ribosomal protein S26

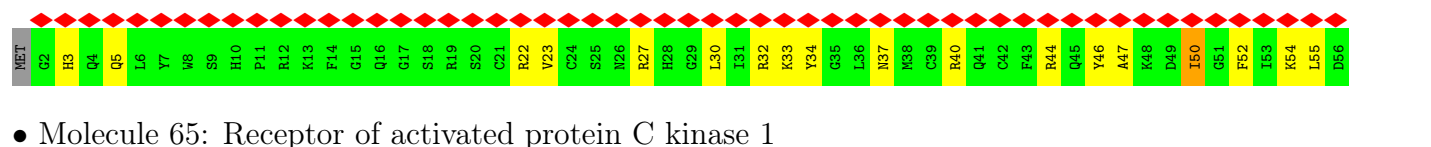




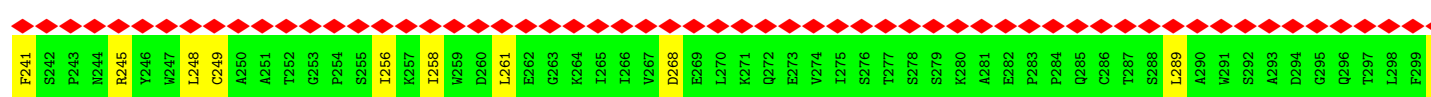
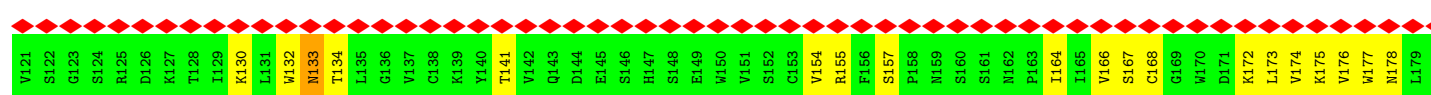
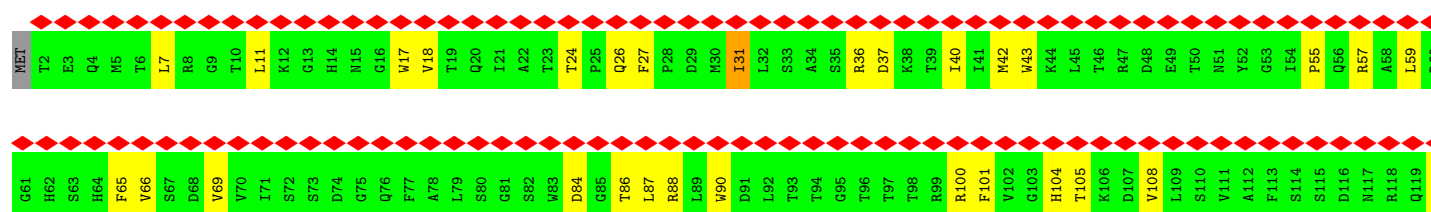
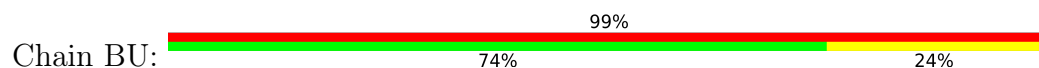
• Molecule 63: 40S ribosomal protein S28



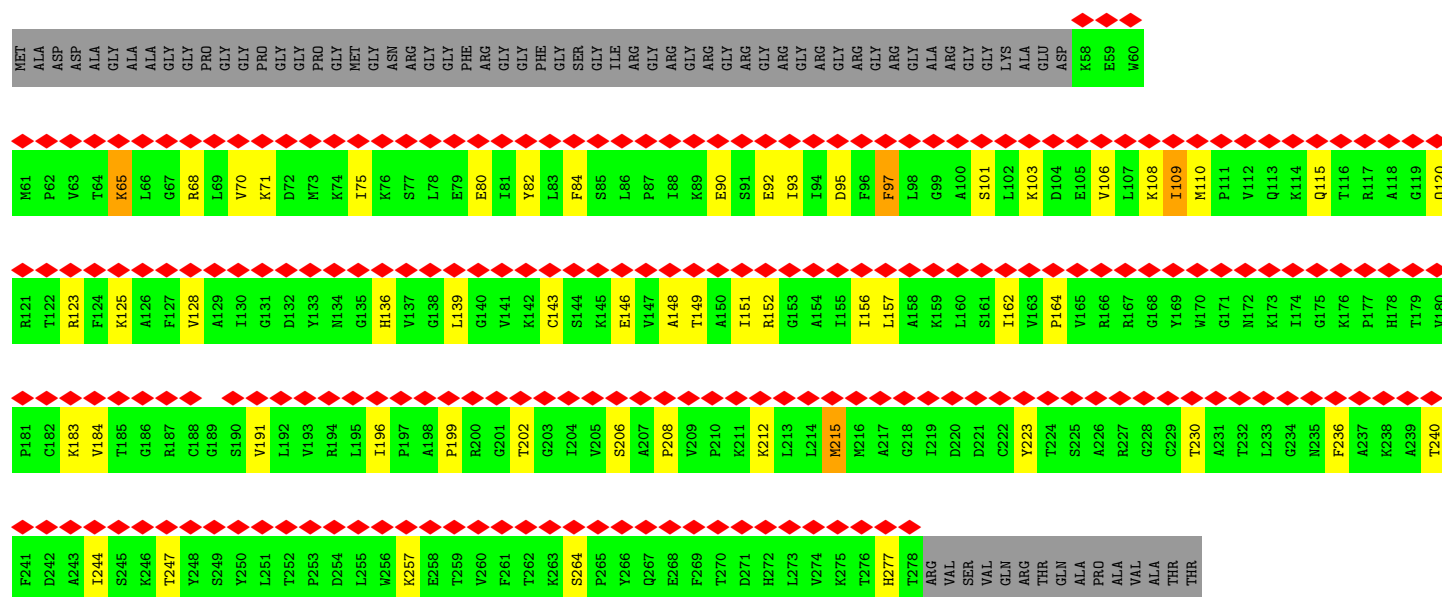
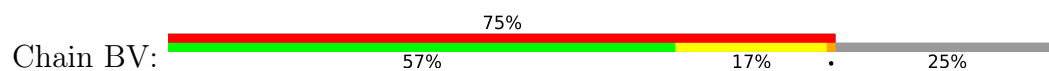
• Molecule 64: 40S ribosomal protein S29



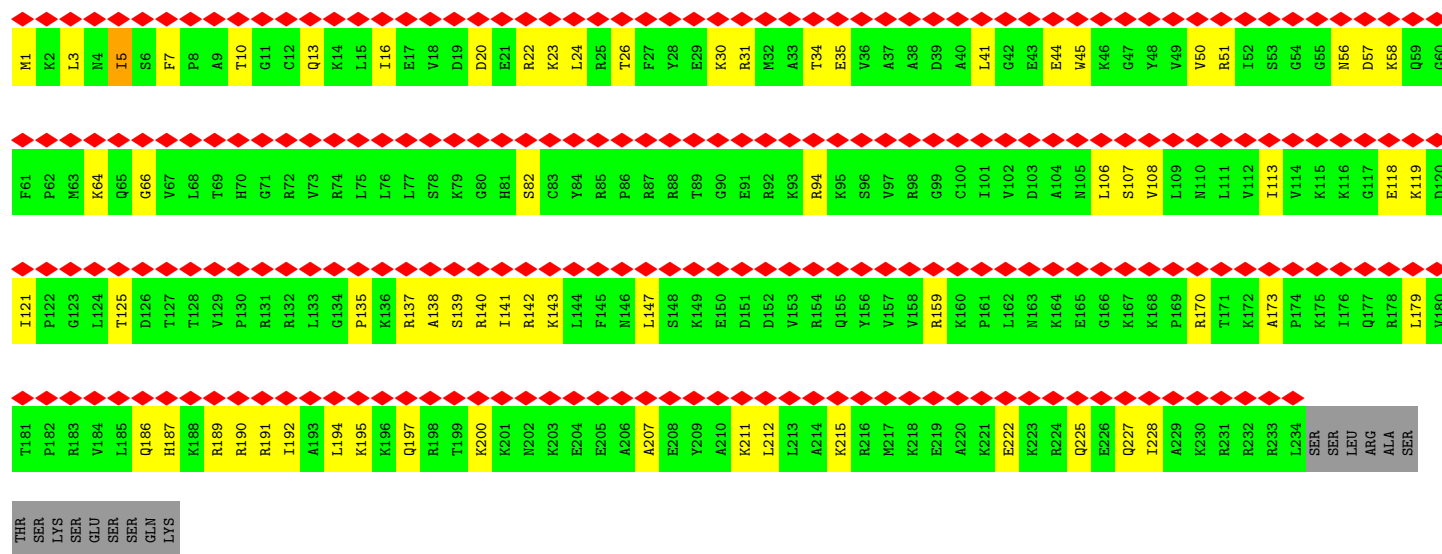
• Molecule 65: Receptor of activated protein C kinase 1



• Molecule 66: 40S ribosomal protein S2



• Molecule 67: 40S ribosomal protein S6

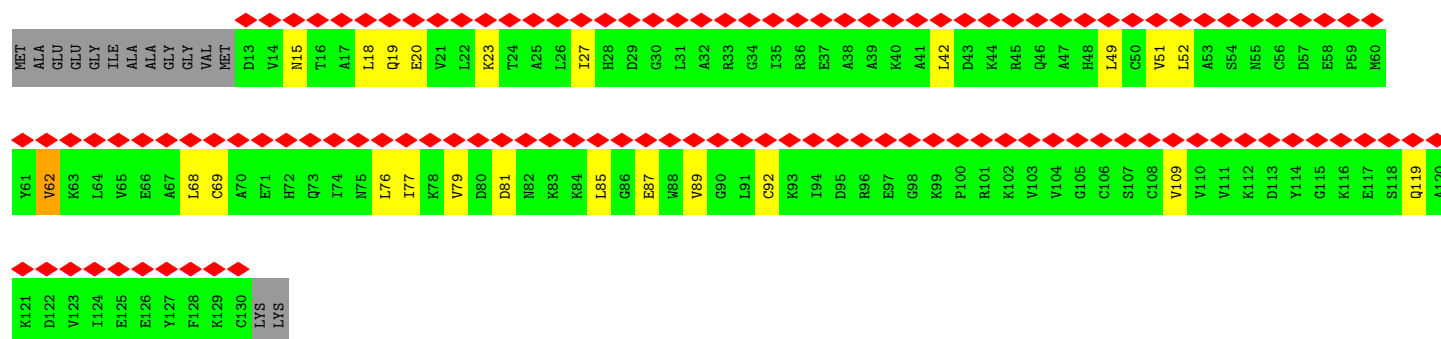
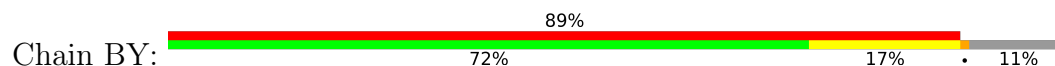


• Molecule 68: 40S ribosomal protein S9





• Molecule 69: 40S ribosomal protein S12

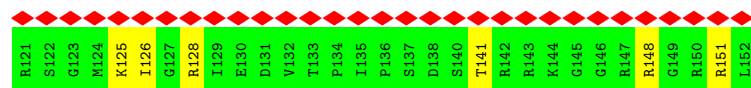


• Molecule 70: 40S ribosomal protein S13



• Molecule 71: Small ribosomal subunit protein uS11





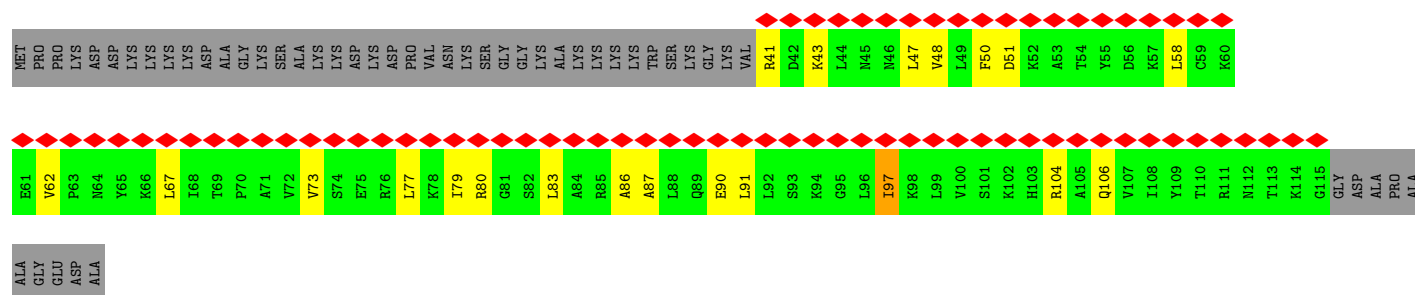
• Molecule 72: 40S ribosomal protein S15a



• Molecule 73: 40S ribosomal protein S24



• Molecule 74: 40S ribosomal protein S25

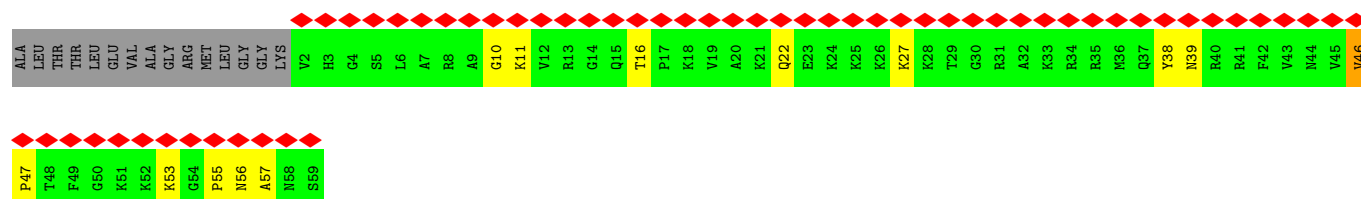
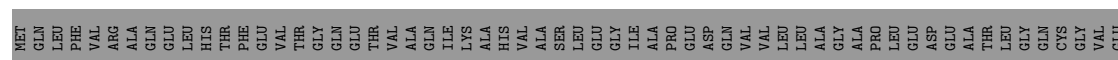
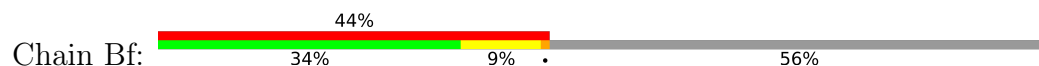


• Molecule 75: 40S ribosomal protein S27

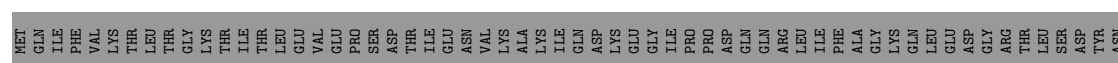
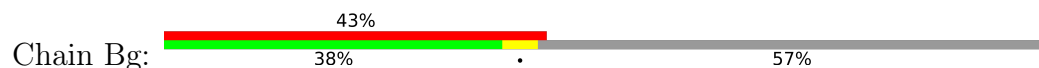




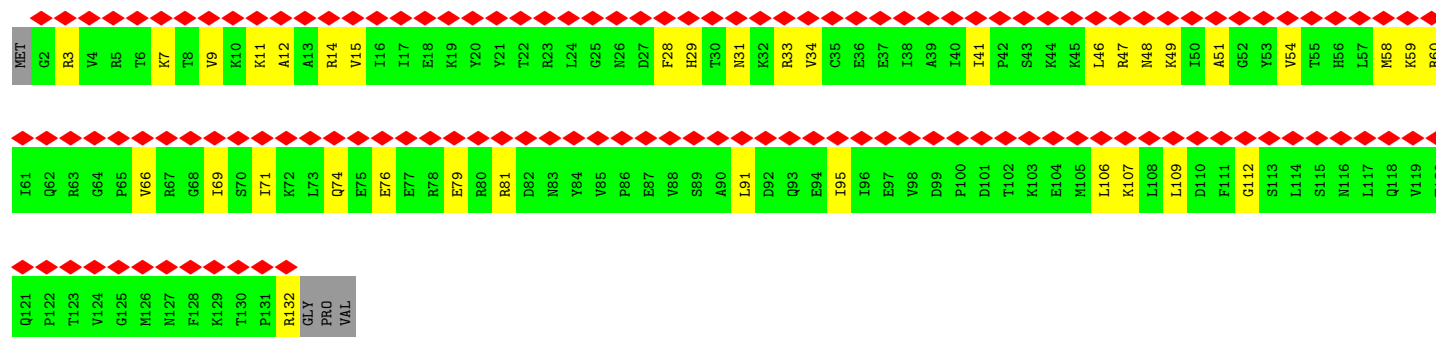
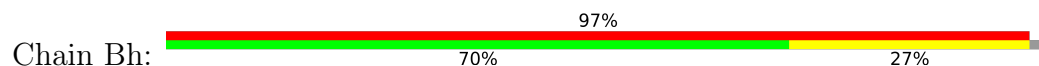
• Molecule 76: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



• Molecule 77: Ubiquitin-40S ribosomal protein S27a



• Molecule 78: 40S ribosomal protein S17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.354	Depositor
Minimum map value	-0.688	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	528.0, 528.0, 528.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMM, UY1, ZN, OMC, MA6, IAS, 1MA, MG, OMG, M7G, 6MZ, A2M, HIC, V5N, K, UR3, 4AC, B8N, OMU, 5MC, PSU

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	AA	0.17	0/86721	0.28	0/135215
2	AB	0.14	0/2858	0.26	0/4455
3	AC	0.17	0/3609	0.26	0/5623
4	AD	0.18	0/1936	0.37	0/2596
5	AE	0.18	0/3294	0.42	0/4406
6	AF	0.16	0/2981	0.33	0/4002
7	AG	0.16	0/2428	0.42	0/3252
8	AH	0.16	0/1942	0.38	0/2606
9	AI	0.18	0/1916	0.37	0/2553
10	AJ	0.20	0/1971	0.47	0/2651
11	AK	0.18	0/1537	0.45	0/2066
12	AL	0.17	0/1753	0.49	0/2343
13	AM	0.15	0/1433	0.47	0/1915
14	AN	0.17	0/1732	0.42	0/2315
15	AO	0.17	0/1125	0.34	0/1505
16	AP	0.21	0/1746	0.34	0/2338
17	AQ	0.18	0/1682	0.40	0/2250
18	AR	0.19	0/1268	0.44	0/1701
19	AS	0.18	0/1537	0.39	0/2052
20	AT	0.15	0/1424	0.34	0/1884
21	AU	0.18	0/1493	0.45	0/2003
22	AV	0.17	0/1326	0.39	0/1770
23	AW	0.17	0/839	0.49	0/1126
24	AX	0.16	0/993	0.40	0/1332
25	AY	0.17	0/532	0.46	0/708
26	AZ	0.16	0/1002	0.33	0/1345
27	Aa	0.16	0/1119	0.39	0/1488
28	Ab	0.14	0/1130	0.33	0/1507
29	Ac	0.18	0/1179	0.36	0/1573
30	Ad	0.17	0/821	0.45	0/1084
31	Ae	0.17	0/774	0.45	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.17	0/894	0.44	1/1204 (0.1%)
33	Ag	0.18	0/1071	0.38	0/1429
34	Ah	0.17	0/895	0.30	0/1198
35	Ai	0.16	0/878	0.33	0/1170
36	Aj	0.14	0/1023	0.35	0/1351
37	Ak	0.16	0/824	0.43	0/1090
38	Al	0.16	0/720	0.31	0/952
39	Am	0.19	0/565	0.49	0/750
40	An	0.15	0/454	0.26	0/599
41	Ao	0.25	0/425	0.52	0/564
42	Aq	0.15	0/858	0.34	0/1131
43	Ar	0.15	0/691	0.34	0/919
44	As	0.18	0/1002	0.36	0/1344
45	BA	0.16	0/39081	0.28	0/60888
46	BB	0.13	0/2101	0.39	0/2830
47	BC	0.17	0/1764	0.49	0/2396
48	BD	0.16	0/1774	0.45	0/2373
49	BE	0.16	0/1790	0.43	0/2410
50	BF	0.17	0/1531	0.49	0/2059
51	BG	0.17	0/1519	0.45	0/2033
52	BH	0.14	0/1715	0.41	0/2287
53	BI	0.15	0/840	0.47	0/1133
54	BJ	0.14	0/1280	0.37	0/1712
55	BK	0.19	0/1047	0.55	0/1399
56	BL	0.18	0/1142	0.51	0/1528
57	BM	0.17	0/1212	0.46	0/1624
58	BN	0.17	0/1116	0.45	0/1495
59	BO	0.15	0/732	0.43	0/980
60	BP	0.17	0/643	0.46	0/860
61	BQ	0.14	0/1116	0.43	0/1490
62	BR	0.12	0/836	0.33	0/1121
63	BS	0.16	0/508	0.45	0/680
64	BT	0.14	0/470	0.40	0/623
65	BU	0.15	0/2493	0.45	0/3394
66	BV	0.19	0/1764	0.52	1/2382 (0.0%)
67	BW	0.18	0/1926	0.50	1/2563 (0.0%)
68	BX	0.24	0/1548	0.61	0/2066
69	BY	0.15	0/916	0.42	0/1233
70	BZ	0.19	0/1232	0.48	0/1656
71	Ba	0.16	0/1011	0.49	0/1355
72	Bb	0.18	0/1051	0.48	0/1406
73	Bc	0.14	0/1068	0.36	0/1418
74	Bd	0.14	0/604	0.41	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Be	0.16	0/665	0.45	0/891
76	Bf	0.15	0/465	0.38	0/612
77	Bg	0.13	0/556	0.40	0/741
78	Bh	0.15	0/1078	0.38	0/1447
All	All	0.17	0/224995	0.34	3/330298 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	BW	22	ARG	CA-CB-CG	5.79	125.69	114.10
32	Af	54	MET	CB-CG-SD	5.77	130.01	112.70
66	BV	215	MET	CA-CB-CG	5.41	124.92	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	80204	0	40485	671	0
2	AB	2558	0	1296	18	0
3	AC	3316	0	1687	29	0
4	AD	1898	0	1993	24	0
5	AE	3239	0	3377	35	0
6	AF	2927	0	3104	28	0
7	AG	2382	0	2410	36	0
8	AH	1904	0	2055	20	0
9	AI	1878	0	2009	24	0
10	AJ	1935	0	2087	18	0
11	AK	1518	0	1601	28	0
12	AL	1713	0	1751	29	0
13	AM	1410	0	1441	19	0
14	AN	1701	0	1818	15	0
15	AO	1103	0	1163	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AP	1701	0	1749	19	0
17	AQ	1650	0	1794	18	0
18	AR	1242	0	1269	9	0
19	AS	1513	0	1628	8	0
20	AT	1408	0	1550	12	0
21	AU	1453	0	1490	19	0
22	AV	1298	0	1366	13	0
23	AW	825	0	850	13	0
24	AX	979	0	1039	4	0
25	AY	519	0	533	2	0
26	AZ	985	0	1066	7	0
27	Aa	1102	0	1189	15	0
28	Ab	1107	0	1182	13	0
29	Ac	1163	0	1206	6	0
30	Ad	808	0	875	11	0
31	Ae	764	0	804	14	0
32	Af	879	0	924	8	0
33	Ag	1053	0	1147	6	0
34	Ah	876	0	910	5	0
35	Ai	868	0	959	7	0
36	Aj	1015	0	1148	14	0
37	Ak	813	0	894	8	0
38	Al	705	0	737	4	0
39	Am	559	0	624	6	0
40	An	444	0	483	3	0
41	Ao	419	0	452	6	0
42	Aq	842	0	914	8	0
43	Ar	681	0	731	8	0
44	As	987	0	1050	10	0
45	BA	36892	0	18630	564	0
46	BB	2059	0	2137	48	0
47	BC	1727	0	1729	48	0
48	BD	1747	0	1822	44	0
49	BE	1762	0	1856	52	0
50	BF	1509	0	1563	43	0
51	BG	1497	0	1590	41	0
52	BH	1686	0	1772	39	0
53	BI	816	0	841	17	0
54	BJ	1258	0	1332	29	0
55	BK	1027	0	1075	27	0
56	BL	1124	0	1193	27	0
57	BM	1194	0	1250	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	BN	1110	0	1138	41	0
59	BO	726	0	782	21	0
60	BP	636	0	637	16	0
61	BQ	1098	0	1167	19	0
62	BR	821	0	870	12	0
63	BS	506	0	536	10	0
64	BT	459	0	448	16	0
65	BU	2436	0	2393	44	0
66	BV	1724	0	1816	38	0
67	BW	1903	0	2068	43	0
68	BX	1520	0	1642	34	0
69	BY	906	0	921	13	0
70	BZ	1208	0	1294	30	0
71	Ba	1007	0	1025	25	0
72	Bb	1034	0	1080	28	0
73	Bc	1048	0	1119	30	0
74	Bd	598	0	656	18	0
75	Be	651	0	672	17	0
76	Bf	459	0	503	6	0
77	Bg	544	0	539	2	0
78	Bh	1064	0	1118	26	0
79	AA	184	0	0	0	0
79	AB	2	0	0	0	0
79	AC	4	0	0	0	0
79	AP	1	0	0	0	0
79	AR	1	0	0	0	0
79	AX	1	0	0	0	0
79	BA	27	0	0	0	0
80	AA	51	0	0	0	0
80	AB	1	0	0	0	0
80	AD	1	0	0	0	0
80	AL	1	0	0	0	0
80	Ag	1	0	0	0	0
80	Ah	1	0	0	0	0
80	Aq	1	0	0	0	0
80	BA	5	0	0	0	0
81	Ai	1	0	0	0	0
81	Al	1	0	0	0	0
81	Ao	1	0	0	0	0
81	Aq	1	0	0	0	0
81	Ar	1	0	0	0	0
81	BR	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	BT	1	0	0	0	0
81	Bg	1	0	0	0	0
82	BA	24	0	16	0	0
All	All	214414	0	158070	2506	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 (2506) 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)
45:BA:3:C:OP2	66:BV:223:TYR:CE2	1.81	1.31
45:BA:3:C:OP2	66:BV:223:TYR:CZ	1.87	1.26
1:AA:2647:A:H62	1:AA:2686:G:N2	1.44	1.15
1:AA:2647:A:N6	1:AA:2686:G:H21	1.50	1.08
14:AN:142:GLU:O	14:AN:146:LEU:HB2	1.52	1.08
45:BA:568:C:N4	45:BA:582:U:H3	1.52	1.05
1:AA:4745:G:H1	1:AA:4955:A:H61	1.06	1.00
45:BA:3:C:OP2	66:BV:223:TYR:OH	1.79	0.99
3:AC:72:A:H61	3:AC:79:G:H1	1.05	0.99
45:BA:1656:G:H1	45:BA:1668:U:H3	1.06	0.98
51:BG:72:PHE:O	51:BG:76:GLN:HB3	1.65	0.96
45:BA:4:C:H5''	45:BA:4:C:H6	1.27	0.96
1:AA:450:G:H1	1:AA:1297:U:H3	1.10	0.95
3:AC:72:A:N6	3:AC:79:G:H1	1.65	0.95
55:BK:38:SER:O	55:BK:42:ARG:HB3	1.69	0.92
45:BA:1099:G:H1	45:BA:1133:A:H2	1.16	0.91
45:BA:678:U:H3	45:BA:1027:A:H62	1.15	0.89
1:AA:752:G:H1	1:AA:911:U:H3	1.21	0.88
45:BA:878:G:H1	45:BA:908:A:H61	1.22	0.86
45:BA:1521:C:H5'	57:BM:129:LEU:HD21	1.56	0.85
45:BA:1560:U:H3	45:BA:1575:G:H1	1.23	0.85
45:BA:1398:G:H1	45:BA:1448:A:H2	1.24	0.83
36:Aj:13:LYS:HE2	36:Aj:16:GLU:HG3	1.61	0.82
5:AE:44:THR:HG21	5:AE:186:ASN:HD22	1.44	0.81
5:AE:300:LYS:O	5:AE:304:SER:HB3	1.79	0.81
1:AA:3944:G:H1	1:AA:4069:U:H3	0.82	0.81
45:BA:3:C:OP2	66:BV:223:TYR:HE2	1.60	0.81
1:AA:4745:G:H1	1:AA:4955:A:N6	1.78	0.80
45:BA:1382:A:H2'	45:BA:1383:A2M:H8	1.61	0.80
1:AA:4757:C:H42	1:AA:4877:G:H1	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BO:35:VAL:HG22	59:BO:107:GLU:HG3	1.65	0.77
45:BA:1415:C:H2'	58:BN:129:ARG:HB2	1.67	0.77
3:AC:83:C:H41	27:Aa:50:ARG:HH21	1.33	0.77
51:BG:137:SER:HB2	51:BG:158:LEU:HB3	1.67	0.76
45:BA:844:U:H2'	45:BA:845:G:H8	1.52	0.75
50:BF:50:PRO:HB3	50:BF:69:VAL:HG23	1.68	0.75
45:BA:1030:A:H2'	45:BA:1031:A2M:H8	1.68	0.74
66:BV:183:LYS:HE2	72:Bb:95:PRO:HA	1.67	0.74
45:BA:1657:G:H1	45:BA:1667:U:H3	1.34	0.74
45:BA:934:G:H1	45:BA:1008:A:H2	1.33	0.74
49:BE:29:LEU:HB3	49:BE:34:TYR:HB2	1.70	0.74
1:AA:3717:A:H2'	1:AA:3718:A2M:H8	1.69	0.73
45:BA:571:U:H5''	73:Bc:37:LYS:HG3	1.69	0.73
45:BA:1778:C:H2'	45:BA:1779:G:H8	1.54	0.73
45:BA:1598:G:H2'	74:Bd:80:ARG:HH21	1.53	0.72
46:BB:48:LEU:HD12	46:BB:61:VAL:HG22	1.71	0.72
45:BA:1453:C:H4'	78:Bh:49:LYS:HA	1.72	0.72
1:AA:1921:C:H42	15:AO:16:SER:HB3	1.53	0.72
1:AA:1870:C:H2'	1:AA:1871:A2M:H8	1.72	0.72
45:BA:3:C:H1'	66:BV:206:SER:C	2.15	0.72
45:BA:4:C:H5''	45:BA:4:C:C6	2.19	0.72
1:AA:966:A:H5''	1:AA:2092:G:H22	1.53	0.71
45:BA:4:C:H6	45:BA:4:C:C5'	2.03	0.71
47:BC:57:LYS:HZ1	60:BP:70:LEU:HD13	1.55	0.71
55:BK:121:ILE:HG12	57:BM:118:ARG:HH22	1.54	0.71
45:BA:377:G:H5'	52:BH:98:LYS:HB3	1.73	0.71
52:BH:97:VAL:H	52:BH:100:CYS:HB3	1.56	0.71
70:BZ:45:LEU:HD23	70:BZ:50:ILE:HG12	1.73	0.71
58:BN:83:GLN:HG2	58:BN:93:SER:HB2	1.73	0.70
45:BA:1849:G:H3'	45:BA:1850:MA6:H8	1.73	0.70
50:BF:128:ILE:HG22	50:BF:135:ARG:HH12	1.56	0.70
45:BA:1096:G:H22	45:BA:1136:PSU:HN3	1.39	0.70
67:BW:5:ILE:HG13	67:BW:113:ILE:HD11	1.74	0.70
65:BU:87:LEU:HB2	65:BU:101:PHE:HB2	1.73	0.70
45:BA:797:C:H3'	45:BA:799:U:H5''	1.74	0.70
54:BJ:57:ASP:HB3	54:BJ:60:CYS:HB2	1.74	0.70
47:BC:63:ARG:HG3	47:BC:185:MET:HE1	1.74	0.70
55:BK:85:ILE:HD12	55:BK:114:HIS:H	1.57	0.70
72:Bb:51:GLU:HB2	72:Bb:62:VAL:O	1.92	0.70
67:BW:30:LYS:HZ3	67:BW:34:THR:HB	1.56	0.69
45:BA:1726:G:H1	45:BA:1808:U:H3	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:185:LYS:HB3	49:BE:187:LYS:HZ3	1.56	0.69
50:BF:69:VAL:HA	50:BF:72:LEU:HD22	1.73	0.69
61:BQ:101:LEU:HB3	61:BQ:124:LYS:HB2	1.74	0.69
62:BR:49:ALA:HB1	71:Ba:117:ARG:HE	1.56	0.69
1:AA:3697:U:H5''	1:AA:3698:G:H5'	1.75	0.69
8:AH:186:LEU:HD21	8:AH:253:VAL:HG21	1.74	0.69
67:BW:119:LYS:HZ3	67:BW:121:ILE:HA	1.56	0.69
70:BZ:99:ARG:HH12	70:BZ:143:SER:HB3	1.56	0.69
45:BA:1244:PSU:H2'	45:BA:1245:G:H8	1.57	0.69
65:BU:212:LYS:HA	65:BU:235:ILE:HG23	1.74	0.69
66:BV:70:VAL:HG11	66:BV:93:ILE:HG13	1.75	0.69
1:AA:1358:G:N7	1:AA:1377:G:N2	2.40	0.69
45:BA:3:C:H1'	66:BV:206:SER:O	1.92	0.69
45:BA:1259:A:H8	45:BA:1264:C:H42	1.40	0.68
1:AA:3963:A:H5'	1:AA:3964:U:H5''	1.75	0.68
1:AA:4041:C:H5'	1:AA:4042:G:H5''	1.74	0.68
45:BA:1592:C:H5''	50:BF:87:LEU:HG	1.75	0.68
65:BU:120:ILE:HD11	65:BU:132:TRP:HB2	1.76	0.68
45:BA:366:PSU:H4'	52:BH:11:ARG:HH12	1.57	0.68
45:BA:574:A:H5''	73:Bc:93:ARG:HH12	1.58	0.68
1:AA:1332:C:H2'	1:AA:1333:A:H8	1.58	0.68
1:AA:1517:G:H22	6:AF:103:ALA:HA	1.58	0.68
1:AA:3718:A2M:HM'2	1:AA:3719:A:H5'	1.75	0.68
45:BA:851:C:H5''	45:BA:852:G:H5'	1.77	0.67
45:BA:1729:U:H3	45:BA:1805:G:H1	1.42	0.67
54:BJ:84:ARG:HH21	54:BJ:115:PRO:HG3	1.59	0.67
73:Bc:8:ARG:HH22	73:Bc:10:ARG:HG3	1.59	0.67
13:AM:18:ARG:HD3	13:AM:135:GLY:HA3	1.76	0.67
75:Be:33:MET:HE2	75:Be:79:PHE:HB2	1.76	0.67
60:BP:71:ARG:HA	60:BP:74:LYS:HD2	1.74	0.67
11:AK:92:MET:HB2	11:AK:144:LEU:HB2	1.77	0.67
45:BA:969:U:H4'	45:BA:971:G:H1'	1.75	0.67
45:BA:1099:G:N1	45:BA:1133:A:C2	2.56	0.67
45:BA:568:C:H2'	45:BA:569:A:H8	1.58	0.67
45:BA:943:U:H2'	45:BA:944:A:H8	1.60	0.67
46:BB:173:ILE:HG23	46:BB:230:LYS:HD2	1.75	0.67
12:AL:86:HIS:HB3	12:AL:139:ARG:HG2	1.76	0.66
45:BA:1396:A:N7	45:BA:1449:G:O6	2.28	0.66
53:BI:1:MET:HE1	53:BI:51:SER:HB2	1.78	0.66
47:BC:10:MET:HE2	78:Bh:109:LEU:HD21	1.78	0.66
70:BZ:142:GLU:HB2	70:BZ:145:THR:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1276:A:H4'	53:BI:1:MET:HE3	1.76	0.66
45:BA:878:G:H1	45:BA:908:A:N6	1.92	0.66
7:AG:232:THR:HG22	7:AG:235:MET:HE1	1.77	0.66
45:BA:975:G:H21	71:Ba:50:LYS:HA	1.60	0.66
45:BA:1707:U:H1'	45:BA:1849:G:H21	1.61	0.66
7:AG:197:LYS:HB2	7:AG:202:GLN:HB2	1.77	0.66
1:AA:1859:C:H42	1:AA:1875:C:H42	1.44	0.66
47:BC:29:ASN:HB2	47:BC:151:ASP:HB3	1.76	0.66
45:BA:532:C:H2'	45:BA:533:A:H8	1.61	0.66
45:BA:678:U:H3	45:BA:1027:A:N6	1.92	0.66
45:BA:1860:A:H3'	62:BR:8:ASN:HB3	1.76	0.66
1:AA:964:A:H62	1:AA:966:A:H1'	1.60	0.66
1:AA:2633:U:H5''	20:AT:61:ALA:HB2	1.78	0.66
45:BA:1099:G:N1	45:BA:1133:A:H2	1.93	0.66
49:BE:105:LEU:HD11	49:BE:184:ILE:HG21	1.78	0.65
53:BI:66:HIS:HB3	53:BI:68:TYR:HE1	1.61	0.65
1:AA:1245:C:H2'	1:AA:1246:G:H8	1.61	0.65
23:AW:20:LYS:HG3	23:AW:73:THR:HG22	1.77	0.65
1:AA:4258:C:H5'	13:AM:68:ILE:HD11	1.78	0.65
65:BU:157:SER:HB2	65:BU:164:ILE:H	1.61	0.65
67:BW:1:MET:HE3	67:BW:24:LEU:HG	1.77	0.65
1:AA:132:G:H2'	1:AA:133:C:H4'	1.78	0.65
51:BG:45:ILE:HD13	51:BG:62:ILE:HG23	1.77	0.65
74:Bd:48:VAL:HA	74:Bd:83:LEU:HD22	1.79	0.65
1:AA:2777:G:H5''	1:AA:2778:G:H5'	1.79	0.65
1:AA:4611:A:H2	11:AK:120:GLU:HB3	1.61	0.65
45:BA:551:U:H4'	76:Bf:39:ASN:HB3	1.78	0.65
45:BA:1398:G:O6	45:BA:1448:A:N1	2.29	0.65
46:BB:71:LYS:HE3	46:BB:76:VAL:HG22	1.78	0.65
47:BC:184:ARG:HD3	47:BC:189:ILE:HG23	1.79	0.65
60:BP:46:PHE:HD1	60:BP:48:GLY:H	1.45	0.65
1:AA:990:C:H1'	1:AA:1064:G:H22	1.61	0.65
1:AA:4906:C:H2'	1:AA:4907:G:H8	1.62	0.65
68:BX:84:ILE:HD11	68:BX:148:ILE:HG13	1.78	0.65
70:BZ:91:LEU:HB3	70:BZ:122:ILE:HG22	1.78	0.65
73:Bc:22:GLN:HB2	73:Bc:72:PHE:HE1	1.61	0.65
1:AA:4415:A:H62	1:AA:4427:G:N2	1.95	0.65
65:BU:87:LEU:HD11	65:BU:108:VAL:HG11	1.79	0.65
45:BA:925:G:H1	45:BA:1017:U:H3	1.43	0.65
45:BA:928:G:H1	45:BA:1013:U:H3	1.44	0.65
45:BA:1821:U:H2'	45:BA:1822:A:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BD:24:PRO:HA	48:BD:27:LYS:HG2	1.79	0.64
1:AA:2575:U:H5''	1:AA:2576:G:H5'	1.78	0.64
16:AP:9:GLU:HB3	37:Ak:44:ILE:HG13	1.79	0.64
55:BK:98:ASN:HB2	55:BK:122:THR:HA	1.78	0.64
1:AA:733:A:H61	1:AA:930:G:H22	1.45	0.64
1:AA:1460:C:H5''	19:AS:144:LYS:HG2	1.79	0.64
47:BC:57:LYS:HD3	47:BC:60:LEU:HD11	1.80	0.64
45:BA:1359:U:H2'	45:BA:1360:PSU:H6	1.61	0.64
45:BA:1445:PSU:H1'	45:BA:1580:A:H61	1.62	0.64
68:BX:106:LEU:HD12	68:BX:109:ARG:HD3	1.78	0.64
45:BA:522:A:H5''	68:BX:145:PRO:HD2	1.79	0.64
66:BV:136:HIS:HB3	66:BV:162:ILE:HD11	1.80	0.64
47:BC:145:ILE:HG23	47:BC:159:ILE:HD11	1.79	0.64
78:Bh:47:ARG:HB2	78:Bh:49:LYS:HZ1	1.63	0.64
1:AA:74:G:H5'	14:AN:59:VAL:HG13	1.80	0.64
8:AH:66:LYS:HE2	8:AH:68:MET:HE2	1.79	0.64
65:BU:172:LYS:HB3	65:BU:191:HIS:HB2	1.78	0.64
1:AA:2745:A:H2'	1:AA:2746:A:H8	1.63	0.63
1:AA:3961:G:N1	1:AA:4048:A:N6	2.46	0.63
1:AA:4859:C:H3'	1:AA:4860:G:H8	1.63	0.63
14:AN:47:ALA:HB1	14:AN:48:PRO:HD2	1.81	0.63
57:BM:44:VAL:HG11	57:BM:71:MET:HE3	1.81	0.63
47:BC:42:LYS:HZ1	47:BC:46:ILE:HB	1.63	0.63
5:AE:191:ALA:HA	5:AE:194:LEU:HB2	1.81	0.63
45:BA:1218:C:H1'	45:BA:1683:C:H42	1.62	0.63
62:BR:53:ILE:HB	71:Ba:117:ARG:HH22	1.62	0.63
45:BA:62:G:H1'	45:BA:172:OMU:HM23	1.81	0.63
65:BU:24:THR:HG23	65:BU:27:PHE:H	1.63	0.63
68:BX:17:ARG:HG2	68:BX:18:ARG:HD2	1.78	0.63
49:BE:142:LEU:HD22	49:BE:148:LYS:HB3	1.80	0.63
78:Bh:71:ILE:HG22	78:Bh:74:GLN:H	1.63	0.63
1:AA:4254:G:H3'	1:AA:4255:A:H3'	1.81	0.63
54:BJ:135:SER:HB3	54:BJ:138:VAL:HG12	1.80	0.63
57:BM:33:ILE:HG12	57:BM:99:LEU:HD12	1.80	0.63
1:AA:450:G:O6	1:AA:1297:U:O4	2.17	0.63
45:BA:988:C:H5'	48:BD:116:LYS:HG3	1.81	0.63
46:BB:191:ARG:HE	46:BB:245:ARG:HD2	1.64	0.63
18:AR:84:PRO:HB2	18:AR:87:SER:HB2	1.81	0.62
57:BM:22:GLY:HA2	57:BM:56:ALA:HB3	1.81	0.62
45:BA:436:OMG:HM22	45:BA:437:G:H5'	1.81	0.62
58:BN:108:GLU:HG3	58:BN:113:VAL:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Bb:14:ILE:HB	72:Bb:25:VAL:HG11	1.81	0.62
47:BC:76:VAL:HG13	47:BC:87:VAL:HG23	1.81	0.62
46:BB:35:PRO:HD2	46:BB:83:PRO:HG2	1.81	0.62
66:BV:90:GLU:HB2	66:BV:93:ILE:HD13	1.81	0.62
65:BU:178:ASN:HB2	65:BU:185:LYS:HB2	1.81	0.62
49:BE:122:VAL:O	49:BE:126:ILE:HD12	1.99	0.62
67:BW:197:GLN:HA	67:BW:200:LYS:HE3	1.82	0.62
5:AE:317:LEU:HD11	5:AE:382:MET:HG3	1.80	0.62
49:BE:109:LEU:HD11	49:BE:175:VAL:HG11	1.81	0.62
6:AF:149:GLU:HG3	44:As:72:LYS:HG2	1.81	0.62
70:BZ:114:ARG:O	70:BZ:118:ILE:HD12	2.00	0.62
45:BA:1655:C:H2'	45:BA:1656:G:H8	1.64	0.62
48:BD:223:PHE:HZ	48:BD:228:LEU:HD22	1.65	0.62
1:AA:1857:C:H2'	1:AA:1858:A:H8	1.64	0.62
70:BZ:98:VAL:HG12	70:BZ:115:LEU:HD23	1.82	0.62
73:Bc:55:ILE:HG12	73:Bc:75:ILE:HG23	1.81	0.62
5:AE:57:VAL:HG22	5:AE:73:VAL:HG12	1.82	0.61
31:Ae:45:LEU:HB3	31:Ae:96:ILE:HG23	1.82	0.61
72:Bb:25:VAL:HG23	72:Bb:65:LEU:HD11	1.82	0.61
1:AA:734:G:H1	1:AA:929:A:H61	1.47	0.61
72:Bb:102:ILE:HG22	72:Bb:128:PHE:HB2	1.82	0.61
11:AK:95:VAL:HG22	41:Ao:82:LEU:HD13	1.83	0.61
45:BA:186:C:H2'	45:BA:187:G:H8	1.66	0.61
26:AZ:124:VAL:HG22	26:AZ:138:VAL:HG12	1.82	0.61
51:BG:160:LYS:HD2	51:BG:191:GLU:HA	1.83	0.61
1:AA:2261:G:H4'	8:AH:112:MET:HE1	1.81	0.61
3:AC:67:U:H2'	3:AC:68:G:H8	1.66	0.61
58:BN:84:ARG:HE	58:BN:86:GLY:H	1.48	0.61
59:BO:78:ASP:HB3	64:BT:54:LYS:HD2	1.82	0.61
23:AW:48:LYS:HG2	23:AW:53:ALA:HB2	1.82	0.61
27:Aa:52:ASP:HB2	27:Aa:110:LYS:HD2	1.83	0.61
45:BA:874:G:H2'	45:BA:875:A:H8	1.63	0.61
46:BB:220:THR:HG22	46:BB:221:ARG:H	1.66	0.61
1:AA:4060:U:H5''	1:AA:4061:G:H5'	1.83	0.61
6:AF:37:VAL:HG21	6:AF:246:VAL:HG13	1.82	0.61
48:BD:71:LEU:HD22	48:BD:74:LEU:HD12	1.83	0.61
50:BF:103:LEU:HD11	74:Bd:67:LEU:HD22	1.82	0.61
73:Bc:108:LYS:HA	73:Bc:111:LYS:HG2	1.83	0.61
31:Ae:48:LEU:HD21	31:Ae:60:ILE:HG21	1.83	0.61
43:Ar:38:THR:HA	43:Ar:45:THR:HA	1.83	0.61
45:BA:921:G:H5'	75:Be:21:LYS:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Am:12:LEU:O	39:Am:16:ARG:HG2	2.01	0.60
45:BA:421:G:H5'	54:BJ:98:LYS:HG2	1.82	0.60
45:BA:1850:MA6:H2'	45:BA:1851:MA6:H8	1.82	0.60
50:BF:144:LEU:HD13	50:BF:148:ASN:HD21	1.65	0.60
43:Ar:47:MET:HE2	43:Ar:57:CYS:HB2	1.84	0.60
7:AG:235:MET:HE3	7:AG:235:MET:H	1.65	0.60
70:BZ:49:GLN:HA	70:BZ:52:VAL:HG12	1.84	0.60
1:AA:4929:C:H2'	1:AA:4930:C:C6	2.37	0.60
1:AA:4314:C:H4'	22:AV:68:THR:HG21	1.82	0.60
45:BA:928:G:H2'	45:BA:929:G:C8	2.37	0.60
45:BA:1183:A:H2'	45:BA:1184:G:H8	1.66	0.60
46:BB:31:PRO:HG2	46:BB:38:LEU:HD22	1.83	0.60
1:AA:2362:U:H2'	1:AA:2363:A2M:H8	1.84	0.60
1:AA:2411:C:H2'	1:AA:2412:A:H8	1.67	0.60
45:BA:1560:U:O2	45:BA:1575:G:N2	2.30	0.60
50:BF:150:ALA:O	50:BF:154:LEU:HD22	2.02	0.60
4:AD:80:GLU:HG3	43:Ar:66:GLY:HA2	1.84	0.60
6:AF:236:ASN:HD22	6:AF:239:LYS:HG2	1.66	0.60
48:BD:36:PRO:HA	48:BD:232:HIS:HA	1.82	0.60
73:Bc:5:VAL:HG13	73:Bc:27:VAL:HG13	1.83	0.60
45:BA:861:A:H4'	45:BA:862:A:H8	1.67	0.60
56:BL:17:LYS:HD2	56:BL:18:THR:H	1.67	0.60
57:BM:16:LEU:HB3	57:BM:33:ILE:HD13	1.84	0.60
68:BX:85:GLY:HA3	68:BX:108:ARG:HE	1.66	0.60
45:BA:822:PSU:HN3	45:BA:826:A:H62	1.50	0.60
50:BF:100:ILE:HD13	50:BF:111:VAL:HG11	1.84	0.60
57:BM:25:LYS:HA	57:BM:55:ARG:HA	1.84	0.60
45:BA:1513:C:H2'	45:BA:1514:G:H8	1.66	0.60
48:BD:186:ASN:HA	48:BD:189:ILE:HD12	1.83	0.60
56:BL:37:ARG:HE	56:BL:41:MET:HE2	1.67	0.60
1:AA:4336:A:H5''	1:AA:4337:C:H5'	1.84	0.59
45:BA:1137:U:H4'	47:BC:155:ARG:HH22	1.68	0.59
57:BM:6:PRO:HG2	57:BM:9:PHE:HB2	1.84	0.59
1:AA:4929:C:H1'	15:AO:118:MET:HE1	1.84	0.59
57:BM:100:ALA:H	57:BM:103:LEU:HD13	1.65	0.59
65:BU:154:VAL:HG12	65:BU:167:SER:HB2	1.85	0.59
1:AA:928:C:H2'	1:AA:929:A:C8	2.38	0.59
1:AA:4750:G:H2'	1:AA:4751:G:H8	1.67	0.59
55:BK:52:LYS:HZ1	55:BK:56:LEU:HB2	1.67	0.59
3:AC:1:C:H3'	3:AC:2:G:H21	1.66	0.59
17:AQ:34:VAL:HG22	17:AQ:103:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AZ:64:SER:HB2	36:Aj:69:LEU:HD13	1.83	0.59
52:BH:83:TYR:HB2	52:BH:202:ILE:HD11	1.85	0.59
52:BH:152:ARG:O	52:BH:156:ALA:HB2	2.02	0.59
1:AA:4992:G:H2'	1:AA:4993:G:C8	2.38	0.59
5:AE:163:ILE:HG22	5:AE:180:LEU:HD22	1.84	0.59
45:BA:609:PSU:H2'	45:BA:610:G:H8	1.66	0.59
60:BP:14:PRO:HG2	60:BP:23:ILE:HD12	1.84	0.59
73:Bc:108:LYS:HG3	73:Bc:111:LYS:HD3	1.83	0.59
1:AA:4723:A:H4'	5:AE:100:ARG:HD2	1.84	0.59
45:BA:1223:A:H2	45:BA:1643:PSU:HN3	1.49	0.59
45:BA:1645:C:H4'	56:BL:138:ARG:HB3	1.85	0.59
47:BC:117:ARG:HG3	47:BC:119:PRO:HD3	1.85	0.59
45:BA:1705:C:H2'	45:BA:1706:G:H8	1.68	0.59
55:BK:18:ARG:HB2	55:BK:36:LEU:HD23	1.85	0.59
1:AA:2568:C:H2'	1:AA:2569:G:H8	1.68	0.59
9:AI:105:VAL:HG13	9:AI:136:VAL:HG12	1.83	0.59
39:Am:26:LYS:HD3	39:Am:69:LEU:HD22	1.84	0.59
45:BA:159:A2M:H2	45:BA:468:A2M:H1'	1.83	0.59
48:BD:187:LYS:HB3	48:BD:193:ILE:HD11	1.85	0.59
54:BJ:61:PRO:HD3	54:BJ:141:ASN:HD21	1.68	0.59
1:AA:3604:A:H5'	20:AT:71:ARG:HD2	1.85	0.59
63:BS:10:LYS:HB2	63:BS:58:LEU:HB2	1.84	0.59
1:AA:1947:U:H2'	41:Ao:109:ASN:HB2	1.85	0.58
45:BA:140:C:H42	45:BA:313:A:H61	1.51	0.58
46:BB:45:ILE:HA	46:BB:61:VAL:HG11	1.84	0.58
1:AA:4933:C:H2'	1:AA:4934:A:H8	1.66	0.58
12:AL:176:PHE:HD2	12:AL:184:MET:HE3	1.67	0.58
23:AW:25:CYS:O	23:AW:29:VAL:HB	2.03	0.58
45:BA:28:U:H2'	45:BA:29:G:H8	1.68	0.58
48:BD:84:PHE:HB3	48:BD:86:LEU:HD23	1.85	0.58
1:AA:268:G:H2'	1:AA:269:G:H8	1.67	0.58
10:AJ:63:LEU:HD11	16:AP:29:GLN:HG3	1.85	0.58
15:AO:5:ARG:HD2	15:AO:57:LEU:HB3	1.85	0.58
60:BP:36:VAL:HG13	60:BP:51:LYS:HG3	1.85	0.58
75:Be:36:LYS:HG2	75:Be:43:ILE:HG22	1.85	0.58
9:AI:31:LYS:HD3	9:AI:34:ARG:HH12	1.67	0.58
12:AL:35:ASP:HB3	12:AL:39:LYS:HZ3	1.67	0.58
45:BA:1486:A:H2'	45:BA:1487:A:H8	1.68	0.58
1:AA:679:C:H2'	1:AA:680:G:H8	1.68	0.58
6:AF:101:MET:HE2	6:AF:104:PRO:HA	1.85	0.58
28:Ab:84:ARG:HH21	35:Ai:102:ILE:HD11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ao:85:LEU:HA	41:Ao:88:LYS:HD2	1.86	0.58
45:BA:115:U:H2'	45:BA:116:OMU:H6	1.85	0.58
65:BU:130:LYS:HG2	65:BU:141:THR:HG22	1.85	0.58
4:AD:181:LYS:HB2	4:AD:184:ARG:HG3	1.84	0.58
21:AU:80:ILE:HG12	21:AU:129:VAL:HG22	1.84	0.58
45:BA:186:C:H2'	45:BA:187:G:C8	2.38	0.58
47:BC:58:LEU:HD23	47:BC:161:ILE:HD12	1.85	0.58
48:BD:48:LEU:HG	71:Ba:51:GLU:HG3	1.85	0.58
9:AI:182:TYR:HB3	9:AI:200:ARG:HG3	1.85	0.58
47:BC:184:ARG:HE	47:BC:191:ARG:HA	1.68	0.58
49:BE:157:MET:HA	49:BE:189:MET:HE3	1.85	0.58
52:BH:74:ARG:HH21	52:BH:112:TRP:HE3	1.52	0.58
66:BV:93:ILE:O	66:BV:97:PHE:HB2	2.03	0.58
1:AA:189:G:H2'	1:AA:190:G:H8	1.68	0.58
1:AA:4537:C:H2'	1:AA:4538:G:H8	1.68	0.58
55:BK:33:LEU:HD22	55:BK:36:LEU:HD13	1.84	0.58
1:AA:1207:C:H2'	1:AA:1208:G:H8	1.67	0.58
51:BG:41:ARG:NH1	51:BG:41:ARG:HA	2.19	0.58
73:Bc:57:VAL:HB	73:Bc:60:PHE:HE2	1.68	0.58
45:BA:861:A:H4'	45:BA:862:A:C8	2.39	0.58
8:AH:164:PHE:HA	8:AH:175:VAL:HG23	1.86	0.57
54:BJ:50:ALA:HB2	54:BJ:116:CYS:HB2	1.87	0.57
76:Bf:53:LYS:HE3	76:Bf:57:ALA:HA	1.86	0.57
1:AA:486:C:H2'	1:AA:487:G:C8	2.40	0.57
1:AA:2411:C:H2'	1:AA:2412:A:C8	2.39	0.57
45:BA:223:C:H2'	45:BA:224:A:C4	2.39	0.57
45:BA:634:A:H2'	45:BA:635:G:H8	1.69	0.57
72:Bb:10:ALA:HB1	72:Bb:27:ILE:HD12	1.85	0.57
1:AA:2521:G:H4'	35:Ai:26:PRO:HD2	1.86	0.57
13:AM:120:ASP:HB3	13:AM:123:ILE:HG13	1.86	0.57
45:BA:551:U:H2'	45:BA:552:G:C8	2.38	0.57
55:BK:38:SER:HB2	55:BK:41:GLN:NE2	2.19	0.57
1:AA:1217:G:H2'	1:AA:1218:G:C8	2.40	0.57
1:AA:4991:U:H2'	1:AA:4992:G:H8	1.69	0.57
45:BA:1227:G:H21	45:BA:1635:C:H4'	1.69	0.57
45:BA:1529:C:H4'	58:BN:89:PRO:HG3	1.86	0.57
1:AA:3861:A:H2'	1:AA:3862:A:H8	1.70	0.57
45:BA:159:A2M:HM'2	45:BA:160:U:H5'	1.85	0.57
45:BA:379:C:H41	52:BH:178:ARG:HH22	1.53	0.57
45:BA:1560:U:H2'	45:BA:1561:A:H8	1.69	0.57
12:AL:36:LEU:HA	12:AL:39:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BB:97:GLU:HG2	46:BB:113:ARG:HE	1.68	0.57
1:AA:678:C:H2'	1:AA:679:C:H6	1.69	0.57
1:AA:3944:G:O6	1:AA:4069:U:O4	2.23	0.57
1:AA:4477:A:H4'	11:AK:174:LYS:HD2	1.85	0.57
27:Aa:4:ASN:HB3	27:Aa:7:VAL:HG22	1.86	0.57
49:BE:123:LEU:HD21	49:BE:136:VAL:HG12	1.86	0.57
1:AA:4571:A2M:HM'2	1:AA:4572:U:H5'	1.87	0.57
1:AA:4761:G:H2'	1:AA:4762:A:H8	1.70	0.57
27:Aa:72:GLN:HB3	27:Aa:81:TYR:HB2	1.87	0.57
45:BA:795:A:H2'	45:BA:796:G:C4	2.40	0.57
55:BK:57:LEU:HD11	55:BK:86:LEU:HD21	1.86	0.57
78:Bh:48:ASN:H	78:Bh:49:LYS:HZ3	1.52	0.57
1:AA:2647:A:H62	1:AA:2686:G:H21	0.67	0.57
1:AA:4618:OMG:H5''	24:AX:15:ARG:HB2	1.86	0.57
45:BA:130:G:H5''	45:BA:132:U:H5''	1.87	0.57
45:BA:388:U:H2'	45:BA:389:A:H8	1.70	0.57
50:BF:34:SER:HA	63:BS:55:VAL:HB	1.86	0.57
45:BA:934:G:O6	45:BA:1008:A:N1	2.38	0.57
72:Bb:6:VAL:HG23	72:Bb:34:ILE:HD11	1.87	0.57
33:Ag:66:THR:HA	33:Ag:69:MET:HE2	1.86	0.56
42:Aq:70:LEU:HB2	42:Aq:81:ARG:HG3	1.87	0.56
45:BA:1616:U:H2'	45:BA:1617:G:C8	2.40	0.56
45:BA:1745:A:H1'	67:BW:66:GLY:HA2	1.86	0.56
1:AA:399:G:H2'	1:AA:400:A2M:H8	1.86	0.56
39:Am:23:VAL:HG22	39:Am:36:VAL:HG22	1.87	0.56
45:BA:1455:A:H2'	45:BA:1456:G:H8	1.70	0.56
47:BC:19:LEU:HD21	78:Bh:106:LEU:HD21	1.87	0.56
60:BP:57:GLY:O	60:BP:61:ARG:HG2	2.05	0.56
1:AA:18:C:H2'	1:AA:19:G:H8	1.70	0.56
1:AA:190:G:H2'	1:AA:191:G:H8	1.70	0.56
1:AA:1914:C:H4'	17:AQ:89:PRO:HD3	1.86	0.56
1:AA:2400:G:H21	35:Ai:6:THR:HG22	1.71	0.56
1:AA:3873:G:H2'	1:AA:3874:G:C8	2.41	0.56
1:AA:3961:G:H1	1:AA:4048:A:N6	2.03	0.56
1:AA:4960:G:H2'	1:AA:4961:G:H8	1.70	0.56
11:AK:7:ASN:HD22	11:AK:56:ARG:HH22	1.52	0.56
52:BH:37:LYS:HB2	52:BH:59:ARG:HG3	1.87	0.56
55:BK:107:ILE:HG23	55:BK:111:MET:HE2	1.86	0.56
70:BZ:19:ARG:HD3	70:BZ:21:SER:HB3	1.88	0.56
44:As:48:THR:HG23	44:As:65:LYS:HD2	1.87	0.56
45:BA:1821:U:H2'	45:BA:1822:A:C8	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:33:ILE:HG22	63:BS:55:VAL:HG21	1.87	0.56
68:BX:32:ILE:HD12	68:BX:37:LEU:HD23	1.87	0.56
45:BA:394:G:H5'	54:BJ:81:LYS:HB2	1.86	0.56
45:BA:509:OMG:HM22	45:BA:510:G:H5'	1.86	0.56
45:BA:690:G:H3'	45:BA:691:G:H21	1.71	0.56
49:BE:197:LYS:HG2	49:BE:198:ILE:HG12	1.88	0.56
57:BM:15:VAL:HB	57:BM:20:ILE:HG13	1.87	0.56
3:AC:72:A:N1	3:AC:79:G:N2	2.51	0.56
36:Aj:80:PRO:HD2	36:Aj:83:LEU:HD12	1.88	0.56
45:BA:948:C:H2'	45:BA:949:G:H8	1.71	0.56
52:BH:25:ARG:HE	52:BH:27:TYR:HE1	1.53	0.56
53:BI:9:ILE:O	53:BI:13:GLU:HG3	2.06	0.56
67:BW:3:LEU:HD21	67:BW:24:LEU:HD11	1.87	0.56
45:BA:1656:G:O6	45:BA:1668:U:O4	2.23	0.56
58:BN:27:LYS:HD2	58:BN:110:LEU:HG	1.87	0.56
65:BU:18:VAL:HB	65:BU:301:GLY:HA3	1.87	0.56
65:BU:258:ILE:HD13	65:BU:268:ASP:HB3	1.86	0.56
9:AI:67:THR:O	9:AI:71:MET:HG2	2.04	0.56
45:BA:1588:A:H2'	45:BA:1589:A:C8	2.41	0.56
65:BU:7:LEU:HD11	65:BU:308:ARG:HD2	1.88	0.56
69:BY:51:VAL:HG22	69:BY:85:LEU:HD11	1.88	0.56
1:AA:1306:C:H2'	1:AA:1307:A:H8	1.69	0.56
1:AA:3664:G:H2'	1:AA:3665:G:H8	1.70	0.56
1:AA:3774:A:H2'	1:AA:3775:A:C8	2.41	0.56
1:AA:5006:U:H4'	1:AA:5007:A:H5'	1.88	0.56
27:Aa:45:ARG:HB2	27:Aa:126:ARG:HH22	1.71	0.56
45:BA:1473:G:H22	45:BA:1475:G:H3'	1.71	0.56
47:BC:74:VAL:HG23	47:BC:121:LEU:HB3	1.88	0.56
50:BF:35:LEU:HD12	50:BF:117:ILE:HG12	1.88	0.56
61:BQ:100:VAL:HA	61:BQ:125:VAL:HA	1.88	0.56
1:AA:4601:U:H2'	1:AA:4602:A:H8	1.71	0.56
8:AH:46:ARG:HH21	8:AH:66:LYS:HG2	1.71	0.56
28:Ab:25:ILE:HA	28:Ab:43:VAL:HG12	1.87	0.56
72:Bb:90:GLN:HA	72:Bb:94:LEU:HD23	1.86	0.56
1:AA:3619:G:H22	1:AA:3624:A:H1'	1.70	0.55
4:AD:83:HIS:HB3	43:Ar:64:VAL:HG22	1.88	0.55
51:BG:34:SER:HA	51:BG:37:LYS:HG3	1.87	0.55
68:BX:63:LEU:HD12	68:BX:70:ARG:HB2	1.88	0.55
1:AA:2770:C:H2'	1:AA:2771:G:H8	1.70	0.55
1:AA:4889:G:H2'	1:AA:4890:G:C8	2.41	0.55
6:AF:328:LEU:HD22	9:AI:187:MET:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:23:LEU:HD11	23:AW:83:LEU:HD12	1.88	0.55
45:BA:49:C:H2'	45:BA:472:C:H41	1.71	0.55
48:BD:146:ARG:HB2	48:BD:149:GLN:HB2	1.88	0.55
52:BH:119:LEU:HD11	52:BH:153:LYS:HG2	1.89	0.55
3:AC:78:G:H2'	3:AC:79:G:C8	2.40	0.55
45:BA:1432:U:H2'	45:BA:1438:A:C8	2.41	0.55
45:BA:1538:C:H2'	45:BA:1539:U:C6	2.42	0.55
45:BA:1562:C:H2'	45:BA:1563:G:C8	2.42	0.55
45:BA:1614:A:H61	45:BA:1625:PSU:HN3	1.54	0.55
46:BB:45:ILE:HG13	46:BB:49:ARG:HH21	1.69	0.55
48:BD:177:GLN:HG3	48:BD:178:THR:HG23	1.89	0.55
67:BW:41:LEU:HD12	67:BW:45:TRP:CD1	2.41	0.55
1:AA:1604:G:H2'	1:AA:1605:G:C8	2.42	0.55
1:AA:2744:A:H2'	1:AA:2745:A:C8	2.41	0.55
1:AA:4642:U:H2'	1:AA:4643:G:H8	1.71	0.55
4:AD:234:LYS:HG2	4:AD:238:ILE:HG12	1.89	0.55
45:BA:116:OMU:HM22	45:BA:117:C:H5'	1.89	0.55
1:AA:3771:C:H2'	1:AA:3772:U:C6	2.41	0.55
45:BA:1594:A:H3'	74:Bd:104:ARG:HD2	1.89	0.55
45:BA:1780:G:H3'	45:BA:1781:A:C8	2.41	0.55
61:BQ:102:VAL:HG12	61:BQ:122:VAL:HA	1.89	0.55
65:BU:212:LYS:HD2	65:BU:235:ILE:HG12	1.88	0.55
1:AA:4754:G:N2	1:AA:4755:G:C2	2.75	0.55
45:BA:382:C:H2'	45:BA:383:G:H8	1.71	0.55
45:BA:946:U:H2'	45:BA:947:G:H8	1.71	0.55
45:BA:952:G:H2'	45:BA:953:C:C6	2.42	0.55
45:BA:1804:OMU:HM22	45:BA:1805:G:H5'	1.89	0.55
69:BY:87:GLU:HG3	69:BY:92:CYS:HB2	1.87	0.55
1:AA:2610:G:H2'	1:AA:2611:A:H8	1.72	0.55
45:BA:367:U:H4'	45:BA:371:A:C8	2.41	0.55
1:AA:2520:C:H2'	1:AA:2521:G:H8	1.72	0.55
45:BA:907:G:H2'	45:BA:908:A:H8	1.71	0.55
49:BE:106:ARG:HH11	49:BE:175:VAL:HG13	1.70	0.55
55:BK:81:ARG:HA	55:BK:116:LEU:HB2	1.87	0.55
58:BN:64:LEU:HB3	58:BN:123:LEU:HD23	1.89	0.55
1:AA:1273:G:H8	30:Ad:117:ARG:HD2	1.72	0.55
1:AA:1749:A:H2'	1:AA:1750:G:C8	2.42	0.55
1:AA:4095:G:H1	1:AA:4114:C:H4'	1.71	0.55
45:BA:1468:C:H2'	45:BA:1469:A:H8	1.70	0.55
53:BI:80:ARG:HG3	53:BI:85:LEU:HB2	1.88	0.55
68:BX:49:THR:O	68:BX:53:ILE:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:388:U:H2'	45:BA:389:A:C8	2.42	0.54
45:BA:1218:C:H2'	45:BA:1219:C:H6	1.70	0.54
56:BL:58:LEU:HB3	56:BL:62:ARG:HD2	1.89	0.54
59:BO:43:ALA:HB1	59:BO:91:LEU:HD21	1.89	0.54
1:AA:2845:A:H61	1:AA:3843:C:H42	1.54	0.54
1:AA:4754:G:H2'	1:AA:4755:G:C8	2.42	0.54
1:AA:4767:C:H2'	1:AA:4768:G:C8	2.42	0.54
5:AE:220:ILE:HG12	5:AE:278:THR:HG23	1.89	0.54
45:BA:1705:C:H2'	45:BA:1706:G:C8	2.41	0.54
47:BC:205:ARG:HD3	47:BC:210:ILE:HD12	1.88	0.54
1:AA:4991:U:H2'	1:AA:4992:G:C8	2.42	0.54
32:Af:54:MET:HE1	32:Af:60:PRO:HA	1.90	0.54
46:BB:29:PRO:HG2	46:BB:46:ILE:HD11	1.89	0.54
51:BG:101:LEU:HD22	51:BG:102:PRO:HD2	1.88	0.54
63:BS:32:VAL:HG23	63:BS:42:ILE:HG13	1.88	0.54
45:BA:4:C:C6	45:BA:4:C:C5'	2.85	0.54
45:BA:184:G:H2'	45:BA:185:G:H8	1.73	0.54
45:BA:1513:C:H2'	45:BA:1514:G:C8	2.43	0.54
47:BC:31:ASP:HB2	47:BC:34:MET:HG3	1.89	0.54
49:BE:141:LYS:HA	49:BE:147:ALA:HA	1.89	0.54
51:BG:55:GLY:H	51:BG:57:ARG:HH12	1.54	0.54
58:BN:107:LEU:HD13	58:BN:110:LEU:HD13	1.89	0.54
78:Bh:31:ASN:HA	78:Bh:34:VAL:HB	1.89	0.54
1:AA:1778:C:H5''	7:AG:5:LYS:HG3	1.89	0.54
1:AA:4537:C:H2'	1:AA:4538:G:C8	2.42	0.54
45:BA:996:A:H5''	70:BZ:7:PRO:HG3	1.89	0.54
45:BA:1740:C:H42	45:BA:1794:C:H42	1.55	0.54
57:BM:33:ILE:HD11	57:BM:99:LEU:HB3	1.90	0.54
1:AA:425:U:H2'	1:AA:426:A:H8	1.73	0.54
1:AA:1577:G:O2'	1:AA:1612:G:H4'	2.07	0.54
31:Ae:38:ILE:HG21	31:Ae:63:TYR:HB3	1.89	0.54
47:BC:24:HIS:HD2	47:BC:51:LEU:HD21	1.71	0.54
48:BD:73:ASP:HB2	71:Ba:128:ARG:HH12	1.73	0.54
53:BI:91:PRO:HG2	53:BI:94:LEU:HD23	1.90	0.54
1:AA:160:G:H2'	1:AA:161:G:C8	2.42	0.54
1:AA:2745:A:H2'	1:AA:2746:A:C8	2.41	0.54
7:AG:256:LYS:HD3	7:AG:257:PRO:HD2	1.88	0.54
23:AW:23:LEU:HD22	23:AW:110:TYR:HB2	1.90	0.54
45:BA:874:G:H2'	45:BA:875:A:C8	2.43	0.54
45:BA:1468:C:H2'	45:BA:1469:A:C8	2.43	0.54
48:BD:71:LEU:HA	48:BD:74:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:41:VAL:HB	50:BF:109:LEU:HD23	1.89	0.54
1:AA:160:G:H2'	1:AA:161:G:H8	1.72	0.54
1:AA:173:C:H5''	14:AN:129:ARG:HH22	1.73	0.54
1:AA:1332:C:H2'	1:AA:1333:A:C8	2.39	0.54
1:AA:3870:C:H2'	1:AA:3871:A:H8	1.73	0.54
1:AA:4723:A:H2'	1:AA:4724:A:C8	2.43	0.54
2:AB:4:U:H2'	2:AB:5:A:H8	1.72	0.54
9:AI:236:ARG:HB2	9:AI:239:GLN:HB2	1.90	0.54
16:AP:138:PHE:HA	16:AP:143:ARG:HD2	1.90	0.54
45:BA:1650:A:H3'	45:BA:1651:A:H8	1.72	0.54
45:BA:1703:OMC:HM22	45:BA:1704:C:H5'	1.89	0.54
45:BA:1845:A:H2'	45:BA:1846:G:C8	2.43	0.54
49:BE:37:VAL:HG12	49:BE:50:ILE:HG12	1.89	0.54
56:BL:86:GLN:O	56:BL:90:LYS:HG2	2.08	0.54
58:BN:76:THR:HG23	58:BN:94:ARG:HD2	1.88	0.54
71:Ba:72:TYR:HA	71:Ba:75:MET:HE3	1.89	0.54
1:AA:678:C:H2'	1:AA:679:C:C6	2.43	0.54
1:AA:1824:G:H2'	1:AA:1825:A:C8	2.43	0.54
1:AA:3848:U:H2'	1:AA:3849:A:C8	2.43	0.54
1:AA:4174:U:H2'	1:AA:4175:G:H8	1.73	0.54
12:AL:139:ARG:HH12	12:AL:195:CYS:HB2	1.73	0.54
66:BV:146:GLU:HB2	66:BV:149:THR:HG22	1.90	0.54
67:BW:50:VAL:HG12	67:BW:113:ILE:HG13	1.90	0.54
1:AA:1339:U:H2'	1:AA:1340:OMC:C6	2.42	0.54
1:AA:4238:G:H2'	1:AA:4239:A:H8	1.71	0.54
1:AA:5054:C:H4'	1:AA:5055:G:H5'	1.89	0.54
7:AG:208:MET:HG2	7:AG:219:TYR:HE1	1.73	0.54
12:AL:36:LEU:HD23	12:AL:87:MET:HB2	1.89	0.54
16:AP:10:LEU:HD13	37:Ak:44:ILE:HD12	1.90	0.54
45:BA:26:U:H2'	45:BA:27:A2M:H8	1.89	0.54
45:BA:528:A:H2'	45:BA:529:A:H8	1.73	0.54
45:BA:1223:A:H2'	45:BA:1224:G:C8	2.43	0.54
45:BA:1575:G:H2'	45:BA:1576:G:C8	2.43	0.54
45:BA:1668:U:H4'	59:BO:64:THR:HG21	1.89	0.54
1:AA:190:G:H2'	1:AA:191:G:C8	2.43	0.53
1:AA:696:C:H5'	1:AA:697:G:H5'	1.89	0.53
1:AA:3910:C:H2'	1:AA:3911:C:H6	1.74	0.53
1:AA:4745:G:N2	1:AA:4955:A:N1	2.45	0.53
5:AE:299:ILE:HB	5:AE:313:SER:HB3	1.90	0.53
11:AK:112:VAL:HB	11:AK:126:VAL:HG23	1.90	0.53
13:AM:95:ARG:O	13:AM:98:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:48:VAL:HG21	22:AV:94:GLU:HG2	1.89	0.53
45:BA:518:G:H2'	45:BA:519:A:H8	1.71	0.53
45:BA:1063:C:H4'	71:Ba:151:ARG:HD3	1.89	0.53
45:BA:1322:G:H5''	45:BA:1323:U:H5	1.72	0.53
65:BU:40:ILE:HB	65:BU:59:LEU:HB2	1.90	0.53
1:AA:3829:G:H2'	1:AA:3830:A2M:H8	1.89	0.53
1:AA:4743:G:H2'	1:AA:4744:A:C8	2.43	0.53
1:AA:4935:C:H2'	1:AA:4936:G:C8	2.43	0.53
12:AL:190:LEU:HD13	12:AL:197:VAL:HG21	1.90	0.53
33:Ag:113:GLU:O	33:Ag:117:GLN:HG3	2.07	0.53
52:BH:165:GLN:HE22	52:BH:195:LEU:HD21	1.73	0.53
1:AA:1182:C:H5'	1:AA:1183:C:H5''	1.91	0.53
1:AA:1193:C:H2'	1:AA:1194:G:H8	1.73	0.53
4:AD:206:PRO:HG3	4:AD:213:GLY:HA3	1.89	0.53
7:AG:280:VAL:HG13	12:AL:206:LEU:HD11	1.90	0.53
1:AA:1921:C:C4	15:AO:17:PHE:HB3	2.44	0.53
46:BB:18:TRP:HB3	46:BB:20:LEU:HD13	1.89	0.53
51:BG:143:ARG:HD3	72:Bb:53:ILE:HG22	1.90	0.53
69:BY:23:LYS:O	69:BY:27:ILE:HG12	2.09	0.53
1:AA:2337:C:H4'	44:As:19:LYS:HB2	1.91	0.53
1:AA:2815:A2M:HM'2	1:AA:2816:G:H5'	1.91	0.53
7:AG:55:VAL:HG23	7:AG:60:ILE:HG12	1.91	0.53
45:BA:1538:C:H2'	45:BA:1539:U:H6	1.73	0.53
68:BX:47:LYS:NZ	68:BX:102:ILE:HD11	2.24	0.53
1:AA:257:C:H2'	1:AA:258:G:C8	2.43	0.53
1:AA:1296:G:H2'	1:AA:1297:U:H6	1.73	0.53
1:AA:3917:A:H2'	1:AA:3918:G:H8	1.73	0.53
15:AO:101:LYS:HB2	17:AQ:200:GLY:HA3	1.91	0.53
23:AW:18:VAL:HG21	23:AW:78:PHE:H	1.73	0.53
35:Ai:56:VAL:HG13	35:Ai:72:LYS:HA	1.90	0.53
45:BA:383:G:H4'	54:BJ:132:ARG:HD2	1.90	0.53
45:BA:1337:4AC:H4'	59:BO:67:LYS:HB3	1.90	0.53
45:BA:1730:U:H3	45:BA:1804:OMU:HN3	1.57	0.53
47:BC:62:ALA:HA	47:BC:65:ILE:HD12	1.90	0.53
1:AA:956:A:H1'	1:AA:2076:G:H5''	1.91	0.53
1:AA:3746:A:H5''	4:AD:244:GLY:HA3	1.90	0.53
3:AC:120:G:H2'	3:AC:121:G:H8	1.74	0.53
21:AU:69:GLU:HG3	21:AU:71:SER:H	1.73	0.53
45:BA:106:C:H2'	45:BA:107:A:H8	1.74	0.53
45:BA:907:G:H2'	45:BA:908:A:C8	2.44	0.53
45:BA:1527:C:H5''	56:BL:142:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Ba:119:LEU:HD21	71:Ba:126:ILE:HD11	1.91	0.53
72:Bb:51:GLU:O	72:Bb:61:ILE:HA	2.08	0.53
1:AA:300:A:H2'	1:AA:301:G:H8	1.72	0.53
1:AA:4253:A:H5'	1:AA:4254:G:C8	2.44	0.53
44:As:66:ARG:HH21	44:As:78:VAL:HG22	1.73	0.53
45:BA:1259:A:H61	45:BA:1519:U:H5'	1.74	0.53
48:BD:192:SER:HA	48:BD:195:LYS:HG3	1.91	0.53
57:BM:124:ARG:HD2	57:BM:131:VAL:HA	1.90	0.53
73:Bc:110:ARG:HG2	73:Bc:113[A]:ARG:HH22	1.74	0.53
1:AA:2648:G:H2'	1:AA:2649:G:H8	1.73	0.53
1:AA:3718:A2M:H2	1:AA:3934:G:O4'	2.09	0.53
1:AA:4238:G:H2'	1:AA:4239:A:C8	2.44	0.53
1:AA:4523:A2M:H5''	1:AA:4524:G:H5'	1.91	0.53
29:Ac:119:LYS:HA	29:Ac:140:VAL:HG13	1.91	0.53
32:Af:41:ARG:HG3	32:Af:78:ARG:HA	1.90	0.53
45:BA:576:A2M:OP2	45:BA:576:A2M:H8	2.09	0.53
46:BB:188:ASN:HD22	46:BB:220:THR:HG23	1.73	0.53
58:BN:4:VAL:HG21	58:BN:136:GLY:HA2	1.91	0.53
1:AA:2699:C:H2'	1:AA:2700:G:H8	1.74	0.53
45:BA:877:C:H2'	45:BA:878:G:C8	2.44	0.53
45:BA:1631:U:H4'	57:BM:34:LYS:HG2	1.92	0.53
47:BC:33:GLN:HB2	47:BC:154:LEU:HD13	1.91	0.53
47:BC:85:ARG:HH11	47:BC:85:ARG:HG3	1.74	0.53
58:BN:11:GLN:HB2	58:BN:62:ARG:HH12	1.74	0.53
45:BA:432:G:H2'	45:BA:433:A:C8	2.44	0.52
51:BG:130:LEU:HA	51:BG:133:LEU:HD12	1.91	0.52
1:AA:710:G:H2'	1:AA:711:A:H8	1.73	0.52
1:AA:1749:A:H4'	12:AL:39:LYS:HE2	1.91	0.52
3:AC:77:A:H2'	3:AC:78:G:O4'	2.09	0.52
45:BA:678:U:O4	45:BA:1027:A:N7	2.42	0.52
45:BA:1539:U:H2'	45:BA:1540:G:H8	1.75	0.52
46:BB:115:THR:HG23	46:BB:118:GLU:H	1.74	0.52
73:Bc:41:ARG:HH12	73:Bc:94:HIS:CD2	2.26	0.52
75:Be:12:PRO:HA	75:Be:15:GLU:HB2	1.91	0.52
1:AA:189:G:H2'	1:AA:190:G:C8	2.44	0.52
1:AA:1942:A:H2'	1:AA:1943:A:C8	2.44	0.52
27:Aa:54:GLU:HB2	27:Aa:108:ARG:HG2	1.91	0.52
51:BG:47:ALA:HB3	51:BG:63:PHE:HB2	1.91	0.52
1:AA:691:C:H2'	1:AA:692:A:C8	2.44	0.52
1:AA:4423:PSU:H2'	41:Ao:97:ARG:HD3	1.91	0.52
3:AC:78:G:H2'	3:AC:79:G:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:58:PRO:HG2	10:AJ:61:ILE:HD12	1.91	0.52
13:AM:112:HIS:CE1	13:AM:126:TYR:H	2.27	0.52
31:Ae:96:ILE:HD11	31:Ae:99:PRO:HB3	1.91	0.52
43:Ar:27:LYS:O	43:Ar:31:ILE:HG13	2.09	0.52
45:BA:1324:G:H1	45:BA:1504:U:H3	1.58	0.52
45:BA:1841:C:H2'	45:BA:1842:4AC:H6	1.90	0.52
46:BB:87:MET:HB3	46:BB:102:ILE:HG22	1.91	0.52
48:BD:30:TRP:HB3	71:Ba:19:PRO:HB3	1.90	0.52
48:BD:182:LYS:HD3	48:BD:231:LEU:HD22	1.92	0.52
7:AG:197:LYS:HA	7:AG:200:MET:HB2	1.91	0.52
45:BA:610:G:H2'	45:BA:611:G:H8	1.74	0.52
45:BA:1486:A:H2'	45:BA:1487:A:C8	2.44	0.52
51:BG:87:PHE:HB3	51:BG:90:LYS:HE3	1.90	0.52
57:BM:55:ARG:HH22	74:Bd:80:ARG:NH1	2.08	0.52
59:BO:20:ILE:HG12	59:BO:98:VAL:HG11	1.90	0.52
67:BW:142:ARG:HA	67:BW:147:LEU:HB2	1.90	0.52
1:AA:700:G:H2'	1:AA:701:G:C8	2.45	0.52
1:AA:700:G:H2'	1:AA:701:G:H8	1.74	0.52
23:AW:93:LYS:HD2	23:AW:94:ASN:OD1	2.10	0.52
25:AY:20:ARG:HG3	25:AY:20:ARG:HH11	1.74	0.52
45:BA:585:C:H3'	45:BA:586:G:H8	1.74	0.52
45:BA:824:C:H1'	68:BX:144:ILE:HD11	1.92	0.52
45:BA:1455:A:H4'	78:Bh:28:PHE:HB2	1.92	0.52
45:BA:1844:U:H2'	45:BA:1845:A:C8	2.45	0.52
50:BF:23:TRP:HZ2	50:BF:101:HIS:CG	2.27	0.52
50:BF:78:MET:HE2	50:BF:159:ARG:NE	2.25	0.52
71:Ba:85:CYS:HB3	71:Ba:90:ILE:HB	1.91	0.52
74:Bd:73:VAL:HG12	74:Bd:79:ILE:HD11	1.91	0.52
1:AA:752:G:O6	1:AA:911:U:O4	2.27	0.52
1:AA:1066:G:H2'	1:AA:1067:G:C8	2.44	0.52
1:AA:4870:G:H5''	15:AO:91:TRP:CE2	2.45	0.52
1:AA:4906:C:H2'	1:AA:4907:G:C8	2.43	0.52
45:BA:435:A:H2'	45:BA:450:C:H5'	1.91	0.52
45:BA:479:C:H2'	45:BA:480:G:H8	1.74	0.52
46:BB:179:ASN:HD21	46:BB:230:LYS:HA	1.74	0.52
67:BW:135:PRO:HB2	67:BW:141:ILE:HG13	1.90	0.52
1:AA:2017:A:H5''	1:AA:2018:C:C5	2.45	0.52
1:AA:2025:A:N3	1:AA:2026:A:H1'	2.25	0.52
12:AL:47:PRO:HD2	12:AL:141:LYS:HA	1.92	0.52
45:BA:1414:A:H2'	45:BA:1415:C:C6	2.44	0.52
56:BL:72:VAL:HG11	56:BL:84:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:3732:A:H2'	1:AA:3733:A:C8	2.43	0.52
1:AA:4483:C:H2'	1:AA:4484:A:H8	1.75	0.52
1:AA:4761:G:H2'	1:AA:4762:A:C8	2.45	0.52
1:AA:4933:C:H2'	1:AA:4934:A:C8	2.45	0.52
6:AF:7:LEU:HD22	6:AF:21:ASN:HB3	1.92	0.52
11:AK:59:LYS:HE2	11:AK:66:GLU:HB3	1.91	0.52
12:AL:36:LEU:HD11	12:AL:73:ASN:HD21	1.75	0.52
45:BA:116:OMU:HN3	45:BA:347:G:H1	1.57	0.52
45:BA:1137:U:H3	45:BA:1148:A:H62	1.58	0.52
45:BA:1432:U:H2'	45:BA:1438:A:H8	1.74	0.52
46:BB:106:LYS:HE3	46:BB:108:ARG:HD3	1.91	0.52
46:BB:201:HIS:HD1	46:BB:206:ASP:HA	1.75	0.52
51:BG:101:LEU:HD12	51:BG:116:ARG:HD3	1.90	0.52
1:AA:272:U:H2'	1:AA:273:U:C6	2.45	0.52
1:AA:2017:A:H5''	1:AA:2018:C:H5	1.75	0.52
1:AA:2335:C:H2'	1:AA:2336:G:H8	1.74	0.52
2:AB:4:U:H2'	2:AB:5:A:C8	2.45	0.52
6:AF:116:ASN:HB2	6:AF:119:GLN:HG3	1.90	0.52
18:AR:116:HIS:HB3	18:AR:149:ILE:HB	1.91	0.52
21:AU:16:CYS:SG	21:AU:54:MET:HE3	2.49	0.52
45:BA:35:C:H2'	45:BA:36:PSU:H6	1.75	0.52
45:BA:149:A:H3'	45:BA:150:A:H8	1.75	0.52
45:BA:680:G:H2'	45:BA:681:PSU:H6	1.75	0.52
52:BH:117:TYR:HB3	52:BH:119:LEU:HD13	1.92	0.52
65:BU:36:ARG:HA	65:BU:65:PHE:HB3	1.91	0.52
65:BU:42:MET:HE3	65:BU:57:ARG:HB2	1.92	0.52
1:AA:1933:G:H2'	1:AA:1934:A:C8	2.45	0.51
1:AA:2699:C:H2'	1:AA:2700:G:C8	2.45	0.51
1:AA:4484:A:H2'	1:AA:4485:C:H6	1.74	0.51
45:BA:568:C:H2'	45:BA:569:A:C8	2.42	0.51
45:BA:1649:U:H5''	56:BL:137:ALA:HB3	1.92	0.51
46:BB:192:ILE:HD11	46:BB:244:ILE:HD13	1.91	0.51
49:BE:17:PHE:HE2	49:BE:39:VAL:HG11	1.75	0.51
59:BO:24:LEU:HD12	59:BO:32:LEU:HD11	1.92	0.51
67:BW:57:ASP:HA	67:BW:106:LEU:HA	1.92	0.51
1:AA:61:A:H5''	16:AP:164:LEU:HD11	1.93	0.51
1:AA:3848:U:H2'	1:AA:3849:A:H8	1.75	0.51
1:AA:4260:U:H2'	1:AA:4261:C:H6	1.75	0.51
1:AA:4897:G:H2'	1:AA:4898:G:H8	1.75	0.51
10:AJ:182:CYS:HB3	10:AJ:222:ILE:HG23	1.91	0.51
13:AM:26:VAL:HG23	13:AM:28:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:116:LEU:HD22	16:AP:135:ILE:HD11	1.92	0.51
20:AT:134:ASN:OD1	20:AT:137:ILE:HG13	2.10	0.51
48:BD:105:LEU:HD11	48:BD:211:PHE:HB2	1.92	0.51
57:BM:31:THR:HG21	57:BM:38:ARG:HG3	1.91	0.51
1:AA:909:A:H2'	1:AA:910:G:H8	1.75	0.51
1:AA:1645:C:H2'	1:AA:1646:A:C8	2.45	0.51
7:AG:52:ILE:O	7:AG:62:CYS:HA	2.10	0.51
45:BA:51:U:H2'	45:BA:52:G:H8	1.76	0.51
45:BA:1654:G:H5'	58:BN:91:HIS:HA	1.92	0.51
1:AA:93:G:H2'	1:AA:94:A:C8	2.45	0.51
1:AA:1188:C:H2'	1:AA:1189:G:H8	1.75	0.51
1:AA:1249:C:H42	1:AA:1261:G:H1	1.58	0.51
1:AA:1751:A:H1'	12:AL:193:ASP:HB2	1.91	0.51
45:BA:946:U:H2'	45:BA:947:G:C8	2.45	0.51
45:BA:1174:PSU:H2'	45:BA:1175:G:C8	2.46	0.51
48:BD:30:TRP:CZ3	48:BD:48:LEU:HB3	2.44	0.51
1:AA:1217:G:H2'	1:AA:1218:G:H8	1.75	0.51
1:AA:1750:G:H22	1:AA:1780:A:H2	1.58	0.51
45:BA:106:C:H2'	45:BA:107:A:C8	2.45	0.51
45:BA:568:C:H42	45:BA:582:U:H3	0.68	0.51
45:BA:808:A:H2'	45:BA:809:A:C4	2.45	0.51
45:BA:1831:A:H2'	45:BA:1832:6MZ:H8	1.93	0.51
59:BO:56:MET:HE3	59:BO:86:LYS:HG2	1.92	0.51
1:AA:2648:G:H2'	1:AA:2649:G:C8	2.45	0.51
1:AA:4483:C:H2'	1:AA:4484:A:C8	2.46	0.51
45:BA:68:A:H2'	45:BA:69:C:H6	1.76	0.51
45:BA:1430:C:H2'	45:BA:1431:G:H8	1.75	0.51
47:BC:57:LYS:HG3	47:BC:161:ILE:HD13	1.93	0.51
61:BQ:94:ILE:HG22	61:BQ:125:VAL:HG21	1.93	0.51
1:AA:2568:C:H2'	1:AA:2569:G:C8	2.45	0.51
10:AJ:106:THR:HG22	10:AJ:107:LYS:H	1.75	0.51
44:As:97:ILE:HD13	44:As:107:ARG:HA	1.92	0.51
45:BA:634:A:H2'	45:BA:635:G:C8	2.46	0.51
45:BA:924:G:H1	45:BA:1018:U:H3	1.58	0.51
45:BA:1605:G:H1'	45:BA:1634:A:H61	1.75	0.51
64:BT:3:HIS:HD2	64:BT:5:GLN:H	1.57	0.51
10:AJ:162:ASP:HB3	10:AJ:163:PRO:HD3	1.91	0.51
45:BA:99:A2M:HM'2	45:BA:100:PSU:H5''	1.93	0.51
45:BA:1708:C:H2'	45:BA:1709:G:H8	1.74	0.51
48:BD:103:MET:HB3	48:BD:215:VAL:HB	1.93	0.51
70:BZ:62:GLN:HB3	70:BZ:65:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:729:G:H1	21:AU:67:VAL:HA	1.75	0.51
45:BA:5:U:H2'	45:BA:6:G:C8	2.46	0.51
45:BA:83:A:H2'	45:BA:84:A:C8	2.45	0.51
49:BE:137:VAL:HB	49:BE:185:LYS:HB2	1.93	0.51
56:BL:90:LYS:HA	56:BL:93:VAL:HG22	1.93	0.51
67:BW:35:GLU:HG3	67:BW:51:ARG:HB2	1.93	0.51
1:AA:3910:C:H2'	1:AA:3911:C:C6	2.45	0.51
10:AJ:114:LEU:HD22	10:AJ:117:ARG:HD2	1.93	0.51
17:AQ:43:ILE:HD11	17:AQ:138:LEU:HD13	1.94	0.51
32:Af:57:MET:HE3	32:Af:88:LEU:HB3	1.93	0.51
45:BA:174:OMC:HM22	45:BA:175:A:H5'	1.92	0.51
50:BF:68:ILE:O	50:BF:72:LEU:HD13	2.11	0.51
52:BH:151:GLU:HA	52:BH:154:LYS:HE2	1.92	0.51
1:AA:743:G:H2'	1:AA:744:G:C8	2.46	0.50
1:AA:4960:G:H2'	1:AA:4961:G:C8	2.46	0.50
13:AM:40:LEU:HD23	13:AM:48:PRO:HB3	1.92	0.50
17:AQ:29:LEU:HB3	34:Ah:10:ILE:HG21	1.93	0.50
23:AW:42:PHE:CD1	23:AW:90:TYR:HB2	2.47	0.50
45:BA:5:U:H2'	45:BA:6:G:H8	1.74	0.50
45:BA:379:C:H2'	45:BA:380:G:C8	2.45	0.50
45:BA:752:G:H4'	45:BA:792:C:H5'	1.93	0.50
45:BA:906:U:H2'	45:BA:907:G:H8	1.75	0.50
45:BA:1112:U:H2'	45:BA:1113:A:C8	2.45	0.50
45:BA:1856:C:H2'	45:BA:1857:G:C8	2.46	0.50
1:AA:710:G:H2'	1:AA:711:A:C8	2.46	0.50
1:AA:1086:C:H2'	1:AA:1087:A:H8	1.75	0.50
1:AA:1346:C:H2'	1:AA:1347:G:H8	1.76	0.50
1:AA:4260:U:H2'	1:AA:4261:C:C6	2.46	0.50
45:BA:1787:G:H2'	45:BA:1788:A:H8	1.76	0.50
1:AA:271:C:H2'	1:AA:272:U:C6	2.46	0.50
1:AA:2333:G:N7	6:AF:189:MET:HE3	2.26	0.50
1:AA:2550:G:H2'	1:AA:2551:A:C8	2.46	0.50
45:BA:1426:U:H4'	58:BN:7:LYS:HD3	1.94	0.50
47:BC:63:ARG:HH21	60:BP:39:VAL:HG13	1.75	0.50
62:BR:30:VAL:HG23	62:BR:34:LYS:HE2	1.92	0.50
1:AA:398:A2M:H8	1:AA:398:A2M:O5'	2.10	0.50
5:AE:56:ILE:O	5:AE:73:VAL:HA	2.12	0.50
15:AO:119:ARG:O	15:AO:123:ILE:HD12	2.11	0.50
45:BA:1475:G:H5'	56:BL:124:PRO:HG3	1.93	0.50
45:BA:1595:U:H5	74:Bd:104:ARG:HG3	1.77	0.50
45:BA:1607:A:N6	45:BA:1632:G:H1'	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1657:G:H2'	45:BA:1658:G:H8	1.76	0.50
49:BE:74:GLN:HA	49:BE:79:PHE:HB2	1.93	0.50
49:BE:75:LYS:HD2	53:BI:22:VAL:HB	1.93	0.50
71:Ba:57:THR:HG23	71:Ba:60:MET:HE3	1.93	0.50
1:AA:4237:C:H2'	1:AA:4238:G:H8	1.75	0.50
45:BA:1415:C:C2'	58:BN:129:ARG:HB2	2.40	0.50
67:BW:207:ALA:O	67:BW:211:LYS:HG2	2.12	0.50
72:Bb:103:VAL:HG23	72:Bb:126:LEU:HD23	1.94	0.50
1:AA:121:A:H62	1:AA:152:U:H3	1.59	0.50
1:AA:2477:A:H2	1:AA:2478:C:H41	1.59	0.50
1:AA:2631:U:H5''	1:AA:2632:PSU:H5''	1.94	0.50
1:AA:5009:G:H2'	1:AA:5010:PSU:H6	1.76	0.50
12:AL:115:MET:O	12:AL:115:MET:HG2	2.11	0.50
13:AM:19:LYS:HG2	13:AM:133:VAL:HB	1.93	0.50
22:AV:68:THR:HG22	22:AV:69:GLN:H	1.76	0.50
45:BA:329:G:H2'	45:BA:330:G:C8	2.47	0.50
45:BA:475:C:H1'	45:BA:507:G:H1'	1.94	0.50
45:BA:562:U:H2'	45:BA:563:G:C8	2.46	0.50
45:BA:1715:A:H61	45:BA:1818:A:H61	1.57	0.50
55:BK:33:LEU:HD12	55:BK:37:TYR:CE2	2.46	0.50
57:BM:39:ARG:HG2	58:BN:45:LEU:HA	1.92	0.50
57:BM:98:VAL:HG22	57:BM:103:LEU:HD12	1.93	0.50
1:AA:426:A:H2'	1:AA:427:A:H8	1.77	0.50
1:AA:1296:G:H2'	1:AA:1297:U:C6	2.47	0.50
1:AA:4879:C:H2'	1:AA:4880:C:C6	2.47	0.50
20:AT:99:MET:HE1	20:AT:127:VAL:O	2.12	0.50
28:Ab:77:TYR:HD2	31:Ae:39:ARG:HD2	1.77	0.50
45:BA:121:OMU:HM22	46:BB:145:ARG:HH21	1.76	0.50
46:BB:201:HIS:HB3	46:BB:204:SER:HB3	1.93	0.50
47:BC:1:MET:SD	60:BP:79:VAL:HA	2.52	0.50
47:BC:30:LEU:HB2	47:BC:47:TYR:CZ	2.46	0.50
47:BC:167:GLY:O	47:BC:171:VAL:HG13	2.12	0.50
49:BE:39:VAL:HG22	49:BE:48:ILE:HG12	1.92	0.50
54:BJ:125:ILE:HG23	54:BJ:146:THR:HB	1.93	0.50
59:BO:48:LEU:HD13	59:BO:93:SER:HB2	1.94	0.50
1:AA:153:G:H2'	1:AA:154:G:H8	1.77	0.50
1:AA:318:A:H2'	1:AA:319:A:H8	1.76	0.50
1:AA:1732:C:H2'	1:AA:1733:G:C8	2.47	0.50
1:AA:1758:G:H2'	1:AA:1759:G:C8	2.47	0.50
1:AA:1857:C:H2'	1:AA:1858:A:C8	2.45	0.50
1:AA:3861:A:H2'	1:AA:3862:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:3932:U:H2'	1:AA:3933:G:H8	1.77	0.50
10:AJ:182:CYS:HB3	10:AJ:222:ILE:HD12	1.93	0.50
20:AT:137:ILE:HA	20:AT:140:GLU:HG2	1.93	0.50
45:BA:562:U:H1'	68:BX:132:GLN:HG2	1.92	0.50
45:BA:1144:A:H2'	45:BA:1145:A:C8	2.47	0.50
45:BA:1415:C:H3'	58:BN:129:ARG:NH2	2.27	0.50
52:BH:158:ILE:HG12	52:BH:162:LEU:HD22	1.94	0.50
69:BY:89:VAL:HG11	69:BY:109:VAL:HG21	1.94	0.50
7:AG:235:MET:HE3	7:AG:235:MET:N	2.27	0.50
28:Ab:66:SER:HB2	28:Ab:122:TYR:HE2	1.76	0.50
36:Aj:6:ALA:O	36:Aj:10:ARG:HG2	2.12	0.50
1:AA:1486:C:H2'	1:AA:1487:G:C8	2.46	0.49
1:AA:4258:C:H2'	1:AA:4259:C:H6	1.77	0.49
1:AA:4890:G:H2'	1:AA:4891:G:C8	2.47	0.49
4:AD:101:VAL:HG22	4:AD:165:VAL:HG22	1.94	0.49
13:AM:51:SER:HB2	13:AM:69:ALA:HB3	1.94	0.49
45:BA:155:G:O6	45:BA:163:U:O2	2.30	0.49
45:BA:223:C:H2'	45:BA:224:A:C5	2.47	0.49
45:BA:1243:U:H2'	45:BA:1244:PSU:O4'	2.13	0.49
45:BA:1633:A:H2'	45:BA:1634:A:C8	2.47	0.49
50:BF:87:LEU:O	50:BF:91:ARG:HG2	2.12	0.49
65:BU:155:ARG:HH12	65:BU:198:VAL:HG23	1.76	0.49
68:BX:77:LEU:O	68:BX:80:ARG:HG2	2.12	0.49
1:AA:1308:C:H2'	1:AA:1309:C:C6	2.47	0.49
1:AA:1683:PSU:H2'	1:AA:1684:A:C8	2.47	0.49
1:AA:3772:U:H2'	1:AA:3773:U:H2'	1.93	0.49
1:AA:4619:U:H2'	1:AA:4620:OMU:H6	1.92	0.49
6:AF:155:GLU:HG3	6:AF:157:LYS:H	1.75	0.49
21:AU:4:SER:HB3	21:AU:111:ARG:HH22	1.76	0.49
45:BA:166:A2M:HM'2	45:BA:167:G:H5'	1.95	0.49
45:BA:1103:C:H2'	45:BA:1104:G:C8	2.48	0.49
45:BA:1643:PSU:H4'	56:BL:143:LYS:H	1.77	0.49
52:BH:190:LEU:HD22	52:BH:194:GLU:HG2	1.94	0.49
53:BI:18:GLU:HG3	53:BI:20:VAL:HG22	1.94	0.49
67:BW:138:ALA:O	67:BW:142:ARG:HG2	2.13	0.49
69:BY:15:ASN:O	69:BY:19:GLN:HG2	2.12	0.49
1:AA:518:G:H1	1:AA:643:C:H2'	1.77	0.49
1:AA:742:G:H2'	1:AA:743:G:H8	1.77	0.49
1:AA:4227:OMU:HM21	1:AA:4336:A:H1'	1.93	0.49
45:BA:77:A:H4'	67:BW:173:ALA:HB3	1.93	0.49
45:BA:1127:C:H5''	75:Be:17:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1687:C:H2'	45:BA:1688:C:C6	2.47	0.49
49:BE:47:GLU:HA	49:BE:85:GLU:HG2	1.94	0.49
53:BI:15:LEU:HD21	53:BI:71:LEU:HD13	1.93	0.49
65:BU:249:CYS:HB3	65:BU:256:ILE:HD11	1.94	0.49
66:BV:208:PRO:O	66:BV:212:LYS:HG2	2.12	0.49
1:AA:743:G:H2'	1:AA:744:G:H8	1.78	0.49
6:AF:318:PRO:HG2	9:AI:155:TYR:HB3	1.94	0.49
46:BB:188:ASN:HA	46:BB:191:ARG:HH22	1.77	0.49
52:BH:65:PHE:HZ	52:BH:175:ILE:HD13	1.78	0.49
59:BO:31:SER:O	59:BO:35:VAL:HG23	2.12	0.49
65:BU:175:LYS:HA	65:BU:187:ASN:HA	1.94	0.49
1:AA:2029:A:H2'	1:AA:2030:A:C8	2.48	0.49
1:AA:3937:C:H1'	16:AP:125:SER:HB2	1.93	0.49
3:AC:19:C:H2'	3:AC:20:A:C8	2.47	0.49
4:AD:117:GLU:HG2	4:AD:124:GLY:H	1.77	0.49
5:AE:168:MET:HA	5:AE:171:LEU:HD12	1.94	0.49
26:AZ:73:HIS:ND1	26:AZ:115:LYS:HD3	2.27	0.49
45:BA:358:C:H5''	61:BQ:18:ARG:HD3	1.93	0.49
45:BA:693:A:H1'	45:BA:739:C:H4'	1.95	0.49
45:BA:796:G:H2'	45:BA:797:C:O4'	2.12	0.49
45:BA:1749:G:N1	45:BA:1786:U:C2	2.81	0.49
52:BH:101:ILE:HG12	52:BH:198:TYR:HE1	1.77	0.49
69:BY:42:LEU:HD13	69:BY:68:LEU:HB3	1.94	0.49
1:AA:5:A:H4'	10:AJ:192:ARG:NH2	2.28	0.49
1:AA:1326:A2M:H5''	1:AA:1326:A2M:H8	1.94	0.49
7:AG:65:ALA:HB2	7:AG:74:ILE:HD13	1.95	0.49
45:BA:857:U:H2'	45:BA:858:A:C8	2.47	0.49
45:BA:1002:U:H2'	45:BA:1003:PSU:H6	1.78	0.49
45:BA:1163:C:H2'	45:BA:1164:G:H8	1.77	0.49
46:BB:205:PHE:HD2	46:BB:221:ARG:HD3	1.76	0.49
51:BG:118:ARG:HA	51:BG:121:THR:HG23	1.95	0.49
52:BH:178:ARG:HB2	52:BH:181:GLN:HB2	1.93	0.49
54:BJ:77:VAL:HG23	54:BJ:122:ILE:HD12	1.95	0.49
69:BY:20:GLU:HG2	69:BY:119:GLN:HB3	1.94	0.49
1:AA:137:G:H2'	1:AA:138:G:H8	1.77	0.49
16:AP:113:LEU:HB2	16:AP:134:LEU:HD12	1.94	0.49
45:BA:996:A:H2'	45:BA:997:A:C8	2.48	0.49
50:BF:108:PRO:O	50:BF:112:LEU:HG	2.13	0.49
1:AA:1333:A:H2'	1:AA:1334:A:C8	2.48	0.49
1:AA:3868:G:H22	1:AA:3900:G:H1'	1.78	0.49
1:AA:4567:G:H2'	1:AA:4568:A:H5'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:4929:C:H5''	15:AO:114:LYS:NZ	2.28	0.49
59:BO:83:ARG:HB3	59:BO:85:HIS:CE1	2.47	0.49
72:Bb:41:MET:HE1	72:Bb:129:PHE:CG	2.48	0.49
75:Be:19:HIS:HD2	75:Be:22:LYS:HG3	1.77	0.49
75:Be:19:HIS:NE2	75:Be:21:LYS:HB2	2.27	0.49
13:AM:103:GLY:HA3	13:AM:157:ILE:HD12	1.95	0.49
41:Ao:94:MET:HG2	41:Ao:105:PRO:HA	1.94	0.49
45:BA:70:G:H21	45:BA:71:G:H22	1.60	0.49
45:BA:431:G:H2'	45:BA:432:G:H8	1.78	0.49
45:BA:1743:G:H1'	45:BA:1791:A:H61	1.77	0.49
48:BD:202:GLN:HA	48:BD:206:PRO:HA	1.95	0.49
49:BE:21:LEU:HD22	49:BE:37:VAL:HG11	1.94	0.49
52:BH:101:ILE:HG12	52:BH:198:TYR:CE1	2.48	0.49
1:AA:2377:C:O2	1:AA:2381:A:N6	2.46	0.49
1:AA:3700:C:H2'	1:AA:3746:A:H61	1.78	0.49
1:AA:4415:A:H62	1:AA:4427:G:H21	1.61	0.49
11:AK:92:MET:O	11:AK:143:GLU:HA	2.13	0.49
45:BA:15:U:H2'	45:BA:16:G:O4'	2.13	0.49
45:BA:1416:C:H2'	45:BA:1417:C:C6	2.48	0.49
56:BL:47:LEU:HD12	56:BL:81:ILE:HG12	1.95	0.49
63:BS:20:ARG:HA	63:BS:28:THR:HA	1.95	0.49
1:AA:318:A:H2'	1:AA:319:A:C8	2.47	0.48
1:AA:488:G:N2	1:AA:668:C:H42	2.10	0.48
1:AA:2493:G:N2	3:AC:126:C:H3'	2.28	0.48
1:AA:4096:C:H41	1:AA:4113:U:H4'	1.78	0.48
12:AL:49:CYS:HA	12:AL:138:ILE:O	2.12	0.48
13:AM:17:ILE:HG23	13:AM:132:VAL:HG23	1.95	0.48
27:Aa:55:VAL:HG12	27:Aa:106:ILE:HA	1.94	0.48
45:BA:432:G:H2'	45:BA:433:A:H8	1.76	0.48
50:BF:134:VAL:HG12	50:BF:135:ARG:H	1.78	0.48
66:BV:110:MET:HB2	66:BV:125:LYS:HD3	1.94	0.48
74:Bd:87:ALA:O	74:Bd:90:GLU:HG3	2.13	0.48
1:AA:742:G:H2'	1:AA:743:G:C8	2.48	0.48
1:AA:2255:C:H5''	9:AI:25:PHE:HE1	1.79	0.48
2:AB:110:G:H2'	2:AB:111:C:C6	2.47	0.48
11:AK:117:PHE:HE1	11:AK:178:GLY:HA2	1.79	0.48
45:BA:222:U:H2'	45:BA:223:C:C6	2.47	0.48
45:BA:494:C:N4	45:BA:509:OMG:HN22	2.11	0.48
45:BA:1858:G:H2'	45:BA:1859:A:H8	1.77	0.48
1:AA:2486:G:H22	1:AA:2494:U:H3	1.59	0.48
1:AA:3684:G:H2'	1:AA:3685:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Ad:55:LYS:HE2	30:Ad:56:LYS:HG2	1.95	0.48
36:Aj:9:LEU:HA	36:Aj:12:LYS:HD3	1.95	0.48
45:BA:381:C:H41	52:BH:27:TYR:HB2	1.79	0.48
45:BA:455:A:H2'	45:BA:456:C:C6	2.49	0.48
45:BA:1183:A:H2'	45:BA:1184:G:C8	2.47	0.48
45:BA:1430:C:H2'	45:BA:1431:G:C8	2.48	0.48
45:BA:1587:G:C5	58:BN:78:ILE:HD11	2.48	0.48
45:BA:1839:U:H2'	45:BA:1840:U:C6	2.48	0.48
48:BD:152:LYS:HB2	78:Bh:132:ARG:HB2	1.96	0.48
50:BF:21:GLY:H	50:BF:48:TYR:HD1	1.60	0.48
65:BU:18:VAL:HG21	65:BU:307:VAL:HG22	1.96	0.48
1:AA:990:C:H1'	1:AA:1064:G:N2	2.27	0.48
1:AA:1333:A:H2'	1:AA:1334:A:H8	1.78	0.48
1:AA:1893:C:H1'	1:AA:1937:C:O2	2.13	0.48
1:AA:2028:C:H2'	1:AA:2029:A:C8	2.49	0.48
1:AA:2610:G:H2'	1:AA:2611:A:C8	2.48	0.48
1:AA:3944:G:N2	1:AA:4069:U:O2	2.37	0.48
1:AA:4239:A:H2'	1:AA:4240:G:C8	2.49	0.48
11:AK:2:LYS:HE3	11:AK:61:TRP:HB3	1.95	0.48
11:AK:41:ILE:HG13	11:AK:43:VAL:HG13	1.95	0.48
45:BA:60:A:H2'	45:BA:61:A:C5	2.49	0.48
45:BA:462:OMC:HM22	45:BA:463:C:H5'	1.94	0.48
73:Bc:56:PHE:HB2	73:Bc:74:MET:HE3	1.95	0.48
1:AA:257:C:H2'	1:AA:258:G:H8	1.79	0.48
1:AA:478:G:H2'	1:AA:479:G:H8	1.79	0.48
1:AA:1316:OMG:HM22	1:AA:1317:U:H5'	1.94	0.48
1:AA:2804:OMC:HM22	1:AA:2805:C:H5'	1.95	0.48
2:AB:24:C:H3'	2:AB:25:G:H8	1.79	0.48
5:AE:224:LYS:HD2	5:AE:340:THR:HG22	1.95	0.48
11:AK:103:VAL:HG11	11:AK:144:LEU:HD11	1.96	0.48
17:AQ:125:LYS:HG3	17:AQ:129:LEU:HD22	1.95	0.48
18:AR:94:MET:HE3	18:AR:94:MET:HB2	1.67	0.48
31:Ae:19:GLN:NE2	31:Ae:20:LEU:HB3	2.29	0.48
36:Aj:28:LEU:O	36:Aj:32:ARG:HG2	2.14	0.48
45:BA:1240:A:C6	55:BK:100:LYS:HB2	2.48	0.48
46:BB:11:ARG:HA	46:BB:28:ALA:HB2	1.95	0.48
46:BB:102:ILE:HD11	46:BB:239:PRO:HG2	1.96	0.48
55:BK:92:SER:H	55:BK:107:ILE:HB	1.77	0.48
62:BR:23:CYS:SG	62:BR:74:CYS:HB3	2.54	0.48
67:BW:64:LYS:HA	67:BW:64:LYS:HD3	1.53	0.48
68:BX:81:LEU:HA	68:BX:84:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Bb:36:ARG:O	72:Bb:40:VAL:HG23	2.14	0.48
1:AA:425:U:H2'	1:AA:426:A:C8	2.49	0.48
1:AA:1803:G:C6	22:AV:109:VAL:HG23	2.49	0.48
1:AA:4734:A:H1'	1:AA:4735:G:C8	2.49	0.48
1:AA:4767:C:H2'	1:AA:4768:G:H8	1.77	0.48
3:AC:94:G:C5	38:Al:84:PRO:HG3	2.48	0.48
7:AG:191:ASN:HB3	7:AG:194:VAL:HB	1.96	0.48
45:BA:1416:C:C4	45:BA:1417:C:N4	2.81	0.48
46:BB:64:ILE:HG23	73:Bc:17:LEU:HD22	1.95	0.48
48:BD:86:LEU:HD12	48:BD:98:THR:HG22	1.95	0.48
49:BE:113:LEU:HD21	49:BE:117:ARG:HH21	1.78	0.48
51:BG:5:SER:N	51:BG:10:LYS:HZ3	2.10	0.48
55:BK:77:LYS:HA	55:BK:95:GLY:O	2.13	0.48
61:BQ:25:LYS:O	61:BQ:29:LYS:HB2	2.13	0.48
71:Ba:34:PHE:HB3	71:Ba:41:PHE:HB2	1.96	0.48
1:AA:1503:A:H4'	1:AA:1504:G:H5'	1.94	0.48
1:AA:2351:OMC:HM22	1:AA:2352:U:H5'	1.95	0.48
1:AA:4627:U:H4'	5:AE:373:LYS:HD2	1.95	0.48
32:Af:44:ARG:O	32:Af:48:GLU:HG2	2.14	0.48
68:BX:124:HIS:O	68:BX:128:VAL:HG23	2.12	0.48
70:BZ:5:HIS:CG	70:BZ:117:LEU:HD12	2.49	0.48
1:AA:2493:G:H21	3:AC:126:C:H3'	1.78	0.48
1:AA:4642:U:H2'	1:AA:4643:G:C8	2.49	0.48
12:AL:79:SER:HB2	12:AL:147:HIS:HB3	1.96	0.48
39:Am:23:VAL:HA	39:Am:35:LYS:O	2.13	0.48
45:BA:1315:U:H4'	53:BI:2:LEU:HD13	1.96	0.48
45:BA:1322:G:H3'	45:BA:1323:U:H6	1.79	0.48
45:BA:1692:PSU:H2'	45:BA:1693:G:C8	2.49	0.48
54:BJ:85:THR:HG22	54:BJ:112:HIS:HA	1.95	0.48
58:BN:33:TRP:HZ3	58:BN:99:VAL:HG12	1.78	0.48
67:BW:222:GLU:HA	67:BW:225:GLN:HG2	1.96	0.48
1:AA:929:A:H2'	1:AA:930:G:C8	2.49	0.48
5:AE:358:ARG:HG3	5:AE:358:ARG:HH11	1.79	0.48
11:AK:96:TYR:HB3	11:AK:101:ILE:HD12	1.94	0.48
12:AL:4:ARG:HH12	12:AL:99:ILE:HD12	1.78	0.48
45:BA:176:U:H2'	45:BA:177:G:C8	2.49	0.48
45:BA:472:C:N3	45:BA:477:G:N1	2.62	0.48
51:BG:66:VAL:HA	51:BG:69:LEU:HD23	1.96	0.48
73:Bc:6:THR:OG1	73:Bc:28:LEU:HB2	2.14	0.48
1:AA:1241:C:H6	30:Ad:120:ARG:H	1.62	0.48
1:AA:2743:A:H2'	1:AA:2744:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:4757:C:N4	1:AA:4877:G:H1	2.06	0.48
3:AC:137:A:H2'	3:AC:138:C:C6	2.49	0.48
8:AH:190:HIS:HB3	8:AH:193:PHE:HD1	1.79	0.48
11:AK:132:VAL:HG13	11:AK:154:VAL:HG12	1.96	0.48
20:AT:95:TRP:CZ2	20:AT:99:MET:HE3	2.49	0.48
26:AZ:87:MET:HE1	26:AZ:156:ILE:HB	1.96	0.48
45:BA:504:G:H2'	45:BA:505:G:H8	1.79	0.48
45:BA:647:U:H2'	45:BA:648:A:H8	1.79	0.48
45:BA:867:OMG:HM23	45:BA:867:OMG:H1'	1.65	0.48
45:BA:1098:C:H2'	45:BA:1099:G:C8	2.49	0.48
47:BC:42:LYS:NZ	47:BC:44:ASP:HB3	2.29	0.48
51:BG:30:LEU:HD11	51:BG:40:LEU:HB2	1.96	0.48
57:BM:52:LEU:HD11	58:BN:48:TYR:HD1	1.79	0.48
71:Ba:71:PRO:O	71:Ba:75:MET:HE2	2.14	0.48
78:Bh:58:MET:HE2	78:Bh:58:MET:HA	1.96	0.48
1:AA:1295:C:H4'	1:AA:1296:G:C8	2.49	0.47
1:AA:1397:A:C8	29:Ac:114:LYS:HD2	2.49	0.47
1:AA:1669:A:H4'	1:AA:1685:G:N2	2.28	0.47
1:AA:2323:C:H2'	1:AA:2324:C:H6	1.78	0.47
4:AD:20:VAL:HA	4:AD:23:ARG:HG3	1.96	0.47
5:AE:165:HIS:HA	5:AE:179:HIS:O	2.13	0.47
12:AL:12:CYS:SG	12:AL:128:ARG:HG2	2.53	0.47
45:BA:526:A:H2'	45:BA:527:C:H6	1.79	0.47
45:BA:1844:U:H2'	45:BA:1845:A:H8	1.79	0.47
57:BM:108:ARG:HA	57:BM:111:LEU:HG	1.95	0.47
58:BN:59:SER:HA	58:BN:62:ARG:HG2	1.95	0.47
66:BV:148:ALA:O	66:BV:151:ILE:HG13	2.13	0.47
1:AA:1563:A:H2'	1:AA:1564:A:C8	2.50	0.47
1:AA:1858:A:H2'	1:AA:1859:C:H6	1.78	0.47
1:AA:1986:U:H4'	1:AA:2003:G:H2'	1.96	0.47
1:AA:2079:G:H2'	1:AA:2080:U:C6	2.49	0.47
1:AA:3893:C:H2'	1:AA:3894:A:C8	2.50	0.47
1:AA:4274:A:H2'	1:AA:4275:G:H8	1.80	0.47
1:AA:4889:G:H2'	1:AA:4890:G:H8	1.79	0.47
28:Ab:52:LYS:HE2	28:Ab:52:LYS:HB3	1.71	0.47
45:BA:28:U:H2'	45:BA:29:G:C8	2.47	0.47
45:BA:868:G:C5	51:BG:115:LYS:HB2	2.49	0.47
53:BI:66:HIS:HB3	53:BI:68:TYR:CE1	2.47	0.47
54:BJ:22:ARG:HH11	54:BJ:31:GLU:HG2	1.79	0.47
1:AA:1084:C:H2'	1:AA:1085:C:C6	2.49	0.47
1:AA:4163:U:H5'	1:AA:4164:C:H5''	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:4192:A:H2'	1:AA:4193:C:H6	1.79	0.47
8:AH:114:ARG:HG3	44:As:86:ALA:HB3	1.95	0.47
17:AQ:159:LYS:O	17:AQ:162:GLU:HG3	2.13	0.47
45:BA:639:C:H2'	45:BA:640:A:C8	2.50	0.47
45:BA:1450:G:H2'	45:BA:1451:G:C8	2.49	0.47
45:BA:1677:U:H5	50:BF:57:ALA:HB1	1.79	0.47
46:BB:154:ILE:HG23	46:BB:158:ASP:HB2	1.97	0.47
47:BC:12:GLU:O	47:BC:16:LEU:HD23	2.14	0.47
78:Bh:31:ASN:HD22	78:Bh:54:VAL:HG23	1.79	0.47
1:AA:965:G:H21	1:AA:2092:G:H1'	1.78	0.47
1:AA:1907:A:H5''	9:AI:220:MET:HB2	1.96	0.47
1:AA:2028:C:H2'	1:AA:2029:A:H8	1.79	0.47
1:AA:2749:C:H2'	1:AA:2750:G:H8	1.79	0.47
1:AA:4392:OMG:HM21	1:AA:4394:A:H2'	1.97	0.47
3:AC:67:U:H2'	3:AC:68:G:C8	2.46	0.47
45:BA:1205:C:H2'	45:BA:1206:G:C8	2.48	0.47
45:BA:1470:C:H2'	45:BA:1471:C:C6	2.49	0.47
45:BA:1541:G:H5''	58:BN:59:SER:HB3	1.97	0.47
45:BA:1605:G:H1'	45:BA:1634:A:N6	2.29	0.47
49:BE:102:ALA:HB2	49:BE:186:VAL:HG11	1.97	0.47
50:BF:175:ASP:HA	50:BF:178:ILE:HG22	1.96	0.47
67:BW:34:THR:O	67:BW:51:ARG:HA	2.14	0.47
1:AA:299:C:H2'	1:AA:300:A:C8	2.49	0.47
1:AA:2550:G:H2'	1:AA:2551:A:H8	1.78	0.47
1:AA:4918:C:H2'	1:AA:4919:G:C8	2.49	0.47
23:AW:72:VAL:HG11	23:AW:83:LEU:HD21	1.96	0.47
24:AX:96:LEU:HD12	25:AY:20:ARG:HD2	1.95	0.47
28:Ab:77:TYR:CD2	31:Ae:39:ARG:HD2	2.50	0.47
35:Ai:98:GLU:O	35:Ai:102:ILE:HG23	2.15	0.47
43:Ar:51:ALA:HB3	43:Ar:54:ILE:HD12	1.96	0.47
45:BA:1099:G:O6	45:BA:1133:A:N1	2.47	0.47
45:BA:1142:G:H21	45:BA:1145:A:H62	1.62	0.47
54:BJ:30:LYS:HZ3	54:BJ:32:LYS:HD3	1.78	0.47
1:AA:137:G:H2'	1:AA:138:G:C8	2.48	0.47
1:AA:1306:C:H2'	1:AA:1307:A:C8	2.49	0.47
1:AA:4415:A:N6	1:AA:4427:G:H21	2.13	0.47
7:AG:152:ARG:HG3	7:AG:154:THR:HG23	1.95	0.47
19:AS:22:ASP:O	19:AS:26:ARG:HG2	2.15	0.47
44:As:97:ILE:HG21	44:As:107:ARG:HB2	1.97	0.47
45:BA:76:U:O2'	45:BA:77:A:H5''	2.15	0.47
45:BA:806:U:H2'	45:BA:807:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1630:A:H5''	57:BM:37:GLY:H	1.78	0.47
46:BB:41:CYS:HA	46:BB:85:GLY:HA2	1.96	0.47
51:BG:93:VAL:HG21	51:BG:133:LEU:HD23	1.95	0.47
58:BN:12:GLN:HB3	58:BN:16:ARG:HH21	1.79	0.47
65:BU:104:HIS:CE1	65:BU:130:LYS:HD2	2.50	0.47
70:BZ:123:HIS:O	70:BZ:127:ARG:HG2	2.15	0.47
1:AA:299:C:H2'	1:AA:300:A:H8	1.80	0.47
1:AA:1438:U:H4'	9:AI:31:LYS:NZ	2.30	0.47
1:AA:1449:C:H2'	1:AA:1450:C:H6	1.78	0.47
1:AA:3717:A:H2'	1:AA:3718:A2M:C8	2.43	0.47
1:AA:3911:C:H2'	1:AA:3912:U:H6	1.80	0.47
1:AA:4940:C:H1'	8:AH:246:ARG:HH22	1.79	0.47
2:AB:2:U:H2'	2:AB:3:C:H6	1.79	0.47
3:AC:141:C:H2'	3:AC:142:U:C6	2.49	0.47
4:AD:2:GLY:HA2	4:AD:207:VAL:HG23	1.96	0.47
11:AK:137:SER:HB3	11:AK:145:ILE:HG12	1.96	0.47
18:AR:126:ARG:NH1	18:AR:126:ARG:HB2	2.30	0.47
30:Ad:114:LYS:O	30:Ad:118:LEU:HB2	2.15	0.47
32:Af:20:VAL:HG12	32:Af:91:LYS:HA	1.97	0.47
32:Af:25:TYR:O	32:Af:85:ARG:HD2	2.15	0.47
36:Aj:52:LYS:HA	36:Aj:52:LYS:HD3	1.73	0.47
45:BA:127:C:H3'	45:BA:128:U:H6	1.80	0.47
45:BA:184:G:H2'	45:BA:185:G:C8	2.49	0.47
45:BA:857:U:H2'	45:BA:858:A:H8	1.79	0.47
45:BA:1277:C:H2'	45:BA:1278:A:H8	1.78	0.47
45:BA:1462:U:H2'	45:BA:1464:C:N4	2.30	0.47
45:BA:1850:MA6:H92	45:BA:1851:MA6:N6	2.29	0.47
46:BB:137:PRO:HG2	46:BB:150:PRO:HD2	1.96	0.47
47:BC:176:TRP:CD1	47:BC:199:PRO:HA	2.50	0.47
49:BE:208:VAL:HG13	78:Bh:41:ILE:HA	1.97	0.47
54:BJ:33:LEU:HD22	54:BJ:34:PRO:HD2	1.96	0.47
58:BN:30:VAL:HA	58:BN:53:PHE:HE1	1.79	0.47
58:BN:114:GLU:HG2	58:BN:115:LYS:N	2.30	0.47
61:BQ:18:ARG:HA	61:BQ:21:LYS:HD3	1.96	0.47
66:BV:196:ILE:HB	66:BV:223:TYR:HB3	1.96	0.47
74:Bd:50:PHE:HE1	74:Bd:79:ILE:HG21	1.78	0.47
1:AA:928:C:H2'	1:AA:929:A:H8	1.79	0.47
1:AA:1179:U:H5''	7:AG:289:ARG:HD2	1.96	0.47
1:AA:1438:U:H5''	1:AA:1439:C:H5''	1.95	0.47
1:AA:1505:C:H2'	1:AA:1506:G:H8	1.79	0.47
1:AA:2521:G:H2'	1:AA:2522:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2608:G:H2'	1:AA:2609:G:H8	1.80	0.47
1:AA:4274:A:H2'	1:AA:4275:G:C8	2.50	0.47
1:AA:4389:C:H2'	1:AA:4390:A:C8	2.49	0.47
1:AA:4474:A:H5'	41:Ao:125:LYS:HB2	1.97	0.47
1:AA:4578:G:H2'	1:AA:4579:PSU:H6	1.79	0.47
1:AA:4861:G:H2'	1:AA:4862:G:C8	2.50	0.47
45:BA:527:C:H2'	45:BA:528:A:C8	2.50	0.47
45:BA:906:U:H2'	45:BA:907:G:C8	2.50	0.47
45:BA:1706:G:H2'	45:BA:1707:U:C6	2.50	0.47
48:BD:144:LYS:HD2	48:BD:146:ARG:HH11	1.80	0.47
51:BG:103:LYS:HD2	51:BG:104:PRO:HD2	1.97	0.47
55:BK:118:GLU:HA	57:BM:120:HIS:HB2	1.97	0.47
67:BW:159:ARG:HG3	67:BW:173:ALA:HB2	1.97	0.47
68:BX:116:LYS:HE2	68:BX:116:LYS:HA	1.95	0.47
1:AA:651:C:H2'	1:AA:652:G:C8	2.50	0.47
1:AA:4434:C:H2'	1:AA:4435:U:C6	2.50	0.47
1:AA:4591:U:H2'	1:AA:4592:C:C6	2.50	0.47
13:AM:42:GLN:NE2	13:AM:117:ILE:HD13	2.30	0.47
22:AV:27:LEU:HB3	22:AV:31:MET:HE3	1.96	0.47
22:AV:106:LEU:O	22:AV:109:VAL:HG12	2.14	0.47
33:Ag:82:VAL:HG13	33:Ag:114:ARG:HG2	1.97	0.47
37:Ak:73:ILE:O	37:Ak:77:VAL:HG22	2.14	0.47
45:BA:527:C:H2'	45:BA:528:A:H8	1.79	0.47
45:BA:1104:G:H2'	45:BA:1105:G:C8	2.50	0.47
45:BA:1408:U:H5''	56:BL:69:ARG:HH21	1.80	0.47
46:BB:126:VAL:HA	46:BB:141:THR:HG22	1.97	0.47
48:BD:71:LEU:HD13	48:BD:74:LEU:HB2	1.97	0.47
66:BV:152:ARG:O	66:BV:156:ILE:HG12	2.15	0.47
1:AA:1494:U:H2'	1:AA:1495:G:H8	1.80	0.47
1:AA:3633:C:H2'	1:AA:3634:G:C8	2.50	0.47
1:AA:4486:C:H2'	1:AA:4487:A:O4'	2.15	0.47
27:Aa:58:VAL:HG23	27:Aa:59:ARG:HG2	1.96	0.47
45:BA:461:U:H2'	45:BA:462:OMC:H6	1.79	0.47
69:BY:49:LEU:HD11	69:BY:77:ILE:HG12	1.96	0.47
1:AA:123:C:H2'	1:AA:124:C:H6	1.81	0.46
1:AA:926:G:H2'	1:AA:927:G:H8	1.79	0.46
1:AA:4507:A:H2'	1:AA:4508:C:C6	2.50	0.46
10:AJ:114:LEU:HA	10:AJ:117:ARG:HE	1.80	0.46
12:AL:38:ARG:HD2	12:AL:38:ARG:HA	1.78	0.46
16:AP:60:VAL:HG23	16:AP:134:LEU:HB2	1.97	0.46
45:BA:951:C:H2'	45:BA:952:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1438:A:H2'	45:BA:1439:A:C8	2.50	0.46
78:Bh:107:LYS:HD2	78:Bh:112:GLY:HA3	1.96	0.46
1:AA:138:G:H2'	1:AA:139:G:H8	1.80	0.46
1:AA:1824:G:H2'	1:AA:1825:A:H8	1.80	0.46
1:AA:2764:A:H2'	1:AA:2765:A:H8	1.81	0.46
1:AA:4897:G:H2'	1:AA:4898:G:C8	2.51	0.46
1:AA:4913:G:H4'	1:AA:4914:C:O5'	2.15	0.46
1:AA:5037:U:H2'	1:AA:5038:A:C8	2.50	0.46
7:AG:179:ARG:HD3	7:AG:179:ARG:HA	1.62	0.46
11:AK:89:ARG:HA	11:AK:146:LEU:O	2.15	0.46
19:AS:154:LYS:HE3	19:AS:161:SER:HB3	1.97	0.46
23:AW:42:PHE:CE2	23:AW:46:ARG:HG3	2.50	0.46
28:Ab:57:MET:SD	28:Ab:61:LYS:HD3	2.54	0.46
45:BA:1016:U:H5''	70:BZ:14:SER:HB2	1.97	0.46
45:BA:1589:A:H2'	45:BA:1590:C:O4'	2.15	0.46
60:BP:24:ILE:HG12	60:BP:56:CYS:HB3	1.98	0.46
62:BR:59:PHE:HB2	62:BR:62:TYR:HB2	1.97	0.46
67:BW:225:GLN:HA	67:BW:228:ILE:HG12	1.98	0.46
69:BY:69:CYS:HB2	69:BY:76:LEU:HD12	1.98	0.46
70:BZ:35:GLU:HA	70:BZ:38:TYR:HD2	1.80	0.46
73:Bc:16:ARG:H	73:Bc:16:ARG:HD2	1.80	0.46
1:AA:733:A:N6	1:AA:930:G:H22	2.12	0.46
1:AA:1080:C:H2'	1:AA:1081:C:C6	2.50	0.46
1:AA:1097:C:H2'	1:AA:1098:G:C8	2.50	0.46
1:AA:1272:C:H5''	9:AI:34:ARG:HG2	1.96	0.46
1:AA:1538:U:H2'	1:AA:1539:G:H8	1.81	0.46
1:AA:1846:G:H2'	1:AA:1847:C:C6	2.51	0.46
1:AA:1954:U:H2'	1:AA:1955:G:H8	1.80	0.46
1:AA:3893:C:H2'	1:AA:3894:A:H8	1.80	0.46
1:AA:4482:U:H2'	1:AA:4483:C:C6	2.50	0.46
1:AA:5026:U:N3	52:BH:124:LYS:HE3	2.31	0.46
31:Ae:30:GLY:O	31:Ae:34:THR:HG22	2.16	0.46
45:BA:350:C:H2'	45:BA:351:G:H8	1.80	0.46
45:BA:1060:A:H4'	45:BA:1061:U:H5'	1.97	0.46
45:BA:1539:U:H2'	45:BA:1540:G:C8	2.50	0.46
45:BA:1737:G:H1	45:BA:1797:U:H3	1.63	0.46
46:BB:139:LEU:HD13	46:BB:150:PRO:HB3	1.97	0.46
52:BH:121:LEU:HB3	52:BH:166:PHE:CD2	2.50	0.46
66:BV:84:PHE:CE1	66:BV:264:SER:HA	2.50	0.46
1:AA:919:C:H2'	1:AA:920:C:C6	2.51	0.46
1:AA:3880:G:H2'	1:AA:3881:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:3952:A:H2	1:AA:4062:A:H61	1.64	0.46
1:AA:4249:G:H2'	1:AA:4250:G:H8	1.81	0.46
14:AN:87:HIS:HB3	14:AN:90:VAL:HG12	1.97	0.46
29:Ac:85:GLN:HA	29:Ac:88:VAL:HG22	1.98	0.46
45:BA:23:G:H1	45:BA:651:PSU:HN3	1.63	0.46
45:BA:54:A:H1'	45:BA:507:G:H2'	1.97	0.46
45:BA:374:G:H2'	45:BA:375:U:C6	2.51	0.46
55:BK:38:SER:HB2	55:BK:41:GLN:HE22	1.79	0.46
68:BX:97:ILE:HA	68:BX:100:LEU:HG	1.96	0.46
1:AA:138:G:H2'	1:AA:139:G:C8	2.50	0.46
1:AA:750:U:H1'	1:AA:917:A:C8	2.51	0.46
1:AA:1921:C:H1'	21:AU:160:ARG:HE	1.80	0.46
1:AA:1954:U:H2'	1:AA:1955:G:C8	2.51	0.46
1:AA:3607:U:H2'	1:AA:3608:A:C8	2.50	0.46
7:AG:63:GLN:HE21	7:AG:74:ILE:HG21	1.81	0.46
8:AH:218:LYS:HE2	8:AH:218:LYS:HB2	1.71	0.46
45:BA:603:C:H1'	45:BA:604:A:N7	2.30	0.46
45:BA:941:C:H2'	45:BA:942:G:C8	2.50	0.46
45:BA:1277:C:H2'	45:BA:1278:A:C8	2.50	0.46
50:BF:122:ARG:HA	50:BF:146:ARG:HD2	1.96	0.46
55:BK:55:SER:HA	55:BK:58:LYS:HE2	1.97	0.46
57:BM:39:ARG:HH11	58:BN:46:ALA:HB2	1.79	0.46
57:BM:88:LYS:HB2	57:BM:95:TYR:CZ	2.51	0.46
67:BW:20:ASP:HB3	67:BW:23:LYS:HG3	1.97	0.46
1:AA:426:A:H2'	1:AA:427:A:C8	2.50	0.46
1:AA:467:U:H5	1:AA:686:A:H61	1.62	0.46
1:AA:907:C:H2'	1:AA:908:G:H8	1.79	0.46
1:AA:1245:C:H2'	1:AA:1246:G:C8	2.46	0.46
1:AA:1263:A:H2'	1:AA:1264:C:C6	2.50	0.46
1:AA:1504:G:H2'	1:AA:1505:C:C6	2.50	0.46
1:AA:4237:C:H2'	1:AA:4238:G:C8	2.50	0.46
1:AA:4402:C:H42	1:AA:4441:A:H61	1.62	0.46
27:Aa:37:GLU:H	27:Aa:37:GLU:CD	2.23	0.46
32:Af:64:ILE:HG23	32:Af:68:LEU:HD23	1.97	0.46
45:BA:504:G:H2'	45:BA:505:G:C8	2.51	0.46
45:BA:1858:G:H2'	45:BA:1859:A:C8	2.51	0.46
1:AA:18:C:H2'	1:AA:19:G:C8	2.50	0.46
1:AA:1095:A:C2	1:AA:1200:G:N1	2.84	0.46
1:AA:1307:A:H2'	1:AA:1308:C:C6	2.51	0.46
1:AA:1733:G:N3	1:AA:4214:A:H2'	2.30	0.46
1:AA:2607:C:H2'	1:AA:2608:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2705:G:H22	1:AA:2710:C:H5	1.64	0.46
1:AA:4070:U:H2'	1:AA:4071:U:C6	2.51	0.46
5:AE:321:VAL:HG12	5:AE:322:HIS:HD1	1.80	0.46
6:AF:62:THR:HG22	6:AF:64:ALA:H	1.80	0.46
12:AL:15:LYS:HG3	12:AL:16:PRO:HD2	1.97	0.46
12:AL:35:ASP:HB3	12:AL:39:LYS:NZ	2.31	0.46
17:AQ:179:LYS:HD3	17:AQ:179:LYS:HA	1.72	0.46
45:BA:1034:A:N7	45:BA:1081:U:O4	2.48	0.46
45:BA:1445:PSU:H4'	59:BO:57:PRO:HG3	1.97	0.46
45:BA:1473:G:N2	45:BA:1475:G:H3'	2.29	0.46
45:BA:1568:C:H2'	45:BA:1569:A:C8	2.51	0.46
47:BC:184:ARG:NE	47:BC:191:ARG:HA	2.31	0.46
49:BE:23:GLU:HG2	64:BT:46:TYR:HE1	1.80	0.46
65:BU:133:ASN:HD22	65:BU:134:THR:H	1.64	0.46
70:BZ:88:LEU:HD13	70:BZ:125:LEU:HD23	1.98	0.46
1:AA:411:G:H4'	1:AA:412:G:H5''	1.98	0.46
1:AA:2870:A:H2'	1:AA:2871:A:C8	2.50	0.46
1:AA:3961:G:N1	1:AA:4048:A:C6	2.84	0.46
1:AA:4258:C:H2'	1:AA:4259:C:C6	2.51	0.46
1:AA:4484:A:H2'	1:AA:4485:C:C6	2.50	0.46
1:AA:5002:U:H2'	1:AA:5003:U:H6	1.80	0.46
27:Aa:89:LYS:HB3	27:Aa:89:LYS:HE3	1.65	0.46
45:BA:1134:G:H2'	45:BA:1135:C:C6	2.49	0.46
51:BG:163:GLN:O	51:BG:167:GLU:HG2	2.15	0.46
1:AA:1431:C:H2'	1:AA:1432:G:O4'	2.15	0.46
1:AA:2701:U:H3	1:AA:2715:G:H1	1.64	0.46
1:AA:2727:C:H2'	1:AA:2728:U:C6	2.50	0.46
5:AE:92:TYR:HB2	5:AE:159:VAL:HB	1.97	0.46
45:BA:144:U:H2'	45:BA:145:G:C8	2.51	0.46
45:BA:288:G:H2'	45:BA:289:G:C8	2.51	0.46
45:BA:945:U:H2'	45:BA:946:U:H6	1.81	0.46
45:BA:1558:C:H2'	45:BA:1559:C:C6	2.50	0.46
46:BB:233:LYS:HD3	46:BB:233:LYS:H	1.80	0.46
50:BF:76:MET:SD	50:BF:78:MET:HE1	2.56	0.46
59:BO:66:ARG:HB2	64:BT:40:ARG:HH12	1.80	0.46
65:BU:166:VAL:HG12	65:BU:176:VAL:HG22	1.97	0.46
67:BW:58:LYS:HA	67:BW:107:SER:HB3	1.98	0.46
67:BW:139:SER:O	67:BW:143:LYS:HG2	2.15	0.46
68:BX:110:LEU:HD13	68:BX:147:PHE:HB3	1.97	0.46
1:AA:4651:A:H2'	1:AA:4652:G:O4'	2.16	0.46
3:AC:140:C:H2'	3:AC:141:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:9:VAL:HG11	15:AO:66:HIS:HA	1.97	0.46
18:AR:125:MET:HE3	18:AR:143:PRO:HG3	1.98	0.46
45:BA:1103:C:H2'	45:BA:1104:G:H8	1.81	0.46
45:BA:1375:G:H2'	45:BA:1376:A:C8	2.51	0.46
45:BA:1415:C:O2	58:BN:129:ARG:HD3	2.16	0.46
50:BF:40:ALA:HB1	50:BF:45:TYR:CG	2.51	0.46
61:BQ:52:LEU:HD11	61:BQ:73:GLN:HB2	1.98	0.46
70:BZ:37:ILE:HG22	70:BZ:54:LEU:HD11	1.98	0.46
71:Ba:34:PHE:HD1	71:Ba:98:ARG:HD2	1.81	0.46
78:Bh:12:ALA:HA	78:Bh:15:VAL:HG12	1.98	0.46
1:AA:10:A:H2'	1:AA:11:G:H8	1.80	0.45
1:AA:325:U:H2'	1:AA:326:C:C6	2.50	0.45
1:AA:676:C:H2'	1:AA:677:G:H8	1.81	0.45
1:AA:1811:G:H2'	1:AA:1812:C:C6	2.51	0.45
1:AA:2521:G:H5'	1:AA:2640:G:H1'	1.98	0.45
1:AA:2539:C:H2'	1:AA:2540:C:C6	2.50	0.45
28:Ab:33:THR:HG23	28:Ab:40:HIS:HE1	1.81	0.45
45:BA:1730:U:H2'	45:BA:1731:A:C8	2.51	0.45
47:BC:51:LEU:HA	47:BC:54:THR:HG22	1.98	0.45
51:BG:172:THR:O	51:BG:176:VAL:HG22	2.16	0.45
55:BK:43:ARG:O	55:BK:47:ARG:HG2	2.16	0.45
65:BU:289:LEU:HD12	65:BU:300:ALA:HB2	1.98	0.45
71:Ba:56:VAL:HB	71:Ba:81:VAL:HG23	1.98	0.45
1:AA:1450:C:H2'	1:AA:1451:G:O4'	2.16	0.45
1:AA:1494:U:H2'	1:AA:1495:G:C8	2.51	0.45
13:AM:50:PHE:HB2	13:AM:67:LYS:HE2	1.97	0.45
28:Ab:81:MET:HE3	28:Ab:82:PRO:HD2	1.97	0.45
37:Ak:43:MET:HA	37:Ak:43:MET:HE2	1.98	0.45
38:Al:46:LYS:HE2	38:Al:46:LYS:HB3	1.69	0.45
45:BA:16:G:H2'	45:BA:17:C:C6	2.51	0.45
45:BA:128:U:C6	45:BA:215:G:H1'	2.51	0.45
45:BA:945:U:H2'	45:BA:946:U:C6	2.51	0.45
45:BA:1788:A:H2'	45:BA:1789:G:O4'	2.16	0.45
45:BA:1805:G:H2'	45:BA:1806:A:C8	2.52	0.45
46:BB:90:ILE:HD11	46:BB:99:PHE:HB2	1.97	0.45
54:BJ:59:LYS:HE2	54:BJ:59:LYS:HB3	1.83	0.45
58:BN:42:HIS:HB3	58:BN:83:GLN:HA	1.98	0.45
65:BU:11:LEU:HB2	65:BU:307:VAL:HB	1.98	0.45
1:AA:7:C:H2'	1:AA:8:U:C6	2.51	0.45
1:AA:161:G:H2'	1:AA:162:A:C8	2.51	0.45
1:AA:478:G:H2'	1:AA:479:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:490:C:H2'	1:AA:491:G:C8	2.52	0.45
1:AA:1193:C:H2'	1:AA:1194:G:C8	2.51	0.45
1:AA:2611:A:H2'	1:AA:2612:G:C8	2.52	0.45
1:AA:4239:A:H2'	1:AA:4240:G:H8	1.81	0.45
1:AA:4459:U:H2'	1:AA:4460:U:C6	2.52	0.45
15:AO:31:ILE:H	15:AO:31:ILE:HD12	1.81	0.45
45:BA:287:U:H2'	45:BA:288:G:C8	2.52	0.45
45:BA:287:U:H3	45:BA:296:PSU:HN3	1.64	0.45
45:BA:617:G:H4'	61:BQ:88:ASP:HA	1.97	0.45
45:BA:1623:A:H5'	45:BA:1624:U:H5''	1.96	0.45
45:BA:1749:G:C2	45:BA:1786:U:O2	2.69	0.45
46:BB:6:LYS:HB2	46:BB:30:ARG:HH12	1.80	0.45
48:BD:33:VAL:HG12	48:BD:44:ILE:HD13	1.98	0.45
50:BF:35:LEU:HD23	50:BF:143:PRO:HB3	1.98	0.45
57:BM:1:MET:HE1	74:Bd:86:ALA:HB1	1.99	0.45
66:BV:199:PRO:HG2	66:BV:202:THR:HG21	1.98	0.45
77:Bg:135:HIS:HB2	77:Bg:138:ARG:HG2	1.98	0.45
1:AA:269:G:H2'	1:AA:270:U:C6	2.52	0.45
1:AA:436:C:H2'	1:AA:437:G:H8	1.82	0.45
1:AA:1183:C:H2'	1:AA:1184:A:C8	2.52	0.45
10:AJ:165:GLU:HA	10:AJ:168:VAL:HG12	1.97	0.45
32:Af:61:ASP:OD1	32:Af:103:TYR:HB2	2.16	0.45
45:BA:526:A:H2'	45:BA:527:C:C6	2.51	0.45
45:BA:1710:C:H2'	45:BA:1711:U:C6	2.52	0.45
54:BJ:60:CYS:HB3	54:BJ:64:GLY:H	1.81	0.45
58:BN:106:ALA:O	58:BN:110:LEU:HD12	2.16	0.45
62:BR:23:CYS:HB2	62:BR:74:CYS:HB3	1.99	0.45
68:BX:24:ARG:O	68:BX:28:GLU:HG3	2.16	0.45
74:Bd:80:ARG:CZ	74:Bd:80:ARG:HB3	2.46	0.45
1:AA:679:C:H2'	1:AA:680:G:C8	2.48	0.45
1:AA:2607:C:H2'	1:AA:2608:G:C8	2.52	0.45
1:AA:4220:6MZ:H8	1:AA:4220:6MZ:O5'	2.17	0.45
1:AA:4903:G:H2'	1:AA:4904:G:C8	2.51	0.45
4:AD:208:GLU:H	4:AD:208:GLU:HG2	1.55	0.45
8:AH:68:MET:HE1	8:AH:71:ARG:HH21	1.82	0.45
36:Aj:89:ARG:O	36:Aj:93:ARG:HG2	2.17	0.45
43:Ar:6:LYS:HE3	43:Ar:6:LYS:HB3	1.73	0.45
45:BA:185:G:H2'	45:BA:186:C:O4'	2.17	0.45
45:BA:913:A:C6	51:BG:98:ARG:HD3	2.51	0.45
45:BA:929:G:N2	45:BA:1104:G:H4'	2.32	0.45
45:BA:1189:A:H2'	45:BA:1190:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1305:C:H2'	45:BA:1306:U:H5	1.82	0.45
54:BJ:138:VAL:O	54:BJ:139:ARG:HD3	2.16	0.45
60:BP:1:MET:HA	60:BP:9:VAL:HB	1.99	0.45
61:BQ:107:ARG:HB3	61:BQ:110:HIS:HB3	1.98	0.45
66:BV:109:ILE:H	66:BV:109:ILE:HG13	1.71	0.45
73:Bc:110:ARG:HH22	73:Bc:126:GLY:HA2	1.80	0.45
1:AA:35:U:H4'	1:AA:1525:A:C2	2.52	0.45
1:AA:137:G:H4'	36:Aj:98:HIS:CG	2.51	0.45
1:AA:1086:C:H2'	1:AA:1087:A:C8	2.51	0.45
1:AA:1183:C:H2'	1:AA:1184:A:H8	1.81	0.45
1:AA:2763:U:H4'	1:AA:2764:A:H5''	1.98	0.45
6:AF:114:ARG:HG3	16:AP:203:TYR:HB3	1.99	0.45
15:AO:6:PHE:H	15:AO:11:ARG:NH2	2.15	0.45
21:AU:92:ASN:HD21	22:AV:156:TYR:H	1.65	0.45
30:Ad:33:LYS:HE2	30:Ad:33:LYS:HB3	1.73	0.45
45:BA:72:C:N4	67:BW:170:ARG:HH21	2.15	0.45
45:BA:76:U:H2'	67:BW:159:ARG:HH12	1.81	0.45
45:BA:831:G:H2'	45:BA:832:G:C8	2.51	0.45
45:BA:1562:C:H2'	45:BA:1563:G:H8	1.81	0.45
52:BH:117:TYR:CD1	52:BH:152:ARG:HB3	2.52	0.45
56:BL:39:LEU:HD23	56:BL:39:LEU:H	1.80	0.45
60:BP:39:VAL:HB	60:BP:44:GLY:HA2	1.99	0.45
72:Bb:24:GLN:HA	72:Bb:63:VAL:O	2.16	0.45
1:AA:268:G:H2'	1:AA:269:G:C8	2.51	0.45
1:AA:699:C:H2'	1:AA:700:G:C8	2.52	0.45
1:AA:989:U:H2'	1:AA:992:C:C4	2.51	0.45
1:AA:1955:G:H2'	1:AA:1956:A:C8	2.51	0.45
1:AA:4139:G:H2'	1:AA:4140:C:H5	1.80	0.45
1:AA:4563:U:H2'	1:AA:4564:A:H8	1.80	0.45
1:AA:4932:U:H2'	1:AA:4933:C:C6	2.51	0.45
3:AC:9:A:H2'	3:AC:10:G:H8	1.81	0.45
3:AC:92:U:H2'	3:AC:93:C:O4'	2.16	0.45
3:AC:122:G:N7	3:AC:123:U:H1'	2.32	0.45
5:AE:45:ALA:HB3	5:AE:183:ILE:HG23	1.98	0.45
7:AG:196:ARG:C	7:AG:198:HIS:H	2.25	0.45
45:BA:68:A:H2'	45:BA:69:C:C6	2.51	0.45
45:BA:1360:PSU:H3'	45:BA:1361:G:C8	2.51	0.45
47:BC:21:ALA:HB2	78:Bh:91:LEU:HD13	1.99	0.45
51:BG:36:LEU:HD12	51:BG:40:LEU:HD11	1.98	0.45
51:BG:43:LEU:HD12	51:BG:72:PHE:CE2	2.52	0.45
67:BW:190:ARG:O	67:BW:194:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:BX:29:LEU:O	68:BX:32:ILE:HG22	2.16	0.45
68:BX:129:LEU:HD12	68:BX:130:ILE:HD12	1.99	0.45
1:AA:267:G:H5'	36:Aj:109:ARG:HH12	1.82	0.45
1:AA:1172:C:H3'	1:AA:1173:G:C8	2.51	0.45
1:AA:2633:U:H2'	1:AA:2634:C:H6	1.82	0.45
1:AA:4578:G:H2'	1:AA:4579:PSU:C6	2.52	0.45
1:AA:4685:U:H2'	1:AA:4686:G:C8	2.51	0.45
17:AQ:191:LYS:HE2	17:AQ:191:LYS:HB2	1.74	0.45
22:AV:107:LYS:HD2	22:AV:107:LYS:HA	1.72	0.45
45:BA:1787:G:H2'	45:BA:1788:A:C8	2.52	0.45
45:BA:1794:C:H2'	45:BA:1795:G:C8	2.52	0.45
57:BM:16:LEU:HD22	57:BM:99:LEU:HG	1.99	0.45
72:Bb:27:ILE:HB	72:Bb:61:ILE:HB	1.99	0.45
1:AA:139:G:H2'	1:AA:140:G:C8	2.52	0.45
1:AA:1066:G:H2'	1:AA:1067:G:H8	1.78	0.45
1:AA:1504:G:H2'	1:AA:1505:C:H6	1.82	0.45
1:AA:2254:G:H5'	1:AA:2255:C:H5'	1.99	0.45
1:AA:4188:U:H2'	1:AA:4189:U:C6	2.52	0.45
3:AC:144:U:H2'	3:AC:145:C:C6	2.52	0.45
6:AF:288:ASP:O	6:AF:292:ILE:HG13	2.17	0.45
7:AG:14:LYS:HB2	7:AG:14:LYS:HE2	1.59	0.45
9:AI:92:VAL:O	9:AI:120:GLY:HA2	2.17	0.45
45:BA:943:U:H2'	45:BA:944:A:C8	2.45	0.45
56:BL:10:VAL:HG12	56:BL:25:CYS:HB3	1.99	0.45
58:BN:98:SER:O	58:BN:101:ARG:HG3	2.17	0.45
69:BY:81:ASP:O	69:BY:85:LEU:HB2	2.17	0.45
73:Bc:40:ILE:HD13	73:Bc:60:PHE:CZ	2.52	0.45
1:AA:252:C:H2'	1:AA:253:G:C2	2.52	0.45
1:AA:1213:G:H5''	1:AA:1214:C:H5''	1.98	0.45
1:AA:1509:C:H5''	29:Ac:2:PRO:HD2	1.97	0.45
1:AA:1811:G:H2'	1:AA:1812:C:H6	1.81	0.45
1:AA:2030:A:H2'	1:AA:2031:C:O4'	2.17	0.45
1:AA:3727:A:H2'	1:AA:3728:A:C8	2.52	0.45
1:AA:4688:C:H2'	1:AA:4689:PSU:C6	2.52	0.45
4:AD:80:GLU:HB2	4:AD:170:ALA:HA	1.98	0.45
7:AG:273:LEU:HD11	7:AG:277:LYS:HE2	1.98	0.45
8:AH:112:MET:HG3	8:AH:113:PRO:HD2	1.98	0.45
12:AL:91:LEU:HD12	12:AL:127:ALA:HB1	1.98	0.45
45:BA:20:G:H5'	45:BA:620:G:C4	2.52	0.45
45:BA:77:A:H2'	45:BA:78:C:C6	2.52	0.45
45:BA:640:A:H2'	45:BA:641:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1104:G:H2'	45:BA:1105:G:H8	1.82	0.45
45:BA:1607:A:H61	45:BA:1632:G:H1'	1.82	0.45
45:BA:1648:G:H2'	56:BL:127:CYS:HA	1.98	0.45
45:BA:1716:C:H2'	45:BA:1717:C:H6	1.81	0.45
52:BH:200:ARG:HA	52:BH:203:LYS:HE3	1.99	0.45
53:BI:27:VAL:HG23	53:BI:28:HIS:CD2	2.52	0.45
66:BV:68:ARG:HD3	66:BV:71:LYS:HD3	1.99	0.45
1:AA:86:U:H2'	1:AA:87:A:H8	1.82	0.44
1:AA:127:G:H2'	1:AA:128:C:C6	2.52	0.44
1:AA:711:A:H2'	1:AA:712:C:C6	2.52	0.44
1:AA:1278:C:H2'	1:AA:1279:A:O4'	2.17	0.44
1:AA:2521:G:H2'	1:AA:2522:G:C8	2.51	0.44
1:AA:4088:C:H2'	1:AA:4089:G:H8	1.81	0.44
1:AA:5018:C:H2'	1:AA:5019:A:C8	2.52	0.44
13:AM:35:ARG:HB3	13:AM:123:ILE:HG22	1.98	0.44
17:AQ:202:LEU:HA	17:AQ:202:LEU:HD12	1.83	0.44
18:AR:131:ARG:HG3	18:AR:137:ASN:OD1	2.17	0.44
45:BA:647:U:H2'	45:BA:648:A:C8	2.52	0.44
45:BA:861:A:C8	51:BG:106:ARG:HD3	2.51	0.44
45:BA:878:G:N2	45:BA:908:A:N1	2.55	0.44
45:BA:1608:U:H5''	57:BM:134:GLN:HE21	1.81	0.44
64:BT:32:ARG:HA	64:BT:37:ASN:H	1.81	0.44
66:BV:103:LYS:HD3	66:BV:103:LYS:N	2.31	0.44
70:BZ:25:TRP:CE2	75:Be:82:LYS:HD3	2.52	0.44
72:Bb:25:VAL:O	72:Bb:62:VAL:HA	2.17	0.44
72:Bb:111:MET:HE1	72:Bb:116:ALA:N	2.32	0.44
1:AA:754:U:H2'	1:AA:755:C:C6	2.52	0.44
1:AA:1358:G:C8	1:AA:1377:G:N1	2.74	0.44
1:AA:3805:U:H2'	1:AA:3806:G:H8	1.83	0.44
1:AA:3917:A:H2'	1:AA:3918:G:C8	2.52	0.44
1:AA:4070:U:H2'	1:AA:4071:U:H6	1.82	0.44
1:AA:4861:G:H2'	1:AA:4862:G:H8	1.82	0.44
1:AA:4887:C:H2'	1:AA:4888:U:O4'	2.17	0.44
12:AL:208:LYS:HA	12:AL:208:LYS:HD2	1.88	0.44
27:Aa:38:LEU:HD11	27:Aa:108:ARG:HA	1.98	0.44
45:BA:655:A:H4'	45:BA:656:G:H3'	1.98	0.44
46:BB:36:HIS:CD2	46:BB:85:GLY:HA3	2.52	0.44
46:BB:63:LYS:HE3	73:Bc:85:ASN:HB3	1.98	0.44
48:BD:172:MET:HA	48:BD:175:GLU:OE1	2.17	0.44
49:BE:29:LEU:HD21	49:BE:52:ALA:HB2	1.99	0.44
49:BE:105:LEU:HB3	49:BE:122:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BG:58:LYS:HB2	51:BG:90:LYS:HG2	1.99	0.44
54:BJ:78:THR:HG23	54:BJ:79:LYS:HG2	2.00	0.44
56:BL:132:PHE:CD1	59:BO:77:TRP:HB2	2.52	0.44
62:BR:23:CYS:HB3	62:BR:27:ALA:N	2.32	0.44
75:Be:5:LYS:HE2	75:Be:7:LEU:HD21	1.99	0.44
1:AA:1338:G:H4'	1:AA:1339:U:H6	1.82	0.44
1:AA:1662:C:H2'	1:AA:1663:C:C6	2.52	0.44
1:AA:2078:C:H2'	1:AA:2079:G:C8	2.53	0.44
1:AA:2757:A:H2'	1:AA:2758:G:C8	2.53	0.44
1:AA:2884:G:H2'	1:AA:2885:A:H8	1.82	0.44
1:AA:3870:C:H2'	1:AA:3871:A:C8	2.51	0.44
1:AA:4551:U:H2'	1:AA:4552:PSU:C6	2.52	0.44
10:AJ:171:PRO:HB3	10:AJ:181:TYR:CE1	2.53	0.44
14:AN:158:ARG:HB3	14:AN:158:ARG:NH1	2.32	0.44
45:BA:319:C:H41	67:BW:186:GLN:HG3	1.82	0.44
45:BA:479:C:H2'	45:BA:480:G:C8	2.53	0.44
45:BA:560:A:H61	45:BA:588:G:H1	1.65	0.44
45:BA:1228:A:H2'	45:BA:1229:G:C8	2.52	0.44
45:BA:1674:G:P	56:BL:78:VAL:HG21	2.57	0.44
47:BC:85:ARG:NH1	47:BC:202:TYR:HA	2.32	0.44
50:BF:187:SER:O	50:BF:191:LYS:HG2	2.17	0.44
52:BH:10:LYS:HE3	52:BH:10:LYS:HB3	1.78	0.44
67:BW:212:LEU:HD12	67:BW:215:LYS:HZ3	1.82	0.44
70:BZ:118:ILE:O	70:BZ:122:ILE:HG23	2.17	0.44
1:AA:10:A:H2'	1:AA:11:G:C8	2.53	0.44
1:AA:4704:C:H2'	1:AA:4705:A:C8	2.52	0.44
1:AA:4934:A:H2'	1:AA:4935:C:H6	1.82	0.44
2:AB:46:C:H2'	2:AB:47:G:H8	1.82	0.44
12:AL:108:ALA:HB1	12:AL:112:GLN:H	1.82	0.44
45:BA:948:C:H2'	45:BA:949:G:C8	2.50	0.44
45:BA:1050:A:H62	45:BA:1068:G:H21	1.64	0.44
55:BK:90:VAL:HA	55:BK:107:ILE:HG21	1.98	0.44
55:BK:116:LEU:HA	55:BK:119:PHE:HD2	1.83	0.44
61:BQ:51:VAL:HG22	61:BQ:97:ASN:H	1.82	0.44
70:BZ:45:LEU:HG	70:BZ:49:GLN:HB2	1.98	0.44
1:AA:347:A:H2'	1:AA:348:G:C8	2.53	0.44
1:AA:734:G:H1	1:AA:929:A:N6	2.16	0.44
1:AA:1218:G:H2'	1:AA:1219:G:C8	2.53	0.44
1:AA:1617:G:H1'	1:AA:2513:A:N6	2.31	0.44
1:AA:2027:U:H2'	1:AA:2028:C:C6	2.52	0.44
1:AA:2870:A:H2'	1:AA:2871:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:3899:OMG:HM22	1:AA:3900:G:H5'	2.00	0.44
1:AA:4293:PSU:H4'	42:Aq:83:LEU:HD11	1.99	0.44
1:AA:4760:G:H2'	1:AA:4761:G:O4'	2.18	0.44
7:AG:208:MET:HG3	7:AG:223:PHE:CE2	2.52	0.44
7:AG:243:ALA:O	7:AG:247:ILE:HG12	2.16	0.44
9:AI:83:VAL:HG22	21:AU:62:VAL:HA	1.99	0.44
15:AO:118:MET:O	15:AO:122:ILE:HG12	2.18	0.44
19:AS:76:GLU:CD	19:AS:76:GLU:H	2.25	0.44
36:Aj:117:ARG:HA	36:Aj:117:ARG:HD2	1.80	0.44
45:BA:1097:G:H4'	47:BC:32:PHE:CG	2.52	0.44
45:BA:1230:C:H2'	45:BA:1231:C:H6	1.83	0.44
45:BA:1425:G:H22	58:BN:129:ARG:HD3	1.83	0.44
45:BA:1464:C:H5''	78:Bh:60:ARG:HH21	1.83	0.44
45:BA:1629:C:H2'	45:BA:1630:A:H8	1.82	0.44
45:BA:1808:U:H2'	45:BA:1809:A:C8	2.52	0.44
61:BQ:40:PRO:HG2	61:BQ:120:PHE:HZ	1.82	0.44
62:BR:44:ILE:HD13	62:BR:44:ILE:HA	1.90	0.44
65:BU:88:ARG:HE	65:BU:100:ARG:NH1	2.15	0.44
72:Bb:111:MET:HE2	72:Bb:111:MET:HB2	1.89	0.44
73:Bc:58:PHE:HB3	73:Bc:90:ARG:HH12	1.82	0.44
73:Bc:114:MET:HE2	73:Bc:122:LYS:HB2	2.00	0.44
1:AA:159:C:H5''	37:Ak:25:ARG:HE	1.83	0.44
1:AA:717:U:H2'	1:AA:718:C:C6	2.53	0.44
1:AA:1346:C:H2'	1:AA:1347:G:C8	2.52	0.44
1:AA:1955:G:H2'	1:AA:1956:A:H8	1.83	0.44
1:AA:2500:U:H2'	1:AA:2501:C:H5'	1.99	0.44
1:AA:3641:U:H5	1:AA:3646:A:N7	2.15	0.44
1:AA:4903:G:H2'	1:AA:4904:G:H8	1.83	0.44
1:AA:5030:U:C2	1:AA:5031:G:C8	3.06	0.44
31:Ae:34:THR:HG21	31:Ae:93:THR:HG22	1.99	0.44
45:BA:291:G:N1	46:BB:203:GLY:HA2	2.33	0.44
45:BA:1392:U:H2'	45:BA:1393:G:C8	2.52	0.44
47:BC:122:LEU:HD22	47:BC:123:VAL:N	2.33	0.44
52:BH:54:LYS:HE2	52:BH:54:LYS:HB2	1.64	0.44
52:BH:83:TYR:HB3	52:BH:101:ILE:HD13	1.98	0.44
67:BW:3:LEU:HB2	67:BW:16:ILE:HG13	2.00	0.44
68:BX:58:ARG:HA	68:BX:61:LEU:HG	2.00	0.44
78:Bh:14:ARG:HG2	78:Bh:69:ILE:HG13	1.99	0.44
1:AA:1772:C:H2'	1:AA:1773:U:C6	2.53	0.44
1:AA:1794:A:H5''	1:AA:4214:A:H61	1.83	0.44
1:AA:3610:A:H2'	1:AA:3611:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:68:ARG:HG3	7:AG:73:MET:HE2	1.99	0.44
8:AH:183:ARG:HA	8:AH:183:ARG:HD2	1.81	0.44
20:AT:159:ALA:O	20:AT:163:ARG:HD3	2.17	0.44
31:Ae:57:LYS:O	31:Ae:61:GLU:HG3	2.17	0.44
40:An:28:ARG:HA	40:An:33:ASN:HD22	1.83	0.44
45:BA:24:C:H2'	45:BA:25:A:C8	2.53	0.44
45:BA:92:A:N6	45:BA:444:G:H1'	2.33	0.44
45:BA:1405:A:H2'	45:BA:1406:G:C8	2.53	0.44
48:BD:105:LEU:HG	48:BD:213:ARG:HA	2.00	0.44
54:BJ:86:ILE:HG13	54:BJ:111:VAL:O	2.18	0.44
58:BN:122:LYS:HD2	58:BN:122:LYS:HA	1.76	0.44
66:BV:184:VAL:HG21	66:BV:247:THR:HG22	1.99	0.44
1:AA:505:G:H2'	1:AA:506:C:H6	1.82	0.44
1:AA:2780:C:H2'	1:AA:2781:G:H8	1.83	0.44
1:AA:4195:G:H1	12:AL:115:MET:HE2	1.82	0.44
1:AA:4768:G:H2'	1:AA:4769:G:C8	2.52	0.44
2:AB:20:U:H2'	2:AB:21:G:H8	1.83	0.44
6:AF:165:LYS:HA	6:AF:168:VAL:HG12	2.00	0.44
8:AH:239:LYS:HD3	8:AH:240:TYR:N	2.32	0.44
9:AI:31:LYS:HG2	9:AI:34:ARG:HH22	1.82	0.44
29:Ac:36:GLY:HA3	29:Ac:40:HIS:CE1	2.53	0.44
46:BB:67:GLN:HE22	73:Bc:18:LEU:HD23	1.83	0.44
48:BD:133:TYR:CE1	48:BD:221:PRO:HD2	2.53	0.44
54:BJ:27:GLU:HG3	54:BJ:29:GLY:H	1.81	0.44
55:BK:83:MET:HE1	55:BK:85:ILE:HG13	2.00	0.44
64:BT:47:ALA:HA	64:BT:50:ILE:HD11	2.00	0.44
64:BT:50:ILE:HD13	64:BT:52:PHE:HD2	1.81	0.44
66:BV:82:TYR:CZ	66:BV:164:PRO:HD3	2.52	0.44
66:BV:257:LYS:HB2	66:BV:257:LYS:HE2	1.75	0.44
67:BW:44:GLU:HB2	67:BW:119:LYS:NZ	2.33	0.44
68:BX:77:LEU:O	68:BX:81:LEU:HD22	2.18	0.44
1:AA:1449:C:H2'	1:AA:1450:C:C6	2.52	0.44
1:AA:3720:G:H1	1:AA:3733:A:N6	2.16	0.44
1:AA:4862:G:H2'	1:AA:4863:G:H8	1.83	0.44
42:Aq:12:CYS:HB3	42:Aq:15:CYS:HB2	2.00	0.44
45:BA:352:U:H2'	45:BA:353:C:C6	2.53	0.44
45:BA:353:C:H2'	45:BA:354:OMU:C6	2.48	0.44
45:BA:1244:PSU:H2'	45:BA:1245:G:C8	2.45	0.44
45:BA:1393:G:H2'	45:BA:1394:G:C8	2.53	0.44
45:BA:1398:G:C6	45:BA:1448:A:N1	2.86	0.44
46:BB:36:HIS:CG	46:BB:85:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BB:104:ASP:HB3	46:BB:110:ALA:HB2	2.00	0.44
47:BC:171:VAL:HA	47:BC:174:MET:SD	2.58	0.44
48:BD:65:ARG:HB2	71:Ba:48:SER:OG	2.17	0.44
51:BG:85:LYS:HE2	51:BG:85:LYS:HB2	1.76	0.44
54:BJ:48:LYS:O	54:BJ:52:GLU:HG3	2.18	0.44
56:BL:112:LEU:HD13	56:BL:119:LEU:HD12	2.00	0.44
70:BZ:85:PRO:HG2	70:BZ:88:LEU:HB2	1.99	0.44
70:BZ:113:PHE:HA	70:BZ:116:ILE:HD12	2.00	0.44
71:Ba:45:THR:HB	71:Ba:51:GLU:O	2.17	0.44
1:AA:3748:A:H5''	4:AD:243:THR:HB	2.00	0.43
1:AA:4635:A:H3'	1:AA:4636:PSU:H4'	2.00	0.43
3:AC:45:C:P	40:An:15:LYS:HD3	2.57	0.43
7:AG:211:LEU:HD12	7:AG:211:LEU:HA	1.89	0.43
45:BA:493:A:H5'	73:Bc:89:HIS:HB3	1.99	0.43
45:BA:598:G:H2'	45:BA:599:A:C8	2.53	0.43
45:BA:867:OMG:H2'	45:BA:868:G:C2	2.53	0.43
45:BA:1230:C:OP2	57:BM:139:THR:HB	2.19	0.43
47:BC:183:LEU:HD23	47:BC:195:TRP:HZ2	1.83	0.43
49:BE:69:LEU:HA	49:BE:72:VAL:HG22	1.99	0.43
51:BG:65:PRO:HB2	51:BG:68:GLN:HE22	1.82	0.43
59:BO:81:GLN:HG3	64:BT:55:LEU:HD12	2.00	0.43
66:BV:123:ARG:HG2	66:BV:143:CYS:SG	2.58	0.43
1:AA:487:G:H2'	1:AA:488:G:C8	2.52	0.43
1:AA:909:A:H2'	1:AA:910:G:C8	2.54	0.43
1:AA:1438:U:H4'	9:Al:31:LYS:HZ1	1.82	0.43
1:AA:1823:G:H2'	1:AA:1824:G:C8	2.52	0.43
1:AA:3607:U:H2'	1:AA:3608:A:H8	1.83	0.43
1:AA:3610:A:H2'	1:AA:3611:A:C8	2.53	0.43
1:AA:4862:G:H2'	1:AA:4863:G:C8	2.54	0.43
2:AB:92:C:H2'	2:AB:93:G:H8	1.83	0.43
11:AK:18:ILE:HG12	11:AK:27:VAL:HG13	2.00	0.43
26:AZ:145:ASP:HB3	26:AZ:148:ASP:HB2	2.00	0.43
45:BA:835:C:H2'	45:BA:837:A:C8	2.53	0.43
45:BA:1512:C:H2'	45:BA:1513:C:H6	1.83	0.43
45:BA:1689:C:H2'	45:BA:1690:U:H6	1.83	0.43
45:BA:1749:G:N1	45:BA:1786:U:N3	2.65	0.43
45:BA:1805:G:H2'	45:BA:1806:A:H8	1.82	0.43
45:BA:1856:C:H2'	45:BA:1857:G:H8	1.83	0.43
47:BC:110:ASN:HB3	47:BC:113:GLN:HG2	1.99	0.43
48:BD:25:PHE:HZ	71:Ba:53:ILE:HA	1.82	0.43
49:BE:55:THR:HB	49:BE:59:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BG:68:GLN:HB2	51:BG:71:SER:HB2	1.99	0.43
51:BG:86:LYS:HE2	51:BG:86:LYS:HB3	1.81	0.43
55:BK:25:LEU:HB3	55:BK:87:PRO:HB2	1.99	0.43
58:BN:140:ALA:O	58:BN:144:LYS:HG3	2.17	0.43
63:BS:63:ARG:HD3	63:BS:63:ARG:HA	1.86	0.43
72:Bb:93:LEU:HG	72:Bb:128:PHE:CD2	2.53	0.43
73:Bc:90:ARG:HE	73:Bc:94:HIS:HE1	1.66	0.43
1:AA:1477:C:H2'	1:AA:1478:C:C6	2.53	0.43
1:AA:4159:C:H2'	1:AA:4160:C:C6	2.53	0.43
9:AI:237:GLU:HG3	21:AU:38:VAL:HG22	1.99	0.43
10:AJ:132:ARG:HA	10:AJ:133:PRO:HD3	1.88	0.43
11:AK:41:ILE:HD12	11:AK:42:ASN:H	1.84	0.43
16:AP:28:TRP:O	16:AP:32:GLN:HG2	2.18	0.43
21:AU:81:TRP:HZ3	21:AU:130:GLU:HG3	1.84	0.43
45:BA:108:G:H2'	45:BA:109:PSU:O4'	2.19	0.43
45:BA:120:U:H2'	45:BA:121:OMU:H6	2.01	0.43
45:BA:1523:C:H2'	45:BA:1524:G:C8	2.53	0.43
48:BD:100:PHE:HE2	48:BD:181:LEU:HD11	1.84	0.43
49:BE:67:ARG:H	49:BE:67:ARG:HG2	1.66	0.43
50:BF:153:LEU:HD21	50:BF:189:ALA:HA	1.99	0.43
53:BI:86:PRO:HG2	53:BI:89:ILE:HG12	2.00	0.43
68:BX:53:ILE:HD12	68:BX:53:ILE:H	1.82	0.43
72:Bb:43:LYS:HD3	72:Bb:43:LYS:HA	1.75	0.43
1:AA:422:C:H2'	1:AA:423:G:H8	1.83	0.43
1:AA:1359:G:H5'	6:AF:114:ARG:HD2	2.00	0.43
1:AA:1662:C:H2'	1:AA:1663:C:H6	1.83	0.43
1:AA:2448:G:H2'	1:AA:2449:A:C8	2.53	0.43
1:AA:5004:C:H2'	1:AA:5005:G:O4'	2.18	0.43
3:AC:76:C:H2'	3:AC:77:A:C8	2.54	0.43
5:AE:302:ASN:HB2	5:AE:313:SER:HA	2.00	0.43
8:AH:281:ILE:HG23	8:AH:286:LEU:HD11	2.01	0.43
33:Ag:109:LYS:HE3	33:Ag:109:LYS:HB2	1.85	0.43
45:BA:374:G:H2'	45:BA:375:U:H6	1.83	0.43
45:BA:430:C:H2'	45:BA:431:G:C8	2.53	0.43
45:BA:1004:PSU:H2'	45:BA:1005:G:H8	1.82	0.43
45:BA:1406:G:H2'	45:BA:1407:U:H6	1.83	0.43
45:BA:1554:C:H42	64:BT:22:ARG:NH2	2.16	0.43
45:BA:1643:PSU:O2'	56:BL:142:GLN:HA	2.19	0.43
45:BA:1806:A:H2'	45:BA:1807:C:H6	1.84	0.43
46:BB:238:LEU:HB2	46:BB:242:LYS:HD2	1.99	0.43
50:BF:187:SER:HB3	50:BF:190:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BI:49:MET:HG2	53:BI:69:TRP:CD2	2.53	0.43
54:BJ:22:ARG:HD2	54:BJ:31:GLU:HG2	1.99	0.43
56:BL:51:LEU:HD21	56:BL:81:ILE:HB	1.99	0.43
57:BM:46:ARG:HD3	58:BN:35:ASP:O	2.19	0.43
72:Bb:87:GLU:HA	72:Bb:90:GLN:HG3	1.99	0.43
1:AA:223:G:H4'	1:AA:225:G:N7	2.34	0.43
1:AA:699:C:H2'	1:AA:700:G:H8	1.83	0.43
1:AA:947:C:H5''	8:AH:51:VAL:HG21	2.00	0.43
1:AA:1179:U:H3'	1:AA:1180:C:H5''	2.01	0.43
1:AA:1845:U:H2'	1:AA:1846:G:H8	1.83	0.43
1:AA:3855:C:H2'	1:AA:3856:A:H8	1.83	0.43
1:AA:4174:U:H2'	1:AA:4175:G:C8	2.53	0.43
1:AA:4422:A:H2'	1:AA:4423:PSU:O4'	2.17	0.43
4:AD:49:ILE:HD11	4:AD:75:LEU:HD11	2.00	0.43
14:AN:48:PRO:HB2	36:Aj:120:ALA:HB2	2.01	0.43
45:BA:881:G:H5'	45:BA:882:U:C6	2.54	0.43
45:BA:1213:C:H2'	45:BA:1214:A:C8	2.54	0.43
45:BA:1398:G:N1	45:BA:1448:A:C2	2.64	0.43
45:BA:1611:G:H21	57:BM:87:GLN:NE2	2.15	0.43
45:BA:1644:C:H2'	45:BA:1645:C:C6	2.53	0.43
47:BC:185:MET:HE3	60:BP:39:VAL:HG12	2.01	0.43
49:BE:157:MET:HE1	49:BE:159:HIS:CG	2.54	0.43
54:BJ:144:LYS:HB3	54:BJ:144:LYS:HE3	1.83	0.43
59:BO:66:ARG:HB2	64:BT:40:ARG:NH1	2.33	0.43
61:BQ:28:LYS:HE2	61:BQ:28:LYS:HB2	1.77	0.43
72:Bb:22:LYS:HG2	75:Be:3:LEU:HD12	2.00	0.43
78:Bh:9:VAL:HG13	78:Bh:51:ALA:HA	2.00	0.43
1:AA:1094:G:H2'	1:AA:1095:A:C8	2.54	0.43
1:AA:1505:C:H2'	1:AA:1506:G:C8	2.53	0.43
1:AA:4314:C:H2'	1:AA:4315:A:H8	1.84	0.43
1:AA:4736:C:H2'	1:AA:4737:G:H8	1.83	0.43
1:AA:4768:G:H2'	1:AA:4769:G:H8	1.83	0.43
3:AC:14:OMU:HM23	3:AC:14:OMU:H1'	1.80	0.43
13:AM:125:ILE:HD13	13:AM:125:ILE:HA	1.87	0.43
17:AQ:46:ASN:HB3	17:AQ:134:LYS:HE2	2.01	0.43
45:BA:319:C:H2'	45:BA:320:G:H8	1.84	0.43
45:BA:1278:A:H2'	45:BA:1279:C:C6	2.54	0.43
45:BA:1598:G:H2'	74:Bd:80:ARG:NH2	2.28	0.43
45:BA:1631:U:H2'	45:BA:1632:G:O4'	2.17	0.43
45:BA:1845:A:H2'	45:BA:1846:G:H8	1.82	0.43
47:BC:89:LYS:HB3	47:BC:89:LYS:HE3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:25:LEU:HG	49:BE:50:ILE:HD13	2.00	0.43
59:BO:21:ARG:HB3	59:BO:88:LEU:HD21	2.01	0.43
73:Bc:29:HIS:HD2	73:Bc:32:LYS:HB3	1.84	0.43
1:AA:64:A:H1'	1:AA:76:A:H1'	2.01	0.43
1:AA:1304:C:H2'	1:AA:1305:C:H6	1.84	0.43
1:AA:2375:A:H2'	1:AA:2376:A:H8	1.83	0.43
1:AA:3720:G:H1	1:AA:3733:A:H61	1.66	0.43
1:AA:3792:OMG:HM22	1:AA:3793:U:H5'	2.01	0.43
1:AA:4935:C:H2'	1:AA:4936:G:H8	1.84	0.43
26:AZ:39:LYS:H	26:AZ:39:LYS:HG2	1.66	0.43
45:BA:586:G:C6	68:BX:172:ARG:HD2	2.53	0.43
45:BA:929:G:H2'	45:BA:930:C:O4'	2.19	0.43
45:BA:1392:U:H3	45:BA:1478:U:H3	1.67	0.43
46:BB:118:GLU:HA	46:BB:121:TYR:HE1	1.83	0.43
49:BE:164:VAL:HA	49:BE:168:VAL:HG12	2.01	0.43
66:BV:68:ARG:HG2	66:BV:277:HIS:HA	2.00	0.43
68:BX:119:LEU:HG	68:BX:159:PHE:CE1	2.54	0.43
68:BX:131:ARG:HD2	68:BX:131:ARG:HA	1.74	0.43
70:BZ:127:ARG:O	70:BZ:131:THR:HG22	2.18	0.43
73:Bc:47:MET:HE2	73:Bc:47:MET:HB2	1.76	0.43
1:AA:943:A:H62	9:AI:151:ASN:HD21	1.67	0.43
1:AA:2845:A:H61	1:AA:3843:C:N4	2.15	0.43
1:AA:4680:G:H2'	1:AA:4681:A:C8	2.54	0.43
1:AA:4750:G:H2'	1:AA:4751:G:C8	2.51	0.43
15:AO:41:PRO:HA	15:AO:70:GLN:HE22	1.83	0.43
15:AO:72:TYR:HA	15:AO:75:GLN:HG3	2.01	0.43
16:AP:140:LYS:HA	16:AP:140:LYS:HD3	1.78	0.43
22:AV:143:THR:HG23	22:AV:145:GLY:H	1.84	0.43
45:BA:19:A:H5'	61:BQ:107:ARG:HH11	1.83	0.43
45:BA:1113:A:O2'	45:BA:1114:U:H5'	2.19	0.43
45:BA:1725:U:H2'	45:BA:1726:G:H8	1.84	0.43
45:BA:1862:G:H1'	45:BA:1863:A:H2'	1.99	0.43
49:BE:185:LYS:HD2	49:BE:185:LYS:HA	1.82	0.43
50:BF:108:PRO:O	50:BF:111:VAL:HG12	2.18	0.43
52:BH:40:PRO:O	52:BH:59:ARG:HB3	2.18	0.43
53:BI:29:MET:HA	53:BI:30:PRO:HD3	1.81	0.43
66:BV:157:LEU:HD23	66:BV:157:LEU:HA	1.81	0.43
67:BW:31:ARG:H	67:BW:31:ARG:HD2	1.83	0.43
73:Bc:101:LYS:HD2	73:Bc:101:LYS:HA	1.79	0.43
1:AA:490:C:H4'	6:AF:4:ALA:HB1	2.01	0.43
1:AA:732:A:H2'	1:AA:733:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:3932:U:H2'	1:AA:3933:G:C8	2.54	0.43
1:AA:5002:U:H2'	1:AA:5003:U:C6	2.54	0.43
6:AF:34:PRO:HA	6:AF:37:VAL:HG22	2.00	0.43
6:AF:190:ARG:HG2	6:AF:191:ALA:H	1.83	0.43
11:AK:152:GLU:CD	11:AK:152:GLU:H	2.26	0.43
14:AN:121:ARG:HD2	14:AN:121:ARG:HA	1.88	0.43
14:AN:154:VAL:HG12	14:AN:155:MET:HG3	2.00	0.43
15:AO:91:TRP:O	15:AO:95:ILE:HD12	2.19	0.43
17:AQ:181:ALA:O	17:AQ:185:VAL:HG22	2.19	0.43
24:AX:87:SER:HA	24:AX:97:TYR:HB3	2.01	0.43
27:Aa:124:LYS:O	27:Aa:128:VAL:HG23	2.19	0.43
38:Al:39:TYR:CD1	38:Al:40:PRO:HA	2.54	0.43
45:BA:49:C:N4	45:BA:472:C:H2'	2.34	0.43
45:BA:458:A:H2'	45:BA:459:C:C6	2.52	0.43
45:BA:638:C:H4'	76:Bf:55:PRO:HB2	2.01	0.43
45:BA:1447:OMG:HM22	45:BA:1448:A:O4'	2.19	0.43
48:BD:229:MET:O	48:BD:229:MET:HE3	2.19	0.43
51:BG:157:HIS:CD2	51:BG:157:HIS:N	2.86	0.43
52:BH:67:TRP:CE3	52:BH:72:CYS:HB3	2.53	0.43
65:BU:175:LYS:HB2	65:BU:177:TRP:HE1	1.83	0.43
67:BW:192:ILE:HA	67:BW:195:LYS:HD2	2.01	0.43
68:BX:139:LYS:HE3	68:BX:139:LYS:HB2	1.92	0.43
72:Bb:62:VAL:HG21	75:Be:7:LEU:HB2	1.99	0.43
1:AA:1089:G:H2'	1:AA:1090:G:C8	2.54	0.43
1:AA:1701:A:H1'	1:AA:2096:G:H1	1.83	0.43
1:AA:2079:G:H2'	1:AA:2080:U:H6	1.83	0.43
1:AA:2749:C:H2'	1:AA:2750:G:C8	2.54	0.43
1:AA:3726:A:H2'	1:AA:3727:A:C8	2.53	0.43
1:AA:4353:PSU:H5'	1:AA:4354:U:H5'	2.01	0.43
2:AB:119:U:C4	7:AG:261:VAL:HG21	2.54	0.43
6:AF:152:LEU:HD12	6:AF:152:LEU:HA	1.90	0.43
15:AO:115:ALA:HB1	17:AQ:192:TYR:HB3	2.01	0.43
17:AQ:183:LYS:HB2	17:AQ:183:LYS:HE3	1.77	0.43
40:An:12:PHE:CD2	40:An:51:LEU:HD13	2.54	0.43
43:Ar:24:LYS:HB2	43:Ar:24:LYS:HE3	1.75	0.43
45:BA:1396:A:N7	45:BA:1449:G:C6	2.86	0.43
45:BA:1817:G:H2'	45:BA:1818:A:C8	2.53	0.43
48:BD:122:GLU:OE2	48:BD:140:VAL:HG12	2.18	0.43
49:BE:80:PRO:HG2	49:BE:83:SER:HB3	2.01	0.43
66:BV:84:PHE:HE1	66:BV:264:SER:HA	1.84	0.43
72:Bb:81:VAL:HG22	72:Bb:104:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1248:C:H2'	1:AA:1249:C:H6	1.84	0.42
1:AA:1307:A:H2'	1:AA:1308:C:H6	1.84	0.42
1:AA:4139:G:H2'	1:AA:4140:C:C5	2.54	0.42
1:AA:4413:C:H2'	1:AA:4414:A:O4'	2.20	0.42
10:AJ:26:LYS:HG3	10:AJ:28:VAL:HG22	2.00	0.42
13:AM:112:HIS:HE1	13:AM:125:ILE:HA	1.84	0.42
18:AR:33:ALA:HB1	18:AR:117:ILE:HG12	1.99	0.42
45:BA:825:A:H2'	45:BA:826:A:C8	2.53	0.42
45:BA:1384:C:C2	45:BA:1385:G:C8	3.07	0.42
45:BA:1452:A:P	45:BA:1452:A:H8	2.41	0.42
45:BA:1852:C:H2'	45:BA:1853:C:C6	2.54	0.42
48:BD:222:LYS:HD3	48:BD:223:PHE:N	2.33	0.42
50:BF:91:ARG:HA	50:BF:94:LYS:HG3	2.00	0.42
50:BF:99:ILE:HA	50:BF:102:LEU:HG	2.00	0.42
51:BG:99:ARG:HH12	51:BG:120:ARG:HB3	1.84	0.42
1:AA:1447:C:H2'	1:AA:1448:G:H8	1.84	0.42
1:AA:3770:PSU:H2'	1:AA:3771:C:C6	2.55	0.42
1:AA:4405:G:H4'	12:AL:4:ARG:NE	2.34	0.42
1:AA:4525:C:H5''	5:AE:245:HIC:HB2	2.01	0.42
1:AA:4759:C:H2'	1:AA:4760:G:C8	2.54	0.42
6:AF:140:LYS:HE3	6:AF:140:LYS:HB3	1.94	0.42
9:AI:110:GLN:HG2	9:AI:115:ARG:CZ	2.49	0.42
10:AJ:137[A]:ARG:HD2	10:AJ:146:LEU:HD21	2.00	0.42
30:Ad:108:ALA:O	30:Ad:112:ILE:HD12	2.19	0.42
45:BA:921:G:N3	75:Be:22:LYS:HG2	2.34	0.42
45:BA:1204:A:H2'	45:BA:1205:C:C6	2.54	0.42
45:BA:1667:U:H2'	45:BA:1668:U:C6	2.55	0.42
45:BA:1678:A2M:H1'	45:BA:1678:A2M:HM'2	1.63	0.42
52:BH:79:ILE:HG13	52:BH:170:LYS:HZ2	1.84	0.42
63:BS:40:ARG:HH22	63:BS:62:GLU:CD	2.26	0.42
78:Bh:41:ILE:HG23	78:Bh:46:LEU:HD12	2.01	0.42
1:AA:1266:G:H5'	30:Ad:99:ILE:HD11	2.02	0.42
1:AA:4178:A:H2'	1:AA:4179:G:C8	2.54	0.42
30:Ad:12:GLN:HB3	30:Ad:16:TRP:CZ2	2.54	0.42
44:As:95:HIS:O	44:As:99:LYS:HB2	2.19	0.42
45:BA:406:PSU:H2'	45:BA:408:A:C8	2.54	0.42
45:BA:572:PSU:H2'	45:BA:573:U:C2	2.54	0.42
45:BA:1592:C:H2'	45:BA:1593:C:C6	2.55	0.42
45:BA:1693:G:H2'	45:BA:1694:U:C6	2.54	0.42
45:BA:1726:G:H2'	45:BA:1727:G:C8	2.54	0.42
48:BD:100:PHE:CE2	48:BD:181:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:192:TRP:CG	49:BE:203:PRO:HA	2.54	0.42
56:BL:57:LEU:HD21	56:BL:111:ILE:HG22	2.00	0.42
58:BN:97:LYS:H	58:BN:97:LYS:HG2	1.55	0.42
64:BT:50:ILE:H	64:BT:50:ILE:HG13	1.47	0.42
65:BU:40:ILE:HG12	65:BU:69:VAL:HG21	2.00	0.42
65:BU:168:CYS:HA	65:BU:173:LEU:O	2.19	0.42
72:Bb:114:GLU:O	72:Bb:118:ARG:HG3	2.19	0.42
1:AA:3832:U:H2'	1:AA:3833:C:H6	1.84	0.42
4:AD:137:ILE:HD11	4:AD:149:LYS:HB2	2.01	0.42
15:AO:130:LEU:HD12	15:AO:130:LEU:HA	1.86	0.42
24:AX:35:LYS:HA	24:AX:35:LYS:HD2	1.81	0.42
45:BA:1689:C:H2'	45:BA:1690:U:C6	2.54	0.42
45:BA:1794:C:H2'	45:BA:1795:G:H8	1.84	0.42
55:BK:33:LEU:HD12	55:BK:37:TYR:CZ	2.54	0.42
61:BQ:68:LYS:HD2	61:BQ:91:LEU:HD22	2.02	0.42
62:BR:83:VAL:HG12	62:BR:84:VAL:HG13	2.01	0.42
68:BX:64:ASP:O	68:BX:70:ARG:HD3	2.20	0.42
70:BZ:114:ARG:HD3	70:BZ:114:ARG:HA	1.77	0.42
78:Bh:41:ILE:HD12	78:Bh:47:ARG:HE	1.83	0.42
1:AA:962:C:H1'	9:AI:32:ARG:HH12	1.84	0.42
1:AA:2676:A:H8	1:AA:2676:A:OP2	2.01	0.42
1:AA:2756:G:H2'	1:AA:2757:A:C8	2.54	0.42
1:AA:4891:G:H3'	1:AA:4892:A:C2	2.54	0.42
3:AC:130:C:H2'	3:AC:131:G:C8	2.55	0.42
10:AJ:100:HIS:HB2	10:AJ:103:ARG:NE	2.34	0.42
14:AN:42:LYS:O	14:AN:46:ILE:HG23	2.19	0.42
20:AT:105:LEU:HD23	20:AT:138:LEU:HD23	2.02	0.42
30:Ad:63:LYS:HZ2	30:Ad:63:LYS:HB3	1.84	0.42
38:Al:67:LEU:HD23	38:Al:67:LEU:HA	1.83	0.42
45:BA:870:A:H62	45:BA:915:G:H2'	1.84	0.42
45:BA:913:A:C6	51:BG:120:ARG:HG3	2.54	0.42
45:BA:1009:A:H2'	45:BA:1010:G:H8	1.83	0.42
45:BA:1206:G:H1	45:BA:1692:PSU:HN3	1.67	0.42
45:BA:1675:A:H5'	50:BF:74:ASN:HD21	1.84	0.42
45:BA:1750:C:H2'	45:BA:1751:C:O4'	2.20	0.42
46:BB:145:ARG:HG3	46:BB:147:ILE:HD11	2.01	0.42
47:BC:62:ALA:O	47:BC:66:VAL:HG13	2.20	0.42
47:BC:210:ILE:HD11	78:Bh:81:ARG:HB3	2.01	0.42
49:BE:12:VAL:HG21	64:BT:34:TYR:HB2	2.01	0.42
57:BM:45:LEU:HB2	57:BM:50:ILE:HB	2.02	0.42
60:BP:22:ARG:NH2	72:Bb:70:ASN:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BQ:89:GLY:HA3	76:Bf:10:GLY:N	2.35	0.42
61:BQ:91:LEU:HD12	61:BQ:94:ILE:HD11	2.01	0.42
70:BZ:29:THR:HG23	70:BZ:31:ASP:H	1.84	0.42
1:AA:460:C:H2'	1:AA:461:G:C8	2.55	0.42
1:AA:694:C:H2'	1:AA:695:G:C8	2.55	0.42
1:AA:1085:C:H2'	1:AA:1086:C:C6	2.54	0.42
1:AA:1577:G:H5'	1:AA:1578:U:H5''	2.02	0.42
1:AA:4392:OMG:N3	1:AA:4447:5MC:HM52	2.35	0.42
1:AA:4456:OMC:HM22	1:AA:4457:PSU:H5''	2.02	0.42
4:AD:145:LYS:HD2	4:AD:157:VAL:HG12	2.01	0.42
16:AP:135:ILE:HD12	16:AP:151:ILE:HD13	2.01	0.42
23:AW:48:LYS:HE3	23:AW:48:LYS:HB3	1.84	0.42
31:Ae:60:ILE:HD12	31:Ae:60:ILE:HA	1.93	0.42
45:BA:176:U:H2'	45:BA:177:G:H8	1.84	0.42
45:BA:648:A:H2'	45:BA:649:PSU:C6	2.55	0.42
45:BA:860:G:H2'	45:BA:861:A:O4'	2.19	0.42
45:BA:1467:C:OP1	78:Bh:3:ARG:HB2	2.19	0.42
45:BA:1529:C:H2'	45:BA:1530:U:H6	1.84	0.42
45:BA:1655:C:H2'	45:BA:1656:G:C8	2.50	0.42
48:BD:137:LEU:HG	48:BD:215:VAL:HG13	2.01	0.42
52:BH:76:THR:HG23	52:BH:104:ILE:HD11	2.02	0.42
57:BM:74:PRO:HA	57:BM:79:ILE:HD13	2.01	0.42
68:BX:55:LYS:HE2	68:BX:55:LYS:HB3	1.80	0.42
74:Bd:47:LEU:H	74:Bd:79:ILE:HA	1.84	0.42
1:AA:175:C:H2'	1:AA:176:G:O4'	2.18	0.42
1:AA:920:C:H2'	1:AA:921:C:C6	2.54	0.42
1:AA:1417:C:H2'	1:AA:1418:C:H6	1.85	0.42
1:AA:1985:G:H2'	1:AA:1986:U:O4'	2.20	0.42
1:AA:2032:U:H5''	12:AL:164:LYS:HZ1	1.84	0.42
1:AA:2521:G:H5''	35:Ai:25:THR:HG22	2.01	0.42
1:AA:4080:C:H2'	1:AA:4081:G:H8	1.84	0.42
6:AF:154:VAL:HG21	6:AF:174:LEU:HD11	2.02	0.42
7:AG:163:LEU:HD21	7:AG:175:HIS:CG	2.55	0.42
8:AH:72:LYS:HE3	8:AH:72:LYS:HB2	1.81	0.42
11:AK:128:MET:HE3	11:AK:157:SER:HB3	2.02	0.42
13:AM:112:HIS:CD2	13:AM:117:ILE:HD11	2.54	0.42
15:AO:58:THR:HG23	15:AO:60:PHE:H	1.85	0.42
20:AT:105:LEU:HD22	20:AT:135:LYS:HG2	2.01	0.42
27:Aa:2:LYS:HB3	27:Aa:2:LYS:HE3	1.82	0.42
45:BA:512:A2M:HM'2	45:BA:513:G:H5'	2.01	0.42
45:BA:600:G:H2'	45:BA:601:OMG:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1135:C:H2'	45:BA:1136:PSU:C6	2.55	0.42
45:BA:1221:G:H2'	45:BA:1222:G:C8	2.54	0.42
45:BA:1528:G:H2'	45:BA:1529:C:H6	1.85	0.42
45:BA:1680:G:H2'	45:BA:1681:U:C6	2.54	0.42
49:BE:25:LEU:HA	49:BE:28:GLU:HB2	2.01	0.42
52:BH:197:PHE:O	52:BH:200:ARG:HG2	2.20	0.42
52:BH:206:LYS:H	52:BH:206:LYS:HG2	1.65	0.42
53:BI:64:TRP:CG	64:BT:23:VAL:HG22	2.55	0.42
58:BN:134:ILE:O	58:BN:138:VAL:HG12	2.20	0.42
63:BS:29:GLN:HE22	63:BS:68:LEU:H	1.68	0.42
65:BU:245:ARG:HB2	65:BU:245:ARG:NH1	2.35	0.42
68:BX:57:ALA:CB	68:BX:97:ILE:HD11	2.49	0.42
1:AA:127:G:H2'	1:AA:128:C:H6	1.83	0.42
1:AA:159:C:H5''	37:Ak:25:ARG:NE	2.35	0.42
1:AA:646:G:H2'	1:AA:647:G:O4'	2.20	0.42
1:AA:1185:G:H2'	1:AA:1186:U:C6	2.54	0.42
1:AA:3673:C:H4'	1:AA:3674:G:O5'	2.19	0.42
1:AA:3787:G:H1'	1:AA:3789:C:N4	2.35	0.42
1:AA:3933:G:H2'	1:AA:3934:G:H8	1.83	0.42
2:AB:59:G:H2'	2:AB:60:G:H8	1.85	0.42
4:AD:92:LYS:HE3	4:AD:92:LYS:HB2	1.78	0.42
9:AI:241:ASN:O	9:AI:245:ARG:HG2	2.19	0.42
13:AM:163:MET:O	13:AM:167:GLN:HG2	2.20	0.42
15:AO:12:VAL:O	15:AO:58:THR:HG22	2.20	0.42
21:AU:15:ARG:HB3	21:AU:27:LEU:HD23	2.02	0.42
28:Ab:11:VAL:HG12	28:Ab:82:PRO:HA	2.02	0.42
45:BA:1568:C:H4'	58:BN:41:LYS:HE2	2.02	0.42
45:BA:1812:U:H2'	45:BA:1813:A:H8	1.85	0.42
65:BU:31:ILE:HG13	65:BU:43:TRP:HD1	1.84	0.42
1:AA:161:G:H2'	1:AA:162:A:H8	1.85	0.42
1:AA:1406:G:N7	1:AA:1408:G:H5'	2.34	0.42
1:AA:1725:U:H2'	1:AA:1726:U:H6	1.85	0.42
1:AA:2730:U:H2'	1:AA:2731:C:C6	2.55	0.42
4:AD:3:ARG:HG2	4:AD:207:VAL:HG22	2.00	0.42
6:AF:33:ARG:O	6:AF:37:VAL:HG13	2.20	0.42
6:AF:230:LEU:HD23	6:AF:230:LEU:HA	1.91	0.42
7:AG:219:TYR:CE2	7:AG:227:ILE:HD11	2.55	0.42
9:AI:162:ILE:HD13	9:AI:174:LEU:HD12	2.02	0.42
14:AN:59:VAL:HG21	14:AN:73:GLY:HA3	2.01	0.42
17:AQ:177:LEU:HD12	17:AQ:177:LEU:HA	1.88	0.42
45:BA:118:C:H2'	45:BA:119:PSU:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:330:G:P	67:BW:189:ARG:HH22	2.43	0.42
45:BA:1533:A:H2	45:BA:1536:G:H21	1.67	0.42
45:BA:1535:U:H3'	45:BA:1536:G:H8	1.84	0.42
47:BC:165:ASN:HA	47:BC:171:VAL:HG12	2.01	0.42
47:BC:183:LEU:HD12	47:BC:183:LEU:HA	1.83	0.42
48:BD:83:LYS:HE2	48:BD:83:LYS:HB2	1.80	0.42
48:BD:168:MET:SD	48:BD:197:ILE:HD13	2.59	0.42
49:BE:176:LEU:HD12	49:BE:176:LEU:HA	1.89	0.42
50:BF:85:LYS:O	50:BF:89:THR:HG23	2.20	0.42
52:BH:43:ILE:HD11	52:BH:55:TYR:HB3	2.00	0.42
65:BU:206:LEU:HD13	65:BU:218:LEU:HD21	2.02	0.42
66:BV:106:VAL:HG22	66:BV:128:VAL:HG12	2.01	0.42
77:Bg:100:LEU:HD11	77:Bg:103:LEU:HD13	2.01	0.42
1:AA:687:U:H3	8:AH:95:PRO:HG2	1.85	0.42
1:AA:1085:C:H2'	1:AA:1086:C:H6	1.84	0.42
1:AA:1327:C:H2'	1:AA:1328:G:C8	2.55	0.42
1:AA:1628:C:OP2	4:AD:9:ARG:HD2	2.20	0.42
1:AA:1802:A:H5''	1:AA:1803:G:H5'	2.02	0.42
1:AA:1906:U:H2'	1:AA:1907:A:H8	1.84	0.42
1:AA:2896:G:H5''	20:AT:134:ASN:HD22	1.85	0.42
1:AA:4611:A:C2	11:AK:120:GLU:HB3	2.49	0.42
7:AG:236:MET:HA	7:AG:239:MET:HE2	2.02	0.42
9:AI:247:MET:HE2	9:AI:247:MET:HB3	1.91	0.42
14:AN:105:LYS:HE2	14:AN:105:LYS:HB3	1.80	0.42
34:Ah:75:THR:HG21	34:Ah:87:LYS:HG3	2.01	0.42
45:BA:53:C:H2'	45:BA:54:A:H8	1.85	0.42
45:BA:344:U:H2'	45:BA:345:U:C6	2.55	0.42
45:BA:981:A:H2'	45:BA:982:G:C8	2.55	0.42
52:BH:13:LYS:HD3	54:BJ:137:THR:HG21	2.01	0.42
63:BS:59:LEU:HD23	63:BS:59:LEU:HA	1.83	0.42
66:BV:75:ILE:HD11	66:BV:80:GLU:HB3	2.01	0.42
67:BW:10:THR:HG21	67:BW:125:THR:HA	2.02	0.42
1:AA:1821:G:H5'	1:AA:1822:U:C6	2.55	0.41
1:AA:4088:C:H2'	1:AA:4089:G:C8	2.54	0.41
1:AA:4967:A:H2'	1:AA:4968:A:C8	2.54	0.41
10:AJ:229:ARG:O	10:AJ:233:ILE:HG13	2.20	0.41
12:AL:139:ARG:HD3	12:AL:173:PHE:CE2	2.54	0.41
28:Ab:83:THR:HG22	35:Ai:95:PHE:CZ	2.55	0.41
45:BA:213:G:H2'	45:BA:214:U:C6	2.56	0.41
45:BA:1320:G:H3'	45:BA:1321:G:C8	2.55	0.41
45:BA:1567:G:H2'	45:BA:1568:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1628:C:H2'	45:BA:1629:C:C6	2.55	0.41
45:BA:1797:U:H2'	45:BA:1798:C:C6	2.55	0.41
47:BC:63:ARG:NH2	60:BP:39:VAL:HG13	2.35	0.41
49:BE:51:LEU:HB3	49:BE:91:VAL:HG22	2.01	0.41
49:BE:137:VAL:HG22	49:BE:151:LYS:HG2	2.02	0.41
55:BK:91:GLY:H	55:BK:107:ILE:HB	1.85	0.41
66:BV:240:THR:O	66:BV:244:ILE:HD13	2.20	0.41
68:BX:33:GLY:HA3	76:Bf:38:TYR:CD2	2.55	0.41
1:AA:1358:G:N7	1:AA:1377:G:C2	2.88	0.41
1:AA:4046:A:H62	1:AA:4048:A:N6	2.18	0.41
1:AA:4601:U:H2'	1:AA:4602:A:C8	2.53	0.41
2:AB:113:G:H2'	2:AB:114:U:C6	2.55	0.41
4:AD:96:LEU:HD23	4:AD:96:LEU:HA	1.89	0.41
5:AE:14:LEU:HD22	5:AE:17:LEU:HD11	2.02	0.41
5:AE:142:GLY:O	5:AE:146:LEU:HG	2.20	0.41
8:AH:92:VAL:HG23	8:AH:109:LEU:HD21	2.02	0.41
9:AI:244:ILE:O	9:AI:248:ASN:HB3	2.20	0.41
15:AO:37:LEU:HD11	15:AO:47:ARG:HG3	2.02	0.41
17:AQ:61:ARG:HA	17:AQ:70:PRO:HD2	2.02	0.41
21:AU:21:LYS:H	21:AU:21:LYS:HD2	1.84	0.41
21:AU:51:LEU:HD13	22:AV:151:LEU:HD22	2.02	0.41
22:AV:84:ILE:HD12	30:Ad:23:LYS:HG2	2.02	0.41
45:BA:372:U:H2'	45:BA:373:G:C8	2.55	0.41
45:BA:569:A:H2'	45:BA:570:C:H6	1.85	0.41
45:BA:609:PSU:H2'	45:BA:610:G:C8	2.52	0.41
45:BA:930:C:O2'	45:BA:1104:G:H5''	2.19	0.41
45:BA:1564:C:H3'	58:BN:101:ARG:HH21	1.85	0.41
45:BA:1606:G:H21	45:BA:1633:A:H62	1.68	0.41
45:BA:1674:G:H5''	50:BF:86:LYS:HD2	2.02	0.41
45:BA:1708:C:H2'	45:BA:1709:G:C8	2.54	0.41
45:BA:1798:C:H2'	45:BA:1799:G:O4'	2.19	0.41
49:BE:33:GLY:O	49:BE:53:THR:HG23	2.20	0.41
50:BF:123:GLU:HG3	50:BF:139:VAL:O	2.20	0.41
58:BN:107:LEU:HD13	58:BN:107:LEU:HA	1.94	0.41
65:BU:196:ASN:HB3	65:BU:211:GLY:HA2	2.01	0.41
66:BV:65:LYS:HG3	66:BV:277:HIS:HD2	1.85	0.41
69:BY:18:LEU:HD13	69:BY:79:VAL:HG22	2.01	0.41
71:Ba:125:LYS:HD3	71:Ba:126:ILE:H	1.84	0.41
74:Bd:41:ARG:HG2	74:Bd:43:LYS:H	1.86	0.41
1:AA:86:U:H2'	1:AA:87:A:C8	2.55	0.41
1:AA:116:G:H2'	1:AA:117:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:275:C:H2'	1:AA:276:C:C6	2.55	0.41
1:AA:1348:U:H2'	1:AA:1349:G:H8	1.85	0.41
1:AA:1588:U:H2'	1:AA:1589:C:C6	2.56	0.41
1:AA:4724:A:O2'	5:AE:104:THR:HG22	2.21	0.41
5:AE:103:LYS:HE2	5:AE:103:LYS:HB2	1.97	0.41
5:AE:291:TYR:CE1	5:AE:299:ILE:HG22	2.56	0.41
11:AK:50:LYS:HD2	11:AK:50:LYS:HA	1.84	0.41
21:AU:143:LYS:HD2	21:AU:143:LYS:HA	1.95	0.41
28:Ab:124:THR:HG23	28:Ab:126:LYS:HG2	2.02	0.41
31:Ae:29:LEU:HD13	31:Ae:91:VAL:HG21	2.02	0.41
45:BA:170:A:O5'	67:BW:137:ARG:HB2	2.20	0.41
45:BA:311:C:H5''	45:BA:312:G:H5''	2.02	0.41
45:BA:556:U:H3'	45:BA:557:U:C5'	2.50	0.41
45:BA:1657:G:H2'	45:BA:1658:G:C8	2.54	0.41
45:BA:1718:G:H22	45:BA:1814:G:H2'	1.85	0.41
47:BC:1:MET:HB2	47:BC:2:SER:H	1.66	0.41
48:BD:223:PHE:CZ	48:BD:228:LEU:HD22	2.50	0.41
49:BE:135:GLU:CD	49:BE:187:LYS:HE3	2.45	0.41
51:BG:158:LEU:HB2	51:BG:189:PHE:CE1	2.55	0.41
57:BM:14:ARG:HD2	57:BM:14:ARG:HA	1.77	0.41
57:BM:129:LEU:HD13	57:BM:130:ARG:N	2.36	0.41
62:BR:10:ARG:HH11	62:BR:12:LYS:HD3	1.84	0.41
71:Ba:61:LYS:HD3	71:Ba:61:LYS:HA	1.79	0.41
1:AA:660:A:C6	1:AA:661:C:N4	2.88	0.41
1:AA:713:C:H2'	1:AA:714:G:H8	1.86	0.41
1:AA:907:C:H2'	1:AA:908:G:C8	2.55	0.41
1:AA:1238:A:H5'	8:AH:59:ARG:HB2	2.01	0.41
1:AA:1345:A:H2'	1:AA:1346:C:C6	2.55	0.41
1:AA:1512:G:H2'	1:AA:1513:U:C6	2.55	0.41
4:AD:68:ARG:HE	4:AD:68:ARG:HB2	1.70	0.41
10:AJ:120:LYS:HZ1	10:AJ:125:LYS:HB3	1.85	0.41
13:AM:50:PHE:HD1	13:AM:70:VAL:HG22	1.86	0.41
39:Am:67:LYS:HE3	39:Am:67:LYS:HB3	1.85	0.41
42:Aq:44:LYS:HE3	42:Aq:52:THR:HB	2.02	0.41
45:BA:518:G:H2'	45:BA:519:A:C8	2.52	0.41
45:BA:1458:G:H2'	45:BA:1459:G:C8	2.55	0.41
45:BA:1801:A:H2'	45:BA:1802:C:C6	2.56	0.41
49:BE:169:ASP:O	49:BE:187:LYS:HA	2.20	0.41
50:BF:80:GLY:HA2	50:BF:83:ASN:CG	2.46	0.41
56:BL:134:GLY:HA2	56:BL:140:ARG:HA	2.02	0.41
65:BU:43:TRP:CZ3	65:BU:55:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BU:177:TRP:CE2	65:BU:184:LEU:HD12	2.56	0.41
71:Ba:31:CYS:HB2	71:Ba:93:LEU:HD13	2.02	0.41
1:AA:5:A:H2'	1:AA:6:C:C6	2.55	0.41
1:AA:1993:C:H2'	1:AA:1994:C:C6	2.55	0.41
1:AA:4524:G:N3	5:AE:252:ALA:HB1	2.36	0.41
1:AA:4918:C:H2'	1:AA:4919:G:H8	1.85	0.41
3:AC:7:U:H2'	3:AC:8:U:C6	2.56	0.41
6:AF:297:GLU:H	6:AF:297:GLU:HG2	1.55	0.41
6:AF:298:ILE:HD13	19:AS:131:PRO:HB3	2.02	0.41
7:AG:164:LYS:HA	7:AG:167:VAL:HG12	2.02	0.41
11:AK:7:ASN:HD22	11:AK:56:ARG:NH2	2.17	0.41
14:AN:19:GLN:HA	14:AN:22:VAL:HG23	2.03	0.41
16:AP:120:TRP:HZ2	16:AP:123:GLU:HB2	1.85	0.41
26:AZ:81:LEU:HG	26:AZ:83:THR:HG23	2.01	0.41
42:Aq:2:VAL:HG23	42:Aq:88:CYS:SG	2.60	0.41
45:BA:454:U:H2'	45:BA:455:A:C8	2.55	0.41
45:BA:519:A:H2'	45:BA:520:A:H8	1.86	0.41
45:BA:651:PSU:H2'	45:BA:652:U:H6	1.85	0.41
45:BA:680:G:H2'	45:BA:681:PSU:C6	2.55	0.41
45:BA:1092:G:H2'	45:BA:1093:A:H8	1.85	0.41
49:BE:65:ARG:HA	49:BE:68:GLU:HG3	2.02	0.41
51:BG:24:SER:O	51:BG:28:LEU:HB2	2.21	0.41
51:BG:101:LEU:HB3	51:BG:116:ARG:HD3	2.01	0.41
75:Be:55:LEU:HD11	75:Be:62:VAL:HG22	2.03	0.41
1:AA:297:U:H2'	1:AA:298:G:H8	1.85	0.41
1:AA:1461:C:H2'	1:AA:1462:A:H8	1.84	0.41
1:AA:1468:C:H2'	1:AA:1469:C:H6	1.86	0.41
1:AA:1801:A:H4'	22:AV:102:ARG:HD3	2.01	0.41
1:AA:4236:G:H2'	1:AA:4237:C:C6	2.55	0.41
3:AC:28:C:H4'	6:AF:51:PRO:HG2	2.01	0.41
5:AE:317:LEU:HD12	5:AE:317:LEU:HA	1.79	0.41
5:AE:354:GLN:HG3	5:AE:359:ALA:HB1	2.03	0.41
12:AL:47:PRO:HA	12:AL:171:TRP:CD1	2.55	0.41
27:Aa:22:PRO:HG2	27:Aa:25:ILE:HD12	2.02	0.41
31:Ae:52:CYS:SG	31:Ae:57:LYS:HD3	2.60	0.41
45:BA:532:C:H2'	45:BA:533:A:C8	2.47	0.41
45:BA:935:G:H2'	45:BA:936:G:H8	1.86	0.41
45:BA:1009:A:H2'	45:BA:1010:G:C8	2.56	0.41
49:BE:28:GLU:HG2	53:BI:61:GLN:HG2	2.01	0.41
52:BH:41:ARG:HA	52:BH:59:ARG:O	2.21	0.41
65:BU:59:LEU:HB3	65:BU:90:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:BZ:4:MET:HE3	70:BZ:4:MET:HA	2.02	0.41
73:Bc:44:LEU:HD23	73:Bc:44:LEU:HA	1.90	0.41
1:AA:116:G:H2'	1:AA:117:C:C6	2.56	0.41
1:AA:978:G:H2'	1:AA:979:C:C6	2.56	0.41
1:AA:1939:A:H5'	1:AA:1940:G:H4'	2.01	0.41
1:AA:2262:G:P	44:As:98:ARG:HH22	2.44	0.41
1:AA:3707:U:H2'	1:AA:3708:C:C6	2.56	0.41
1:AA:4071:U:H2'	1:AA:4072:C:H6	1.85	0.41
1:AA:4584:A:H2'	1:AA:4585:U:O4'	2.20	0.41
1:AA:4990:C:H5'	1:AA:4991:U:H5''	2.01	0.41
1:AA:5018:C:H2'	1:AA:5019:A:H8	1.86	0.41
1:AA:5026:U:H1'	1:AA:5027:C:H5	1.85	0.41
2:AB:16:A:H2'	2:AB:17:C:C6	2.56	0.41
2:AB:20:U:H2'	2:AB:21:G:C8	2.56	0.41
5:AE:92:TYR:HB3	5:AE:99:LEU:HD22	2.03	0.41
5:AE:231:VAL:HG21	5:AE:251:VAL:HG23	2.02	0.41
37:Ak:25:ARG:HD2	37:Ak:25:ARG:HA	1.90	0.41
45:BA:354:OMU:HM22	45:BA:355:G:O4'	2.21	0.41
45:BA:921:G:C2	75:Be:22:LYS:HG2	2.55	0.41
45:BA:1019:C:H5''	70:BZ:72:LEU:HD22	2.01	0.41
45:BA:1310:U:H2'	45:BA:1311:C:H5	1.86	0.41
45:BA:1390:U:H2'	45:BA:1391:OMC:H6	1.85	0.41
45:BA:1405:A:H2'	45:BA:1406:G:H8	1.85	0.41
48:BD:39:PHE:CD1	48:BD:74:LEU:HD22	2.55	0.41
52:BH:103:LEU:HD12	52:BH:170:LYS:HD3	2.02	0.41
59:BO:65:THR:HB	59:BO:80:PHE:HE1	1.85	0.41
65:BU:174:VAL:CG1	65:BU:188:HIS:HB2	2.50	0.41
66:BV:92:GLU:HA	66:BV:95:ASP:HB2	2.03	0.41
66:BV:108:LYS:HE3	66:BV:108:LYS:HB3	1.87	0.41
1:AA:26:C:N4	1:AA:56:A:H61	2.18	0.41
1:AA:937:U:H2'	1:AA:938:C:C6	2.56	0.41
1:AA:1341:U:H2'	1:AA:1342:A:C8	2.56	0.41
1:AA:1512:G:H2'	1:AA:1513:U:H6	1.85	0.41
1:AA:1895:G:H2'	1:AA:1896:A:O4'	2.21	0.41
1:AA:2864:A:H2'	1:AA:2865:U:C6	2.55	0.41
1:AA:2901:G:H2'	1:AA:2902:G:H4'	2.03	0.41
1:AA:4458:C:H2'	1:AA:4459:U:C6	2.55	0.41
1:AA:4500:PSU:H2'	1:AA:4501:U:H6	1.85	0.41
1:AA:4570:G:H2'	1:AA:4571:A2M:H8	2.03	0.41
6:AF:279:LEU:HD23	6:AF:279:LEU:HA	1.87	0.41
7:AG:256:LYS:HD3	7:AG:256:LYS:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:82:LYS:HG2	11:AK:88:PHE:CZ	2.55	0.41
16:AP:16:SER:O	16:AP:20:ARG:HB2	2.21	0.41
21:AU:118:ARG:HD3	21:AU:118:ARG:HA	1.72	0.41
29:Ac:102:ASP:HA	29:Ac:125:LYS:HB2	2.01	0.41
42:Aq:82:MET:HE3	42:Aq:82:MET:HB3	1.85	0.41
45:BA:158:A:H2'	45:BA:159:A2M:O4'	2.20	0.41
45:BA:1203:G:H2'	45:BA:1204:A:C8	2.56	0.41
45:BA:1232:PSU:H2'	45:BA:1233:G:H8	1.85	0.41
45:BA:1302:G:H4'	45:BA:1303:C:C2	2.55	0.41
49:BE:98:ALA:HA	49:BE:188:ILE:HD13	2.02	0.41
54:BJ:22:ARG:NH1	54:BJ:26:GLY:HA3	2.36	0.41
58:BN:132:ASP:HA	58:BN:135:ALA:HB3	2.02	0.41
62:BR:53:ILE:HD12	62:BR:53:ILE:HA	1.90	0.41
65:BU:261:LEU:HD23	65:BU:261:LEU:HA	1.93	0.41
68:BX:171:GLY:O	68:BX:175:ARG:HG2	2.20	0.41
72:Bb:18:GLU:HA	72:Bb:18:GLU:OE2	2.21	0.41
72:Bb:38:LEU:HA	72:Bb:41:MET:HB2	2.01	0.41
1:AA:481:G:H2'	1:AA:482:G:C8	2.56	0.41
1:AA:1309:C:H2'	1:AA:1310:C:C6	2.56	0.41
1:AA:1778:C:H2'	1:AA:1779:PSU:C6	2.56	0.41
1:AA:1971:C:H41	1:AA:2017:A:H61	1.69	0.41
1:AA:2063:G:H2'	1:AA:2064:G:C8	2.56	0.41
1:AA:2080:U:H2'	1:AA:2081:C:C6	2.56	0.41
1:AA:3961:G:H21	1:AA:3965:A:N6	2.18	0.41
1:AA:3973:G:H2'	1:AA:3974:G:C8	2.55	0.41
1:AA:4232:U:H4'	1:AA:4233:A:O4'	2.21	0.41
5:AE:135:LYS:HB3	5:AE:135:LYS:HE3	1.83	0.41
5:AE:138:GLN:H	5:AE:138:GLN:HG2	1.66	0.41
9:AI:36:LYS:HE3	9:AI:36:LYS:HB3	1.88	0.41
11:AK:41:ILE:HG21	11:AK:73:ILE:HD11	2.03	0.41
11:AK:129:ARG:HA	11:AK:129:ARG:HD2	1.95	0.41
14:AN:130:LYS:HD2	14:AN:130:LYS:HA	1.92	0.41
16:AP:178:HIS:HA	16:AP:181:HIS:NE2	2.36	0.41
20:AT:95:TRP:CH2	20:AT:99:MET:HE3	2.56	0.41
20:AT:153:LYS:HE2	20:AT:153:LYS:HB2	1.79	0.41
21:AU:13:VAL:HG22	21:AU:29:ARG:HB2	2.03	0.41
21:AU:28:TYR:HB3	22:AV:151:LEU:HD12	2.02	0.41
42:Aq:67:VAL:HG11	42:Aq:82:MET:HE3	2.03	0.41
45:BA:184:G:C2	45:BA:185:G:C5	3.09	0.41
45:BA:628:A:N6	49:BE:179:GLN:HB2	2.36	0.41
45:BA:1098:C:H2'	45:BA:1099:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1349:G:H2'	45:BA:1350:U:C6	2.56	0.41
45:BA:1537:A:H1'	45:BA:1604:G:H4'	2.02	0.41
45:BA:1590:C:H4'	45:BA:1653:U:H4'	2.02	0.41
45:BA:1716:C:H2'	45:BA:1717:C:C6	2.56	0.41
46:BB:95:THR:HG23	46:BB:97:GLU:HB2	2.03	0.41
48:BD:199:LYS:HB3	48:BD:199:LYS:HE2	1.85	0.41
49:BE:40:ARG:NH1	59:BO:108:PRO:HA	2.36	0.41
51:BG:45:ILE:HD12	51:BG:46:THR:H	1.86	0.41
51:BG:142:LYS:HE2	51:BG:142:LYS:HB3	1.83	0.41
52:BH:65:PHE:HA	52:BH:187:GLY:O	2.21	0.41
54:BJ:7:GLU:OE2	54:BJ:11:GLN:HG2	2.21	0.41
55:BK:103:ASN:HD22	55:BK:103:ASN:HA	1.70	0.41
56:BL:16:LYS:HG3	56:BL:17:LYS:H	1.86	0.41
57:BM:66:ARG:O	57:BM:70:ILE:HG13	2.20	0.41
58:BN:40:ALA:HB2	58:BN:95:GLY:HA2	2.03	0.41
61:BQ:68:LYS:HB3	61:BQ:91:LEU:HD22	2.03	0.41
65:BU:241:PHE:CE2	65:BU:248:LEU:HD13	2.55	0.41
66:BV:191:VAL:HG11	66:BV:236:PHE:HA	2.02	0.41
67:BW:137:ARG:HD2	67:BW:140:ARG:HG2	2.01	0.41
68:BX:28:GLU:HB3	68:BX:40:LYS:HE2	2.03	0.41
70:BZ:73:ARG:O	70:BZ:76:LYS:HG3	2.20	0.41
70:BZ:89:TYR:CE1	70:BZ:93:LYS:HD2	2.56	0.41
71:Ba:38:ASN:C	71:Ba:69:SER:HB3	2.46	0.41
73:Bc:91:LEU:HD22	73:Bc:96:LEU:HD13	2.03	0.41
76:Bf:46:VAL:HA	76:Bf:47:PRO:HD3	1.92	0.41
78:Bh:76:GLU:O	78:Bh:79:GLU:HG3	2.21	0.41
1:AA:4389:C:H2'	1:AA:4390:A:H8	1.86	0.41
1:AA:4508:C:N3	1:AA:4512:U:H5	2.19	0.41
1:AA:4678:G:N2	1:AA:4713:G:H1'	2.36	0.41
1:AA:4967:A:H2'	1:AA:4968:A:H8	1.86	0.41
19:AS:69:LYS:HA	19:AS:69:LYS:HD3	1.86	0.41
30:Ad:107:ARG:NH1	30:Ad:111:ARG:HB2	2.37	0.41
45:BA:14:C:H2'	45:BA:15:U:C6	2.56	0.41
45:BA:153:G:H21	67:BW:13:GLN:NE2	2.19	0.41
45:BA:349:A:H2'	45:BA:350:C:O4'	2.20	0.41
45:BA:484:A2M:H8	45:BA:484:A2M:O5'	2.21	0.41
45:BA:904:A:H4'	54:BJ:48:LYS:NZ	2.36	0.41
45:BA:1205:C:H2'	45:BA:1206:G:H8	1.86	0.41
45:BA:1318:G:H2'	45:BA:1319:U:C6	2.56	0.41
45:BA:1542:C:H5'	58:BN:62:ARG:HD3	2.02	0.41
45:BA:1781:A:H8	45:BA:1781:A:OP2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1788:A:H3'	45:BA:1789:G:H8	1.86	0.41
47:BC:111:GLN:HA	47:BC:116:PHE:CG	2.56	0.41
48:BD:73:ASP:HB2	71:Ba:128:ARG:HH22	1.86	0.41
49:BE:106:ARG:HD3	49:BE:173:ARG:HD3	2.03	0.41
54:BJ:35:ARG:HB3	54:BJ:37:TYR:HE1	1.86	0.41
54:BJ:120:VAL:HG22	54:BJ:145:VAL:HG11	2.03	0.41
65:BU:168:CYS:HA	65:BU:174:VAL:HA	2.03	0.41
66:BV:115:GLN:HA	66:BV:120:GLN:HG3	2.04	0.41
71:Ba:148:ARG:HB2	71:Ba:151:ARG:HH21	1.86	0.41
78:Bh:29:HIS:HB3	78:Bh:33:ARG:HH21	1.85	0.41
1:AA:6:C:H2'	1:AA:7:C:H6	1.86	0.40
1:AA:674:G:H2'	1:AA:675:C:C6	2.56	0.40
1:AA:1243:C:C2	1:AA:1244:G:C8	3.09	0.40
1:AA:2633:U:H2'	1:AA:2634:C:C6	2.56	0.40
1:AA:2669:C:H2'	1:AA:2670:C:O4'	2.21	0.40
1:AA:3747:A:C8	4:AD:245:ARG:HB2	2.56	0.40
1:AA:3916:G:H2'	1:AA:3917:A:C8	2.55	0.40
2:AB:92:C:H2'	2:AB:93:G:C8	2.55	0.40
3:AC:66:A:H2'	3:AC:67:U:C6	2.57	0.40
7:AG:223:PHE:O	7:AG:227:ILE:HG12	2.22	0.40
11:AK:128:MET:HE2	11:AK:134:CYS:HB2	2.04	0.40
11:AK:129:ARG:HB3	11:AK:153:LEU:HD22	2.02	0.40
12:AL:175:LYS:HD3	12:AL:175:LYS:HA	1.67	0.40
16:AP:9:GLU:O	16:AP:13:LYS:HG2	2.20	0.40
18:AR:126:ARG:NH2	18:AR:140:MET:HE1	2.36	0.40
19:AS:178:ARG:HA	19:AS:184:ARG:O	2.20	0.40
37:Ak:36:HIS:O	37:Ak:40:VAL:HG23	2.21	0.40
45:BA:118:C:H1'	45:BA:445:A:C5	2.55	0.40
45:BA:333:G:H2'	45:BA:334:C:C6	2.56	0.40
45:BA:972:A:H61	71:Ba:55:ARG:HH21	1.70	0.40
45:BA:1005:G:H2'	45:BA:1006:C:C6	2.56	0.40
45:BA:1030:A:H2'	45:BA:1031:A2M:C8	2.46	0.40
45:BA:1406:G:H2'	45:BA:1407:U:C6	2.55	0.40
45:BA:1611:G:H1'	57:BM:86:ARG:HH21	1.87	0.40
45:BA:1658:G:H5'	64:BT:33:LYS:HD3	2.03	0.40
45:BA:1784:G:H2'	45:BA:1785:C:O4'	2.21	0.40
46:BB:175:PHE:HE2	46:BB:225:ILE:HG21	1.86	0.40
51:BG:163:GLN:HE21	51:BG:163:GLN:HB3	1.63	0.40
59:BO:65:THR:HG23	64:BT:40:ARG:HB2	2.02	0.40
67:BW:23:LYS:HD2	67:BW:41:LEU:HD22	2.03	0.40
68:BX:13:TYR:HB2	68:BX:44:TRP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:Bd:91:LEU:HB3	74:Bd:97:ILE:HD13	2.03	0.40
1:AA:178:C:H2'	1:AA:179:G:C8	2.56	0.40
1:AA:319:A:H1'	1:AA:3726:A:N3	2.37	0.40
1:AA:1721:G:H2'	1:AA:1722:C:H6	1.86	0.40
1:AA:1820:C:H5'	7:AG:139:PRO:HB3	2.03	0.40
1:AA:1884:C:H2'	1:AA:1885:G:H8	1.86	0.40
1:AA:2520:C:H2'	1:AA:2521:G:C8	2.52	0.40
1:AA:2683:C:H2'	1:AA:2684:C:C6	2.57	0.40
1:AA:2770:C:H2'	1:AA:2771:G:C8	2.54	0.40
1:AA:4192:A:H2'	1:AA:4193:C:C6	2.56	0.40
1:AA:4413:C:H42	1:AA:4429:C:H42	1.69	0.40
14:AN:92:ARG:NH1	14:AN:98:VAL:HB	2.36	0.40
16:AP:104:GLU:HA	16:AP:160:GLU:HG3	2.02	0.40
17:AQ:130:LYS:HB2	17:AQ:133:ARG:HG2	2.03	0.40
39:Am:56:LEU:HD22	39:Am:56:LEU:HA	1.96	0.40
45:BA:12:U:H2'	45:BA:13:C:C6	2.56	0.40
45:BA:809:A:H2'	45:BA:810:A:O4'	2.21	0.40
45:BA:822:PSU:H3'	45:BA:823:U:H5'	2.03	0.40
45:BA:1218:C:H2'	45:BA:1219:C:C6	2.54	0.40
45:BA:1696:C:H2'	45:BA:1697:A:C8	2.56	0.40
46:BB:9:LEU:HB2	46:BB:28:ALA:HB3	2.03	0.40
46:BB:179:ASN:HD22	46:BB:179:ASN:HA	1.66	0.40
48:BD:227:LYS:HD2	48:BD:227:LYS:HA	1.84	0.40
50:BF:91:ARG:HA	50:BF:91:ARG:HD3	1.93	0.40
50:BF:204:ARG:HH12	63:BS:63:ARG:HG3	1.86	0.40
51:BG:130:LEU:O	51:BG:134:VAL:HG12	2.21	0.40
56:BL:90:LYS:HG2	56:BL:90:LYS:H	1.77	0.40
57:BM:47:LYS:HB2	57:BM:47:LYS:HE2	1.85	0.40
65:BU:258:ILE:HB	65:BU:268:ASP:HB3	2.03	0.40
67:BW:56:ASN:H	67:BW:108:VAL:HB	1.86	0.40
1:AA:642:G:H2'	1:AA:643:C:C6	2.56	0.40
1:AA:1317:U:H2'	1:AA:1318:C:C6	2.56	0.40
1:AA:1613:A:H5'	4:AD:183:GLY:HA2	2.04	0.40
1:AA:2323:C:H2'	1:AA:2324:C:C6	2.56	0.40
1:AA:2391:G:H2'	1:AA:2392:C:C6	2.56	0.40
1:AA:3856:A:H5''	18:AR:83:TRP:O	2.22	0.40
1:AA:5030:U:H2'	1:AA:5031:G:H8	1.85	0.40
2:AB:65:G:H2'	2:AB:66:G:O4'	2.21	0.40
5:AE:389:MET:HB3	5:AE:389:MET:HE3	1.82	0.40
8:AH:192:LYS:HD2	34:Ah:107:PRO:HB3	2.03	0.40
10:AJ:120:LYS:NZ	10:AJ:125:LYS:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:6:PHE:H	15:AO:11:ARG:HH21	1.70	0.40
15:AO:31:ILE:HG23	21:AU:75:VAL:HG13	2.02	0.40
16:AP:146:PRO:HB2	36:Aj:104:THR:HG23	2.04	0.40
45:BA:43:U:H2'	45:BA:44:U:H5	1.86	0.40
45:BA:129:C:H5'	45:BA:130:G:C5	2.57	0.40
45:BA:306:C:P	52:BH:41:ARG:HE	2.44	0.40
45:BA:580:U:H1'	73:Bc:62:THR:HB	2.04	0.40
45:BA:1458:G:H2'	45:BA:1459:G:H8	1.86	0.40
45:BA:1499:U:H4'	49:BE:176:LEU:HD11	2.03	0.40
45:BA:1686:G:H2'	45:BA:1687:C:O4'	2.21	0.40
45:BA:1747:C:H2'	45:BA:1748:G:C8	2.56	0.40
46:BB:59:ASP:O	46:BB:63:LYS:HG3	2.21	0.40
48:BD:97:LEU:HB3	48:BD:228:LEU:HD21	2.03	0.40
49:BE:23:GLU:HG2	64:BT:46:TYR:CE1	2.56	0.40
50:BF:102:LEU:HD11	74:Bd:67:LEU:HD13	2.03	0.40
50:BF:121:PRO:HB3	50:BF:193:LYS:HG3	2.03	0.40
57:BM:87:GLN:HB3	57:BM:95:TYR:CE2	2.57	0.40
59:BO:17:ILE:HD13	59:BO:17:ILE:HA	1.89	0.40
60:BP:61:ARG:HG2	60:BP:61:ARG:H	1.65	0.40
61:BQ:28:LYS:HB3	61:BQ:32:LEU:HG	2.02	0.40
65:BU:17:TRP:O	65:BU:36:ARG:HG2	2.21	0.40
66:BV:65:LYS:HG3	66:BV:277:HIS:CD2	2.56	0.40
70:BZ:25:TRP:CH2	75:Be:32:PHE:HD1	2.39	0.40
70:BZ:52:VAL:HG13	70:BZ:53:ILE:HD13	2.04	0.40
73:Bc:12:PHE:HB2	73:Bc:23:MET:HE3	2.02	0.40
74:Bd:58:LEU:O	74:Bd:62:VAL:HB	2.22	0.40
1:AA:713:C:H2'	1:AA:714:G:C8	2.57	0.40
1:AA:1304:C:H2'	1:AA:1305:C:C6	2.57	0.40
1:AA:1514:U:H2'	1:AA:1515:A:C8	2.57	0.40
1:AA:2406:G:H1'	1:AA:2791:C:H5''	2.03	0.40
1:AA:2884:G:H2'	1:AA:2885:A:C8	2.57	0.40
1:AA:4549:G:H2'	1:AA:4550:G:H8	1.86	0.40
1:AA:4748:U:H5''	34:Ah:54:LYS:HE3	2.03	0.40
1:AA:4754:G:N1	1:AA:4755:G:C6	2.90	0.40
1:AA:4934:A:H2'	1:AA:4935:C:C6	2.56	0.40
4:AD:42:LYS:HE2	4:AD:87:PHE:CD1	2.57	0.40
7:AG:51:MET:HE2	7:AG:51:MET:HB3	1.97	0.40
27:Aa:77:LYS:HB3	27:Aa:79:VAL:HG22	2.04	0.40
28:Ab:28:ASN:HB2	28:Ab:77:TYR:OH	2.21	0.40
33:Ag:91:CYS:HB3	33:Ag:95:TYR:HD2	1.85	0.40
36:Aj:13:LYS:HE2	36:Aj:13:LYS:HB3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:220:U:H2'	45:BA:221:A:C8	2.56	0.40
45:BA:484:A2M:H1'	45:BA:484:A2M:HM'2	1.87	0.40
45:BA:648:A:H2'	45:BA:649:PSU:H6	1.85	0.40
45:BA:833:C:C4	45:BA:834:C:N4	2.90	0.40
45:BA:840:C:H5'	45:BA:841:G:H5''	2.04	0.40
45:BA:1303:C:H2'	45:BA:1304:U:C2	2.57	0.40
45:BA:1389:C:H2'	45:BA:1390:U:C6	2.56	0.40
45:BA:1476:A:H4'	45:BA:1477:U:H5''	2.04	0.40
45:BA:1600:G:C5	45:BA:1602:U:H1'	2.56	0.40
45:BA:1736:G:H4'	67:BW:94:ARG:HH22	1.86	0.40
47:BC:85:ARG:CZ	47:BC:202:TYR:HA	2.51	0.40
49:BE:96:LEU:HD23	49:BE:190:LEU:HD23	2.04	0.40
50:BF:122:ARG:HG3	50:BF:146:ARG:HD2	2.03	0.40
55:BK:45:LEU:HD23	55:BK:49:LEU:HD21	2.03	0.40
56:BL:104:SER:HA	56:BL:107:GLU:CD	2.47	0.40
57:BM:113:ARG:O	57:BM:116:LYS:HG3	2.21	0.40
67:BW:118:GLU:HG2	67:BW:119:LYS:N	2.36	0.40
67:BW:187:HIS:CE1	67:BW:191:ARG:HE	2.40	0.40
78:Bh:48:ASN:H	78:Bh:49:LYS:NZ	2.17	0.40
1:AA:1172:C:H5'	1:AA:1173:G:N7	2.36	0.40
1:AA:1325:C:C4	1:AA:3879:G:H5''	2.57	0.40
1:AA:2374:A:H2'	1:AA:2375:A:H8	1.86	0.40
1:AA:2563:C:H2'	1:AA:2564:G:C8	2.56	0.40
1:AA:2671:C:H2'	1:AA:2672:C:C6	2.57	0.40
1:AA:4249:G:H2'	1:AA:4250:G:C8	2.57	0.40
1:AA:4372:U:OP2	42:Aq:61:LYS:HG2	2.21	0.40
1:AA:4457:PSU:H1'	5:AE:252:ALA:HB3	2.03	0.40
1:AA:4499:OMG:N2	1:AA:4529:G:H1'	2.36	0.40
2:AB:46:C:H2'	2:AB:47:G:C8	2.56	0.40
2:AB:119:U:N3	7:AG:261:VAL:HG21	2.36	0.40
2:AB:120:U:H5'	7:AG:261:VAL:HG12	2.04	0.40
5:AE:161:ARG:HG2	5:AE:184:GLN:HA	2.02	0.40
7:AG:108:ARG:CZ	7:AG:253:TYR:HB2	2.52	0.40
17:AQ:81:TRP:HB2	17:AQ:104:VAL:HG21	2.04	0.40
19:AS:24:TYR:CZ	44:As:5:LEU:HD11	2.56	0.40
21:Au:12:VAL:O	21:Au:29:ARG:HA	2.21	0.40
23:AW:83:LEU:HA	23:AW:83:LEU:HD13	1.88	0.40
23:AW:89:LYS:O	23:AW:93:LYS:HG3	2.22	0.40
31:Ae:18:LEU:HA	31:Ae:21:VAL:HG12	2.04	0.40
33:Ag:89:LEU:HD13	33:Ag:118:LEU:HD22	2.03	0.40
34:Ah:87:LYS:HB3	34:Ah:87:LYS:HE3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:353:C:H2'	45:BA:354:OMU:H6	2.03	0.40
45:BA:500:A:O2'	45:BA:501:C:H5'	2.21	0.40
45:BA:570:C:C2	45:BA:571:U:C5	3.09	0.40
45:BA:575:A:H2'	45:BA:576:A2M:C8	2.52	0.40
45:BA:902:G:H1'	45:BA:903:A:C8	2.57	0.40
45:BA:1304:U:H2'	45:BA:1305:C:C6	2.56	0.40
49:BE:132:LYS:C	49:BE:132:LYS:HD2	2.46	0.40
50:BF:42:LYS:HB3	50:BF:43:GLU:H	1.81	0.40
50:BF:95:HIS:HB3	74:Bd:106:GLN:HG2	2.03	0.40
56:BL:78:VAL:O	56:BL:82:TYR:HD2	2.05	0.40
60:BP:71:ARG:NH2	75:Be:4:ALA:HB2	2.36	0.40
65:BU:168:CYS:HB2	65:BU:195:LEU:HD13	2.04	0.40
69:BY:15:ASN:HA	69:BY:18:LEU:HD12	2.03	0.40
69:BY:52:LEU:HD21	69:BY:62:VAL:HG23	2.03	0.40
75:Be:34:ASP:O	75:Be:79:PHE:HA	2.21	0.40
78:Bh:59:LYS:HE2	78:Bh:59:LYS:HB3	1.98	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	
4	AD	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
5	AE	399/402 (99%)	391 (98%)	8 (2%)	0	100	100
6	AF	366/368 (100%)	360 (98%)	6 (2%)	0	100	100
7	AG	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
8	AH	232/247 (94%)	220 (95%)	12 (5%)	0	100	100
9	AI	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
10	AJ	240/266 (90%)	228 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
12	AL	211/214 (99%)	197 (93%)	14 (7%)	0	100	100
13	AM	174/178 (98%)	160 (92%)	14 (8%)	0	100	100
14	AN	208/211 (99%)	196 (94%)	10 (5%)	2 (1%)	12	37
15	AO	132/215 (61%)	129 (98%)	3 (2%)	0	100	100
16	AP	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	AQ	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
18	AR	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
19	AS	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	AT	167/196 (85%)	164 (98%)	3 (2%)	0	100	100
21	AU	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
22	AV	157/160 (98%)	151 (96%)	5 (3%)	1 (1%)	21	50
23	AW	99/128 (77%)	90 (91%)	9 (9%)	0	100	100
24	AX	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
25	AY	60/157 (38%)	56 (93%)	4 (7%)	0	100	100
26	AZ	118/156 (76%)	117 (99%)	1 (1%)	0	100	100
27	Aa	130/145 (90%)	127 (98%)	3 (2%)	0	100	100
28	Ab	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	Ac	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
30	Ad	95/159 (60%)	92 (97%)	3 (3%)	0	100	100
31	Ae	96/115 (84%)	90 (94%)	6 (6%)	0	100	100
32	Af	104/125 (83%)	102 (98%)	2 (2%)	0	100	100
33	Ag	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
34	Ah	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	Ai	107/117 (92%)	107 (100%)	0	0	100	100
36	Aj	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Ak	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
38	Al	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
39	Am	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	An	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	Ao	49/128 (38%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Aq	101/106 (95%)	94 (93%)	7 (7%)	0	100	100
43	Ar	86/92 (94%)	84 (98%)	2 (2%)	0	100	100
44	As	121/137 (88%)	116 (96%)	5 (4%)	0	100	100
46	BB	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
47	BC	217/295 (74%)	209 (96%)	8 (4%)	0	100	100
48	BD	213/264 (81%)	203 (95%)	10 (5%)	0	100	100
49	BE	225/243 (93%)	214 (95%)	11 (5%)	0	100	100
50	BF	189/204 (93%)	172 (91%)	17 (9%)	0	100	100
51	BG	182/194 (94%)	169 (93%)	13 (7%)	0	100	100
52	BH	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
53	BI	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
54	BJ	152/158 (96%)	144 (95%)	8 (5%)	0	100	100
55	BK	123/145 (85%)	113 (92%)	10 (8%)	0	100	100
56	BL	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
57	BM	143/152 (94%)	134 (94%)	9 (6%)	0	100	100
58	BN	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
59	BO	85/119 (71%)	77 (91%)	8 (9%)	0	100	100
60	BP	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
61	BQ	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
62	BR	100/115 (87%)	99 (99%)	1 (1%)	0	100	100
63	BS	62/69 (90%)	58 (94%)	4 (6%)	0	100	100
64	BT	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
65	BU	311/317 (98%)	288 (93%)	23 (7%)	0	100	100
66	BV	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
67	BW	232/249 (93%)	226 (97%)	6 (3%)	0	100	100
68	BX	181/194 (93%)	175 (97%)	6 (3%)	0	100	100
69	BY	116/132 (88%)	109 (94%)	7 (6%)	0	100	100
70	BZ	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
71	Ba	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
72	Bb	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
73	Bc	127/133 (96%)	124 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Bd	73/125 (58%)	64 (88%)	9 (12%)	0	100	100
75	Be	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
76	Bf	56/133 (42%)	49 (88%)	7 (12%)	0	100	100
77	Bg	65/156 (42%)	59 (91%)	6 (9%)	0	100	100
78	Bh	129/135 (96%)	123 (95%)	6 (5%)	0	100	100
All	All	11164/12632 (88%)	10690 (96%)	471 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	AN	47	ALA
14	AN	64	VAL
22	AV	82	GLY

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	
4	AD	190/199 (96%)	186 (98%)	4 (2%)	47	76
5	AE	347/347 (100%)	342 (99%)	5 (1%)	59	83
6	AF	306/306 (100%)	300 (98%)	6 (2%)	48	77
7	AG	246/247 (100%)	240 (98%)	6 (2%)	43	73
8	AH	209/220 (95%)	202 (97%)	7 (3%)	33	65
9	AI	195/215 (91%)	194 (100%)	1 (0%)	81	93
10	AJ	204/223 (92%)	198 (97%)	6 (3%)	37	69
11	AK	169/171 (99%)	162 (96%)	7 (4%)	27	60
12	AL	181/182 (100%)	175 (97%)	6 (3%)	33	65
13	AM	148/149 (99%)	140 (95%)	8 (5%)	20	49
14	AN	176/177 (99%)	174 (99%)	2 (1%)	65	86
15	AO	114/161 (71%)	111 (97%)	3 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AP	171/172 (99%)	166 (97%)	5 (3%)	37	69
17	AQ	173/174 (99%)	164 (95%)	9 (5%)	21	50
18	AR	134/163 (82%)	129 (96%)	5 (4%)	30	63
19	AS	164/165 (99%)	162 (99%)	2 (1%)	63	85
20	AT	149/175 (85%)	145 (97%)	4 (3%)	39	71
21	AU	156/157 (99%)	154 (99%)	2 (1%)	61	84
22	AV	139/140 (99%)	132 (95%)	7 (5%)	22	52
23	AW	91/115 (79%)	85 (93%)	6 (7%)	15	41
24	AX	101/107 (94%)	96 (95%)	5 (5%)	22	52
25	AY	54/126 (43%)	53 (98%)	1 (2%)	50	78
26	AZ	108/133 (81%)	104 (96%)	4 (4%)	30	63
27	Aa	123/135 (91%)	121 (98%)	2 (2%)	55	81
28	Ab	117/118 (99%)	116 (99%)	1 (1%)	70	88
29	Ac	119/120 (99%)	116 (98%)	3 (2%)	42	73
30	Ad	83/126 (66%)	80 (96%)	3 (4%)	31	63
31	Ae	83/97 (86%)	77 (93%)	6 (7%)	13	37
32	Af	97/110 (88%)	94 (97%)	3 (3%)	35	67
33	Ag	114/121 (94%)	111 (97%)	3 (3%)	40	72
34	Ah	88/89 (99%)	87 (99%)	1 (1%)	65	86
35	Ai	94/100 (94%)	90 (96%)	4 (4%)	26	58
36	Aj	109/110 (99%)	107 (98%)	2 (2%)	51	79
37	Ak	85/89 (96%)	81 (95%)	4 (5%)	23	55
38	Al	73/80 (91%)	70 (96%)	3 (4%)	27	60
39	Am	63/65 (97%)	58 (92%)	5 (8%)	11	33
40	An	47/48 (98%)	46 (98%)	1 (2%)	47	76
41	Ao	47/116 (40%)	45 (96%)	2 (4%)	26	58
42	Aq	91/94 (97%)	88 (97%)	3 (3%)	33	65
43	Ar	71/75 (95%)	68 (96%)	3 (4%)	26	59
44	As	107/121 (88%)	106 (99%)	1 (1%)	70	88
46	BB	219/225 (97%)	210 (96%)	9 (4%)	27	60
47	BC	182/243 (75%)	171 (94%)	11 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BD	196/231 (85%)	187 (95%)	9 (5%)	24	56
49	BE	189/202 (94%)	183 (97%)	6 (3%)	34	66
50	BF	161/170 (95%)	157 (98%)	4 (2%)	42	73
51	BG	166/174 (95%)	161 (97%)	5 (3%)	36	68
52	BH	178/180 (99%)	172 (97%)	6 (3%)	32	65
53	BI	88/136 (65%)	85 (97%)	3 (3%)	32	65
54	BJ	138/142 (97%)	134 (97%)	4 (3%)	37	69
55	BK	111/130 (85%)	108 (97%)	3 (3%)	39	71
56	BL	117/121 (97%)	113 (97%)	4 (3%)	32	65
57	BM	125/132 (95%)	117 (94%)	8 (6%)	16	43
58	BN	111/114 (97%)	106 (96%)	5 (4%)	24	56
59	BO	83/107 (78%)	80 (96%)	3 (4%)	31	63
60	BP	67/67 (100%)	64 (96%)	3 (4%)	24	56
61	BQ	113/115 (98%)	104 (92%)	9 (8%)	11	32
62	BR	89/98 (91%)	88 (99%)	1 (1%)	65	86
63	BS	57/62 (92%)	56 (98%)	1 (2%)	51	79
64	BT	48/49 (98%)	44 (92%)	4 (8%)	10	30
65	BU	272/275 (99%)	260 (96%)	12 (4%)	25	57
66	BV	188/225 (84%)	181 (96%)	7 (4%)	30	63
67	BW	204/218 (94%)	198 (97%)	6 (3%)	37	69
68	BX	162/168 (96%)	158 (98%)	4 (2%)	42	73
69	BY	98/108 (91%)	97 (99%)	1 (1%)	68	87
70	BZ	130/131 (99%)	119 (92%)	11 (8%)	10	29
71	Ba	103/118 (87%)	100 (97%)	3 (3%)	37	69
72	Bb	112/113 (99%)	100 (89%)	12 (11%)	6	21
73	Bc	111/115 (96%)	109 (98%)	2 (2%)	51	79
74	Bd	66/103 (64%)	63 (96%)	3 (4%)	24	56
75	Be	75/76 (99%)	73 (97%)	2 (3%)	39	71
76	Bf	47/104 (45%)	41 (87%)	6 (13%)	4	13
77	Bg	59/140 (42%)	56 (95%)	3 (5%)	21	51
78	Bh	119/122 (98%)	115 (97%)	4 (3%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9720/10752 (90%)	9385 (97%)	335 (3%)	33 65

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AD	102	LEU
4	AD	142	GLU
4	AD	208	GLU
4	AD	243	THR
5	AE	5	LYS
5	AE	31	SER
5	AE	74	GLU
5	AE	90	VAL
5	AE	353	VAL
6	AF	5	ARG
6	AF	23	THR
6	AF	56	GLU
6	AF	169	LEU
6	AF	170	LEU
6	AF	209	ILE
7	AG	4	VAL
7	AG	7	VAL
7	AG	125	VAL
7	AG	155	THR
7	AG	255	LYS
7	AG	278	ASP
8	AH	49	VAL
8	AH	70	LYS
8	AH	111	LYS
8	AH	175	VAL
8	AH	186	LEU
8	AH	243	THR
8	AH	250	GLN
9	AI	53	LYS
10	AJ	31	LEU
10	AJ	55	VAL
10	AJ	100	HIS
10	AJ	114	LEU
10	AJ	190	LEU
10	AJ	231	ASP
11	AK	11	ASP
11	AK	42	ASN

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Mol	Chain	Res	Type
11	AK	46	SER
11	AK	86	LEU
11	AK	126	VAL
11	AK	151	ILE
11	AK	183	GLU
12	AL	4	ARG
12	AL	102	MET
12	AL	126	VAL
12	AL	131	ILE
12	AL	149	ILE
12	AL	212	LEU
13	AM	29	SER
13	AM	34	THR
13	AM	40	LEU
13	AM	47	THR
13	AM	88	LYS
13	AM	132	VAL
13	AM	148	THR
13	AM	163	MET
14	AN	92	ARG
14	AN	138	ASP
15	AO	43	THR
15	AO	56	GLN
15	AO	69	HIS
16	AP	9	GLU
16	AP	15	GLN
16	AP	20	ARG
16	AP	161	MET
16	AP	189	ARG
17	AQ	6	VAL
17	AQ	32	LYS
17	AQ	132	THR
17	AQ	134	LYS
17	AQ	141	LEU
17	AQ	169	ARG
17	AQ	182	GLU
17	AQ	186	GLU
17	AQ	203	VAL
18	AR	79	THR
18	AR	94	MET
18	AR	100	SER
18	AR	107	LEU

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Mol	Chain	Res	Type
18	AR	110	ASP
19	AS	49	LYS
19	AS	82	VAL
20	AT	66	ASN
20	AT	96	MET
20	AT	140	GLU
20	AT	155	LEU
21	AU	159	LEU
21	AU	169	THR
22	AV	29	THR
22	AV	52	MET
22	AV	76	VAL
22	AV	83	LYS
22	AV	124	THR
22	AV	152	GLU
22	AV	157	GLU
23	AW	18	VAL
23	AW	41	GLN
23	AW	47	ILE
23	AW	49	VAL
23	AW	65	ARG
23	AW	101	ARG
24	AX	43	LYS
24	AX	45	ILE
24	AX	48	ARG
24	AX	73	ARG
24	AX	87	SER
25	AY	4	GLU
26	AZ	91	GLU
26	AZ	119	ILE
26	AZ	147	LEU
26	AZ	156	ILE
27	Aa	49	ILE
27	Aa	94	THR
28	Ab	62	ILE
29	Ac	65	ARG
29	Ac	95	THR
29	Ac	120	GLN
30	Ad	7	HIS
30	Ad	9	THR
30	Ad	93	LEU
31	Ae	9	LYS

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Mol	Chain	Res	Type
31	Ae	19	GLN
31	Ae	40	GLN
31	Ae	55	LEU
31	Ae	94	LEU
31	Ae	96	ILE
32	Af	84	ILE
32	Af	98	SER
32	Af	113	THR
33	Ag	13	VAL
33	Ag	83	LYS
33	Ag	123	THR
34	Ah	58	VAL
35	Ai	48	VAL
35	Ai	71	LYS
35	Ai	73	HIS
35	Ai	82	MET
36	Aj	36	VAL
36	Aj	67	GLU
37	Ak	9	VAL
37	Ak	21	VAL
37	Ak	30	ARG
37	Ak	46	GLU
38	Al	6	SER
38	Al	59	THR
38	Al	83	THR
39	Am	8	ILE
39	Am	45	LEU
39	Am	56	LEU
39	Am	60	LEU
39	Am	69	LEU
40	An	39	SER
41	Ao	84	GLN
41	Ao	103	LEU
42	Aq	68	LEU
42	Aq	79	SER
42	Aq	82	MET
43	Ar	3	LYS
43	Ar	69	TRP
43	Ar	70	THR
44	As	64	ILE
46	BB	17	HIS
46	BB	42	LEU

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Mol	Chain	Res	Type
46	BB	57	THR
46	BB	76	VAL
46	BB	80	ILE
46	BB	101	LEU
46	BB	164	LEU
46	BB	179	ASN
46	BB	192	ILE
47	BC	1	MET
47	BC	75	SER
47	BC	81	ASN
47	BC	99	ILE
47	BC	122	LEU
47	BC	140	VAL
47	BC	151	ASP
47	BC	165	ASN
47	BC	182	VAL
47	BC	188	THR
47	BC	192	GLU
48	BD	47	THR
48	BD	106	THR
48	BD	108	ASP
48	BD	119	THR
48	BD	135	LEU
48	BD	153	THR
48	BD	172	MET
48	BD	175	GLU
48	BD	184	VAL
49	BE	1	MET
49	BE	24	PHE
49	BE	54	ARG
49	BE	84	VAL
49	BE	115	VAL
49	BE	170	THR
50	BF	88	MET
50	BF	134	VAL
50	BF	142	SER
50	BF	144	LEU
51	BG	80	VAL
51	BG	86	LYS
51	BG	120	ARG
51	BG	144	ILE
51	BG	184	ASP

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Mol	Chain	Res	Type
52	BH	14	THR
52	BH	29	LEU
52	BH	43	ILE
52	BH	61	ASP
52	BH	76	THR
52	BH	151	GLU
53	BI	21	MET
53	BI	46	MET
53	BI	94	LEU
54	BJ	24	LEU
54	BJ	78	THR
54	BJ	125	ILE
54	BJ	127	THR
55	BK	56	LEU
55	BK	70	MET
55	BK	122	THR
56	BL	34	VAL
56	BL	42	ILE
56	BL	119	LEU
56	BL	142	GLN
57	BM	26	ILE
57	BM	33	ILE
57	BM	39	ARG
57	BM	59	LEU
57	BM	71	MET
57	BM	75	ARG
57	BM	78	LYS
57	BM	129	LEU
58	BN	14	PHE
58	BN	97	LYS
58	BN	110	LEU
58	BN	123	LEU
58	BN	129	ARG
59	BO	56	MET
59	BO	79	ARG
59	BO	84	ILE
60	BP	22	ARG
60	BP	36	VAL
60	BP	43	THR
61	BQ	4	CYS
61	BQ	7	LEU
61	BQ	18	ARG

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Mol	Chain	Res	Type
61	BQ	21	LYS
61	BQ	51	VAL
61	BQ	70	VAL
61	BQ	96	GLU
61	BQ	100	VAL
61	BQ	115	ILE
62	BR	52	ASP
63	BS	32	VAL
64	BT	27	ARG
64	BT	30	LEU
64	BT	44	ARG
64	BT	50	ILE
65	BU	26	GLN
65	BU	31	ILE
65	BU	37	ASP
65	BU	66	VAL
65	BU	84	ASP
65	BU	86	THR
65	BU	105	THR
65	BU	133	ASN
65	BU	206	LEU
65	BU	215	GLN
65	BU	309	VAL
65	BU	313	THR
66	BV	65	LYS
66	BV	97	PHE
66	BV	101	SER
66	BV	109	ILE
66	BV	139	LEU
66	BV	215	MET
66	BV	230	THR
67	BW	5	ILE
67	BW	7	PHE
67	BW	26	THR
67	BW	82	SER
67	BW	179	LEU
67	BW	227	GLN
68	BX	8	VAL
68	BX	81	LEU
68	BX	125	HIS
68	BX	129	LEU
69	BY	62	VAL

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Mol	Chain	Res	Type
70	BZ	22	VAL
70	BZ	33	VAL
70	BZ	37	ILE
70	BZ	64	ARG
70	BZ	67	THR
70	BZ	92	ILE
70	BZ	109	LYS
70	BZ	110	ASP
70	BZ	119	GLU
70	BZ	122	ILE
70	BZ	134	VAL
71	Ba	95	ILE
71	Ba	105	THR
71	Ba	141	THR
72	Bb	2	VAL
72	Bb	14	ILE
72	Bb	26	LEU
72	Bb	31	SER
72	Bb	42	MET
72	Bb	46	TYR
72	Bb	63	VAL
72	Bb	66	THR
72	Bb	81	VAL
72	Bb	90	GLN
72	Bb	103	VAL
72	Bb	111	MET
73	Bc	74	MET
73	Bc	89	HIS
74	Bd	51	ASP
74	Bd	77	LEU
74	Bd	97	ILE
75	Be	8	LEU
75	Be	74	THR
76	Bf	11	LYS
76	Bf	16	THR
76	Bf	22	GLN
76	Bf	27	LYS
76	Bf	46	VAL
76	Bf	56	ASN
77	Bg	86	THR
77	Bg	105	TYR
77	Bg	144	CYS

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Mol	Chain	Res	Type
78	Bh	7	LYS
78	Bh	11	LYS
78	Bh	66	VAL
78	Bh	95	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	121	ASN
5	AE	186	ASN
5	AE	208	ASN
6	AF	43	ASN
6	AF	212	ASN
6	AF	236	ASN
6	AF	299	GLN
6	AF	329	ASN
7	AG	63	GLN
8	AH	205	ASN
8	AH	250	GLN
9	AI	56	HIS
9	AI	80	ASN
9	AI	110	GLN
9	AI	206	ASN
10	AJ	85	GLN
11	AK	7	ASN
12	AL	143	GLN
13	AM	65	ASN
13	AM	112	HIS
13	AM	155	HIS
14	AN	104	ASN
16	AP	145	ASN
17	AQ	42	ASN
17	AQ	50	ASN
18	AR	56	GLN
19	AS	125	GLN
24	AX	135	ASN
27	Aa	14	ASN
27	Aa	18	HIS
27	Aa	86	GLN
29	Ac	44	ASN
30	Ad	11	ASN
30	Ad	42	ASN

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Mol	Chain	Res	Type
32	Af	116	ASN
33	Ag	34	ASN
33	Ag	57	ASN
34	Ah	21	GLN
38	Al	13	ASN
38	Al	57	ASN
41	Ao	84	GLN
44	As	23	GLN
44	As	85	ASN
46	BB	67	GLN
46	BB	98	ASN
46	BB	179	ASN
48	BD	157	GLN
50	BF	74	ASN
50	BF	82	ASN
50	BF	148	ASN
51	BG	12	ASN
51	BG	68	GLN
52	BH	9	HIS
52	BH	99	ASN
52	BH	111	GLN
52	BH	165	GLN
53	BI	50	GLN
53	BI	84	HIS
54	BJ	39	ASN
55	BK	54	HIS
56	BL	142	GLN
58	BN	10	ASN
58	BN	142	ASN
59	BO	47	ASN
60	BP	49	GLN
61	BQ	31	HIS
63	BS	29	GLN
64	BT	3	HIS
65	BU	133	ASN
65	BU	159	ASN
67	BW	146	ASN
70	BZ	69	ASN
73	Bc	94	HIS
74	Bd	45	ASN
76	Bf	22	GLN
78	Bh	116	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3705/5069 (73%)	846 (22%)	10 (0%)
2	AB	119/120 (99%)	12 (10%)	0
3	AC	155/157 (98%)	27 (17%)	1 (0%)
45	BA	1711/1869 (91%)	467 (27%)	4 (0%)
All	All	5690/7215 (78%)	1352 (23%)	15 (0%)

All (1352) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	21	G
1	AA	25	A
1	AA	39	A
1	AA	42	A
1	AA	48	G
1	AA	56	A
1	AA	59	A
1	AA	63	G
1	AA	64	A
1	AA	65	A
1	AA	66	A
1	AA	72	C
1	AA	74	G
1	AA	91	G
1	AA	104	G
1	AA	108	A
1	AA	109	G
1	AA	110	C
1	AA	112	C
1	AA	119	G
1	AA	133	C
1	AA	134	G
1	AA	135	G
1	AA	136	C
1	AA	141	C
1	AA	144	G
1	AA	146	G
1	AA	152	U
1	AA	158	A
1	AA	159	C
1	AA	173	C
1	AA	175	C

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Mol	Chain	Res	Type
1	AA	177	G
1	AA	179	G
1	AA	183	C
1	AA	184	U
1	AA	185	C
1	AA	186	G
1	AA	188	G
1	AA	189	G
1	AA	195	C
1	AA	200	U
1	AA	205	C
1	AA	210	C
1	AA	213	G
1	AA	216	C
1	AA	218	A
1	AA	219	G
1	AA	234	G
1	AA	246	G
1	AA	251	C
1	AA	253	G
1	AA	255	C
1	AA	256	G
1	AA	259	C
1	AA	261	G
1	AA	262	G
1	AA	264	C
1	AA	265	C
1	AA	266	C
1	AA	267	G
1	AA	272	U
1	AA	275	C
1	AA	276	C
1	AA	280	G
1	AA	297	U
1	AA	306	A
1	AA	315	G
1	AA	316	U
1	AA	340	C
1	AA	341	G
1	AA	373	G
1	AA	387	G
1	AA	399	G

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Mol	Chain	Res	Type
1	AA	407	A
1	AA	408	A
1	AA	409	G
1	AA	410	A
1	AA	412	G
1	AA	413	G
1	AA	415	G
1	AA	449	C
1	AA	450	G
1	AA	452	A
1	AA	453	G
1	AA	454	U
1	AA	456	C
1	AA	457	G
1	AA	464	G
1	AA	467	U
1	AA	483	G
1	AA	484	U
1	AA	485	C
1	AA	486	C
1	AA	487	G
1	AA	490	C
1	AA	491	G
1	AA	493	G
1	AA	494	U
1	AA	497	G
1	AA	498	C
1	AA	499	G
1	AA	500	G
1	AA	501	C
1	AA	502	C
1	AA	503	C
1	AA	504	G
1	AA	507	G
1	AA	509	A
1	AA	513	U
1	AA	514	U
1	AA	515	C
1	AA	516	C
1	AA	517	C
1	AA	518	G
1	AA	643	C

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Mol	Chain	Res	Type
1	AA	644	G
1	AA	645	G
1	AA	653	U
1	AA	654	C
1	AA	656	C
1	AA	657	C
1	AA	659	G
1	AA	660	A
1	AA	664	G
1	AA	665	C
1	AA	666	G
1	AA	667	A
1	AA	668	C
1	AA	669	C
1	AA	670	G
1	AA	671	G
1	AA	673	C
1	AA	685	C
1	AA	686	A
1	AA	687	U
1	AA	696	C
1	AA	703	G
1	AA	704	C
1	AA	730	G
1	AA	731	G
1	AA	738	C
1	AA	739	G
1	AA	740	G
1	AA	742	G
1	AA	746	A
1	AA	747	A
1	AA	750	U
1	AA	758	G
1	AA	904	C
1	AA	905	C
1	AA	913	U
1	AA	914	U
1	AA	915	A
1	AA	917	A
1	AA	918	G
1	AA	923	C
1	AA	924	C

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Mol	Chain	Res	Type
1	AA	926	G
1	AA	932	A
1	AA	933	G
1	AA	934	C
1	AA	935	A
1	AA	937	U
1	AA	943	A
1	AA	945	U
1	AA	946	C
1	AA	956	A
1	AA	959	G
1	AA	960	A
1	AA	961	G
1	AA	962	C
1	AA	965	G
1	AA	966	A
1	AA	967	C
1	AA	968	C
1	AA	970	G
1	AA	971	U
1	AA	972	C
1	AA	982	U
1	AA	984	C
1	AA	986	C
1	AA	989	U
1	AA	990	C
1	AA	991	C
1	AA	992	C
1	AA	994	G
1	AA	995	C
1	AA	1048	G
1	AA	1049	C
1	AA	1067	G
1	AA	1070	G
1	AA	1071	C
1	AA	1078	A
1	AA	1082	C
1	AA	1084	C
1	AA	1090	G
1	AA	1092	G
1	AA	1168	G
1	AA	1171	G

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Mol	Chain	Res	Type
1	AA	1173	G
1	AA	1178	G
1	AA	1179	U
1	AA	1180	C
1	AA	1181	C
1	AA	1182	C
1	AA	1183	C
1	AA	1200	G
1	AA	1202	C
1	AA	1203	G
1	AA	1205	G
1	AA	1211	G
1	AA	1215	C
1	AA	1220	G
1	AA	1221	G
1	AA	1222	A
1	AA	1240	G
1	AA	1241	C
1	AA	1255	A
1	AA	1266	G
1	AA	1271	G
1	AA	1272	C
1	AA	1273	G
1	AA	1275	G
1	AA	1277	G
1	AA	1280	C
1	AA	1284	G
1	AA	1287	G
1	AA	1293	G
1	AA	1294	A
1	AA	1296	G
1	AA	1300	G
1	AA	1302	U
1	AA	1326	A2M
1	AA	1337	A
1	AA	1339	U
1	AA	1354	A
1	AA	1358	G
1	AA	1359	G
1	AA	1365	C
1	AA	1367	C
1	AA	1379	C

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Mol	Chain	Res	Type
1	AA	1381	U
1	AA	1387	A
1	AA	1394	G
1	AA	1397	A
1	AA	1398	A
1	AA	1403	G
1	AA	1404	G
1	AA	1407	C
1	AA	1408	G
1	AA	1409	C
1	AA	1410	U
1	AA	1411	C
1	AA	1412	G
1	AA	1415	G
1	AA	1420	A
1	AA	1421	G
1	AA	1435	G
1	AA	1437	C
1	AA	1439	C
1	AA	1442	C
1	AA	1443	A
1	AA	1444	G
1	AA	1445	U
1	AA	1446	C
1	AA	1447	C
1	AA	1449	C
1	AA	1458	C
1	AA	1480	C
1	AA	1482	G
1	AA	1483	C
1	AA	1485	C
1	AA	1486	C
1	AA	1493	G
1	AA	1498	G
1	AA	1501	C
1	AA	1502	G
1	AA	1514	U
1	AA	1516	G
1	AA	1525	A
1	AA	1534	A2M
1	AA	1547	A
1	AA	1553	A

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Mol	Chain	Res	Type
1	AA	1566	C
1	AA	1573	G
1	AA	1574	G
1	AA	1578	U
1	AA	1591	U
1	AA	1596	U
1	AA	1612	G
1	AA	1624	G
1	AA	1625	OMG
1	AA	1626	G
1	AA	1631	A
1	AA	1633	G
1	AA	1634	A
1	AA	1638	A
1	AA	1641	G
1	AA	1650	A
1	AA	1654	G
1	AA	1661	C
1	AA	1676	C
1	AA	1691	G
1	AA	1698	C
1	AA	1699	A
1	AA	1700	G
1	AA	1701	A
1	AA	1702	C
1	AA	1703	C
1	AA	1704	C
1	AA	1705	G
1	AA	1708	G
1	AA	1731	C
1	AA	1741	G
1	AA	1742	A
1	AA	1757	U
1	AA	1758	G
1	AA	1759	G
1	AA	1760	G
1	AA	1761	G
1	AA	1762	C
1	AA	1763	C
1	AA	1764	G
1	AA	1765	A
1	AA	1766	A

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Mol	Chain	Res	Type
1	AA	1768	C
1	AA	1771	U
1	AA	1772	C
1	AA	1780	A
1	AA	1781	PSU
1	AA	1785	C
1	AA	1787	A
1	AA	1803	G
1	AA	1804	A
1	AA	1806	G
1	AA	1810	G
1	AA	1821	G
1	AA	1833	G
1	AA	1834	U
1	AA	1836	G
1	AA	1837	A
1	AA	1842	G
1	AA	1855	G
1	AA	1869	G
1	AA	1881	OMC
1	AA	1893	C
1	AA	1897	A
1	AA	1917	A
1	AA	1918	U
1	AA	1919	G
1	AA	1921	C
1	AA	1922	G
1	AA	1925	G
1	AA	1931	C
1	AA	1932	A
1	AA	1938	C
1	AA	1940	G
1	AA	1945	G
1	AA	1947	U
1	AA	1959	U
1	AA	1960	A
1	AA	1961	G
1	AA	1963	C
1	AA	1966	C
1	AA	1967	A
1	AA	1968	G
1	AA	1971	C

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Mol	Chain	Res	Type
1	AA	1972	G
1	AA	1973	G
1	AA	1974	U
1	AA	1975	G
1	AA	1978	C
1	AA	1979	A
1	AA	1980	U
1	AA	1981	G
1	AA	1982	G
1	AA	1983	A
1	AA	1984	A
1	AA	1985	G
1	AA	1987	C
1	AA	1988	G
1	AA	1990	A
1	AA	1991	A
1	AA	1993	C
1	AA	1994	C
1	AA	1995	G
1	AA	1996	C
1	AA	1997	U
1	AA	1998	A
1	AA	2000	G
1	AA	2001	G
1	AA	2002	A
1	AA	2003	G
1	AA	2004	U
1	AA	2007	G
1	AA	2009	A
1	AA	2010	A
1	AA	2011	C
1	AA	2012	A
1	AA	2013	A
1	AA	2014	C
1	AA	2015	U
1	AA	2016	C
1	AA	2018	C
1	AA	2019	C
1	AA	2020	U
1	AA	2022	C
1	AA	2023	C
1	AA	2024	G

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Mol	Chain	Res	Type
1	AA	2025	A
1	AA	2026	A
1	AA	2031	C
1	AA	2046	G
1	AA	2048	U
1	AA	2055	G
1	AA	2056	G
1	AA	2069	A
1	AA	2071	A
1	AA	2083	C
1	AA	2084	C
1	AA	2085	G
1	AA	2092	G
1	AA	2093	A
1	AA	2095	A
1	AA	2096	G
1	AA	2097	U
1	AA	2098	G
1	AA	2100	A
1	AA	2101	C
1	AA	2102	G
1	AA	2104	G
1	AA	2105	A
1	AA	2106	G
1	AA	2108	G
1	AA	2110	C
1	AA	2111	G
1	AA	2112	G
1	AA	2113	G
1	AA	2252	G
1	AA	2253	A
1	AA	2255	C
1	AA	2256	C
1	AA	2258	C
1	AA	2259	G
1	AA	2262	G
1	AA	2289	C
1	AA	2300	A
1	AA	2301	G
1	AA	2306	G
1	AA	2313	A
1	AA	2316	G

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Mol	Chain	Res	Type
1	AA	2333	G
1	AA	2345	G
1	AA	2348	G
1	AA	2351	OMC
1	AA	2364	OMG
1	AA	2392	C
1	AA	2395	A
1	AA	2397	G
1	AA	2410	C
1	AA	2416	G
1	AA	2421	G
1	AA	2422	OMC
1	AA	2425	U
1	AA	2441	C
1	AA	2450	G
1	AA	2470	C
1	AA	2475	G
1	AA	2483	G
1	AA	2484	A
1	AA	2485	U
1	AA	2486	G
1	AA	2487	G
1	AA	2488	C
1	AA	2489	C
1	AA	2491	C
1	AA	2492	C
1	AA	2493	G
1	AA	2501	C
1	AA	2503	G
1	AA	2504	C
1	AA	2505	C
1	AA	2506	G
1	AA	2507	A
1	AA	2513	A
1	AA	2514	G
1	AA	2518	G
1	AA	2519	U
1	AA	2529	A
1	AA	2544	G
1	AA	2546	G
1	AA	2547	G
1	AA	2553	A

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Mol	Chain	Res	Type
1	AA	2555	G
1	AA	2560	C
1	AA	2573	A
1	AA	2574	G
1	AA	2583	C
1	AA	2586	G
1	AA	2587	A
1	AA	2589	C
1	AA	2601	A
1	AA	2619	G
1	AA	2627	C
1	AA	2632	PSU
1	AA	2652	G
1	AA	2653	C
1	AA	2658	G
1	AA	2662	G
1	AA	2669	C
1	AA	2670	C
1	AA	2675	G
1	AA	2676	A
1	AA	2686	G
1	AA	2687	U
1	AA	2688	G
1	AA	2694	G
1	AA	2695	A
1	AA	2696	A
1	AA	2700	G
1	AA	2710	C
1	AA	2711	G
1	AA	2712	G
1	AA	2719	C
1	AA	2724	G
1	AA	2726	G
1	AA	2727	C
1	AA	2739	C
1	AA	2742	G
1	AA	2743	A
1	AA	2759	G
1	AA	2760	G
1	AA	2761	U
1	AA	2763	U
1	AA	2764	A

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Mol	Chain	Res	Type
1	AA	2770	C
1	AA	2788	U
1	AA	2790	U
1	AA	2791	C
1	AA	2806	A
1	AA	2814	C
1	AA	2815	A2M
1	AA	2826	U
1	AA	2827	G
1	AA	2855	G
1	AA	2892	C
1	AA	2899	C
1	AA	2902	G
1	AA	2903	G
1	AA	2904	U
1	AA	2906	G
1	AA	2908	U
1	AA	2910	G
1	AA	3585	G
1	AA	3586	G
1	AA	3593	C
1	AA	3594	C
1	AA	3595	U
1	AA	3596	A
1	AA	3597	G
1	AA	3604	A
1	AA	3606	U
1	AA	3615	G
1	AA	3618	C
1	AA	3626	G
1	AA	3635	A
1	AA	3646	A
1	AA	3648	A
1	AA	3662	A
1	AA	3663	A
1	AA	3670	C
1	AA	3673	C
1	AA	3674	G
1	AA	3710	G
1	AA	3711	A
1	AA	3712	A
1	AA	3713	U

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Mol	Chain	Res	Type
1	AA	3714	G
1	AA	3727	A
1	AA	3748	A
1	AA	3756	A
1	AA	3757	G
1	AA	3758	U
1	AA	3759	A
1	AA	3761	C
1	AA	3764	PSU
1	AA	3771	C
1	AA	3773	U
1	AA	3774	A
1	AA	3776	G
1	AA	3777	G
1	AA	3785	A2M
1	AA	3786	U
1	AA	3788	C
1	AA	3811	G
1	AA	3812	C
1	AA	3814	U
1	AA	3817	A
1	AA	3819	G
1	AA	3838	U
1	AA	3839	G
1	AA	3840	U
1	AA	3844	PSU
1	AA	3877	A
1	AA	3878	C
1	AA	3879	G
1	AA	3893	C
1	AA	3897	G
1	AA	3901	A
1	AA	3906	A
1	AA	3907	G
1	AA	3908	A
1	AA	3909	C
1	AA	3915	U
1	AA	3938	G
1	AA	3947	A
1	AA	3949	A
1	AA	3956	G
1	AA	3957	U

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Mol	Chain	Res	Type
1	AA	3958	G
1	AA	3960	A
1	AA	3961	G
1	AA	3963	A
1	AA	3964	U
1	AA	3966	A
1	AA	3967	G
1	AA	3969	G
1	AA	3971	G
1	AA	3972	A
1	AA	3973	G
1	AA	3977	C
1	AA	4035	G
1	AA	4038	C
1	AA	4042	G
1	AA	4044	U
1	AA	4045	G
1	AA	4048	A
1	AA	4049	U
1	AA	4050	A
1	AA	4051	C
1	AA	4052	C
1	AA	4053	A
1	AA	4054	C
1	AA	4055	U
1	AA	4056	A
1	AA	4057	C
1	AA	4058	U
1	AA	4059	C
1	AA	4062	A
1	AA	4063	U
1	AA	4064	C
1	AA	4065	G
1	AA	4068	U
1	AA	4069	U
1	AA	4076	G
1	AA	4084	G
1	AA	4094	G
1	AA	4095	G
1	AA	4099	G
1	AA	4100	C
1	AA	4102	C

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Mol	Chain	Res	Type
1	AA	4103	C
1	AA	4104	G
1	AA	4105	A
1	AA	4106	G
1	AA	4107	G
1	AA	4108	G
1	AA	4109	G
1	AA	4110	C
1	AA	4112	C
1	AA	4113	U
1	AA	4115	G
1	AA	4119	C
1	AA	4120	U
1	AA	4121	G
1	AA	4122	G
1	AA	4127	A
1	AA	4133	C
1	AA	4139	G
1	AA	4140	C
1	AA	4141	G
1	AA	4142	C
1	AA	4143	G
1	AA	4144	C
1	AA	4146	G
1	AA	4147	G
1	AA	4150	G
1	AA	4162	C
1	AA	4163	U
1	AA	4170	A
1	AA	4183	G
1	AA	4184	G
1	AA	4191	G
1	AA	4203	A
1	AA	4222	G
1	AA	4228	OMG
1	AA	4229	U
1	AA	4233	A
1	AA	4234	A
1	AA	4243	C
1	AA	4251	A
1	AA	4254	G
1	AA	4255	A

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Mol	Chain	Res	Type
1	AA	4256	A
1	AA	4266	G
1	AA	4268	A
1	AA	4271	A
1	AA	4273	A
1	AA	4281	A
1	AA	4291	G
1	AA	4295	U
1	AA	4297	G
1	AA	4304	A
1	AA	4305	G
1	AA	4314	C
1	AA	4329	G
1	AA	4330	G
1	AA	4332	C
1	AA	4349	C
1	AA	4354	U
1	AA	4377	G
1	AA	4378	A
1	AA	4379	A
1	AA	4387	C
1	AA	4391	G
1	AA	4394	A
1	AA	4405	G
1	AA	4419	U
1	AA	4421	C
1	AA	4422	A
1	AA	4427	G
1	AA	4428	A
1	AA	4437	U
1	AA	4444	C
1	AA	4448	G
1	AA	4449	A
1	AA	4464	A
1	AA	4466	C
1	AA	4474	A
1	AA	4475	G
1	AA	4478	G
1	AA	4480	A
1	AA	4485	C
1	AA	4486	C
1	AA	4488	A

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Mol	Chain	Res	Type
1	AA	4500	PSU
1	AA	4512	U
1	AA	4513	A
1	AA	4518	A
1	AA	4519	C
1	AA	4524	G
1	AA	4525	C
1	AA	4545	G
1	AA	4548	A
1	AA	4549	G
1	AA	4560	C
1	AA	4567	G
1	AA	4568	A
1	AA	4573	G
1	AA	4575	G
1	AA	4590	A2M
1	AA	4599	A
1	AA	4601	U
1	AA	4627	U
1	AA	4636	PSU
1	AA	4637	OMG
1	AA	4652	G
1	AA	4656	A
1	AA	4670	C
1	AA	4672	A
1	AA	4694	G
1	AA	4695	C
1	AA	4699	U
1	AA	4708	A
1	AA	4709	U
1	AA	4730	C
1	AA	4731	G
1	AA	4733	C
1	AA	4734	A
1	AA	4741	C
1	AA	4742	G
1	AA	4743	G
1	AA	4745	G
1	AA	4750	G
1	AA	4755	G
1	AA	4757	C
1	AA	4758	U

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Mol	Chain	Res	Type
1	AA	4759	C
1	AA	4761	G
1	AA	4765	G
1	AA	4770	U
1	AA	4774	C
1	AA	4775	C
1	AA	4859	C
1	AA	4870	G
1	AA	4871	C
1	AA	4875	G
1	AA	4876	U
1	AA	4882	U
1	AA	4883	C
1	AA	4889	G
1	AA	4890	G
1	AA	4895	C
1	AA	4896	G
1	AA	4900	C
1	AA	4901	G
1	AA	4906	C
1	AA	4910	A
1	AA	4911	A
1	AA	4912	G
1	AA	4913	G
1	AA	4914	C
1	AA	4927	G
1	AA	4928	C
1	AA	4937	C
1	AA	4938	A
1	AA	4940	C
1	AA	4941	G
1	AA	4943	A
1	AA	4949	G
1	AA	4960	G
1	AA	4963	G
1	AA	4964	C
1	AA	4966	A
1	AA	4976	U
1	AA	4979	A
1	AA	4990	C
1	AA	4991	U
1	AA	5006	U

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Mol	Chain	Res	Type
1	AA	5013	C
1	AA	5014	A
1	AA	5017	G
1	AA	5023	C
1	AA	5024	C
1	AA	5025	C
1	AA	5030	U
1	AA	5032	C
1	AA	5034	A
1	AA	5041	G
1	AA	5050	C
1	AA	5054	C
1	AA	5055	G
1	AA	5061	A
1	AA	5062	G
1	AA	5069	U
2	AB	11	A
2	AB	21	G
2	AB	22	A
2	AB	27	G
2	AB	53	U
2	AB	54	A
2	AB	64	G
2	AB	74	A
2	AB	85	G
2	AB	100	A
2	AB	110	G
2	AB	116	G
3	AC	23	C
3	AC	34	U
3	AC	35	C
3	AC	52	A
3	AC	59	A
3	AC	62	A
3	AC	63	U
3	AC	80	A
3	AC	82	A
3	AC	84	A
3	AC	85	U
3	AC	86	U
3	AC	87	G
3	AC	94	G

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Mol	Chain	Res	Type
3	AC	103	A
3	AC	105	C
3	AC	110	U
3	AC	114	G
3	AC	123	U
3	AC	124	U
3	AC	125	C
3	AC	126	C
3	AC	127	U
3	AC	128	C
3	AC	150	C
3	AC	151	G
3	AC	156	U
45	BA	4	C
45	BA	13	C
45	BA	20	G
45	BA	26	U
45	BA	27	A2M
45	BA	33	G
45	BA	41	G
45	BA	42	A
45	BA	44	U
45	BA	46	A
45	BA	56	G
45	BA	59	U
45	BA	60	A
45	BA	61	A
45	BA	62	G
45	BA	65	C
45	BA	67	C
45	BA	68	A
45	BA	71	G
45	BA	72	C
45	BA	73	C
45	BA	74	G
45	BA	75	G
45	BA	76	U
45	BA	80	G
45	BA	103	A
45	BA	113	G
45	BA	114	G
45	BA	115	U

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Mol	Chain	Res	Type
45	BA	126	G
45	BA	127	C
45	BA	130	G
45	BA	140	C
45	BA	142	C
45	BA	143	U
45	BA	145	G
45	BA	149	A
45	BA	151	C
45	BA	155	G
45	BA	156	G
45	BA	158	A
45	BA	159	A2M
45	BA	160	U
45	BA	162	C
45	BA	166	A2M
45	BA	170	A
45	BA	173	A
45	BA	182	C
45	BA	187	G
45	BA	190	G
45	BA	197	U
45	BA	198	U
45	BA	199	C
45	BA	200	G
45	BA	202	G
45	BA	203	G
45	BA	204	G
45	BA	215	G
45	BA	220	U
45	BA	224	A
45	BA	288	G
45	BA	291	G
45	BA	294	U
45	BA	295	C
45	BA	301	A
45	BA	305	U
45	BA	306	C
45	BA	307	G
45	BA	308	G
45	BA	309	G
45	BA	318	A

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Mol	Chain	Res	Type
45	BA	319	C
45	BA	321	C
45	BA	322	C
45	BA	324	C
45	BA	325	C
45	BA	326	C
45	BA	327	G
45	BA	328	U
45	BA	329	G
45	BA	335	G
45	BA	336	A
45	BA	347	G
45	BA	351	G
45	BA	353	C
45	BA	360	A
45	BA	362	C
45	BA	364	A
45	BA	368	U
45	BA	370	G
45	BA	380	G
45	BA	385	G
45	BA	386	C
45	BA	400	C
45	BA	407	G
45	BA	408	A
45	BA	409	C
45	BA	410	G
45	BA	436	OMG
45	BA	448	A
45	BA	450	C
45	BA	452	G
45	BA	462	OMC
45	BA	464	A
45	BA	471	G
45	BA	472	C
45	BA	473	A
45	BA	474	G
45	BA	482	G
45	BA	483	C
45	BA	485	A
45	BA	487	U
45	BA	488	U

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Mol	Chain	Res	Type
45	BA	492	C
45	BA	493	A
45	BA	496	C
45	BA	500	A
45	BA	501	C
45	BA	512	A2M
45	BA	516	A
45	BA	532	C
45	BA	533	A
45	BA	536	A
45	BA	537	C
45	BA	538	U
45	BA	539	C
45	BA	545	A
45	BA	546	G
45	BA	554	A
45	BA	555	A
45	BA	557	U
45	BA	558	G
45	BA	559	G
45	BA	563	G
45	BA	570	C
45	BA	573	U
45	BA	580	U
45	BA	583	A
45	BA	588	G
45	BA	589	G
45	BA	590	A2M
45	BA	591	U
45	BA	592	C
45	BA	593	C
45	BA	594	A
45	BA	601	OMG
45	BA	604	A
45	BA	606	G
45	BA	607	U
45	BA	614	C
45	BA	617	G
45	BA	623	G
45	BA	627	U
45	BA	628	A
45	BA	631	U

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Mol	Chain	Res	Type
45	BA	643	A
45	BA	655	A
45	BA	659	G
45	BA	660	C
45	BA	662	G
45	BA	667	PSU
45	BA	668	A2M
45	BA	669	A
45	BA	671	A
45	BA	673	G
45	BA	689	U
45	BA	692	G
45	BA	694	G
45	BA	696	G
45	BA	697	G
45	BA	698	G
45	BA	731	G
45	BA	732	U
45	BA	736	C
45	BA	737	G
45	BA	738	C
45	BA	747	U
45	BA	748	C
45	BA	749	U
45	BA	750	C
45	BA	751	G
45	BA	752	G
45	BA	753	C
45	BA	787	G
45	BA	788	G
45	BA	791	C
45	BA	792	C
45	BA	793	G
45	BA	797	C
45	BA	798	G
45	BA	799	U
45	BA	801	PSU
45	BA	807	G
45	BA	808	A
45	BA	811	A
45	BA	821	G
45	BA	823	U

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Mol	Chain	Res	Type
45	BA	830	A
45	BA	836	G
45	BA	837	A
45	BA	838	G
45	BA	839	C
45	BA	842	C
45	BA	847	A
45	BA	852	G
45	BA	861	A
45	BA	862	A
45	BA	867	OMG
45	BA	869	A
45	BA	870	A
45	BA	872	A
45	BA	873	G
45	BA	881	G
45	BA	883	U
45	BA	884	C
45	BA	887	U
45	BA	888	U
45	BA	891	G
45	BA	892	U
45	BA	893	U
45	BA	894	G
45	BA	895	G
45	BA	896	U
45	BA	898	U
45	BA	899	U
45	BA	900	C
45	BA	901	G
45	BA	905	C
45	BA	909	G
45	BA	912	C
45	BA	913	A
45	BA	917	U
45	BA	919	A
45	BA	920	A
45	BA	922	A
45	BA	933	G
45	BA	953	C
45	BA	955	A
45	BA	968	U

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Mol	Chain	Res	Type
45	BA	970	G
45	BA	971	G
45	BA	990	A
45	BA	992	A
45	BA	1017	U
45	BA	1019	C
45	BA	1023	A
45	BA	1027	A
45	BA	1042	A
45	BA	1060	A
45	BA	1061	U
45	BA	1062	A
45	BA	1064	C
45	BA	1067	C
45	BA	1080	A
45	BA	1083	A
45	BA	1085	C
45	BA	1086	G
45	BA	1087	A
45	BA	1097	G
45	BA	1109	C
45	BA	1115	U
45	BA	1116	C
45	BA	1118	C
45	BA	1120	U
45	BA	1121	G
45	BA	1123	C
45	BA	1126	G
45	BA	1131	G
45	BA	1134	G
45	BA	1138	C
45	BA	1139	C
45	BA	1146	C
45	BA	1149	A
45	BA	1153	C
45	BA	1154	U
45	BA	1155	U
45	BA	1166	G
45	BA	1170	A
45	BA	1184	G
45	BA	1194	A
45	BA	1195	A

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Mol	Chain	Res	Type
45	BA	1200	A
45	BA	1207	G
45	BA	1208	A
45	BA	1213	C
45	BA	1215	C
45	BA	1216	C
45	BA	1217	A
45	BA	1224	G
45	BA	1227	G
45	BA	1235	G
45	BA	1242	U
45	BA	1243	U
45	BA	1247	C
45	BA	1249	C
45	BA	1251	A
45	BA	1253	A
45	BA	1256	G
45	BA	1257	G
45	BA	1259	A
45	BA	1263	U
45	BA	1266	C
45	BA	1271	C
45	BA	1273	C
45	BA	1274	G
45	BA	1275	G
45	BA	1282	A
45	BA	1284	A
45	BA	1285	G
45	BA	1286	G
45	BA	1290	G
45	BA	1298	G
45	BA	1300	U
45	BA	1301	A
45	BA	1302	G
45	BA	1303	C
45	BA	1308	U
45	BA	1310	U
45	BA	1311	C
45	BA	1313	A
45	BA	1327	G
45	BA	1331	C
45	BA	1333	U

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Mol	Chain	Res	Type
45	BA	1337	4AC
45	BA	1341	C
45	BA	1342	U
45	BA	1343	U
45	BA	1360	PSU
45	BA	1361	G
45	BA	1371	U
45	BA	1372	U
45	BA	1378	A
45	BA	1396	A
45	BA	1397	U
45	BA	1402	A
45	BA	1403	C
45	BA	1404	U
45	BA	1413	G
45	BA	1414	A
45	BA	1415	C
45	BA	1418	C
45	BA	1419	C
45	BA	1421	A
45	BA	1422	G
45	BA	1424	G
45	BA	1427	C
45	BA	1429	G
45	BA	1434	C
45	BA	1435	C
45	BA	1436	C
45	BA	1438	A
45	BA	1449	G
45	BA	1452	A
45	BA	1454	A
45	BA	1455	A
45	BA	1461	G
45	BA	1462	U
45	BA	1463	U
45	BA	1465	A
45	BA	1466	G
45	BA	1473	G
45	BA	1489	A
45	BA	1491	G
45	BA	1494	U
45	BA	1495	G

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Mol	Chain	Res	Type
45	BA	1498	A
45	BA	1508	A
45	BA	1509	U
45	BA	1519	U
45	BA	1521	C
45	BA	1522	A
45	BA	1528	G
45	BA	1531	A
45	BA	1533	A
45	BA	1535	U
45	BA	1545	A
45	BA	1547	C
45	BA	1548	G
45	BA	1551	U
45	BA	1552	G
45	BA	1553	C
45	BA	1554	C
45	BA	1556	A
45	BA	1557	C
45	BA	1560	U
45	BA	1566	G
45	BA	1570	G
45	BA	1579	A
45	BA	1580	A
45	BA	1581	C
45	BA	1584	G
45	BA	1585	U
45	BA	1587	G
45	BA	1588	A
45	BA	1591	C
45	BA	1597	C
45	BA	1599	U
45	BA	1601	A
45	BA	1604	G
45	BA	1605	G
45	BA	1606	G
45	BA	1607	A
45	BA	1615	U
45	BA	1620	A
45	BA	1621	U
45	BA	1623	A
45	BA	1637	A

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Mol	Chain	Res	Type
45	BA	1642	U
45	BA	1643	PSU
45	BA	1646	C
45	BA	1648	G
45	BA	1649	U
45	BA	1654	G
45	BA	1664	A
45	BA	1665	G
45	BA	1670	C
45	BA	1671	G
45	BA	1673	U
45	BA	1680	G
45	BA	1682	C
45	BA	1686	G
45	BA	1695	A
45	BA	1696	C
45	BA	1698	C
45	BA	1699	A
45	BA	1701	C
45	BA	1721	U
45	BA	1722	G
45	BA	1724	A
45	BA	1741	U
45	BA	1742	C
45	BA	1744	G
45	BA	1745	A
45	BA	1750	C
45	BA	1752	C
45	BA	1753	C
45	BA	1754	G
45	BA	1757	G
45	BA	1758	G
45	BA	1761	U
45	BA	1773	C
45	BA	1774	C
45	BA	1776	G
45	BA	1777	G
45	BA	1778	C
45	BA	1780	G
45	BA	1781	A
45	BA	1782	G
45	BA	1786	U

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Mol	Chain	Res	Type
45	BA	1809	A
45	BA	1820	G
45	BA	1825	A
45	BA	1826	G
45	BA	1831	A
45	BA	1835	A
45	BA	1836	G
45	BA	1838	U
45	BA	1839	U
45	BA	1849	G
45	BA	1850	MA6
45	BA	1851	MA6
45	BA	1852	C
45	BA	1861	G
45	BA	1862	G
45	BA	1863	A
45	BA	1865	C
45	BA	1866	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	406	C
1	AA	914	U
1	AA	1633	G
1	AA	2391	G
1	AA	2675	G
1	AA	2760	G
1	AA	3614	G
1	AA	3673	C
1	AA	4120	U
1	AA	4913	G
3	AC	84	A
45	BA	369	C
45	BA	688	U
45	BA	866	PSU
45	BA	1520	G

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

223 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
1	A2M	AA	400	1	22,25,26	1.46	4 (18%)	31,36,39	2.04	7 (22%)
1	OMC	AA	3887	1	19,22,23	0.84	0	26,31,34	0.90	1 (3%)
45	PSU	BA	1596	45	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	4571	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	7 (22%)
29	V5N	Ac	39	29	9,11,12	0.82	0	9,14,16	1.50	2 (22%)
1	OMG	AA	3792	1	23,26,27	1.22	3 (13%)	33,38,41	1.96	6 (18%)
1	PSU	AA	4673	80,1	18,21,22	1.40	3 (16%)	22,30,33	1.85	3 (13%)
1	PSU	AA	4521	79,1	18,21,22	1.40	3 (16%)	22,30,33	1.90	3 (13%)
1	A2M	AA	3718	1	22,25,26	1.48	4 (18%)	31,36,39	1.98	7 (22%)
1	PSU	AA	3764	1	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
45	PSU	BA	815	45	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	AA	1782	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	AA	1326	1	22,25,26	1.45	4 (18%)	31,36,39	2.09	8 (25%)
45	PSU	BA	1174	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
45	6MZ	BA	1832	79,45	22,25,26	1.42	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	AA	3822	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
45	A2M	BA	668	79,45	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
58	NMM	BN	67	58	9,11,12	1.68	1 (11%)	6,12,14	1.25	1 (16%)
1	OMG	AA	2364	79,1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	4576	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	4 (18%)
1	A2M	AA	2363	79,1	22,25,26	1.44	4 (18%)	31,36,39	2.07	9 (29%)
1	OMC	AA	1340	1	19,22,23	0.85	0	26,31,34	0.87	0
1	PSU	AA	5001	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	OMG	AA	2424	1	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	AA	4532	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	AA	3844	1	18,21,22	1.38	3 (16%)	22,30,33	1.87	3 (13%)
45	PSU	BA	866	45	18,21,22	1.32	2 (11%)	22,30,33	2.04	5 (22%)
45	OMC	BA	1391	45	19,22,23	0.84	0	26,31,34	0.94	1 (3%)
1	OMU	AA	2415	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	4552	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
45	A2M	BA	484	45	22,25,26	1.48	4 (18%)	31,36,39	2.28	8 (25%)
45	PSU	BA	1136	45	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	AA	4689	1	18,21,22	1.36	2 (11%)	22,30,33	1.75	3 (13%)
1	OMU	AA	2837	1	19,22,23	1.25	3 (15%)	26,31,34	1.74	4 (15%)
1	OMC	AA	4456	1	19,22,23	0.84	0	26,31,34	0.99	1 (3%)
1	PSU	AA	3695	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
45	PSU	BA	36	45	18,21,22	1.33	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	AA	1744	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	AA	2422	79,1	19,22,23	0.80	0	26,31,34	0.80	0
1	PSU	AA	4296	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
45	PSU	BA	1046	45	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	AA	2365	1	19,22,23	0.80	0	26,31,34	0.76	0
1	OMG	AA	1522	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	5 (15%)
1	OMG	AA	3899	79,1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	4442	1	18,21,22	1.38	3 (16%)	22,30,33	1.96	4 (18%)
1	OMG	AA	4499	1	23,26,27	1.24	3 (13%)	33,38,41	1.97	6 (18%)
45	MA6	BA	1851	45	23,26,27	1.48	4 (17%)	34,38,41	2.41	13 (38%)
1	OMU	AA	4620	1	19,22,23	1.25	3 (15%)	26,31,34	1.66	4 (15%)
1	OMC	AA	2351	79,1	19,22,23	0.83	0	26,31,34	0.98	2 (7%)
45	OMU	BA	1288	45	19,22,23	1.17	3 (15%)	26,31,34	1.73	4 (15%)
1	PSU	AA	4471	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4579	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	1524	1	22,25,26	1.44	4 (18%)	31,36,39	2.15	11 (35%)
1	OMG	AA	4637	80,1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	AA	3701	80,1	19,22,23	0.80	0	26,31,34	0.76	0
3	PSU	AC	69	3	18,21,22	1.39	2 (11%)	22,30,33	1.91	4 (18%)
45	OMU	BA	428	45	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
1	A2M	AA	4523	79,1	22,25,26	1.41	4 (18%)	31,36,39	2.15	10 (32%)
3	PSU	AC	55	3	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4361	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	AA	4628	1	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
45	OMU	BA	172	45	19,22,23	1.19	3 (15%)	26,31,34	1.71	4 (15%)
45	OMC	BA	174	45	19,22,23	0.81	0	26,31,34	0.84	0
45	PSU	BA	609	45	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PSU	BA	1186	45	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	AA	3715	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
45	A2M	BA	27	45	22,25,26	1.49	4 (18%)	31,36,39	2.12	9 (29%)
45	PSU	BA	300	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
45	OMC	BA	1272	45	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
45	OMG	BA	1447	45	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
45	PSU	BA	63	45	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	AA	2824	1	19,22,23	0.82	0	26,31,34	0.89	1 (3%)
1	PSU	AA	3920	79,1	18,21,22	1.39	3 (16%)	22,30,33	1.89	4 (18%)
1	PSU	AA	3768	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
45	PSU	BA	1625	45	18,21,22	1.39	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	1781	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	34	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
45	OMG	BA	509	79,45	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
45	A2M	BA	1678	45	22,25,26	1.48	4 (18%)	31,36,39	2.14	10 (32%)
45	A2M	BA	99	45	22,25,26	1.45	4 (18%)	31,36,39	2.15	8 (25%)
45	PSU	BA	651	45	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	4493	80,1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
45	PSU	BA	1003	45	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
45	A2M	BA	1031	45	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
45	PSU	BA	801	45	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	A2M	AA	2401	1	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
1	OMC	AA	3869	1	19,22,23	0.83	0	26,31,34	0.73	0
1	OMG	AA	4228	1	23,26,27	1.18	4 (17%)	33,38,41	1.95	6 (18%)
1	A2M	AA	1534	79,1	22,25,26	1.44	4 (18%)	31,36,39	2.09	9 (29%)
45	OMG	BA	683	45	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	AA	3724	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
45	OMU	BA	354	45	19,22,23	1.18	3 (15%)	26,31,34	1.71	5 (19%)
45	A2M	BA	159	45	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
1	1MA	AA	1322	79,1	21,25,26	1.38	4 (19%)	31,37,40	1.66	6 (19%)
45	4AC	BA	1337	45	21,24,25	1.09	1 (4%)	29,34,37	1.60	5 (17%)
1	OMC	AA	3808	1	19,22,23	0.84	0	26,31,34	1.00	1 (3%)
45	PSU	BA	1045	45	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	AA	3825	1	22,25,26	1.46	4 (18%)	31,36,39	2.05	8 (25%)
1	OMU	AA	4498	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	AA	2787	79,1	22,25,26	1.43	4 (18%)	31,36,39	2.13	8 (25%)
45	PSU	BA	822	45	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
45	PSU	BA	1445	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
45	OMU	BA	1804	45	19,22,23	1.24	4 (21%)	26,31,34	1.68	5 (19%)
1	PSU	AA	1862	1	18,21,22	1.35	3 (16%)	22,30,33	1.86	3 (13%)
45	A2M	BA	590	45	22,25,26	1.47	4 (18%)	31,36,39	2.26	6 (19%)
1	PSU	AA	4431	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	1347	45	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
1	OMG	AA	4623	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	5MC	AA	4447	80,1	18,22,23	0.99	2 (11%)	26,32,35	1.22	2 (7%)
1	PSU	AA	2632	1	18,21,22	1.39	2 (11%)	22,30,33	1.78	3 (13%)
1	PSU	AA	3639	1	18,21,22	1.38	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	406	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	1677	79,1	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	UR3	AA	4530	1	19,22,23	0.98	0	26,32,35	1.40	1 (3%)
1	PSU	AA	2508	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	AA	4618	1	23,26,27	1.18	3 (13%)	33,38,41	1.98	6 (18%)
45	PSU	BA	105	45	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
45	PSU	BA	1367	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	AA	4590	1	22,25,26	1.45	4 (18%)	31,36,39	2.07	9 (29%)
45	PSU	BA	1056	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
1	PSU	AA	3770	1	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	AA	5010	1	18,21,22	1.35	2 (11%)	22,30,33	1.80	3 (13%)
1	OMG	AA	3627	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
45	A2M	BA	576	45	22,25,26	1.49	4 (18%)	31,36,39	2.05	8 (25%)
45	OMU	BA	121	45	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
1	PSU	AA	3730	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	AA	2843	1	18,21,22	1.38	3 (16%)	22,30,33	1.87	3 (13%)
45	OMC	BA	462	45	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
45	PSU	BA	366	45	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	AA	1683	1	18,21,22	1.42	3 (16%)	22,30,33	1.89	3 (13%)
1	OMG	AA	1625	80,1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	A2M	AA	1323	1	22,25,26	1.46	4 (18%)	31,36,39	2.08	8 (25%)
45	PSU	BA	109	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	AA	1860	1	18,21,22	1.38	3 (16%)	22,30,33	1.82	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	4500	1	18,21,22	1.36	2 (11%)	22,30,33	1.96	4 (18%)
45	PSU	BA	966	45	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	AA	3853	79,1	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
45	PSU	BA	218	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	AA	3867	1	22,25,26	1.46	4 (18%)	31,36,39	2.09	7 (22%)
1	OMG	AA	4196	79,1	23,26,27	1.23	3 (13%)	33,38,41	1.95	6 (18%)
45	OMG	BA	601	45	23,26,27	1.23	3 (13%)	33,38,41	2.01	6 (18%)
45	OMG	BA	867	45	23,26,27	1.24	3 (13%)	33,38,41	1.94	6 (18%)
45	PSU	BA	1244	45	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
5	HIC	AE	245	5	10,11,12	0.52	0	8,14,16	0.49	0
1	OMC	AA	2861	1	19,22,23	0.84	0	26,31,34	0.99	2 (7%)
1	OMG	AA	4494	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
45	PSU	BA	1238	45	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
45	PSU	BA	649	45	18,21,22	1.34	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	AA	1582	1	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
45	PSU	BA	572	45	18,21,22	1.37	3 (16%)	22,30,33	1.93	4 (18%)
1	A2M	AA	1871	79,1	22,25,26	1.47	4 (18%)	31,36,39	2.07	8 (25%)
45	PSU	BA	119	45	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
45	OMU	BA	116	45	19,22,23	1.22	3 (15%)	26,31,34	1.65	5 (19%)
1	PSU	AA	4353	1	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
45	PSU	BA	100	45	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	6MZ	AA	4220	1	22,25,26	1.42	4 (18%)	30,36,39	2.15	9 (30%)
1	PSU	AA	3884	1	18,21,22	1.38	3 (16%)	22,30,33	1.88	3 (13%)
1	PSU	AA	4973	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
1	OMC	AA	1881	79,1	19,22,23	0.82	0	26,31,34	0.86	0
45	PSU	BA	686	45	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	AA	3744	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	AA	1316	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
45	A2M	BA	1383	45	22,25,26	1.47	4 (18%)	31,36,39	2.25	10 (32%)
1	OMG	AA	4370	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
71	IAS	Ba	138	71	6,7,8	1.07	0	6,8,10	1.47	0
1	PSU	AA	1792	1	18,21,22	1.39	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	3851	1	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
3	OMG	AC	75	3	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	OMU	AA	4306	1	19,22,23	1.26	3 (15%)	26,31,34	1.63	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	AA	398	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
45	OMC	BA	1703	45	19,22,23	0.80	0	26,31,34	0.77	0
1	PSU	AA	1536	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	AA	2804	1	19,22,23	0.82	0	26,31,34	0.76	0
1	A2M	AA	2815	1	22,25,26	1.47	4 (18%)	31,36,39	2.18	7 (22%)
1	PSU	AA	4293	1	18,21,22	1.36	3 (16%)	22,30,33	1.89	4 (18%)
45	OMG	BA	436	45	23,26,27	1.18	3 (13%)	33,38,41	1.98	6 (18%)
1	A2M	AA	3830	1	22,25,26	1.45	4 (18%)	31,36,39	2.14	8 (25%)
1	PSU	AA	4403	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	5 (22%)
45	4AC	BA	1842	45	21,24,25	1.06	1 (4%)	29,34,37	1.49	5 (17%)
45	PSU	BA	1692	45	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
3	OMU	AC	14	3,1	19,22,23	1.27	3 (15%)	26,31,34	1.83	5 (19%)
45	PSU	BA	681	45	18,21,22	1.37	2 (11%)	22,30,33	1.80	3 (13%)
45	OMG	BA	1328	45	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
45	OMG	BA	644	45	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
45	PSU	BA	1232	45	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	AA	3925	1	19,22,23	1.23	3 (15%)	26,31,34	1.73	5 (19%)
1	UY1	AA	3818	80,1	19,22,23	4.31	7 (36%)	22,31,34	1.78	5 (22%)
1	OMG	AA	4392	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	5 (15%)
1	5MC	AA	3782	79,1	18,22,23	0.95	2 (11%)	26,32,35	1.18	3 (11%)
45	PSU	BA	814	45	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	1004	45	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	4972	1	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
45	OMU	BA	1442	45	19,22,23	1.30	4 (21%)	26,31,34	1.78	6 (23%)
45	PSU	BA	1360	45	18,21,22	1.42	5 (27%)	22,30,33	1.90	4 (18%)
1	OMC	AA	4536	1	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
1	PSU	AA	1779	1	18,21,22	1.31	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	3637	80,1	18,21,22	1.43	3 (16%)	22,30,33	1.95	5 (22%)
45	PSU	BA	863	45	18,21,22	1.34	2 (11%)	22,30,33	1.74	3 (13%)
45	OMG	BA	1490	45	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
45	PSU	BA	918	45	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
45	OMC	BA	517	45	19,22,23	0.83	0	26,31,34	0.99	1 (3%)
45	B8N	BA	1248	45	24,29,30	0.91	1 (4%)	29,42,45	1.32	2 (6%)
1	PSU	AA	4312	1	18,21,22	1.39	2 (11%)	22,30,33	1.90	3 (13%)
45	PSU	BA	1177	45	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	2839	1	18,21,22	1.38	3 (16%)	22,30,33	1.85	3 (13%)
1	A2M	AA	3785	1	22,25,26	1.41	4 (18%)	31,36,39	2.29	11 (35%)
45	A2M	BA	468	45	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
45	A2M	BA	166	45	22,25,26	1.44	4 (18%)	31,36,39	2.25	9 (29%)
1	PSU	AA	3762	1	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
1	PSU	AA	4423	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	AA	2876	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	AA	4299	1	18,21,22	1.38	3 (16%)	22,30,33	1.82	3 (13%)
45	MA6	BA	1850	45	23,26,27	1.47	4 (17%)	34,38,41	2.40	13 (38%)
45	UY1	BA	1326	45	19,22,23	4.40	7 (36%)	22,31,34	1.75	5 (22%)
45	PSU	BA	93	45	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
45	A2M	BA	512	45	22,25,26	1.47	4 (18%)	31,36,39	2.20	8 (25%)
1	PSU	AA	4457	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	OMC	AA	3841	1	19,22,23	0.81	0	26,31,34	0.74	0
1	OMU	AA	4227	1	19,22,23	1.25	3 (15%)	26,31,34	1.73	4 (15%)
45	PSU	BA	296	45	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
45	PSU	BA	667	45	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
45	PSU	BA	1643	45	18,21,22	1.41	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4636	1	18,21,22	1.38	2 (11%)	22,30,33	1.94	5 (22%)

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
1	A2M	AA	400	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3887	1	-	1/9/27/28	0/2/2/2
45	PSU	BA	1596	45	-	1/7/25/26	0/2/2/2
1	A2M	AA	4571	1	-	0/9/27/28	0/3/3/3
29	V5N	Ac	39	29	-	0/9/10/12	0/1/1/1
1	OMG	AA	3792	1	-	1/9/27/28	0/3/3/3
1	PSU	AA	4673	80,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4521	79,1	-	1/7/25/26	0/2/2/2
1	A2M	AA	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3764	1	-	2/7/25/26	0/2/2/2
45	PSU	BA	815	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1782	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	AA	1326	1	-	3/9/27/28	0/3/3/3
45	PSU	BA	1174	45	-	0/7/25/26	0/2/2/2
45	6MZ	BA	1832	79,45	-	2/9/27/28	0/3/3/3
1	PSU	AA	3822	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	668	79,45	-	4/9/27/28	0/3/3/3
58	NMM	BN	67	58	-	1/9/11/13	-
1	OMG	AA	2364	79,1	-	2/9/27/28	0/3/3/3
1	PSU	AA	4576	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	2363	79,1	-	0/9/27/28	0/3/3/3
1	OMC	AA	1340	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	5001	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2424	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4532	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3844	1	-	3/7/25/26	0/2/2/2
45	PSU	BA	866	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	1391	45	-	0/9/27/28	0/2/2/2
1	OMU	AA	2415	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4552	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	484	45	-	1/9/27/28	0/3/3/3
45	PSU	BA	1136	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4689	1	-	0/7/25/26	0/2/2/2
1	OMU	AA	2837	1	-	1/9/27/28	0/2/2/2
1	OMC	AA	4456	1	-	1/9/27/28	0/2/2/2
1	PSU	AA	3695	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	36	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1744	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2422	79,1	-	1/9/27/28	0/2/2/2
1	PSU	AA	4296	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1046	45	-	0/7/25/26	0/2/2/2
1	OMC	AA	2365	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	1522	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	3899	79,1	-	2/9/27/28	0/3/3/3
1	PSU	AA	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4499	1	-	0/9/27/28	0/3/3/3
45	MA6	BA	1851	45	-	4/11/29/30	0/3/3/3
1	OMU	AA	4620	1	-	0/9/27/28	0/2/2/2
1	OMC	AA	2351	79,1	-	1/9/27/28	0/2/2/2
45	OMU	BA	1288	45	-	2/9/27/28	0/2/2/2
1	PSU	AA	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4579	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	AA	1524	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	4637	80,1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3701	80,1	-	4/9/27/28	0/2/2/2
3	PSU	AC	69	3	-	0/7/25/26	0/2/2/2
45	OMU	BA	428	45	-	4/9/27/28	0/2/2/2
1	A2M	AA	4523	79,1	-	1/9/27/28	0/3/3/3
3	PSU	AC	55	3	-	0/7/25/26	0/2/2/2
1	PSU	AA	4361	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4628	1	-	0/7/25/26	0/2/2/2
45	OMU	BA	172	45	-	0/9/27/28	0/2/2/2
45	OMC	BA	174	45	-	2/9/27/28	0/2/2/2
45	PSU	BA	609	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1186	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	3715	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	27	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	300	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	1272	45	-	0/9/27/28	0/2/2/2
45	OMG	BA	1447	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	63	45	-	0/7/25/26	0/2/2/2
1	OMC	AA	2824	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	3920	79,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3768	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1625	45	-	1/7/25/26	0/2/2/2
1	PSU	AA	1781	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	34	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	509	79,45	-	1/9/27/28	0/3/3/3
45	A2M	BA	1678	45	-	1/9/27/28	0/3/3/3
45	A2M	BA	99	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	651	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4493	80,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1003	45	-	0/7/25/26	0/2/2/2
45	A2M	BA	1031	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	801	45	-	1/7/25/26	0/2/2/2
1	A2M	AA	2401	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3869	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4228	1	-	0/9/27/28	0/3/3/3
1	A2M	AA	1534	79,1	-	1/9/27/28	0/3/3/3
45	OMG	BA	683	45	-	2/9/27/28	0/3/3/3
1	A2M	AA	3724	1	-	0/9/27/28	0/3/3/3
45	OMU	BA	354	45	-	0/9/27/28	0/2/2/2
45	A2M	BA	159	45	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MA	AA	1322	79,1	-	1/7/25/26	0/3/3/3
45	4AC	BA	1337	45	-	2/11/29/30	0/2/2/2
1	OMC	AA	3808	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	1045	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	3825	1	-	0/9/27/28	0/3/3/3
1	OMU	AA	4498	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	2787	79,1	-	5/9/27/28	0/3/3/3
45	PSU	BA	822	45	-	1/7/25/26	0/2/2/2
45	PSU	BA	1445	45	-	0/7/25/26	0/2/2/2
45	OMU	BA	1804	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	1862	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	590	45	-	5/9/27/28	0/3/3/3
1	PSU	AA	4431	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1347	45	-	0/7/25/26	0/2/2/2
1	OMG	AA	4623	1	-	2/9/27/28	0/3/3/3
1	5MC	AA	4447	80,1	-	4/7/25/26	0/2/2/2
1	PSU	AA	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3639	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	406	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1677	79,1	-	4/7/25/26	0/2/2/2
1	UR3	AA	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2508	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4618	1	-	0/9/27/28	0/3/3/3
45	PSU	BA	105	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1367	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	4590	1	-	3/9/27/28	0/3/3/3
45	PSU	BA	1056	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	3770	1	-	2/7/25/26	0/2/2/2
1	PSU	AA	5010	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	3627	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	576	45	-	0/9/27/28	0/3/3/3
45	OMU	BA	121	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	3730	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2843	1	-	0/7/25/26	0/2/2/2
45	OMC	BA	462	45	-	0/9/27/28	0/2/2/2
45	PSU	BA	366	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1683	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	1625	80,1	-	2/9/27/28	0/3/3/3
1	A2M	AA	1323	1	-	2/9/27/28	0/3/3/3
45	PSU	BA	109	45	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4500	1	-	3/7/25/26	0/2/2/2
45	PSU	BA	966	45	-	1/7/25/26	0/2/2/2
1	PSU	AA	3853	79,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	218	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	3867	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	4196	79,1	-	0/9/27/28	0/3/3/3
45	OMG	BA	601	45	-	2/9/27/28	0/3/3/3
45	OMG	BA	867	45	-	1/9/27/28	0/3/3/3
45	PSU	BA	1244	45	-	0/7/25/26	0/2/2/2
5	HIC	AE	245	5	-	0/5/6/8	0/1/1/1
1	OMC	AA	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4494	1	-	0/9/27/28	0/3/3/3
45	PSU	BA	1238	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	649	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1582	1	-	2/7/25/26	0/2/2/2
45	PSU	BA	572	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	1871	79,1	-	0/9/27/28	0/3/3/3
45	PSU	BA	119	45	-	0/7/25/26	0/2/2/2
45	OMU	BA	116	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	4353	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	100	45	-	2/7/25/26	0/2/2/2
1	6MZ	AA	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3884	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4973	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	1881	79,1	-	2/9/27/28	0/2/2/2
45	PSU	BA	686	45	-	0/7/25/26	0/2/2/2
1	OMG	AA	3744	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	1316	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	1383	45	-	0/9/27/28	0/3/3/3
1	OMG	AA	4370	1	-	0/9/27/28	0/3/3/3
71	IAS	Ba	138	71	-	1/7/7/8	-
1	PSU	AA	1792	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3851	1	-	2/7/25/26	0/2/2/2
3	OMG	AC	75	3	-	1/9/27/28	0/3/3/3
1	OMU	AA	4306	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	398	1	-	2/9/27/28	0/3/3/3
45	OMC	BA	1703	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	1536	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2804	1	-	1/9/27/28	0/2/2/2
1	A2M	AA	2815	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	4293	1	-	0/7/25/26	0/2/2/2
45	OMG	BA	436	45	-	4/9/27/28	0/3/3/3
1	A2M	AA	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4403	1	-	0/7/25/26	0/2/2/2
45	4AC	BA	1842	45	-	0/11/29/30	0/2/2/2
45	PSU	BA	1692	45	-	0/7/25/26	0/2/2/2
3	OMU	AC	14	3,1	-	0/9/27/28	0/2/2/2
45	PSU	BA	681	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	1328	45	-	0/9/27/28	0/3/3/3
45	OMG	BA	644	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	1232	45	-	0/7/25/26	0/2/2/2
1	OMU	AA	3925	1	-	0/9/27/28	0/2/2/2
1	UY1	AA	3818	80,1	-	2/9/27/28	0/2/2/2
1	OMG	AA	4392	1	-	0/9/27/28	0/3/3/3
1	5MC	AA	3782	79,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	814	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1004	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4972	1	-	0/7/25/26	0/2/2/2
45	OMU	BA	1442	45	-	2/9/27/28	0/2/2/2
45	PSU	BA	1360	45	-	4/7/25/26	0/2/2/2
1	OMC	AA	4536	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	1779	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3637	80,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	863	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	1490	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	918	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	517	45	-	0/9/27/28	0/2/2/2
45	B8N	BA	1248	45	-	8/16/34/35	0/2/2/2
1	PSU	AA	4312	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1177	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	2839	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3785	1	-	2/9/27/28	0/3/3/3
45	A2M	BA	468	45	-	2/9/27/28	0/3/3/3
45	A2M	BA	166	45	-	2/9/27/28	0/3/3/3
1	PSU	AA	3762	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4423	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2876	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4299	1	-	0/7/25/26	0/2/2/2
45	MA6	BA	1850	45	-	5/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	UY1	BA	1326	45	-	5/9/27/28	0/2/2/2
45	PSU	BA	93	45	-	0/7/25/26	0/2/2/2
45	A2M	BA	512	45	-	2/9/27/28	0/3/3/3
1	PSU	AA	4457	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	3841	1	-	0/9/27/28	0/2/2/2
1	OMU	AA	4227	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	296	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	667	45	-	4/7/25/26	0/2/2/2
45	PSU	BA	1643	45	-	2/7/25/26	0/2/2/2
1	PSU	AA	4636	1	-	4/7/25/26	0/2/2/2

All (544) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	1326	UY1	C6-C5	11.87	1.49	1.35
1	AA	3818	UY1	C6-C5	11.51	1.48	1.35
45	BA	1326	UY1	C2-N1	9.54	1.49	1.36
1	AA	3818	UY1	C2-N1	9.37	1.49	1.36
45	BA	1326	UY1	C2-N3	7.79	1.50	1.37
1	AA	3818	UY1	C2-N3	7.65	1.50	1.37
45	BA	1326	UY1	C6-N1	5.56	1.45	1.36
1	AA	3818	UY1	C6-N1	5.45	1.45	1.36
45	BA	1851	MA6	C5-C4	4.67	1.47	1.39
45	BA	27	A2M	C5-C4	4.65	1.47	1.39
45	BA	576	A2M	C5-C4	4.65	1.47	1.39
45	BA	590	A2M	C5-C4	4.65	1.47	1.39
45	BA	484	A2M	C5-C4	4.62	1.47	1.39
45	BA	512	A2M	C5-C4	4.60	1.47	1.39
45	BA	159	A2M	C5-C4	4.58	1.47	1.39
45	BA	1850	MA6	C5-C4	4.56	1.47	1.39
1	AA	3718	A2M	C5-C4	4.56	1.47	1.39
1	AA	4571	A2M	C5-C4	4.55	1.47	1.39
45	BA	468	A2M	C5-C4	4.54	1.47	1.39
45	BA	1383	A2M	C5-C4	4.51	1.47	1.39
1	AA	2815	A2M	C5-C4	4.51	1.47	1.39
45	BA	1832	6MZ	C5-C4	4.47	1.47	1.39
45	BA	1678	A2M	C5-C4	4.46	1.47	1.39
1	AA	398	A2M	C5-C4	4.45	1.47	1.39
45	BA	99	A2M	C5-C4	4.44	1.47	1.39
45	BA	1031	A2M	C5-C4	4.44	1.47	1.39
45	BA	166	A2M	C5-C4	4.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	668	A2M	C5-C4	4.42	1.47	1.39
1	AA	3867	A2M	C5-C4	4.41	1.47	1.39
1	AA	3724	A2M	C5-C4	4.39	1.47	1.39
1	AA	400	A2M	C5-C4	4.38	1.47	1.39
1	AA	4220	6MZ	C5-C4	4.38	1.47	1.39
58	BN	67	NMM	CZ-NH2	4.37	1.44	1.34
1	AA	3830	A2M	C5-C4	4.36	1.47	1.39
1	AA	1323	A2M	C5-C4	4.35	1.47	1.39
1	AA	3825	A2M	C5-C4	4.35	1.47	1.39
1	AA	4590	A2M	C5-C4	4.35	1.47	1.39
1	AA	2787	A2M	C5-C4	4.34	1.47	1.39
1	AA	2363	A2M	C5-C4	4.34	1.47	1.39
1	AA	1326	A2M	C5-C4	4.34	1.47	1.39
1	AA	1871	A2M	C5-C4	4.33	1.47	1.39
1	AA	1524	A2M	C5-C4	4.33	1.47	1.39
1	AA	2401	A2M	C5-C4	4.29	1.47	1.39
1	AA	3785	A2M	C5-C4	4.22	1.46	1.39
1	AA	1534	A2M	C5-C4	4.21	1.46	1.39
1	AA	4523	A2M	C5-C4	4.20	1.46	1.39
45	BA	1326	UY1	C4-N3	4.15	1.46	1.38
1	AA	3818	UY1	C4-N3	3.95	1.46	1.38
45	BA	1337	4AC	C5-C4	3.79	1.48	1.40
45	BA	1842	4AC	C5-C4	3.77	1.48	1.40
45	BA	667	PSU	C6-C5	3.33	1.39	1.35
45	BA	1056	PSU	C6-C5	3.31	1.39	1.35
45	BA	1244	PSU	C6-C5	3.31	1.39	1.35
1	AA	3715	PSU	C6-C5	3.28	1.39	1.35
1	AA	4423	PSU	C6-C5	3.28	1.39	1.35
45	BA	34	PSU	C6-C5	3.28	1.39	1.35
45	BA	1625	PSU	C6-C5	3.27	1.39	1.35
45	BA	1596	PSU	C6-C5	3.26	1.39	1.35
45	BA	218	PSU	C6-C5	3.25	1.39	1.35
45	BA	867	OMG	C5-C4	3.25	1.47	1.38
1	AA	2632	PSU	C6-C5	3.24	1.39	1.35
45	BA	300	PSU	C6-C5	3.24	1.39	1.35
45	BA	109	PSU	C6-C5	3.23	1.39	1.35
1	AA	1744	PSU	C6-C5	3.23	1.39	1.35
45	BA	100	PSU	C6-C5	3.23	1.39	1.35
45	BA	1692	PSU	C6-C5	3.22	1.39	1.35
45	BA	966	PSU	C6-C5	3.22	1.39	1.35
45	BA	1367	PSU	C6-C5	3.22	1.39	1.35
1	AA	3764	PSU	C6-C5	3.21	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	1174	PSU	C6-C5	3.20	1.39	1.35
45	BA	866	PSU	C6-C5	3.20	1.39	1.35
1	AA	3768	PSU	C6-C5	3.19	1.39	1.35
45	BA	1232	PSU	C6-C5	3.19	1.39	1.35
45	BA	1490	OMG	C5-C4	3.19	1.47	1.38
1	AA	1792	PSU	C6-C5	3.19	1.39	1.35
45	BA	119	PSU	C6-C5	3.18	1.39	1.35
45	BA	1046	PSU	C6-C5	3.18	1.39	1.35
45	BA	822	PSU	C6-C5	3.18	1.39	1.35
45	BA	1347	PSU	C6-C5	3.18	1.39	1.35
45	BA	814	PSU	C6-C5	3.17	1.39	1.35
1	AA	4500	PSU	C6-C5	3.16	1.39	1.35
45	BA	651	PSU	C6-C5	3.16	1.39	1.35
1	AA	1782	PSU	C6-C5	3.16	1.39	1.35
1	AA	1781	PSU	C6-C5	3.16	1.39	1.35
45	BA	601	OMG	C5-C4	3.16	1.47	1.38
45	BA	93	PSU	C6-C5	3.15	1.39	1.35
1	AA	3770	PSU	C6-C5	3.15	1.39	1.35
45	BA	686	PSU	C6-C5	3.14	1.39	1.35
1	AA	3762	PSU	C6-C5	3.13	1.39	1.35
1	AA	1322	1MA	C6-N6	3.13	1.35	1.28
45	BA	63	PSU	C6-C5	3.13	1.39	1.35
45	BA	1003	PSU	C6-C5	3.13	1.39	1.35
45	BA	644	OMG	C5-C4	3.13	1.47	1.38
1	AA	3637	PSU	C4-N3	-3.13	1.33	1.38
45	BA	609	PSU	C6-C5	3.13	1.39	1.35
45	BA	296	PSU	C6-C5	3.13	1.39	1.35
45	BA	801	PSU	C6-C5	3.13	1.39	1.35
45	BA	509	OMG	C5-C4	3.12	1.47	1.38
45	BA	1328	OMG	C5-C4	3.12	1.47	1.38
45	BA	1445	PSU	C6-C5	3.12	1.39	1.35
45	BA	1238	PSU	C6-C5	3.12	1.39	1.35
1	AA	1683	PSU	C6-C5	3.12	1.39	1.35
45	BA	1447	OMG	C5-C4	3.12	1.47	1.38
1	AA	4471	PSU	C6-C5	3.12	1.39	1.35
45	BA	1643	PSU	C6-C5	3.11	1.38	1.35
45	BA	1045	PSU	C6-C5	3.11	1.38	1.35
45	BA	1136	PSU	C6-C5	3.11	1.38	1.35
1	AA	4499	OMG	C5-C4	3.10	1.47	1.38
45	BA	366	PSU	C6-C5	3.10	1.38	1.35
1	AA	3851	PSU	C6-C5	3.10	1.38	1.35
45	BA	1177	PSU	C6-C5	3.10	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1677	PSU	C6-C5	3.09	1.38	1.35
1	AA	4431	PSU	C6-C5	3.08	1.38	1.35
45	BA	105	PSU	C6-C5	3.08	1.38	1.35
45	BA	815	PSU	C6-C5	3.08	1.38	1.35
1	AA	4521	PSU	C6-C5	3.08	1.38	1.35
1	AA	4196	OMG	C5-C4	3.07	1.47	1.38
45	BA	1004	PSU	C6-C5	3.06	1.38	1.35
3	AC	75	OMG	C5-C4	3.06	1.47	1.38
1	AA	4576	PSU	C6-C5	3.05	1.38	1.35
45	BA	1360	PSU	C6-C5	3.05	1.38	1.35
45	BA	406	PSU	C6-C5	3.04	1.38	1.35
1	AA	4532	PSU	C6-C5	3.04	1.38	1.35
1	AA	1536	PSU	C6-C5	3.04	1.38	1.35
1	AA	3730	PSU	C6-C5	3.04	1.38	1.35
1	AA	4673	PSU	C6-C5	3.04	1.38	1.35
45	BA	918	PSU	C6-C5	3.04	1.38	1.35
1	AA	3792	OMG	C5-C4	3.03	1.47	1.38
45	BA	1186	PSU	C6-C5	3.03	1.38	1.35
1	AA	3822	PSU	C6-C5	3.03	1.38	1.35
45	BA	683	OMG	C5-C4	3.03	1.47	1.38
45	BA	436	OMG	C5-C4	3.03	1.47	1.38
1	AA	1625	OMG	C5-C4	3.03	1.47	1.38
1	AA	4636	PSU	C6-C5	3.03	1.38	1.35
1	AA	3744	OMG	C5-C4	3.02	1.47	1.38
1	AA	4312	PSU	C6-C5	3.02	1.38	1.35
1	AA	4353	PSU	C6-C5	3.02	1.38	1.35
1	AA	1322	1MA	C5-C4	3.01	1.47	1.38
1	AA	4493	PSU	C6-C5	3.01	1.38	1.35
45	BA	36	PSU	C6-C5	3.01	1.38	1.35
3	AC	55	PSU	C6-C5	3.01	1.38	1.35
1	AA	1779	PSU	C6-C5	3.01	1.38	1.35
45	BA	572	PSU	C6-C5	3.01	1.38	1.35
1	AA	5001	PSU	C6-C5	3.01	1.38	1.35
1	AA	4293	PSU	C6-C5	3.00	1.38	1.35
1	AA	4494	OMG	C5-C4	3.00	1.47	1.38
1	AA	2364	OMG	C5-C4	3.00	1.47	1.38
1	AA	4370	OMG	C5-C4	2.99	1.47	1.38
1	AA	3853	PSU	C6-C5	2.98	1.38	1.35
45	BA	863	PSU	C6-C5	2.98	1.38	1.35
45	BA	649	PSU	C6-C5	2.98	1.38	1.35
1	AA	1860	PSU	C6-C5	2.97	1.38	1.35
1	AA	2876	OMG	C5-C4	2.97	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	4361	PSU	C6-C5	2.97	1.38	1.35
1	AA	2424	OMG	C5-C4	2.96	1.47	1.38
3	AC	69	PSU	C6-C5	2.96	1.38	1.35
1	AA	3637	PSU	C6-C5	2.96	1.38	1.35
1	AA	4628	PSU	C6-C5	2.96	1.38	1.35
1	AA	1582	PSU	C6-C5	2.96	1.38	1.35
1	AA	3920	PSU	C6-C5	2.95	1.38	1.35
1	AA	4973	PSU	C6-C5	2.95	1.38	1.35
1	AA	4392	OMG	C5-C4	2.95	1.46	1.38
1	AA	4623	OMG	C5-C4	2.94	1.46	1.38
1	AA	4403	PSU	C6-C5	2.94	1.38	1.35
1	AA	3627	OMG	C5-C4	2.93	1.46	1.38
1	AA	3695	PSU	C6-C5	2.93	1.38	1.35
1	AA	4972	PSU	C6-C5	2.93	1.38	1.35
1	AA	4296	PSU	C6-C5	2.93	1.38	1.35
1	AA	3844	PSU	C6-C5	2.93	1.38	1.35
1	AA	1862	PSU	C6-C5	2.93	1.38	1.35
1	AA	4552	PSU	C6-C5	2.93	1.38	1.35
1	AA	2843	PSU	C4-N3	-2.92	1.33	1.38
1	AA	4618	OMG	C5-C4	2.92	1.46	1.38
1	AA	3818	UY1	C1'-C5	2.91	1.56	1.50
1	AA	4637	OMG	C5-C4	2.91	1.46	1.38
1	AA	5010	PSU	C6-C5	2.91	1.38	1.35
1	AA	4673	PSU	C4-N3	-2.90	1.33	1.38
45	BA	681	PSU	C6-C5	2.89	1.38	1.35
1	AA	2843	PSU	C6-C5	2.89	1.38	1.35
45	BA	1643	PSU	C4-N3	-2.89	1.33	1.38
1	AA	4457	PSU	C6-C5	2.89	1.38	1.35
1	AA	3844	PSU	C4-N3	-2.88	1.33	1.38
1	AA	1316	OMG	C5-C4	2.88	1.46	1.38
1	AA	3899	OMG	C5-C4	2.88	1.46	1.38
1	AA	3639	PSU	C6-C5	2.87	1.38	1.35
1	AA	3884	PSU	C6-C5	2.87	1.38	1.35
1	AA	4299	PSU	C6-C5	2.86	1.38	1.35
1	AA	4312	PSU	C4-N3	-2.86	1.33	1.38
1	AA	4689	PSU	C6-C5	2.86	1.38	1.35
1	AA	4552	PSU	C4-N3	-2.86	1.33	1.38
1	AA	2508	PSU	C6-C5	2.86	1.38	1.35
45	BA	1326	UY1	C1'-C5	2.85	1.56	1.50
1	AA	4403	PSU	C4-N3	-2.85	1.33	1.38
1	AA	3639	PSU	C4-N3	-2.85	1.33	1.38
1	AA	2839	PSU	C6-C5	2.85	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2839	PSU	C4-N3	-2.85	1.33	1.38
1	AA	3920	PSU	C4-N3	-2.84	1.33	1.38
1	AA	4299	PSU	C4-N3	-2.84	1.33	1.38
1	AA	4521	PSU	C4-N3	-2.84	1.33	1.38
45	BA	366	PSU	C4-N3	-2.83	1.33	1.38
1	AA	4579	PSU	C6-C5	2.83	1.38	1.35
1	AA	1522	OMG	C5-C4	2.83	1.46	1.38
1	AA	4493	PSU	C4-N3	-2.82	1.33	1.38
1	AA	1862	PSU	C4-N3	-2.82	1.33	1.38
1	AA	4228	OMG	C5-C4	2.82	1.46	1.38
1	AA	4457	PSU	C4-N3	-2.82	1.33	1.38
1	AA	1683	PSU	C4-N3	-2.82	1.33	1.38
1	AA	3822	PSU	C4-N3	-2.82	1.33	1.38
3	AC	55	PSU	C4-N3	-2.82	1.33	1.38
1	AA	4353	PSU	C4-N3	-2.82	1.33	1.38
45	BA	1851	MA6	C5-C6	2.82	1.48	1.41
1	AA	3884	PSU	C4-N3	-2.81	1.33	1.38
1	AA	4392	OMG	C6-N1	-2.81	1.33	1.38
1	AA	4447	5MC	C6-C5	2.81	1.39	1.34
1	AA	3851	PSU	C4-N3	-2.80	1.33	1.38
1	AA	4296	PSU	C4-N3	-2.80	1.33	1.38
1	AA	4636	PSU	C4-N3	-2.80	1.33	1.38
1	AA	4442	PSU	C6-C5	2.80	1.38	1.35
1	AA	1536	PSU	C4-N3	-2.79	1.33	1.38
1	AA	4973	PSU	C4-N3	-2.79	1.33	1.38
1	AA	2508	PSU	C4-N3	-2.79	1.33	1.38
1	AA	4293	PSU	C4-N3	-2.79	1.33	1.38
1	AA	3818	UY1	O4-C4	-2.79	1.18	1.23
1	AA	3695	PSU	C4-N3	-2.78	1.33	1.38
45	BA	681	PSU	C4-N3	-2.78	1.33	1.38
1	AA	4306	OMU	C4-N3	-2.78	1.33	1.38
1	AA	1860	PSU	C4-N3	-2.78	1.33	1.38
1	AA	1677	PSU	C4-N3	-2.77	1.33	1.38
45	BA	1136	PSU	C4-N3	-2.77	1.33	1.38
1	AA	1582	PSU	C4-N3	-2.77	1.33	1.38
1	AA	4442	PSU	C4-N3	-2.77	1.33	1.38
1	AA	4628	PSU	C4-N3	-2.76	1.33	1.38
45	BA	667	PSU	C4-N3	-2.76	1.33	1.38
45	BA	1004	PSU	C4-N3	-2.76	1.33	1.38
45	BA	406	PSU	C4-N3	-2.76	1.33	1.38
3	AC	69	PSU	C4-N3	-2.76	1.33	1.38
1	AA	4689	PSU	C4-N3	-2.76	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	14	OMU	C4-N3	-2.74	1.33	1.38
45	BA	1442	OMU	C2-N1	2.73	1.42	1.38
45	BA	1678	A2M	C5-C6	2.72	1.48	1.41
1	AA	4361	PSU	C4-N3	-2.72	1.33	1.38
1	AA	3853	PSU	C4-N3	-2.72	1.33	1.38
45	BA	576	A2M	C5-C6	2.72	1.48	1.41
1	AA	5001	PSU	C4-N3	-2.71	1.33	1.38
1	AA	4579	PSU	C4-N3	-2.71	1.33	1.38
1	AA	4431	PSU	C4-N3	-2.71	1.33	1.38
45	BA	572	PSU	C4-N3	-2.71	1.33	1.38
45	BA	468	A2M	C5-C6	2.71	1.48	1.41
1	AA	4532	PSU	C4-N3	-2.71	1.33	1.38
45	BA	686	PSU	C4-N3	-2.71	1.33	1.38
45	BA	34	PSU	C4-N3	-2.71	1.33	1.38
45	BA	159	A2M	C5-C6	2.70	1.48	1.41
45	BA	100	PSU	C4-N3	-2.70	1.33	1.38
45	BA	1596	PSU	C4-N3	-2.70	1.33	1.38
45	BA	866	PSU	C4-N3	-2.70	1.33	1.38
45	BA	1177	PSU	C4-N3	-2.70	1.33	1.38
1	AA	3925	OMU	C4-N3	-2.70	1.33	1.38
1	AA	3730	PSU	C4-N3	-2.69	1.33	1.38
1	AA	1792	PSU	C4-N3	-2.69	1.33	1.38
1	AA	4620	OMU	C4-N3	-2.69	1.33	1.38
45	BA	1625	PSU	C4-N3	-2.69	1.33	1.38
1	AA	4500	PSU	C4-N3	-2.69	1.33	1.38
45	BA	814	PSU	C4-N3	-2.69	1.33	1.38
45	BA	27	A2M	C5-C6	2.69	1.48	1.41
1	AA	4471	PSU	C4-N3	-2.69	1.33	1.38
1	AA	1316	OMG	C6-N1	-2.69	1.33	1.38
45	BA	1232	PSU	C4-N3	-2.69	1.33	1.38
45	BA	590	A2M	C5-C6	2.68	1.48	1.41
45	BA	815	PSU	C4-N3	-2.68	1.33	1.38
45	BA	1326	UY1	O4-C4	-2.68	1.18	1.23
45	BA	484	A2M	C5-C6	2.67	1.48	1.41
45	BA	1186	PSU	C4-N3	-2.67	1.33	1.38
45	BA	36	PSU	C4-N3	-2.67	1.33	1.38
45	BA	863	PSU	C4-N3	-2.67	1.33	1.38
1	AA	3724	A2M	C5-C6	2.67	1.48	1.41
1	AA	4972	PSU	C4-N3	-2.67	1.33	1.38
45	BA	93	PSU	C4-N3	-2.66	1.33	1.38
1	AA	5010	PSU	C4-N3	-2.66	1.33	1.38
45	BA	1850	MA6	C5-C6	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	1445	PSU	C4-N3	-2.65	1.33	1.38
1	AA	1781	PSU	C4-N3	-2.65	1.33	1.38
1	AA	4576	PSU	C4-N3	-2.65	1.33	1.38
45	BA	1046	PSU	C4-N3	-2.65	1.33	1.38
1	AA	4196	OMG	C6-N1	-2.65	1.33	1.38
45	BA	1383	A2M	C5-C6	2.65	1.48	1.41
1	AA	4499	OMG	C6-N1	-2.65	1.33	1.38
45	BA	668	A2M	C5-C6	2.64	1.48	1.41
1	AA	2837	OMU	C4-N3	-2.64	1.33	1.38
45	BA	867	OMG	C6-N1	-2.64	1.33	1.38
1	AA	3899	OMG	C6-N1	-2.64	1.33	1.38
1	AA	2876	OMG	C6-N1	-2.64	1.33	1.38
3	AC	75	OMG	C6-N1	-2.64	1.33	1.38
45	BA	1003	PSU	C4-N3	-2.64	1.33	1.38
45	BA	296	PSU	C4-N3	-2.64	1.33	1.38
45	BA	1347	PSU	C4-N3	-2.64	1.33	1.38
45	BA	651	PSU	C4-N3	-2.63	1.33	1.38
1	AA	1782	PSU	C4-N3	-2.63	1.34	1.38
45	BA	1045	PSU	C4-N3	-2.63	1.34	1.38
45	BA	1442	OMU	C4-N3	-2.63	1.33	1.38
1	AA	1744	PSU	C4-N3	-2.62	1.34	1.38
1	AA	3744	OMG	C6-N1	-2.62	1.34	1.38
45	BA	601	OMG	C6-N1	-2.62	1.34	1.38
1	AA	4623	OMG	C6-N1	-2.62	1.34	1.38
1	AA	3768	PSU	C4-N3	-2.62	1.34	1.38
45	BA	918	PSU	C4-N3	-2.62	1.34	1.38
1	AA	4370	OMG	C6-N1	-2.62	1.34	1.38
1	AA	1323	A2M	C5-C6	2.61	1.48	1.41
1	AA	3782	5MC	C6-C5	2.61	1.38	1.34
45	BA	105	PSU	C4-N3	-2.61	1.34	1.38
45	BA	1360	PSU	C4-N3	-2.61	1.34	1.38
1	AA	1522	OMG	C6-N1	-2.61	1.34	1.38
45	BA	1031	A2M	C5-C6	2.61	1.48	1.41
1	AA	4227	OMU	C4-N3	-2.61	1.33	1.38
45	BA	1692	PSU	C4-N3	-2.61	1.34	1.38
1	AA	3770	PSU	C4-N3	-2.61	1.34	1.38
45	BA	609	PSU	C4-N3	-2.61	1.34	1.38
1	AA	2815	A2M	C5-C6	2.61	1.48	1.41
1	AA	4494	OMG	C6-N1	-2.60	1.34	1.38
45	BA	512	A2M	C5-C6	2.60	1.48	1.41
45	BA	1174	PSU	C4-N3	-2.60	1.34	1.38
1	AA	1625	OMG	C6-N1	-2.60	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	109	PSU	C4-N3	-2.60	1.34	1.38
45	BA	218	PSU	C4-N3	-2.59	1.34	1.38
1	AA	4637	OMG	C6-N1	-2.59	1.34	1.38
45	BA	119	PSU	C4-N3	-2.59	1.34	1.38
45	BA	63	PSU	C4-N3	-2.59	1.34	1.38
45	BA	1244	PSU	C4-N3	-2.59	1.34	1.38
45	BA	1367	PSU	C4-N3	-2.59	1.34	1.38
1	AA	1534	A2M	C5-C6	2.59	1.48	1.41
1	AA	2401	A2M	C5-C6	2.59	1.48	1.41
1	AA	2632	PSU	C4-N3	-2.59	1.34	1.38
45	BA	822	PSU	C4-N3	-2.58	1.34	1.38
45	BA	300	PSU	C4-N3	-2.58	1.34	1.38
45	BA	1238	PSU	C4-N3	-2.58	1.34	1.38
1	AA	3792	OMG	C6-N1	-2.58	1.34	1.38
45	BA	649	PSU	C4-N3	-2.58	1.34	1.38
45	BA	509	OMG	C6-N1	-2.58	1.34	1.38
1	AA	1524	A2M	C5-C6	2.58	1.48	1.41
1	AA	4423	PSU	C4-N3	-2.57	1.34	1.38
45	BA	801	PSU	C4-N3	-2.57	1.34	1.38
1	AA	2415	OMU	C4-N3	-2.57	1.34	1.38
45	BA	966	PSU	C4-N3	-2.57	1.34	1.38
45	BA	1248	B8N	C4-N3	-2.57	1.35	1.40
1	AA	2364	OMG	C6-N1	-2.57	1.34	1.38
1	AA	4498	OMU	C4-N3	-2.57	1.34	1.38
1	AA	3867	A2M	C5-C6	2.57	1.48	1.41
1	AA	398	A2M	C5-C6	2.57	1.48	1.41
1	AA	4571	A2M	C5-C6	2.56	1.48	1.41
1	AA	3718	A2M	C5-C6	2.56	1.48	1.41
1	AA	3715	PSU	C4-N3	-2.56	1.34	1.38
1	AA	3825	A2M	C5-C6	2.56	1.48	1.41
1	AA	2424	OMG	C6-N1	-2.56	1.34	1.38
1	AA	4590	A2M	C5-C6	2.55	1.48	1.41
45	BA	1490	OMG	C6-N1	-2.55	1.34	1.38
1	AA	3830	A2M	C5-C6	2.54	1.48	1.41
45	BA	166	A2M	C5-C6	2.54	1.48	1.41
45	BA	99	A2M	C5-C6	2.53	1.48	1.41
1	AA	3764	PSU	C4-N3	-2.53	1.34	1.38
1	AA	3762	PSU	C4-N3	-2.53	1.34	1.38
45	BA	116	OMU	C4-N3	-2.52	1.34	1.38
1	AA	1326	A2M	C5-C6	2.52	1.48	1.41
1	AA	4228	OMG	C6-N1	-2.51	1.34	1.38
1	AA	3627	OMG	C6-N1	-2.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1779	PSU	C4-N3	-2.51	1.34	1.38
45	BA	1804	OMU	C4-N3	-2.50	1.34	1.38
1	AA	1871	A2M	C5-C6	2.50	1.48	1.41
45	BA	121	OMU	C4-N3	-2.50	1.34	1.38
45	BA	644	OMG	C6-N1	-2.50	1.34	1.38
1	AA	2363	A2M	C5-C6	2.49	1.48	1.41
1	AA	400	A2M	C5-C6	2.48	1.48	1.41
45	BA	1328	OMG	C6-N1	-2.48	1.34	1.38
1	AA	4220	6MZ	C5-N7	-2.48	1.34	1.39
1	AA	3785	A2M	C5-C6	2.47	1.48	1.41
45	BA	172	OMU	C4-N3	-2.47	1.34	1.38
1	AA	4499	OMG	C5-N7	-2.47	1.34	1.39
45	BA	1056	PSU	C4-N3	-2.47	1.34	1.38
45	BA	428	OMU	C4-N3	-2.46	1.34	1.38
45	BA	1447	OMG	C6-N1	-2.45	1.34	1.38
1	AA	3718	A2M	C5-N7	-2.44	1.34	1.39
1	AA	4618	OMG	C6-N1	-2.44	1.34	1.38
45	BA	468	A2M	C8-N7	2.44	1.36	1.31
1	AA	2787	A2M	C5-C6	2.44	1.47	1.41
45	BA	668	A2M	C8-N7	2.43	1.36	1.31
45	BA	354	OMU	C4-N3	-2.43	1.34	1.38
1	AA	4196	OMG	C5-N7	-2.42	1.34	1.39
1	AA	4523	A2M	C5-C6	2.42	1.47	1.41
45	BA	683	OMG	C6-N1	-2.42	1.34	1.38
1	AA	400	A2M	C5-N7	-2.41	1.34	1.39
1	AA	2815	A2M	C5-N7	-2.41	1.34	1.39
1	AA	2787	A2M	C5-N7	-2.41	1.34	1.39
45	BA	1678	A2M	C8-N7	2.41	1.36	1.31
1	AA	4220	6MZ	C5-C6	2.40	1.48	1.41
1	AA	3792	OMG	C5-N7	-2.39	1.34	1.39
1	AA	3724	A2M	C8-N7	2.39	1.36	1.31
45	BA	484	A2M	C8-N7	2.39	1.36	1.31
45	BA	1383	A2M	C8-N7	2.39	1.36	1.31
1	AA	1326	A2M	C5-N7	-2.39	1.34	1.39
45	BA	1851	MA6	C8-N7	2.38	1.36	1.31
1	AA	4306	OMU	C2-N3	-2.38	1.33	1.38
1	AA	3925	OMU	C2-N3	-2.38	1.33	1.38
45	BA	436	OMG	C6-N1	-2.38	1.34	1.38
1	AA	4571	A2M	C5-N7	-2.37	1.34	1.39
1	AA	3830	A2M	C5-N7	-2.37	1.34	1.39
45	BA	1832	6MZ	C5-C6	2.36	1.48	1.41
45	BA	1288	OMU	C4-N3	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1871	A2M	C5-N7	-2.35	1.34	1.39
45	BA	166	A2M	C5-N7	-2.35	1.34	1.39
1	AA	2363	A2M	C5-N7	-2.34	1.34	1.39
1	AA	3867	A2M	C5-N7	-2.34	1.34	1.39
1	AA	4590	A2M	C8-N7	2.34	1.36	1.31
1	AA	3825	A2M	C5-N7	-2.34	1.34	1.39
45	BA	576	A2M	C8-N7	2.33	1.36	1.31
1	AA	1534	A2M	C8-N7	2.33	1.36	1.31
1	AA	2876	OMG	C5-N7	-2.33	1.34	1.39
1	AA	1316	OMG	C5-N7	-2.32	1.34	1.39
1	AA	1534	A2M	C5-N7	-2.32	1.34	1.39
45	BA	99	A2M	C8-N7	2.32	1.36	1.31
1	AA	4523	A2M	C5-N7	-2.32	1.34	1.39
45	BA	27	A2M	C8-N7	2.32	1.36	1.31
45	BA	1850	MA6	C8-N7	2.32	1.36	1.31
1	AA	398	A2M	C5-N7	-2.31	1.34	1.39
1	AA	4620	OMU	C2-N3	-2.31	1.33	1.38
45	BA	512	A2M	C5-N7	-2.31	1.34	1.39
1	AA	4447	5MC	C6-N1	-2.31	1.34	1.38
1	AA	1524	A2M	C5-N7	-2.31	1.34	1.39
1	AA	3782	5MC	C6-N1	-2.31	1.34	1.38
1	AA	2401	A2M	C5-N7	-2.31	1.34	1.39
45	BA	99	A2M	C5-N7	-2.31	1.34	1.39
1	AA	4494	OMG	C5-N7	-2.30	1.34	1.39
45	BA	867	OMG	C5-N7	-2.30	1.34	1.39
1	AA	398	A2M	C8-N7	2.30	1.36	1.31
1	AA	4498	OMU	C2-N3	-2.30	1.33	1.38
3	AC	14	OMU	C2-N3	-2.30	1.33	1.38
1	AA	1322	1MA	C5-N7	-2.30	1.34	1.39
1	AA	2364	OMG	C5-N7	-2.30	1.34	1.39
1	AA	1323	A2M	C5-N7	-2.30	1.34	1.39
1	AA	2424	OMG	C5-N7	-2.29	1.34	1.39
45	BA	590	A2M	C5-N7	-2.29	1.34	1.39
45	BA	601	OMG	C5-N7	-2.29	1.34	1.39
1	AA	2401	A2M	C8-N7	2.28	1.35	1.31
45	BA	1031	A2M	C8-N7	2.28	1.35	1.31
45	BA	1031	A2M	C5-N7	-2.28	1.34	1.39
1	AA	3744	OMG	C5-N7	-2.28	1.34	1.39
1	AA	3785	A2M	C8-N7	2.27	1.35	1.31
45	BA	159	A2M	C8-N7	2.27	1.35	1.31
1	AA	3825	A2M	C8-N7	2.27	1.35	1.31
1	AA	3867	A2M	C8-N7	2.27	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	1832	6MZ	C5-N7	-2.27	1.34	1.39
1	AA	2815	A2M	C8-N7	2.26	1.35	1.31
1	AA	1625	OMG	C5-N7	-2.26	1.34	1.39
3	AC	14	OMU	C5-C4	-2.26	1.38	1.43
1	AA	4571	A2M	C8-N7	2.26	1.35	1.31
45	BA	512	A2M	C8-N7	2.26	1.35	1.31
1	AA	4637	OMG	C5-N7	-2.26	1.34	1.39
1	AA	3637	PSU	C2-N3	-2.26	1.33	1.37
45	BA	572	PSU	O4'-C1'	-2.25	1.40	1.43
1	AA	1524	A2M	C8-N7	2.25	1.35	1.31
3	AC	75	OMG	C5-N7	-2.25	1.34	1.39
1	AA	2363	A2M	C8-N7	2.25	1.35	1.31
1	AA	3785	A2M	C5-N7	-2.25	1.34	1.39
1	AA	2837	OMU	C2-N3	-2.24	1.34	1.38
1	AA	1522	OMG	C5-N7	-2.24	1.34	1.39
1	AA	3724	A2M	C5-N7	-2.24	1.34	1.39
1	AA	400	A2M	C8-N7	2.24	1.35	1.31
1	AA	4590	A2M	C5-N7	-2.23	1.34	1.39
45	BA	159	A2M	C5-N7	-2.23	1.34	1.39
1	AA	3899	OMG	C5-N7	-2.23	1.34	1.39
45	BA	484	A2M	C5-N7	-2.23	1.34	1.39
1	AA	1323	A2M	C8-N7	2.23	1.35	1.31
1	AA	4523	A2M	C8-N7	2.23	1.35	1.31
45	BA	590	A2M	C8-N7	2.23	1.35	1.31
1	AA	3830	A2M	C8-N7	2.23	1.35	1.31
1	AA	3627	OMG	C5-N7	-2.23	1.34	1.39
45	BA	509	OMG	C5-N7	-2.23	1.34	1.39
1	AA	1326	A2M	C8-N7	2.23	1.35	1.31
1	AA	2415	OMU	C2-N3	-2.23	1.34	1.38
1	AA	1871	A2M	C8-N7	2.22	1.35	1.31
45	BA	576	A2M	C5-N7	-2.22	1.34	1.39
1	AA	4392	OMG	C5-N7	-2.22	1.34	1.39
45	BA	27	A2M	C5-N7	-2.21	1.34	1.39
45	BA	1832	6MZ	C8-N7	2.21	1.35	1.31
45	BA	668	A2M	C5-N7	-2.21	1.34	1.39
45	BA	166	A2M	C8-N7	2.21	1.35	1.31
45	BA	1490	OMG	C5-N7	-2.20	1.34	1.39
1	AA	4227	OMU	C2-N3	-2.19	1.34	1.38
1	AA	4370	OMG	C5-N7	-2.19	1.34	1.39
1	AA	4623	OMG	C5-N7	-2.19	1.34	1.39
1	AA	4618	OMG	C5-N7	-2.17	1.34	1.39
45	BA	1383	A2M	C5-N7	-2.17	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1582	PSU	C2-N3	-2.17	1.33	1.37
45	BA	436	OMG	C5-N7	-2.17	1.34	1.39
1	AA	2787	A2M	C8-N7	2.17	1.35	1.31
45	BA	116	OMU	C2-N3	-2.17	1.34	1.38
1	AA	4220	6MZ	C8-N7	2.16	1.35	1.31
45	BA	1851	MA6	C5-N7	-2.16	1.34	1.39
1	AA	3718	A2M	C8-N7	2.16	1.35	1.31
45	BA	1447	OMG	C5-N7	-2.16	1.34	1.39
45	BA	1328	OMG	C5-N7	-2.16	1.34	1.39
45	BA	1678	A2M	C5-N7	-2.16	1.34	1.39
45	BA	1804	OMU	C2-N1	2.16	1.41	1.38
45	BA	1442	OMU	C2-N3	-2.16	1.34	1.38
45	BA	1360	PSU	C2-N1	-2.14	1.33	1.36
45	BA	644	OMG	C5-N7	-2.14	1.34	1.39
45	BA	1804	OMU	C2-N3	-2.13	1.34	1.38
45	BA	1850	MA6	C5-N7	-2.13	1.35	1.39
1	AA	4306	OMU	C5-C4	-2.12	1.38	1.43
1	AA	4620	OMU	C5-C4	-2.12	1.38	1.43
45	BA	1360	PSU	C4-C5	2.12	1.50	1.44
1	AA	4228	OMG	C4-N9	-2.11	1.32	1.38
45	BA	121	OMU	C2-N3	-2.11	1.34	1.38
1	AA	4228	OMG	C5-N7	-2.11	1.35	1.39
1	AA	4299	PSU	C2-N3	-2.11	1.33	1.37
45	BA	428	OMU	C2-N3	-2.11	1.34	1.38
45	BA	683	OMG	C5-N7	-2.11	1.35	1.39
1	AA	1322	1MA	C2-N3	2.10	1.34	1.30
45	BA	468	A2M	C5-N7	-2.09	1.35	1.39
1	AA	2843	PSU	C2-N3	-2.08	1.33	1.37
45	BA	1288	OMU	C5-C4	-2.08	1.39	1.43
45	BA	116	OMU	C5-C4	-2.08	1.39	1.43
1	AA	2837	OMU	C5-C4	-2.08	1.39	1.43
1	AA	1683	PSU	C2-N3	-2.07	1.34	1.37
45	BA	354	OMU	C2-N3	-2.07	1.34	1.38
45	BA	1442	OMU	C5-C4	-2.06	1.39	1.43
1	AA	3844	PSU	C2-N3	-2.05	1.34	1.37
1	AA	4227	OMU	C2-N1	2.04	1.41	1.38
45	BA	172	OMU	C2-N3	-2.04	1.34	1.38
45	BA	1288	OMU	C2-N3	-2.04	1.34	1.38
1	AA	4442	PSU	O4'-C1'	-2.04	1.41	1.43
1	AA	1862	PSU	C2-N3	-2.03	1.34	1.37
45	BA	1804	OMU	C5-C4	-2.03	1.39	1.43
45	BA	1360	PSU	C2-N3	-2.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1860	PSU	C2-N3	-2.03	1.34	1.37
1	AA	4498	OMU	C5-C4	-2.02	1.39	1.43
1	AA	2415	OMU	C5-C4	-2.02	1.39	1.43
1	AA	4293	PSU	C2-N3	-2.02	1.34	1.37
1	AA	3925	OMU	C5-C4	-2.02	1.39	1.43
1	AA	4673	PSU	C2-N3	-2.02	1.34	1.37
1	AA	3920	PSU	C2-N3	-2.01	1.34	1.37
1	AA	2839	PSU	C2-N3	-2.01	1.34	1.37
45	BA	667	PSU	C2-N3	-2.01	1.34	1.37
1	AA	3884	PSU	C2-N3	-2.00	1.34	1.37
1	AA	4521	PSU	C2-N3	-2.00	1.34	1.37
45	BA	354	OMU	C5-C4	-2.00	1.39	1.43
45	BA	172	OMU	C2-N1	2.00	1.41	1.38

All (976) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	590	A2M	C5-C4-N3	-7.19	117.37	126.75
1	AA	2815	A2M	C5-C4-N3	-6.91	117.73	126.75
45	BA	867	OMG	C5-C4-N3	-6.62	117.71	128.46
45	BA	512	A2M	C5-C4-N3	-6.61	118.12	126.75
45	BA	601	OMG	C5-C4-N3	-6.58	117.79	128.46
1	AA	4499	OMG	C5-C4-N3	-6.57	117.80	128.46
45	BA	159	A2M	C5-C4-N3	-6.56	118.19	126.75
45	BA	166	A2M	C5-C4-N3	-6.51	118.26	126.75
1	AA	4571	A2M	C5-C4-N3	-6.50	118.27	126.75
1	AA	3867	A2M	C5-C4-N3	-6.48	118.30	126.75
45	BA	1832	6MZ	C5-C4-N3	-6.48	118.30	126.75
1	AA	4196	OMG	C5-C4-N3	-6.44	118.01	128.46
45	BA	27	A2M	C5-C4-N3	-6.43	118.36	126.75
45	BA	484	A2M	C5-C4-N3	-6.42	118.37	126.75
1	AA	3637	PSU	N1-C2-N3	6.42	122.41	115.13
1	AA	1323	A2M	C5-C4-N3	-6.40	118.40	126.75
45	BA	99	A2M	C5-C4-N3	-6.40	118.40	126.75
1	AA	3830	A2M	C5-C4-N3	-6.36	118.45	126.75
1	AA	3792	OMG	C5-C4-N3	-6.35	118.15	128.46
45	BA	576	A2M	C5-C4-N3	-6.35	118.47	126.75
45	BA	1851	MA6	C5-C4-N3	-6.35	118.47	126.75
1	AA	3724	A2M	C5-C4-N3	-6.34	118.48	126.75
1	AA	3718	A2M	C5-C4-N3	-6.31	118.52	126.75
45	BA	509	OMG	C5-C4-N3	-6.30	118.23	128.46
3	AC	75	OMG	C5-C4-N3	-6.29	118.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	3825	A2M	C5-C4-N3	-6.29	118.55	126.75
45	BA	1031	A2M	C5-C4-N3	-6.27	118.56	126.75
1	AA	1326	A2M	C5-C4-N3	-6.27	118.57	126.75
1	AA	2363	A2M	C5-C4-N3	-6.26	118.59	126.75
45	BA	1328	OMG	C5-C4-N3	-6.25	118.31	128.46
45	BA	1447	OMG	C5-C4-N3	-6.25	118.31	128.46
45	BA	1490	OMG	C5-C4-N3	-6.25	118.33	128.46
1	AA	400	A2M	C5-C4-N3	-6.23	118.62	126.75
45	BA	1136	PSU	N1-C2-N3	6.23	122.19	115.13
1	AA	398	A2M	C5-C4-N3	-6.23	118.62	126.75
1	AA	2364	OMG	C5-C4-N3	-6.23	118.35	128.46
1	AA	4628	PSU	N1-C2-N3	6.22	122.18	115.13
1	AA	4220	6MZ	C5-C4-N3	-6.22	118.63	126.75
1	AA	4500	PSU	N1-C2-N3	6.21	122.17	115.13
1	AA	2401	A2M	C5-C4-N3	-6.21	118.65	126.75
45	BA	668	A2M	C5-C4-N3	-6.21	118.65	126.75
1	AA	3785	A2M	C5-C4-N3	-6.19	118.67	126.75
45	BA	436	OMG	C5-C4-N3	-6.18	118.43	128.46
1	AA	1524	A2M	C5-C4-N3	-6.18	118.69	126.75
1	AA	1534	A2M	C5-C4-N3	-6.17	118.70	126.75
1	AA	4523	A2M	C5-C4-N3	-6.16	118.71	126.75
45	BA	1383	A2M	C5-C4-N3	-6.16	118.71	126.75
1	AA	2876	OMG	C5-C4-N3	-6.15	118.49	128.46
1	AA	3744	OMG	C5-C4-N3	-6.14	118.50	128.46
1	AA	4457	PSU	N1-C2-N3	6.14	122.08	115.13
1	AA	4636	PSU	N1-C2-N3	6.14	122.08	115.13
45	BA	1643	PSU	N1-C2-N3	6.12	122.07	115.13
1	AA	4442	PSU	N1-C2-N3	6.12	122.07	115.13
1	AA	3822	PSU	N1-C2-N3	6.12	122.06	115.13
1	AA	1871	A2M	C5-C4-N3	-6.12	118.77	126.75
1	AA	2787	A2M	C5-C4-N3	-6.11	118.78	126.75
1	AA	4532	PSU	N1-C2-N3	6.11	122.05	115.13
1	AA	4296	PSU	N1-C2-N3	6.10	122.04	115.13
1	AA	4590	A2M	C5-C4-N3	-6.10	118.79	126.75
45	BA	822	PSU	N1-C2-N3	6.10	122.04	115.13
1	AA	4494	OMG	C5-C4-N3	-6.08	118.59	128.46
1	AA	4973	PSU	N1-C2-N3	6.08	122.02	115.13
45	BA	649	PSU	N1-C2-N3	6.08	122.02	115.13
45	BA	644	OMG	C5-C4-N3	-6.08	118.60	128.46
1	AA	5001	PSU	N1-C2-N3	6.08	122.01	115.13
45	BA	815	PSU	N1-C2-N3	6.07	122.01	115.13
1	AA	3851	PSU	N1-C2-N3	6.07	122.00	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	4521	PSU	N1-C2-N3	6.07	122.00	115.13
1	AA	4392	OMG	C5-C4-N3	-6.06	118.63	128.46
1	AA	1625	OMG	C5-C4-N3	-6.06	118.63	128.46
1	AA	4493	PSU	N1-C2-N3	6.06	121.99	115.13
1	AA	3920	PSU	N1-C2-N3	6.05	121.98	115.13
1	AA	4353	PSU	N1-C2-N3	6.04	121.98	115.13
45	BA	406	PSU	N1-C2-N3	6.04	121.98	115.13
1	AA	4637	OMG	C5-C4-N3	-6.04	118.66	128.46
1	AA	4312	PSU	N1-C2-N3	6.03	121.97	115.13
3	AC	69	PSU	N1-C2-N3	6.03	121.96	115.13
1	AA	3853	PSU	N1-C2-N3	6.03	121.96	115.13
1	AA	4403	PSU	N1-C2-N3	6.02	121.95	115.13
45	BA	1347	PSU	N1-C2-N3	6.02	121.95	115.13
45	BA	866	PSU	N1-C2-N3	6.02	121.95	115.13
45	BA	1177	PSU	N1-C2-N3	6.02	121.95	115.13
45	BA	34	PSU	N1-C2-N3	6.02	121.94	115.13
45	BA	1850	MA6	C5-C4-N3	-6.01	118.91	126.75
1	AA	3695	PSU	N1-C2-N3	6.01	121.94	115.13
45	BA	651	PSU	N1-C2-N3	6.01	121.94	115.13
1	AA	4623	OMG	C5-C4-N3	-6.01	118.72	128.46
1	AA	4552	PSU	N1-C2-N3	6.00	121.93	115.13
1	AA	1677	PSU	N1-C2-N3	6.00	121.92	115.13
1	AA	4618	OMG	C5-C4-N3	-5.99	118.74	128.46
1	AA	1683	PSU	N1-C2-N3	5.99	121.91	115.13
1	AA	4361	PSU	N1-C2-N3	5.99	121.91	115.13
45	BA	1678	A2M	C5-C4-N3	-5.99	118.94	126.75
45	BA	218	PSU	N1-C2-N3	5.98	121.91	115.13
45	BA	93	PSU	N1-C2-N3	5.97	121.90	115.13
1	AA	2508	PSU	N1-C2-N3	5.97	121.89	115.13
45	BA	1174	PSU	N1-C2-N3	5.97	121.89	115.13
45	BA	1596	PSU	N1-C2-N3	5.97	121.89	115.13
1	AA	1744	PSU	N1-C2-N3	5.97	121.89	115.13
45	BA	686	PSU	N1-C2-N3	5.96	121.89	115.13
1	AA	4293	PSU	N1-C2-N3	5.96	121.89	115.13
1	AA	3844	PSU	N1-C2-N3	5.96	121.89	115.13
45	BA	468	A2M	C5-C4-N3	-5.96	118.97	126.75
45	BA	1046	PSU	N1-C2-N3	5.96	121.88	115.13
1	AA	2424	OMG	C5-C4-N3	-5.96	118.79	128.46
45	BA	572	PSU	N1-C2-N3	5.96	121.88	115.13
45	BA	1003	PSU	N1-C2-N3	5.96	121.88	115.13
1	AA	3730	PSU	N1-C2-N3	5.95	121.88	115.13
45	BA	683	OMG	C5-C4-N3	-5.95	118.80	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	966	PSU	N1-C2-N3	5.95	121.87	115.13
1	AA	3884	PSU	N1-C2-N3	5.95	121.87	115.13
45	BA	1238	PSU	N1-C2-N3	5.95	121.87	115.13
1	AA	4370	OMG	C5-C4-N3	-5.95	118.81	128.46
45	BA	1232	PSU	N1-C2-N3	5.94	121.86	115.13
1	AA	4673	PSU	N1-C2-N3	5.94	121.86	115.13
1	AA	1316	OMG	C5-C4-N3	-5.94	118.83	128.46
1	AA	3715	PSU	N1-C2-N3	5.93	121.85	115.13
45	BA	1045	PSU	N1-C2-N3	5.93	121.85	115.13
1	AA	2843	PSU	N1-C2-N3	5.93	121.85	115.13
45	BA	109	PSU	N1-C2-N3	5.93	121.85	115.13
1	AA	4972	PSU	N1-C2-N3	5.93	121.84	115.13
1	AA	4423	PSU	N1-C2-N3	5.92	121.84	115.13
1	AA	4579	PSU	N1-C2-N3	5.92	121.84	115.13
1	AA	1536	PSU	N1-C2-N3	5.92	121.84	115.13
1	AA	2839	PSU	N1-C2-N3	5.92	121.84	115.13
1	AA	3639	PSU	N1-C2-N3	5.92	121.83	115.13
45	BA	1056	PSU	N1-C2-N3	5.92	121.83	115.13
1	AA	4431	PSU	N1-C2-N3	5.91	121.83	115.13
45	BA	1625	PSU	N1-C2-N3	5.91	121.83	115.13
1	AA	1781	PSU	N1-C2-N3	5.91	121.82	115.13
1	AA	4576	PSU	N1-C2-N3	5.90	121.81	115.13
45	BA	609	PSU	N1-C2-N3	5.90	121.81	115.13
1	AA	1779	PSU	N1-C2-N3	5.90	121.81	115.13
1	AA	4471	PSU	N1-C2-N3	5.90	121.81	115.13
1	AA	1782	PSU	N1-C2-N3	5.89	121.81	115.13
45	BA	918	PSU	N1-C2-N3	5.89	121.81	115.13
45	BA	100	PSU	N1-C2-N3	5.89	121.80	115.13
45	BA	814	PSU	N1-C2-N3	5.89	121.80	115.13
45	BA	119	PSU	N1-C2-N3	5.89	121.80	115.13
1	AA	1862	PSU	N1-C2-N3	5.88	121.80	115.13
45	BA	1445	PSU	N1-C2-N3	5.88	121.79	115.13
1	AA	1792	PSU	N1-C2-N3	5.87	121.78	115.13
45	BA	63	PSU	N1-C2-N3	5.87	121.78	115.13
45	BA	1692	PSU	N1-C2-N3	5.87	121.78	115.13
45	BA	366	PSU	N1-C2-N3	5.86	121.77	115.13
45	BA	1004	PSU	N1-C2-N3	5.86	121.77	115.13
1	AA	3899	OMG	C5-C4-N3	-5.86	118.95	128.46
45	BA	36	PSU	N1-C2-N3	5.86	121.77	115.13
45	BA	296	PSU	N1-C2-N3	5.86	121.77	115.13
3	AC	55	PSU	N1-C2-N3	5.86	121.77	115.13
1	AA	1860	PSU	N1-C2-N3	5.86	121.77	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	801	PSU	N1-C2-N3	5.85	121.76	115.13
45	BA	1186	PSU	N1-C2-N3	5.85	121.75	115.13
1	AA	3627	OMG	C5-C4-N3	-5.85	118.98	128.46
45	BA	1367	PSU	N1-C2-N3	5.84	121.74	115.13
45	BA	300	PSU	N1-C2-N3	5.84	121.74	115.13
1	AA	3768	PSU	N1-C2-N3	5.83	121.74	115.13
45	BA	681	PSU	N1-C2-N3	5.80	121.70	115.13
1	AA	3770	PSU	N1-C2-N3	5.79	121.69	115.13
45	BA	105	PSU	N1-C2-N3	5.78	121.67	115.13
45	BA	1244	PSU	N1-C2-N3	5.77	121.67	115.13
1	AA	3764	PSU	N1-C2-N3	5.77	121.67	115.13
1	AA	4299	PSU	N1-C2-N3	5.77	121.66	115.13
1	AA	5010	PSU	N1-C2-N3	5.74	121.64	115.13
1	AA	3762	PSU	N1-C2-N3	5.74	121.63	115.13
1	AA	1522	OMG	C5-C4-N3	-5.73	119.17	128.46
45	BA	667	PSU	N1-C2-N3	5.71	121.60	115.13
1	AA	4530	UR3	C4-N3-C2	-5.71	119.19	124.56
45	BA	590	A2M	N3-C4-N9	5.68	136.45	127.08
1	AA	2632	PSU	N1-C2-N3	5.66	121.54	115.13
1	AA	1582	PSU	N1-C2-N3	5.66	121.54	115.13
45	BA	1360	PSU	N1-C2-N3	5.65	121.53	115.13
1	AA	4689	PSU	N1-C2-N3	5.56	121.42	115.13
1	AA	4228	OMG	C5-C4-N3	-5.50	119.53	128.46
45	BA	863	PSU	N1-C2-N3	5.49	121.35	115.13
45	BA	1832	6MZ	N3-C4-N9	5.41	135.99	127.08
45	BA	512	A2M	N3-C4-N9	5.34	135.89	127.08
1	AA	2815	A2M	N3-C4-N9	5.33	135.87	127.08
1	AA	1322	1MA	C5-C4-N3	-5.20	119.50	127.26
45	BA	166	A2M	N3-C4-N9	5.18	135.62	127.08
1	AA	4571	A2M	N3-C4-N9	5.18	135.61	127.08
45	BA	159	A2M	N3-C4-N9	5.11	135.51	127.08
45	BA	601	OMG	C2-N3-C4	5.08	121.35	112.30
1	AA	3867	A2M	N3-C4-N9	5.08	135.45	127.08
45	BA	601	OMG	N9-C4-N3	5.06	136.10	125.94
45	BA	99	A2M	N3-C4-N9	5.05	135.41	127.08
1	AA	4618	OMG	C2-N3-C4	5.03	121.27	112.30
45	BA	27	A2M	N3-C4-N9	5.03	135.37	127.08
45	BA	436	OMG	C2-N3-C4	5.01	121.23	112.30
1	AA	2364	OMG	C2-N3-C4	5.01	121.22	112.30
1	AA	3830	A2M	N3-C4-N9	4.99	135.30	127.08
1	AA	3785	A2M	N3-C4-N9	4.97	135.27	127.08
45	BA	484	A2M	N3-C4-N9	4.96	135.25	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	3792	OMG	C2-N3-C4	4.96	121.13	112.30
45	BA	867	OMG	N9-C4-N3	4.95	135.88	125.94
45	BA	1328	OMG	C2-N3-C4	4.95	121.12	112.30
45	BA	1383	A2M	N3-C4-N9	4.95	135.23	127.08
1	AA	4499	OMG	C2-N3-C4	4.95	121.11	112.30
45	BA	576	A2M	N3-C4-N9	4.95	135.23	127.08
45	BA	1031	A2M	N3-C4-N9	4.94	135.22	127.08
45	BA	1447	OMG	C2-N3-C4	4.94	121.09	112.30
1	AA	1323	A2M	N3-C4-N9	4.93	135.21	127.08
1	AA	4523	A2M	N3-C4-N9	4.93	135.20	127.08
1	AA	4196	OMG	N9-C4-N3	4.92	135.82	125.94
1	AA	400	A2M	N3-C4-N9	4.92	135.19	127.08
1	AA	3792	OMG	N9-C4-N3	4.91	135.79	125.94
1	AA	1326	A2M	N3-C4-N9	4.91	135.16	127.08
1	AA	2876	OMG	C2-N3-C4	4.90	121.03	112.30
1	AA	3744	OMG	C2-N3-C4	4.90	121.02	112.30
1	AA	4196	OMG	C2-N3-C4	4.89	121.02	112.30
3	AC	75	OMG	C2-N3-C4	4.89	121.01	112.30
45	BA	683	OMG	C2-N3-C4	4.89	121.01	112.30
1	AA	1871	A2M	N3-C4-N9	4.88	135.12	127.08
45	BA	867	OMG	C2-N3-C4	4.88	120.99	112.30
1	AA	4392	OMG	C2-N3-C4	4.87	120.98	112.30
1	AA	3724	A2M	N3-C4-N9	4.87	135.11	127.08
45	BA	509	OMG	N9-C4-N3	4.87	135.72	125.94
45	BA	509	OMG	C2-N3-C4	4.87	120.97	112.30
1	AA	2363	A2M	N3-C4-N9	4.86	135.10	127.08
45	BA	1851	MA6	N3-C4-N9	4.86	135.09	127.08
1	AA	3825	A2M	N3-C4-N9	4.86	135.08	127.08
1	AA	1316	OMG	C2-N3-C4	4.85	120.95	112.30
1	AA	398	A2M	N3-C4-N9	4.85	135.08	127.08
1	AA	4499	OMG	N9-C4-N3	4.85	135.68	125.94
1	AA	2401	A2M	N3-C4-N9	4.84	135.06	127.08
1	AA	2424	OMG	C2-N3-C4	4.84	120.92	112.30
1	AA	2787	A2M	N3-C4-N9	4.84	135.05	127.08
45	BA	644	OMG	C2-N3-C4	4.84	120.92	112.30
1	AA	3899	OMG	C2-N3-C4	4.83	120.91	112.30
1	AA	3627	OMG	C2-N3-C4	4.83	120.91	112.30
1	AA	3718	A2M	N3-C4-N9	4.83	135.04	127.08
1	AA	4623	OMG	C2-N3-C4	4.83	120.90	112.30
1	AA	4637	OMG	C2-N3-C4	4.83	120.90	112.30
1	AA	4494	OMG	C2-N3-C4	4.82	120.89	112.30
1	AA	4220	6MZ	N3-C4-N9	4.82	135.02	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	4370	OMG	C2-N3-C4	4.81	120.87	112.30
1	AA	1625	OMG	C2-N3-C4	4.81	120.87	112.30
1	AA	4590	A2M	N3-C4-N9	4.81	135.00	127.08
1	AA	4228	OMG	C2-N3-C4	4.80	120.86	112.30
45	BA	1490	OMG	C2-N3-C4	4.77	120.80	112.30
1	AA	1524	A2M	N3-C4-N9	4.76	134.93	127.08
1	AA	1522	OMG	C2-N3-C4	4.76	120.78	112.30
3	AC	75	OMG	N9-C4-N3	4.72	135.42	125.94
45	BA	1490	OMG	N9-C4-N3	4.72	135.42	125.94
45	BA	668	A2M	N3-C4-N9	4.70	134.83	127.08
45	BA	468	A2M	N3-C4-N9	4.68	134.80	127.08
45	BA	436	OMG	N9-C4-N3	4.67	135.32	125.94
45	BA	644	OMG	N9-C4-N3	4.66	135.30	125.94
45	BA	1328	OMG	N9-C4-N3	4.66	135.29	125.94
1	AA	1625	OMG	N9-C4-N3	4.66	135.29	125.94
1	AA	1534	A2M	N3-C4-N9	4.66	134.75	127.08
45	BA	1850	MA6	N3-C4-N9	4.66	134.75	127.08
1	AA	4494	OMG	N9-C4-N3	4.65	135.27	125.94
45	BA	1678	A2M	N3-C4-N9	4.64	134.73	127.08
1	AA	3818	UY1	C4-N3-C2	-4.63	119.67	126.34
45	BA	1447	OMG	N9-C4-N3	4.62	135.22	125.94
1	AA	1322	1MA	C2-N3-C4	4.62	121.49	112.41
1	AA	2364	OMG	N9-C4-N3	4.59	135.16	125.94
1	AA	2876	OMG	N9-C4-N3	4.56	135.09	125.94
45	BA	1383	A2M	C2'-C1'-N9	-4.55	105.86	113.53
1	AA	4498	OMU	C4-N3-C2	-4.55	120.58	126.58
1	AA	2424	OMG	N9-C4-N3	4.54	135.06	125.94
45	BA	1337	4AC	O7-C7-N4	4.54	129.17	121.82
1	AA	3925	OMU	C4-N3-C2	-4.53	120.61	126.58
45	BA	428	OMU	C4-N3-C2	-4.50	120.64	126.58
1	AA	2415	OMU	C4-N3-C2	-4.50	120.65	126.58
45	BA	1288	OMU	C4-N3-C2	-4.49	120.65	126.58
1	AA	3744	OMG	N9-C4-N3	4.49	134.96	125.94
3	AC	14	OMU	C4-N3-C2	-4.49	120.66	126.58
45	BA	1842	4AC	O7-C7-N4	4.47	129.06	121.82
1	AA	4227	OMU	C4-N3-C2	-4.46	120.70	126.58
1	AA	4637	OMG	N9-C4-N3	4.45	134.88	125.94
1	AA	4370	OMG	N9-C4-N3	4.44	134.85	125.94
1	AA	2837	OMU	C4-N3-C2	-4.42	120.75	126.58
1	AA	1316	OMG	N9-C4-N3	4.41	134.79	125.94
45	BA	172	OMU	C4-N3-C2	-4.40	120.77	126.58
45	BA	354	OMU	C4-N3-C2	-4.39	120.79	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	4623	OMG	N9-C4-N3	4.39	134.75	125.94
45	BA	683	OMG	N9-C4-N3	4.38	134.73	125.94
45	BA	1326	UY1	C4-N3-C2	-4.35	120.07	126.34
45	BA	1850	MA6	C2-N1-C6	4.34	122.00	111.75
1	AA	4392	OMG	N9-C4-N3	4.32	134.62	125.94
45	BA	1851	MA6	C2-N1-C6	4.30	121.91	111.75
1	AA	4618	OMG	N9-C4-N3	4.27	134.52	125.94
45	BA	1804	OMU	C4-N3-C2	-4.26	120.96	126.58
45	BA	590	A2M	C2-N3-C4	4.26	121.81	111.75
45	BA	121	OMU	C4-N3-C2	-4.25	120.97	126.58
1	AA	3899	OMG	N9-C4-N3	4.25	134.47	125.94
45	BA	1248	B8N	C4-N3-C2	-4.23	120.11	125.46
1	AA	4227	OMU	N3-C2-N1	4.22	120.49	114.89
1	AA	3925	OMU	N3-C2-N1	4.22	120.49	114.89
1	AA	4498	OMU	N3-C2-N1	4.21	120.48	114.89
1	AA	3627	OMG	N9-C4-N3	4.21	134.38	125.94
45	BA	354	OMU	N3-C2-N1	4.20	120.46	114.89
1	AA	2837	OMU	N3-C2-N1	4.17	120.43	114.89
3	AC	14	OMU	N3-C2-N1	4.17	120.42	114.89
1	AA	4620	OMU	C4-N3-C2	-4.16	121.09	126.58
45	BA	1850	MA6	C10-N6-C6	-4.14	109.66	120.40
45	BA	484	A2M	C2'-C1'-N9	-4.13	106.58	113.53
45	BA	866	PSU	C4-N3-C2	-4.12	120.40	126.34
45	BA	1851	MA6	C10-N6-C6	-4.12	109.72	120.40
45	BA	428	OMU	N3-C2-N1	4.11	120.34	114.89
1	AA	4973	PSU	C4-N3-C2	-4.10	120.44	126.34
1	AA	2415	OMU	N3-C2-N1	4.10	120.33	114.89
45	BA	1337	4AC	N4-C4-N3	4.09	120.72	113.85
1	AA	4306	OMU	C4-N3-C2	-4.09	121.18	126.58
1	AA	4296	PSU	C4-N3-C2	-4.09	120.45	126.34
1	AA	4457	PSU	C4-N3-C2	-4.07	120.48	126.34
1	AA	4972	PSU	C4-N3-C2	-4.06	120.48	126.34
1	AA	4500	PSU	C4-N3-C2	-4.06	120.48	126.34
1	AA	4447	5MC	C5-C6-N1	-4.06	119.16	123.34
45	BA	1804	OMU	N3-C2-N1	4.05	120.27	114.89
1	AA	1522	OMG	N9-C4-N3	4.05	134.07	125.94
1	AA	2815	A2M	C2-N3-C4	4.05	121.31	111.75
45	BA	815	PSU	C4-N3-C2	-4.03	120.53	126.34
1	AA	3637	PSU	C4-N3-C2	-4.03	120.53	126.34
45	BA	172	OMU	N3-C2-N1	4.03	120.24	114.89
1	AA	4442	PSU	C4-N3-C2	-4.03	120.53	126.34
45	BA	116	OMU	C4-N3-C2	-4.02	121.27	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	512	A2M	C2-N3-C4	4.02	121.26	111.75
45	BA	649	PSU	O2-C2-N1	-4.02	118.36	122.79
1	AA	3695	PSU	C4-N3-C2	-4.02	120.55	126.34
1	AA	4620	OMU	N3-C2-N1	4.02	120.23	114.89
1	AA	4636	PSU	C4-N3-C2	-4.02	120.55	126.34
45	BA	1177	PSU	C4-N3-C2	-4.02	120.55	126.34
1	AA	5001	PSU	C4-N3-C2	-4.02	120.55	126.34
1	AA	1782	PSU	C4-N3-C2	-4.01	120.56	126.34
1	AA	1677	PSU	C4-N3-C2	-4.01	120.56	126.34
1	AA	4293	PSU	C4-N3-C2	-4.01	120.57	126.34
1	AA	4403	PSU	C4-N3-C2	-4.01	120.57	126.34
45	BA	1850	MA6	N1-C6-N6	3.99	121.45	117.08
45	BA	121	OMU	N3-C2-N1	3.99	120.19	114.89
1	AA	4493	PSU	C4-N3-C2	-3.98	120.60	126.34
45	BA	1842	4AC	N4-C4-N3	3.98	120.54	113.85
45	BA	1326	UY1	N1-C2-N3	3.98	119.64	115.13
1	AA	3822	PSU	C4-N3-C2	-3.97	120.61	126.34
45	BA	1442	OMU	C4-N3-C2	-3.97	121.34	126.58
45	BA	651	PSU	C4-N3-C2	-3.97	120.62	126.34
1	AA	4353	PSU	C4-N3-C2	-3.97	120.62	126.34
45	BA	1347	PSU	C4-N3-C2	-3.97	120.62	126.34
45	BA	406	PSU	C4-N3-C2	-3.95	120.65	126.34
1	AA	4628	PSU	C4-N3-C2	-3.95	120.65	126.34
1	AA	3724	A2M	C2-N3-C4	3.94	121.07	111.75
1	AA	4571	A2M	C2-N3-C4	3.94	121.06	111.75
45	BA	1232	PSU	C4-N3-C2	-3.94	120.66	126.34
1	AA	3818	UY1	N1-C2-N3	3.94	119.59	115.13
45	BA	159	A2M	C2-N3-C4	3.94	121.06	111.75
45	BA	572	PSU	C4-N3-C2	-3.94	120.66	126.34
1	AA	2508	PSU	C4-N3-C2	-3.94	120.67	126.34
1	AA	4306	OMU	N3-C2-N1	3.93	120.11	114.89
1	AA	1323	A2M	C2-N3-C4	3.93	121.04	111.75
45	BA	1186	PSU	C4-N3-C2	-3.93	120.68	126.34
45	BA	27	A2M	C2-N3-C4	3.93	121.03	111.75
1	AA	2401	A2M	C2-N3-C4	3.93	121.03	111.75
45	BA	99	A2M	C2-N3-C4	3.93	121.02	111.75
45	BA	1851	MA6	C2-N3-C4	3.92	121.02	111.75
45	BA	34	PSU	C4-N3-C2	-3.92	120.69	126.34
45	BA	93	PSU	C4-N3-C2	-3.92	120.69	126.34
1	AA	3730	PSU	C4-N3-C2	-3.92	120.69	126.34
45	BA	966	PSU	C4-N3-C2	-3.92	120.69	126.34
1	AA	1536	PSU	C4-N3-C2	-3.91	120.70	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1779	PSU	C4-N3-C2	-3.91	120.70	126.34
45	BA	166	A2M	C2-N3-C4	3.91	120.99	111.75
1	AA	4532	PSU	C4-N3-C2	-3.91	120.70	126.34
45	BA	1238	PSU	C4-N3-C2	-3.91	120.71	126.34
1	AA	1534	A2M	C2-N3-C4	3.91	120.98	111.75
45	BA	1832	6MZ	C2-N3-C4	3.91	120.98	111.75
1	AA	2843	PSU	C4-N3-C2	-3.91	120.71	126.34
1	AA	1326	A2M	C2-N3-C4	3.91	120.98	111.75
45	BA	1692	PSU	C4-N3-C2	-3.90	120.72	126.34
45	BA	576	A2M	C2-N3-C4	3.90	120.95	111.75
1	AA	3884	PSU	C4-N3-C2	-3.89	120.73	126.34
45	BA	218	PSU	C4-N3-C2	-3.89	120.73	126.34
45	BA	116	OMU	N3-C2-N1	3.89	120.05	114.89
45	BA	814	PSU	C4-N3-C2	-3.89	120.73	126.34
45	BA	1383	A2M	C2-N3-C4	3.89	120.94	111.75
3	AC	69	PSU	C4-N3-C2	-3.89	120.74	126.34
1	AA	1862	PSU	C4-N3-C2	-3.89	120.74	126.34
45	BA	484	A2M	C2-N3-C4	3.88	120.92	111.75
1	AA	4590	A2M	C2-N3-C4	3.88	120.91	111.75
45	BA	686	PSU	C4-N3-C2	-3.88	120.75	126.34
1	AA	3853	PSU	C4-N3-C2	-3.88	120.75	126.34
1	AA	4431	PSU	C4-N3-C2	-3.88	120.75	126.34
1	AA	4552	PSU	C4-N3-C2	-3.88	120.75	126.34
1	AA	1781	PSU	C4-N3-C2	-3.87	120.76	126.34
45	BA	1031	A2M	C2-N3-C4	3.87	120.89	111.75
1	AA	4521	PSU	C4-N3-C2	-3.87	120.77	126.34
1	AA	4579	PSU	C4-N3-C2	-3.86	120.77	126.34
1	AA	3825	A2M	C2-N3-C4	3.86	120.87	111.75
1	AA	4523	A2M	C2-N3-C4	3.86	120.87	111.75
1	AA	4312	PSU	C4-N3-C2	-3.86	120.78	126.34
45	BA	109	PSU	C4-N3-C2	-3.86	120.78	126.34
1	AA	3830	A2M	C2-N3-C4	3.86	120.87	111.75
45	BA	668	A2M	C2-N3-C4	3.86	120.87	111.75
1	AA	3785	A2M	C2-N3-C4	3.86	120.87	111.75
45	BA	63	PSU	C4-N3-C2	-3.85	120.79	126.34
1	AA	4361	PSU	C4-N3-C2	-3.85	120.79	126.34
1	AA	3920	PSU	C4-N3-C2	-3.85	120.79	126.34
45	BA	1174	PSU	C4-N3-C2	-3.85	120.79	126.34
1	AA	3851	PSU	C4-N3-C2	-3.85	120.80	126.34
1	AA	3844	PSU	C4-N3-C2	-3.85	120.80	126.34
1	AA	4423	PSU	C4-N3-C2	-3.85	120.80	126.34
45	BA	918	PSU	C4-N3-C2	-3.85	120.80	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	55	PSU	C4-N3-C2	-3.85	120.80	126.34
1	AA	1683	PSU	C4-N3-C2	-3.84	120.80	126.34
45	BA	1678	A2M	C2-N3-C4	3.84	120.83	111.75
1	AA	4471	PSU	C4-N3-C2	-3.84	120.81	126.34
1	AA	2363	A2M	C2-N3-C4	3.84	120.82	111.75
1	AA	3867	A2M	C2-N3-C4	3.84	120.82	111.75
45	BA	667	PSU	C4-N3-C2	-3.84	120.81	126.34
1	AA	4220	6MZ	C2-N3-C4	3.83	120.81	111.75
1	AA	3768	PSU	C4-N3-C2	-3.83	120.82	126.34
45	BA	36	PSU	C4-N3-C2	-3.83	120.83	126.34
1	AA	400	A2M	C2-N3-C4	3.82	120.79	111.75
1	AA	4576	PSU	C4-N3-C2	-3.82	120.83	126.34
45	BA	1136	PSU	C4-N3-C2	-3.82	120.83	126.34
1	AA	4228	OMG	C6-C5-N7	3.82	137.35	130.25
45	BA	1367	PSU	C4-N3-C2	-3.82	120.84	126.34
45	BA	1288	OMU	N3-C2-N1	3.82	119.95	114.89
1	AA	398	A2M	C2-N3-C4	3.81	120.76	111.75
45	BA	1288	OMU	C5-C4-N3	3.81	120.54	114.84
45	BA	1596	PSU	C4-N3-C2	-3.81	120.85	126.34
45	BA	1244	PSU	C4-N3-C2	-3.80	120.86	126.34
1	AA	3639	PSU	C4-N3-C2	-3.80	120.86	126.34
45	BA	468	A2M	C2-N3-C4	3.80	120.73	111.75
45	BA	822	PSU	O2-C2-N1	-3.80	118.61	122.79
45	BA	649	PSU	C4-N3-C2	-3.80	120.87	126.34
45	BA	1045	PSU	C4-N3-C2	-3.80	120.87	126.34
1	AA	2787	A2M	C2-N3-C4	3.80	120.72	111.75
45	BA	1046	PSU	C4-N3-C2	-3.79	120.87	126.34
45	BA	1850	MA6	C2-N3-C4	3.79	120.70	111.75
1	AA	1744	PSU	C4-N3-C2	-3.79	120.88	126.34
1	AA	4673	PSU	C4-N3-C2	-3.79	120.88	126.34
45	BA	609	PSU	C4-N3-C2	-3.78	120.89	126.34
1	AA	3715	PSU	C4-N3-C2	-3.78	120.89	126.34
45	BA	822	PSU	C4-N3-C2	-3.77	120.90	126.34
1	AA	1871	A2M	C2-N3-C4	3.77	120.66	111.75
45	BA	300	PSU	C4-N3-C2	-3.77	120.91	126.34
1	AA	1524	A2M	C2-N3-C4	3.77	120.65	111.75
45	BA	1003	PSU	C4-N3-C2	-3.76	120.92	126.34
45	BA	1445	PSU	C4-N3-C2	-3.76	120.93	126.34
45	BA	1004	PSU	C4-N3-C2	-3.75	120.93	126.34
45	BA	366	PSU	C4-N3-C2	-3.74	120.94	126.34
1	AA	4299	PSU	C4-N3-C2	-3.74	120.95	126.34
45	BA	1442	OMU	N3-C2-N1	3.74	119.85	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2839	PSU	C4-N3-C2	-3.74	120.96	126.34
1	AA	4220	6MZ	C9-N6-C6	-3.73	119.66	122.87
1	AA	1779	PSU	O2-C2-N1	-3.73	118.69	122.79
1	AA	4228	OMG	N9-C4-N3	3.72	133.42	125.94
45	BA	100	PSU	C4-N3-C2	-3.72	120.97	126.34
45	BA	1056	PSU	C4-N3-C2	-3.72	120.98	126.34
45	BA	1850	MA6	C9-N6-C6	-3.69	110.82	120.40
45	BA	119	PSU	C4-N3-C2	-3.69	121.03	126.34
3	AC	14	OMU	C5-C4-N3	3.69	120.35	114.84
45	BA	1442	OMU	C1'-N1-C2	3.68	124.22	117.57
45	BA	296	PSU	C4-N3-C2	-3.67	121.05	126.34
1	AA	4628	PSU	O2-C2-N1	-3.67	118.75	122.79
45	BA	1851	MA6	N1-C6-N6	3.66	121.09	117.08
1	AA	3925	OMU	C5-C4-N3	3.66	120.31	114.84
1	AA	3718	A2M	C2-N3-C4	3.66	120.39	111.75
45	BA	801	PSU	C4-N3-C2	-3.65	121.08	126.34
45	BA	105	PSU	C4-N3-C2	-3.65	121.08	126.34
1	AA	1860	PSU	C4-N3-C2	-3.65	121.08	126.34
1	AA	1582	PSU	C4-N3-C2	-3.65	121.08	126.34
45	BA	1643	PSU	C4-N3-C2	-3.65	121.08	126.34
45	BA	166	A2M	C2'-C1'-N9	-3.65	107.39	113.53
1	AA	2415	OMU	C5-C4-N3	3.64	120.28	114.84
1	AA	4532	PSU	O2-C2-N1	-3.63	118.79	122.79
45	BA	1056	PSU	O2-C2-N1	-3.60	118.83	122.79
1	AA	3770	PSU	C4-N3-C2	-3.60	121.16	126.34
1	AA	4523	A2M	C2'-C1'-N9	-3.60	107.47	113.53
45	BA	428	OMU	C5-C4-N3	3.60	120.22	114.84
1	AA	1792	PSU	C4-N3-C2	-3.59	121.17	126.34
1	AA	2837	OMU	C5-C4-N3	3.59	120.20	114.84
45	BA	1625	PSU	C4-N3-C2	-3.58	121.18	126.34
1	AA	5010	PSU	C4-N3-C2	-3.58	121.18	126.34
45	BA	172	OMU	C5-C4-N3	3.58	120.19	114.84
1	AA	4442	PSU	O2-C2-N1	-3.57	118.86	122.79
1	AA	4498	OMU	C5-C4-N3	3.57	120.17	114.84
45	BA	1442	OMU	C5-C4-N3	3.56	120.17	114.84
1	AA	4312	PSU	O2-C2-N1	-3.56	118.87	122.79
45	BA	121	OMU	C5-C4-N3	3.56	120.17	114.84
45	BA	109	PSU	O2-C2-N1	-3.56	118.87	122.79
1	AA	3762	PSU	C4-N3-C2	-3.54	121.23	126.34
1	AA	3853	PSU	O2-C2-N1	-3.54	118.89	122.79
45	BA	1851	MA6	C9-N6-C6	-3.54	111.21	120.40
1	AA	1536	PSU	O2-C2-N1	-3.53	118.91	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	3785	A2M	C2'-C1'-N9	-3.52	107.60	113.53
1	AA	1522	OMG	C6-C5-N7	3.51	136.78	130.25
45	BA	354	OMU	C5-C4-N3	3.51	120.09	114.84
3	AC	69	PSU	O2-C2-N1	-3.51	118.92	122.79
45	BA	966	PSU	O2-C2-N1	-3.51	118.93	122.79
45	BA	116	OMU	C5-C4-N3	3.50	120.07	114.84
45	BA	300	PSU	O2-C2-N1	-3.49	118.94	122.79
45	BA	801	PSU	O2-C2-N1	-3.49	118.95	122.79
45	BA	93	PSU	O2-C2-N1	-3.48	118.96	122.79
45	BA	1232	PSU	O2-C2-N1	-3.48	118.96	122.79
1	AA	3764	PSU	C4-N3-C2	-3.48	121.33	126.34
1	AA	2632	PSU	C4-N3-C2	-3.48	121.33	126.34
45	BA	918	PSU	O2-C2-N1	-3.47	118.97	122.79
1	AA	4306	OMU	C5-C4-N3	3.47	120.03	114.84
1	AA	1744	PSU	O2-C2-N1	-3.47	118.97	122.79
1	AA	4500	PSU	O2-C2-N1	-3.47	118.97	122.79
45	BA	681	PSU	C4-N3-C2	-3.47	121.34	126.34
45	BA	1678	A2M	C4-C5-N7	-3.47	106.40	110.62
1	AA	4620	OMU	C5-C4-N3	3.46	120.02	114.84
45	BA	1288	OMU	O4-C4-C5	-3.46	119.07	125.16
1	AA	4227	OMU	C5-C4-N3	3.46	120.02	114.84
1	AA	1792	PSU	O2-C2-N1	-3.46	118.98	122.79
1	AA	4423	PSU	O2-C2-N1	-3.46	118.98	122.79
45	BA	1804	OMU	C5-C4-N3	3.46	120.01	114.84
1	AA	4296	PSU	O2-C2-N1	-3.45	118.99	122.79
45	BA	36	PSU	O2-C2-N1	-3.45	119.00	122.79
45	BA	863	PSU	C4-N3-C2	-3.44	121.38	126.34
45	BA	1692	PSU	O2-C2-N1	-3.44	119.00	122.79
45	BA	1174	PSU	O2-C2-N1	-3.44	119.00	122.79
45	BA	406	PSU	O2-C2-N1	-3.43	119.02	122.79
45	BA	105	PSU	O2-C2-N1	-3.43	119.02	122.79
1	AA	3785	A2M	O4'-C1'-N9	3.43	114.81	108.06
45	BA	119	PSU	O2-C2-N1	-3.43	119.02	122.79
45	BA	218	PSU	O2-C2-N1	-3.42	119.02	122.79
45	BA	1367	PSU	O2-C2-N1	-3.42	119.03	122.79
1	AA	4618	OMG	C6-C5-N7	3.42	136.61	130.25
45	BA	99	A2M	C2'-C1'-N9	-3.42	107.78	113.53
45	BA	34	PSU	O2-C2-N1	-3.41	119.03	122.79
1	AA	1683	PSU	O2-C2-N1	-3.41	119.04	122.79
1	AA	4552	PSU	O2-C2-N1	-3.41	119.04	122.79
1	AA	3822	PSU	O2-C2-N1	-3.40	119.05	122.79
45	BA	668	A2M	C4-C5-N7	-3.40	106.48	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	100	PSU	O2-C2-N1	-3.40	119.05	122.79
45	BA	1851	MA6	C4-C5-N7	-3.40	106.48	110.62
1	AA	1677	PSU	O2-C2-N1	-3.39	119.06	122.79
1	AA	4636	PSU	O2-C2-N1	-3.39	119.06	122.79
1	AA	3764	PSU	O2-C2-N1	-3.39	119.06	122.79
1	AA	3627	OMG	C6-C5-N7	3.39	136.55	130.25
45	BA	1045	PSU	O2-C2-N1	-3.39	119.06	122.79
1	AA	5001	PSU	O2-C2-N1	-3.39	119.06	122.79
1	AA	4392	OMG	C6-C5-N7	3.38	136.54	130.25
1	AA	3730	PSU	O2-C2-N1	-3.38	119.06	122.79
1	AA	4457	PSU	O2-C2-N1	-3.38	119.07	122.79
45	BA	609	PSU	O2-C2-N1	-3.38	119.07	122.79
1	AA	3770	PSU	O2-C2-N1	-3.38	119.07	122.79
45	BA	1136	PSU	O2-C2-N1	-3.38	119.07	122.79
45	BA	686	PSU	O2-C2-N1	-3.38	119.07	122.79
1	AA	3715	PSU	O2-C2-N1	-3.37	119.08	122.79
1	AA	3851	PSU	O2-C2-N1	-3.37	119.08	122.79
45	BA	1383	A2M	N3-C2-N1	-3.37	123.33	128.60
45	BA	1360	PSU	C6-C5-C4	-3.37	115.84	118.20
1	AA	3899	OMG	C6-C5-N7	3.37	136.51	130.25
1	AA	3762	PSU	O2-C2-N1	-3.37	119.08	122.79
45	BA	1360	PSU	O2-C2-N1	-3.37	119.08	122.79
45	BA	296	PSU	O2-C2-N1	-3.36	119.09	122.79
45	BA	815	PSU	O2-C2-N1	-3.36	119.09	122.79
45	BA	1238	PSU	O2-C2-N1	-3.35	119.10	122.79
45	BA	1046	PSU	O2-C2-N1	-3.35	119.10	122.79
1	AA	4579	PSU	O2-C2-N1	-3.35	119.10	122.79
45	BA	683	OMG	C6-C5-N7	3.35	136.48	130.25
45	BA	63	PSU	O2-C2-N1	-3.34	119.11	122.79
45	BA	1643	PSU	O2-C2-N1	-3.34	119.11	122.79
1	AA	4361	PSU	O2-C2-N1	-3.34	119.11	122.79
1	AA	4353	PSU	O2-C2-N1	-3.34	119.11	122.79
45	BA	1850	MA6	C4-C5-N7	-3.34	106.55	110.62
1	AA	3830	A2M	C2'-C1'-N9	-3.34	107.91	113.53
45	BA	651	PSU	O2-C2-N1	-3.34	119.12	122.79
45	BA	1003	PSU	O2-C2-N1	-3.34	119.12	122.79
1	AA	1534	A2M	C4-C5-N7	-3.34	106.56	110.62
45	BA	814	PSU	O2-C2-N1	-3.33	119.12	122.79
1	AA	3724	A2M	C4-C5-N7	-3.33	106.56	110.62
3	AC	14	OMU	C1'-N1-C2	3.33	123.60	117.57
45	BA	1360	PSU	C4-N3-C2	-3.33	121.54	126.34
45	BA	1445	PSU	O2-C2-N1	-3.33	119.13	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1524	A2M	C4-C5-N7	-3.33	106.57	110.62
1	AA	3782	5MC	C5-C6-N1	-3.32	119.92	123.34
1	AA	4576	PSU	O2-C2-N1	-3.32	119.13	122.79
45	BA	1186	PSU	O2-C2-N1	-3.32	119.13	122.79
1	AA	4972	PSU	O2-C2-N1	-3.32	119.14	122.79
1	AA	4689	PSU	C4-N3-C2	-3.32	121.56	126.34
1	AA	4493	PSU	O2-C2-N1	-3.31	119.15	122.79
45	BA	1244	PSU	O2-C2-N1	-3.31	119.15	122.79
1	AA	4590	A2M	N3-C2-N1	-3.31	123.43	128.60
1	AA	3695	PSU	O2-C2-N1	-3.30	119.15	122.79
1	AA	4431	PSU	O2-C2-N1	-3.30	119.15	122.79
1	AA	3768	PSU	O2-C2-N1	-3.30	119.15	122.79
1	AA	3884	PSU	O2-C2-N1	-3.30	119.15	122.79
1	AA	4973	PSU	O2-C2-N1	-3.30	119.16	122.79
1	AA	4623	OMG	C6-C5-N7	3.30	136.39	130.25
1	AA	2508	PSU	O2-C2-N1	-3.30	119.16	122.79
45	BA	866	PSU	O2-C2-N1	-3.30	119.16	122.79
45	BA	1177	PSU	O2-C2-N1	-3.29	119.16	122.79
45	BA	27	A2M	C4-C5-N7	-3.29	106.61	110.62
1	AA	1323	A2M	C4-C5-N7	-3.29	106.61	110.62
45	BA	512	A2M	N3-C2-N1	-3.29	123.45	128.60
1	AA	4521	PSU	O2-C2-N1	-3.29	119.17	122.79
1	AA	3920	PSU	O2-C2-N1	-3.28	119.18	122.79
1	AA	3639	PSU	O2-C2-N1	-3.28	119.18	122.79
45	BA	159	A2M	C4-C5-N7	-3.28	106.62	110.62
1	AA	2401	A2M	C2'-C1'-N9	-3.27	108.02	113.53
1	AA	1782	PSU	O2-C2-N1	-3.27	119.19	122.79
1	AA	2401	A2M	C4-C5-N7	-3.27	106.64	110.62
45	BA	1625	PSU	O2-C2-N1	-3.27	119.19	122.79
45	BA	681	PSU	O2-C2-N1	-3.26	119.21	122.79
45	BA	166	A2M	C4-C5-N7	-3.25	106.65	110.62
1	AA	4370	OMG	C6-C5-N7	3.25	136.30	130.25
1	AA	4403	PSU	O2-C2-N1	-3.25	119.21	122.79
1	AA	1316	OMG	C6-C5-N7	3.25	136.29	130.25
45	BA	468	A2M	C4-C5-N7	-3.25	106.67	110.62
1	AA	2401	A2M	N3-C2-N1	-3.25	123.53	128.60
1	AA	398	A2M	C4-C5-N7	-3.25	106.67	110.62
1	AA	4471	PSU	O2-C2-N1	-3.24	119.22	122.79
45	BA	468	A2M	N3-C2-N1	-3.24	123.53	128.60
3	AC	55	PSU	O2-C2-N1	-3.24	119.22	122.79
45	BA	1596	PSU	O2-C2-N1	-3.24	119.23	122.79
45	BA	1031	A2M	C4-C5-N7	-3.24	106.68	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	4637	OMG	C6-C5-N7	3.23	136.26	130.25
1	AA	5010	PSU	O2-C2-N1	-3.23	119.23	122.79
45	BA	1678	A2M	N3-C2-N1	-3.23	123.55	128.60
1	AA	2815	A2M	C4-C5-N7	-3.23	106.68	110.62
1	AA	3867	A2M	C4-C5-N7	-3.23	106.69	110.62
45	BA	1347	PSU	O2-C2-N1	-3.22	119.25	122.79
45	BA	576	A2M	C4-C5-N7	-3.22	106.70	110.62
1	AA	3825	A2M	C4-C5-N7	-3.21	106.71	110.62
1	AA	4673	PSU	O2-C2-N1	-3.21	119.25	122.79
1	AA	1326	A2M	N3-C2-N1	-3.21	123.58	128.60
1	AA	3830	A2M	C4-C5-N7	-3.21	106.71	110.62
1	AA	2839	PSU	O2-C2-N1	-3.21	119.26	122.79
1	AA	1781	PSU	O2-C2-N1	-3.21	119.26	122.79
45	BA	1004	PSU	O2-C2-N1	-3.21	119.26	122.79
1	AA	3744	OMG	C6-C5-N7	3.21	136.21	130.25
1	AA	1534	A2M	N3-C2-N1	-3.21	123.59	128.60
45	BA	484	A2M	C4-C5-N7	-3.20	106.72	110.62
1	AA	1326	A2M	C4-C5-N7	-3.20	106.73	110.62
45	BA	590	A2M	N3-C2-N1	-3.19	123.61	128.60
1	AA	1860	PSU	O2-C2-N1	-3.19	119.28	122.79
45	BA	1850	MA6	N1-C2-N3	-3.19	123.62	128.60
1	AA	3844	PSU	O2-C2-N1	-3.18	119.28	122.79
1	AA	1862	PSU	O2-C2-N1	-3.18	119.29	122.79
1	AA	1322	1MA	N9-C4-N3	3.18	134.35	126.94
1	AA	2363	A2M	C4-C5-N7	-3.18	106.75	110.62
45	BA	1383	A2M	C4-C5-N7	-3.18	106.75	110.62
1	AA	4523	A2M	N3-C2-N1	-3.17	123.65	128.60
1	AA	2787	A2M	N3-C2-N1	-3.16	123.66	128.60
1	AA	3718	A2M	C4-C5-N7	-3.16	106.77	110.62
1	AA	4590	A2M	C4-C5-N7	-3.16	106.77	110.62
1	AA	4689	PSU	O2-C2-N1	-3.15	119.33	122.79
45	BA	572	PSU	O2-C2-N1	-3.15	119.33	122.79
1	AA	400	A2M	N3-C2-N1	-3.14	123.68	128.60
45	BA	99	A2M	N3-C2-N1	-3.14	123.69	128.60
1	AA	4293	PSU	O2-C2-N1	-3.14	119.33	122.79
45	BA	644	OMG	C6-C5-N7	3.14	136.09	130.25
45	BA	1031	A2M	N3-C2-N1	-3.14	123.70	128.60
1	AA	4220	6MZ	N1-C2-N3	-3.14	123.70	128.60
1	AA	3724	A2M	N3-C2-N1	-3.13	123.70	128.60
45	BA	590	A2M	C4-C5-N7	-3.13	106.80	110.62
45	BA	1851	MA6	N1-C2-N3	-3.13	123.70	128.60
3	AC	14	OMU	O4-C4-C5	-3.13	119.66	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	512	A2M	C2'-C1'-N9	-3.13	108.26	113.53
1	AA	1871	A2M	N3-C2-N1	-3.13	123.71	128.60
1	AA	2787	A2M	C2'-C1'-N9	-3.13	108.27	113.53
45	BA	468	A2M	C2'-C1'-N9	-3.12	108.27	113.53
45	BA	166	A2M	N3-C2-N1	-3.12	123.72	128.60
1	AA	2364	OMG	C6-C5-N7	3.11	136.04	130.25
1	AA	398	A2M	C2'-C1'-N9	-3.11	108.29	113.53
1	AA	2363	A2M	N3-C2-N1	-3.11	123.74	128.60
1	AA	4571	A2M	N3-C2-N1	-3.11	123.74	128.60
45	BA	436	OMG	C6-C5-N7	3.11	136.03	130.25
1	AA	2843	PSU	O2-C2-N1	-3.10	119.37	122.79
1	AA	1323	A2M	N3-C2-N1	-3.10	123.75	128.60
45	BA	27	A2M	N3-C2-N1	-3.10	123.75	128.60
45	BA	1447	OMG	C6-C5-N7	3.10	136.01	130.25
1	AA	1871	A2M	C4-C5-N7	-3.09	106.85	110.62
1	AA	398	A2M	N3-C2-N1	-3.09	123.77	128.60
1	AA	3785	A2M	C4-C5-N7	-3.09	106.86	110.62
1	AA	3785	A2M	N3-C2-N1	-3.09	123.77	128.60
1	AA	4299	PSU	O2-C2-N1	-3.09	119.39	122.79
1	AA	400	A2M	C4-C5-N7	-3.08	106.86	110.62
45	BA	1328	OMG	C6-C5-N7	3.08	135.98	130.25
1	AA	3830	A2M	N3-C2-N1	-3.08	123.79	128.60
45	BA	1832	6MZ	N1-C2-N3	-3.08	123.79	128.60
1	AA	1625	OMG	C6-C5-N7	3.07	135.96	130.25
45	BA	99	A2M	C4-C5-N7	-3.07	106.88	110.62
45	BA	484	A2M	N3-C2-N1	-3.06	123.81	128.60
45	BA	668	A2M	N3-C2-N1	-3.06	123.81	128.60
1	AA	4571	A2M	C4-C5-N7	-3.06	106.89	110.62
1	AA	3825	A2M	N3-C2-N1	-3.06	123.82	128.60
45	BA	576	A2M	N3-C2-N1	-3.06	123.82	128.60
45	BA	354	OMU	O4-C4-C5	-3.06	119.78	125.16
1	AA	2632	PSU	O2-C2-N1	-3.05	119.44	122.79
1	AA	2837	OMU	O4-C4-C5	-3.05	119.81	125.16
45	BA	121	OMU	O4-C4-C5	-3.04	119.81	125.16
45	BA	1031	A2M	C2'-C1'-N9	-3.04	108.41	113.53
1	AA	2424	OMG	C6-C5-N7	3.04	135.90	130.25
1	AA	2876	OMG	C6-C5-N7	3.04	135.89	130.25
1	AA	2815	A2M	N3-C2-N1	-3.03	123.86	128.60
1	AA	4523	A2M	C4-C5-N7	-3.03	106.92	110.62
1	AA	2787	A2M	C4-C5-N7	-3.03	106.92	110.62
45	BA	1326	UY1	C6-C5-C4	3.02	120.31	118.20
45	BA	512	A2M	C4-C5-N7	-3.02	106.94	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	863	PSU	O2-C2-N1	-3.02	119.47	122.79
1	AA	4494	OMG	C6-C5-N7	3.01	135.85	130.25
45	BA	159	A2M	N3-C2-N1	-3.01	123.89	128.60
1	AA	4220	6MZ	C4-C5-N7	-3.01	106.95	110.62
1	AA	1524	A2M	C2'-C1'-N9	-3.00	108.48	113.53
45	BA	116	OMU	O4-C4-C5	-3.00	119.88	125.16
45	BA	172	OMU	O4-C4-C5	-3.00	119.89	125.16
1	AA	4220	6MZ	C6-C5-N7	2.99	135.63	132.39
45	BA	428	OMU	O4-C4-C5	-2.98	119.91	125.16
45	BA	1678	A2M	C5-N7-C8	2.98	107.74	103.51
45	BA	166	A2M	C5-N7-C8	2.96	107.71	103.51
3	AC	75	OMG	C6-C5-N7	2.96	135.75	130.25
1	AA	1582	PSU	O2-C2-N1	-2.95	119.54	122.79
45	BA	1248	B8N	N3-C2-N1	2.94	120.92	116.76
1	AA	1524	A2M	N3-C2-N1	-2.94	124.00	128.60
1	AA	4498	OMU	O4-C4-C5	-2.94	119.99	125.16
1	AA	2415	OMU	O4-C4-C5	-2.94	120.00	125.16
45	BA	1804	OMU	O4-C4-C5	-2.91	120.03	125.16
1	AA	3637	PSU	O2-C2-N1	-2.91	119.58	122.79
45	BA	667	PSU	O2-C2-N1	-2.91	119.58	122.79
1	AA	3785	A2M	C4-N9-C8	2.91	108.88	105.73
1	AA	3925	OMU	O4-C4-C5	-2.91	120.05	125.16
45	BA	1442	OMU	O4-C4-C5	-2.90	120.06	125.16
29	Ac	39	V5N	O2-CB-CG	-2.88	105.53	110.73
1	AA	3818	UY1	C6-C5-C4	2.88	120.21	118.20
45	BA	1326	UY1	C6-N1-C2	-2.86	119.76	122.68
1	AA	4620	OMU	O4-C4-C5	-2.86	120.14	125.16
45	BA	366	PSU	O2-C2-N1	-2.85	119.65	122.79
1	AA	3867	A2M	N3-C2-N1	-2.85	124.15	128.60
1	AA	4227	OMU	O4-C4-C5	-2.84	120.17	125.16
45	BA	509	OMG	C6-C5-N7	2.84	135.53	130.25
45	BA	1851	MA6	C5-N7-C8	2.83	107.53	103.51
1	AA	4306	OMU	O4-C4-C5	-2.82	120.20	125.16
45	BA	159	A2M	C5-N7-C8	2.82	107.51	103.51
1	AA	4228	OMG	C4-C5-N7	-2.82	106.27	110.72
1	AA	3724	A2M	C5-N7-C8	2.80	107.49	103.51
45	BA	668	A2M	C5-N7-C8	2.80	107.49	103.51
1	AA	3792	OMG	C6-C5-N7	2.79	135.44	130.25
1	AA	1522	OMG	C4-C5-N7	-2.79	106.31	110.72
45	BA	1678	A2M	C4-N9-C8	2.78	108.74	105.73
45	BA	1490	OMG	C6-C5-N7	2.78	135.41	130.25
45	BA	601	OMG	C6-C5-N7	2.76	135.38	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1524	A2M	C5-N7-C8	2.75	107.42	103.51
45	BA	1832	6MZ	C9-N6-C6	-2.75	120.51	122.87
1	AA	4618	OMG	C4-C5-N7	-2.74	106.38	110.72
45	BA	468	A2M	C5-N7-C8	2.74	107.40	103.51
45	BA	1832	6MZ	C4-C5-N7	-2.74	107.28	110.62
45	BA	1383	A2M	C4-N9-C8	2.74	108.69	105.73
1	AA	1534	A2M	C5-N7-C8	2.73	107.39	103.51
1	AA	4392	OMG	C4-C5-N7	-2.73	106.40	110.72
45	BA	27	A2M	C5-N7-C8	2.73	107.39	103.51
1	AA	4499	OMG	C6-C5-N7	2.73	135.33	130.25
1	AA	4196	OMG	C6-C5-N7	2.72	135.31	130.25
45	BA	590	A2M	C5-N7-C8	2.72	107.37	103.51
45	BA	468	A2M	C4-N9-C8	2.72	108.67	105.73
45	BA	1383	A2M	C5-N7-C8	2.71	107.36	103.51
1	AA	3867	A2M	C5-N7-C8	2.71	107.36	103.51
45	BA	1031	A2M	C5-N7-C8	2.71	107.36	103.51
1	AA	1323	A2M	C5-N7-C8	2.70	107.35	103.51
29	Ac	39	V5N	O2-CB-CA	2.70	112.97	107.28
1	AA	4523	A2M	C4-N9-C8	2.70	108.65	105.73
1	AA	2401	A2M	C5-N7-C8	2.70	107.34	103.51
1	AA	3830	A2M	C5-N7-C8	2.70	107.34	103.51
1	AA	4623	OMG	C4-C5-N7	-2.69	106.46	110.72
45	BA	1337	4AC	C1'-N1-C2	2.69	124.43	118.42
1	AA	1326	A2M	C5-N7-C8	2.69	107.33	103.51
1	AA	2815	A2M	C5-N7-C8	2.69	107.32	103.51
45	BA	1832	6MZ	C4-N9-C8	2.68	108.64	105.73
1	AA	398	A2M	C5-N7-C8	2.68	107.32	103.51
1	AA	3744	OMG	C4-C5-N7	-2.68	106.48	110.72
45	BA	683	OMG	C4-C5-N7	-2.68	106.48	110.72
1	AA	4637	OMG	C4-C5-N7	-2.67	106.49	110.72
45	BA	1850	MA6	C5-N7-C8	2.67	107.30	103.51
1	AA	3627	OMG	C4-C5-N7	-2.67	106.50	110.72
1	AA	3785	A2M	C5-N7-C8	2.66	107.28	103.51
1	AA	4456	OMC	O2-C2-N3	-2.65	118.02	122.33
1	AA	3825	A2M	C5-N7-C8	2.64	107.26	103.51
1	AA	4590	A2M	C5-N7-C8	2.64	107.26	103.51
45	BA	867	OMG	C6-C5-N7	2.64	135.16	130.25
1	AA	4590	A2M	C4-N9-C8	2.64	108.59	105.73
1	AA	2861	OMC	O2-C2-N3	-2.64	118.04	122.33
45	BA	484	A2M	C5-N7-C8	2.63	107.25	103.51
45	BA	576	A2M	C5-N7-C8	2.63	107.24	103.51
1	AA	1871	A2M	C4-N9-C8	2.63	108.57	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	3899	OMG	C4-C5-N7	-2.63	106.57	110.72
1	AA	4447	5MC	C5-C4-N3	-2.62	118.84	121.67
1	AA	2401	A2M	C4-N9-C8	2.62	108.57	105.73
1	AA	2363	A2M	C5-N7-C8	2.62	107.23	103.51
45	BA	1447	OMG	C4-C5-N7	-2.61	106.58	110.72
1	AA	3718	A2M	N3-C2-N1	-2.61	124.52	128.60
45	BA	99	A2M	C5-N7-C8	2.61	107.21	103.51
1	AA	4523	A2M	C5-N7-C8	2.59	107.19	103.51
45	BA	512	A2M	C5-N7-C8	2.59	107.19	103.51
1	AA	3782	5MC	C5-C4-N3	-2.59	118.88	121.67
1	AA	4571	A2M	C5-N7-C8	2.59	107.19	103.51
45	BA	159	A2M	C2'-C1'-N9	-2.59	109.18	113.53
45	BA	166	A2M	C4-N9-C8	2.58	108.53	105.73
1	AA	4370	OMG	C4-C5-N7	-2.58	106.64	110.72
45	BA	1328	OMG	C4-C5-N7	-2.58	106.64	110.72
1	AA	2787	A2M	C5-N7-C8	2.58	107.17	103.51
1	AA	1524	A2M	C4-N9-C8	2.58	108.52	105.73
1	AA	1316	OMG	C4-C5-N7	-2.57	106.65	110.72
1	AA	2364	OMG	C4-C5-N7	-2.57	106.66	110.72
3	AC	75	OMG	C4-C5-N7	-2.56	106.66	110.72
1	AA	400	A2M	C5-N7-C8	2.56	107.15	103.51
45	BA	644	OMG	C4-C5-N7	-2.56	106.68	110.72
1	AA	1871	A2M	C5-N7-C8	2.55	107.13	103.51
45	BA	517	OMC	O2-C2-N3	-2.54	118.19	122.33
1	AA	4499	OMG	C4-C5-N7	-2.54	106.69	110.72
45	BA	1031	A2M	C4-N9-C8	2.54	108.48	105.73
45	BA	436	OMG	C4-C5-N7	-2.54	106.70	110.72
1	AA	3818	UY1	C6-N1-C2	-2.52	120.11	122.68
1	AA	2876	OMG	C4-C5-N7	-2.51	106.75	110.72
45	BA	668	A2M	C4-N9-C8	2.51	108.45	105.73
45	BA	1832	6MZ	C6-C5-N7	2.50	135.10	132.39
1	AA	1322	1MA	C4-C5-N7	-2.50	106.76	110.72
1	AA	4220	6MZ	C5-N7-C8	2.47	107.02	103.51
1	AA	1625	OMG	C4-C5-N7	-2.47	106.82	110.72
1	AA	3830	A2M	C4-N9-C8	2.46	108.39	105.73
1	AA	398	A2M	C4-N9-C8	2.45	108.38	105.73
1	AA	3724	A2M	C4-N9-C8	2.45	108.38	105.73
1	AA	3782	5MC	O2-C2-N3	-2.45	118.35	122.33
45	BA	1850	MA6	C5-C6-N6	-2.44	121.04	125.30
1	AA	4494	OMG	C4-C5-N7	-2.44	106.86	110.72
1	AA	2787	A2M	C4-N9-C8	2.44	108.37	105.73
45	BA	1832	6MZ	C5-N7-C8	2.43	106.97	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	3867	A2M	C4-N9-C8	2.43	108.37	105.73
45	BA	1337	4AC	CM7-C7-N4	-2.43	111.09	115.29
45	BA	1326	UY1	O2-C2-N1	-2.43	120.12	122.79
45	BA	99	A2M	C4-N9-C8	2.43	108.36	105.73
1	AA	1326	A2M	C4-N9-C8	2.43	108.36	105.73
1	AA	3808	OMC	O2-C2-N3	-2.42	118.39	122.33
1	AA	1871	A2M	C2'-C1'-N9	-2.42	109.45	113.53
1	AA	1534	A2M	C4-N9-C8	2.41	108.34	105.73
45	BA	667	PSU	C6-C5-C4	-2.41	116.51	118.20
1	AA	400	A2M	C4-N9-C8	2.41	108.34	105.73
1	AA	4196	OMG	C4-C5-N7	-2.40	106.92	110.72
1	AA	3718	A2M	C5-N7-C8	2.40	106.92	103.51
45	BA	1678	A2M	C6-C5-N7	2.40	136.48	132.02
45	BA	867	OMG	C4-C5-N7	-2.40	106.93	110.72
45	BA	509	OMG	C4-C5-N7	-2.39	106.93	110.72
45	BA	601	OMG	C4-C5-N7	-2.39	106.93	110.72
45	BA	1850	MA6	C4-N9-C8	2.39	108.32	105.73
1	AA	2363	A2M	C4-N9-C8	2.39	108.31	105.73
45	BA	512	A2M	C4-N9-C8	2.39	108.31	105.73
45	BA	572	PSU	O4'-C1'-C2'	2.38	108.50	105.14
1	AA	3792	OMG	C4-C5-N7	-2.38	106.96	110.72
45	BA	1490	OMG	C4-C5-N7	-2.38	106.96	110.72
1	AA	3825	A2M	C4-N9-C8	2.37	108.29	105.73
1	AA	2424	OMG	C4-C5-N7	-2.36	106.99	110.72
1	AA	1524	A2M	O4'-C1'-N9	2.35	112.69	108.06
45	BA	1337	4AC	C5-C4-N4	-2.34	118.85	122.92
45	BA	1842	4AC	CM7-C7-N4	-2.34	111.25	115.29
45	BA	436	OMG	O6-C6-C5	-2.34	120.40	126.60
1	AA	1323	A2M	C4-N9-C8	2.34	108.26	105.73
45	BA	116	OMU	C1'-N1-C2	2.34	121.80	117.57
1	AA	2351	OMC	O2-C2-N3	-2.33	118.54	122.33
45	BA	27	A2M	C4-N9-C8	2.33	108.25	105.73
45	BA	1442	OMU	O2-C2-N3	-2.33	117.17	121.50
45	BA	1851	MA6	C10-N6-C9	-2.32	108.63	116.12
45	BA	1678	A2M	O4'-C1'-N9	2.31	112.61	108.06
45	BA	1842	4AC	C5-C4-N4	-2.29	118.94	122.92
45	BA	1136	PSU	O4'-C1'-C2'	2.29	108.38	105.14
45	BA	1391	OMC	O2-C2-N3	-2.29	118.61	122.33
1	AA	4571	A2M	C4-N9-C8	2.29	108.21	105.73
1	AA	3818	UY1	O2-C2-N1	-2.29	120.27	122.79
45	BA	159	A2M	C4-N9-C8	2.29	108.21	105.73
45	BA	1678	A2M	N9-C8-N7	-2.28	110.79	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BN	67	NMM	CAA-NH2-CZ	-2.28	118.83	123.86
45	BA	866	PSU	O3'-C3'-C2'	2.27	119.17	111.82
45	BA	428	OMU	O2-C2-N1	-2.27	119.77	122.79
45	BA	576	A2M	C4-N9-C8	2.26	108.18	105.73
1	AA	4442	PSU	O4'-C1'-C2'	2.26	108.33	105.14
45	BA	27	A2M	C2'-C1'-N9	-2.25	109.73	113.53
1	AA	2824	OMC	O2-C2-N3	-2.25	118.67	122.33
1	AA	1534	A2M	C6-C5-N7	2.25	136.21	132.02
45	BA	668	A2M	C6-C5-N7	2.25	136.21	132.02
45	BA	468	A2M	C6-C5-N7	2.24	136.20	132.02
45	BA	1851	MA6	C4-N9-C8	2.24	108.16	105.73
1	AA	2363	A2M	C2'-C1'-N9	-2.24	109.77	113.53
45	BA	1851	MA6	C5-C6-N6	-2.23	121.41	125.30
1	AA	3792	OMG	O6-C6-C5	-2.23	120.68	126.60
1	AA	4403	PSU	O4'-C1'-C2'	2.23	108.29	105.14
1	AA	2424	OMG	O6-C6-C5	-2.23	120.69	126.60
45	BA	509	OMG	O6-C6-C5	-2.22	120.72	126.60
1	AA	4494	OMG	O6-C6-C5	-2.22	120.72	126.60
45	BA	1804	OMU	C1'-N1-C2	2.20	121.56	117.57
45	BA	354	OMU	O2-C2-N1	-2.20	119.86	122.79
1	AA	1625	OMG	O6-C6-C5	-2.20	120.77	126.60
45	BA	1056	PSU	O4'-C1'-C2'	2.20	108.24	105.14
1	AA	3785	A2M	N9-C8-N7	-2.20	110.91	113.91
45	BA	601	OMG	O6-C6-C5	-2.19	120.78	126.60
45	BA	644	OMG	O6-C6-C5	-2.19	120.79	126.60
45	BA	668	A2M	C2'-C1'-N9	-2.18	109.85	113.53
1	AA	3724	A2M	C6-C5-N7	2.18	136.08	132.02
1	AA	2351	OMC	C1'-N1-C2	2.17	123.27	118.42
45	BA	484	A2M	C4-N9-C8	2.17	108.08	105.73
1	AA	1582	PSU	C6-C5-C4	-2.16	116.69	118.20
3	AC	69	PSU	O4'-C1'-C2'	2.16	108.19	105.14
45	BA	109	PSU	O4'-C1'-C2'	2.16	108.19	105.14
1	AA	3637	PSU	C5-C6-N1	-2.16	118.87	122.11
1	AA	4590	A2M	C6-C5-N7	2.16	136.04	132.02
1	AA	1524	A2M	C6-C5-N7	2.16	136.04	132.02
1	AA	1322	1MA	C6-C5-N7	2.16	136.12	132.20
1	AA	3887	OMC	O2-C2-N3	-2.15	118.83	122.33
1	AA	2401	A2M	C6-C5-N7	2.14	136.01	132.02
1	AA	2364	OMG	O6-C6-C5	-2.14	120.92	126.60
1	AA	4636	PSU	C5-C6-N1	-2.14	118.89	122.11
45	BA	1447	OMG	O6-C6-C5	-2.14	120.92	126.60
45	BA	1383	A2M	C6-C5-N7	2.14	136.01	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	683	OMG	O6-C6-C5	-2.14	120.92	126.60
1	AA	2876	OMG	O6-C6-C5	-2.14	120.93	126.60
1	AA	2415	OMU	O2-C2-N1	-2.13	119.95	122.79
1	AA	4618	OMG	O6-C6-C5	-2.13	120.94	126.60
45	BA	166	A2M	N9-C8-N7	-2.13	111.00	113.91
1	AA	4500	PSU	C5-C6-N1	-2.13	118.91	122.11
1	AA	4457	PSU	O4'-C1'-C2'	2.12	108.13	105.14
1	AA	3899	OMG	O6-C6-C5	-2.12	120.98	126.60
1	AA	4499	OMG	O6-C6-C5	-2.12	120.99	126.60
1	AA	1677	PSU	O4'-C1'-C2'	2.11	108.13	105.14
45	BA	866	PSU	C5-C6-N1	-2.11	118.94	122.11
45	BA	1490	OMG	O6-C6-C5	-2.11	121.01	126.60
45	BA	468	A2M	N9-C8-N7	-2.11	111.03	113.91
1	AA	4228	OMG	O6-C6-C5	-2.11	121.02	126.60
1	AA	1323	A2M	C6-C5-N7	2.10	135.94	132.02
45	BA	27	A2M	C6-C5-N7	2.10	135.94	132.02
1	AA	4196	OMG	O6-C6-C5	-2.10	121.03	126.60
1	AA	3785	A2M	C6-C5-N7	2.10	135.93	132.02
45	BA	1850	MA6	C10-N6-C9	-2.10	109.37	116.12
1	AA	4498	OMU	O2-C2-N1	-2.10	120.00	122.79
45	BA	1328	OMG	O6-C6-C5	-2.10	121.04	126.60
45	BA	1347	PSU	C5-C6-N1	-2.10	118.97	122.11
1	AA	4636	PSU	O4'-C1'-C2'	2.09	108.10	105.14
45	BA	867	OMG	O6-C6-C5	-2.09	121.05	126.60
1	AA	3825	A2M	C6-C5-N7	2.09	135.92	132.02
1	AA	3718	A2M	C2'-C1'-N9	-2.09	110.01	113.53
1	AA	1326	A2M	C6-C5-N7	2.09	135.91	132.02
1	AA	3627	OMG	O6-C6-C5	-2.09	121.06	126.60
1	AA	4220	6MZ	C4-N9-C8	2.09	107.99	105.73
1	AA	4293	PSU	C5-C6-N1	-2.08	118.98	122.11
1	AA	398	A2M	C6-C5-N7	2.08	135.90	132.02
45	BA	668	A2M	N9-C8-N7	-2.08	111.07	113.91
1	AA	3925	OMU	O2-C2-N1	-2.08	120.03	122.79
1	AA	4973	PSU	C5-C6-N1	-2.07	119.00	122.11
45	BA	1031	A2M	C6-C5-N7	2.07	135.88	132.02
1	AA	4536	OMC	O2-C2-N3	-2.07	118.96	122.33
45	BA	1842	4AC	C1'-N1-C2	2.07	123.03	118.42
1	AA	4403	PSU	C5-C6-N1	-2.07	119.01	122.11
1	AA	4370	OMG	O6-C6-C5	-2.06	121.13	126.60
1	AA	4637	OMG	O6-C6-C5	-2.06	121.13	126.60
45	BA	576	A2M	C6-C5-N7	2.06	135.86	132.02
1	AA	1316	OMG	O6-C6-C5	-2.06	121.14	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1524	A2M	N9-C8-N7	-2.05	111.11	113.91
3	AC	75	OMG	O6-C6-C5	-2.05	121.16	126.60
1	AA	4623	OMG	O6-C6-C5	-2.05	121.16	126.60
45	BA	462	OMC	O2-C2-N3	-2.05	119.00	122.33
1	AA	3744	OMG	O6-C6-C5	-2.04	121.19	126.60
1	AA	3920	PSU	O4'-C1'-C2'	2.04	108.02	105.14
1	AA	1322	1MA	N1-C2-N3	-2.03	123.58	126.00
1	AA	2363	A2M	C6-C5-N7	2.03	135.81	132.02
45	BA	1383	A2M	N9-C8-N7	-2.03	111.13	113.91
1	AA	4523	A2M	N9-C8-N7	-2.03	111.14	113.91
1	AA	3822	PSU	C5-C6-N1	-2.02	119.08	122.11
1	AA	4523	A2M	C6-C5-N7	2.02	135.79	132.02
45	BA	36	PSU	O4'-C1'-C2'	2.02	107.99	105.14
1	AA	1534	A2M	N9-C8-N7	-2.02	111.15	113.91
1	AA	3724	A2M	N9-C8-N7	-2.02	111.15	113.91
1	AA	3637	PSU	O2-C2-N3	-2.02	118.01	121.82
1	AA	2815	A2M	C4-N9-C8	2.02	107.91	105.73
45	BA	1177	PSU	C5-C6-N1	-2.02	119.08	122.11
1	AA	3695	PSU	O4'-C1'-C2'	2.02	107.99	105.14
1	AA	2401	A2M	N9-C8-N7	-2.02	111.16	113.91
45	BA	159	A2M	C6-C5-N7	2.01	135.77	132.02
45	BA	815	PSU	C5-C6-N1	-2.01	119.09	122.11
1	AA	2861	OMC	C1'-N1-C2	2.01	122.91	118.42
1	AA	4576	PSU	O4'-C1'-C2'	2.01	107.98	105.14
45	BA	121	OMU	C1'-N1-C2	2.01	121.21	117.57
1	AA	4590	A2M	N9-C8-N7	-2.01	111.17	113.91
45	BA	1272	OMC	O2-C2-N3	-2.01	119.07	122.33

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1582	PSU	O4'-C1'-C5-C4
1	AA	1582	PSU	O4'-C1'-C5-C6
1	AA	1625	OMG	O4'-C4'-C5'-O5'
1	AA	1625	OMG	C3'-C4'-C5'-O5'
1	AA	1677	PSU	C2'-C1'-C5-C4
1	AA	1677	PSU	C2'-C1'-C5-C6
1	AA	2364	OMG	O4'-C4'-C5'-O5'
1	AA	2364	OMG	C3'-C4'-C5'-O5'
1	AA	3701	OMC	C2'-C1'-N1-C2
1	AA	3701	OMC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	AA	3764	PSU	C3'-C4'-C5'-O5'
1	AA	3764	PSU	O4'-C4'-C5'-O5'
1	AA	3818	UY1	C1'-C2'-O2'-CM2
1	AA	3867	A2M	C1'-C2'-O2'-CM'
1	AA	4500	PSU	C3'-C4'-C5'-O5'
1	AA	4500	PSU	O4'-C4'-C5'-O5'
1	AA	4636	PSU	C2'-C1'-C5-C6
1	AA	4636	PSU	C3'-C4'-C5'-O5'
1	AA	4636	PSU	O4'-C4'-C5'-O5'
45	BA	27	A2M	O4'-C4'-C5'-O5'
45	BA	166	A2M	C3'-C4'-C5'-O5'
45	BA	428	OMU	C2'-C1'-N1-C2
45	BA	428	OMU	C2'-C1'-N1-C6
45	BA	484	A2M	C1'-C2'-O2'-CM'
45	BA	512	A2M	O4'-C4'-C5'-O5'
45	BA	601	OMG	O4'-C4'-C5'-O5'
45	BA	667	PSU	C2'-C1'-C5-C4
45	BA	667	PSU	O4'-C1'-C5-C4
45	BA	667	PSU	O4'-C1'-C5-C6
45	BA	668	A2M	O4'-C4'-C5'-O5'
45	BA	867	OMG	C1'-C2'-O2'-CM2
45	BA	1248	B8N	C2'-C1'-C5-C6
45	BA	1248	B8N	C31-C32-C33-C34
45	BA	1326	UY1	C2'-C1'-C5-C4
45	BA	1337	4AC	O4'-C4'-C5'-O5'
45	BA	1337	4AC	C3'-C4'-C5'-O5'
45	BA	1360	PSU	C2'-C1'-C5-C4
45	BA	1360	PSU	C2'-C1'-C5-C6
45	BA	1678	A2M	C1'-C2'-O2'-CM'
45	BA	1832	6MZ	C5-C6-N6-C9
45	BA	1832	6MZ	N1-C6-N6-C9
45	BA	1851	MA6	O4'-C4'-C5'-O5'
45	BA	1851	MA6	C5-C6-N6-C9
1	AA	4447	5MC	C2'-C1'-N1-C6
1	AA	1323	A2M	O4'-C4'-C5'-O5'
1	AA	1323	A2M	C3'-C4'-C5'-O5'
1	AA	1326	A2M	C3'-C4'-C5'-O5'
1	AA	3770	PSU	C3'-C4'-C5'-O5'
1	AA	3785	A2M	O4'-C4'-C5'-O5'
1	AA	3785	A2M	C3'-C4'-C5'-O5'
1	AA	3844	PSU	O4'-C4'-C5'-O5'
45	BA	27	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
45	BA	512	A2M	C3'-C4'-C5'-O5'
45	BA	590	A2M	O4'-C4'-C5'-O5'
45	BA	601	OMG	C3'-C4'-C5'-O5'
45	BA	1851	MA6	C3'-C4'-C5'-O5'
1	AA	4590	A2M	C4'-C5'-O5'-P
1	AA	3770	PSU	O4'-C4'-C5'-O5'
1	AA	3844	PSU	C3'-C4'-C5'-O5'
45	BA	99	A2M	O4'-C4'-C5'-O5'
45	BA	668	A2M	C3'-C4'-C5'-O5'
45	BA	683	OMG	O4'-C4'-C5'-O5'
1	AA	4447	5MC	C2'-C1'-N1-C2
1	AA	3851	PSU	C3'-C4'-C5'-O5'
45	BA	166	A2M	O4'-C4'-C5'-O5'
45	BA	468	A2M	C3'-C4'-C5'-O5'
58	BN	67	NMM	NE-CD-CG-CB
1	AA	1326	A2M	O4'-C4'-C5'-O5'
45	BA	100	PSU	O4'-C4'-C5'-O5'
45	BA	468	A2M	O4'-C4'-C5'-O5'
45	BA	590	A2M	C3'-C4'-C5'-O5'
45	BA	1643	PSU	C3'-C4'-C5'-O5'
45	BA	1643	PSU	O4'-C4'-C5'-O5'
45	BA	1851	MA6	N1-C6-N6-C9
1	AA	398	A2M	O4'-C4'-C5'-O5'
45	BA	99	A2M	C3'-C4'-C5'-O5'
45	BA	1850	MA6	C5-C6-N6-C9
1	AA	3818	UY1	C4'-C5'-O5'-P
45	BA	436	OMG	O4'-C4'-C5'-O5'
45	BA	1490	OMG	O4'-C4'-C5'-O5'
45	BA	1288	OMU	C3'-C2'-O2'-CM2
45	BA	1490	OMG	C3'-C4'-C5'-O5'
45	BA	436	OMG	C3'-C4'-C5'-O5'
45	BA	1248	B8N	O4'-C4'-C5'-O5'
1	AA	2787	A2M	C1'-C2'-O2'-CM'
45	BA	1248	B8N	C31-C32-C33-N34
45	BA	1850	MA6	C4'-C5'-O5'-P
45	BA	590	A2M	C2'-C1'-N9-C4
1	AA	2787	A2M	C2'-C1'-N9-C8
45	BA	590	A2M	C2'-C1'-N9-C8
45	BA	668	A2M	C2'-C1'-N9-C8
1	AA	2804	OMC	C3'-C2'-O2'-CM2
45	BA	1326	UY1	C3'-C2'-O2'-CM2
1	AA	4447	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	AA	4500	PSU	C4'-C5'-O5'-P
1	AA	3851	PSU	O4'-C4'-C5'-O5'
1	AA	4590	A2M	C3'-C4'-C5'-O5'
45	BA	683	OMG	C3'-C4'-C5'-O5'
45	BA	1850	MA6	O4'-C4'-C5'-O5'
45	BA	1850	MA6	C3'-C4'-C5'-O5'
1	AA	3844	PSU	C4'-C5'-O5'-P
1	AA	4447	5MC	O4'-C1'-N1-C2
45	BA	801	PSU	C4'-C5'-O5'-P
45	BA	1360	PSU	C4'-C5'-O5'-P
1	AA	1881	OMC	O4'-C4'-C5'-O5'
45	BA	509	OMG	O4'-C4'-C5'-O5'
45	BA	822	PSU	O4'-C4'-C5'-O5'
1	AA	3887	OMC	C4'-C5'-O5'-P
45	BA	436	OMG	C4'-C5'-O5'-P
1	AA	2787	A2M	C3'-C2'-O2'-CM'
45	BA	436	OMG	C3'-C2'-O2'-CM2
1	AA	3701	OMC	O4'-C1'-N1-C6
45	BA	428	OMU	O4'-C1'-N1-C6
1	AA	1326	A2M	C4'-C5'-O5'-P
45	BA	966	PSU	C4'-C5'-O5'-P
71	Ba	138	IAS	CA-CB-CG-OD1
45	BA	1248	B8N	C3'-C4'-C5'-O5'
1	AA	1677	PSU	O4'-C1'-C5-C4
1	AA	4521	PSU	O4'-C1'-C5-C4
45	BA	1248	B8N	O4'-C1'-C5-C4
45	BA	1326	UY1	O4'-C1'-C5-C4
45	BA	1596	PSU	O4'-C1'-C5-C4
1	AA	1522	OMG	C3'-C2'-O2'-CM2
1	AA	2837	OMU	C3'-C2'-O2'-CM2
1	AA	3792	OMG	C3'-C2'-O2'-CM2
1	AA	3899	OMG	C3'-C2'-O2'-CM2
45	BA	1326	UY1	C1'-C2'-O2'-CM2
45	BA	1442	OMU	C2'-C1'-N1-C6
1	AA	2351	OMC	O4'-C4'-C5'-O5'
1	AA	2787	A2M	O4'-C1'-N9-C8
3	AC	75	OMG	C4'-C5'-O5'-P
45	BA	1625	PSU	O4'-C4'-C5'-O5'
45	BA	668	A2M	O4'-C1'-N9-C8
45	BA	1850	MA6	N1-C6-N6-C9
1	AA	1881	OMC	C3'-C4'-C5'-O5'
1	AA	4590	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
45	BA	100	PSU	C3'-C4'-C5'-O5'
1	AA	3899	OMG	C1'-C2'-O2'-CM2
1	AA	4623	OMG	C1'-C2'-O2'-CM2
45	BA	174	OMC	C1'-C2'-O2'-CM2
45	BA	644	OMG	C1'-C2'-O2'-CM2
1	AA	4623	OMG	C3'-C2'-O2'-CM2
45	BA	644	OMG	C3'-C2'-O2'-CM2
45	BA	1248	B8N	N34-C33-C34-O36
1	AA	1524	A2M	O4'-C1'-N9-C8
45	BA	428	OMU	O4'-C1'-N1-C2
1	AA	398	A2M	C3'-C4'-C5'-O5'
1	AA	1322	1MA	C2'-C1'-N9-C8
1	AA	1677	PSU	O4'-C1'-C5-C6
1	AA	4636	PSU	O4'-C1'-C5-C6
45	BA	1248	B8N	O4'-C1'-C5-C6
45	BA	1326	UY1	O4'-C1'-C5-C6
45	BA	1360	PSU	O4'-C1'-C5-C6
45	BA	1442	OMU	C2'-C1'-N1-C2
1	AA	3701	OMC	O4'-C1'-N1-C2
1	AA	2422	OMC	O4'-C4'-C5'-O5'
1	AA	4523	A2M	O4'-C4'-C5'-O5'
1	AA	4456	OMC	C2'-C1'-N1-C2
45	BA	174	OMC	C3'-C2'-O2'-CM2
1	AA	1534	A2M	O4'-C4'-C5'-O5'
45	BA	590	A2M	O4'-C1'-N9-C8
45	BA	667	PSU	C4'-C5'-O5'-P
45	BA	1288	OMU	C4'-C5'-O5'-P
1	AA	2787	A2M	C2'-C1'-N9-C4

There are no ring outliers.

94 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	400	A2M	1	0
1	AA	4571	A2M	2	0
1	AA	3792	OMG	1	0
1	AA	3718	A2M	4	0
1	AA	1326	A2M	1	0
45	BA	1174	PSU	1	0
45	BA	1832	6MZ	1	0
1	AA	2363	A2M	1	0
1	AA	1340	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	1391	OMC	1	0
1	AA	4552	PSU	1	0
45	BA	484	A2M	2	0
45	BA	1136	PSU	2	0
1	AA	4689	PSU	1	0
1	AA	4456	OMC	1	0
45	BA	36	PSU	1	0
1	AA	3899	OMG	1	0
1	AA	4499	OMG	1	0
45	BA	1851	MA6	2	0
1	AA	4620	OMU	1	0
1	AA	2351	OMC	1	0
1	AA	4579	PSU	2	0
1	AA	4523	A2M	1	0
45	BA	172	OMU	1	0
45	BA	174	OMC	1	0
45	BA	609	PSU	2	0
45	BA	27	A2M	1	0
45	BA	1447	OMG	1	0
45	BA	1625	PSU	1	0
45	BA	509	OMG	2	0
45	BA	1678	A2M	1	0
45	BA	99	A2M	1	0
45	BA	651	PSU	2	0
45	BA	1003	PSU	1	0
45	BA	1031	A2M	2	0
45	BA	354	OMU	3	0
45	BA	159	A2M	3	0
45	BA	1337	4AC	1	0
45	BA	822	PSU	2	0
45	BA	1445	PSU	2	0
45	BA	1804	OMU	2	0
1	AA	4447	5MC	1	0
1	AA	2632	PSU	1	0
45	BA	406	PSU	1	0
1	AA	4618	OMG	1	0
1	AA	3770	PSU	1	0
1	AA	5010	PSU	1	0
45	BA	576	A2M	2	0
45	BA	121	OMU	2	0
45	BA	462	OMC	2	0
45	BA	366	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1683	PSU	1	0
45	BA	109	PSU	1	0
1	AA	4500	PSU	1	0
45	BA	601	OMG	1	0
45	BA	867	OMG	2	0
45	BA	1244	PSU	3	0
5	AE	245	HIC	1	0
45	BA	649	PSU	2	0
45	BA	572	PSU	1	0
1	AA	1871	A2M	1	0
45	BA	119	PSU	1	0
45	BA	116	OMU	3	0
1	AA	4353	PSU	1	0
45	BA	100	PSU	1	0
1	AA	4220	6MZ	1	0
1	AA	1316	OMG	1	0
45	BA	1383	A2M	1	0
1	AA	398	A2M	1	0
45	BA	1703	OMC	1	0
1	AA	2804	OMC	1	0
1	AA	2815	A2M	1	0
1	AA	4293	PSU	1	0
45	BA	436	OMG	1	0
1	AA	3830	A2M	1	0
45	BA	1842	4AC	1	0
45	BA	1692	PSU	2	0
3	AC	14	OMU	1	0
45	BA	681	PSU	2	0
45	BA	1232	PSU	1	0
1	AA	4392	OMG	2	0
45	BA	1004	PSU	1	0
45	BA	1360	PSU	2	0
1	AA	1779	PSU	1	0
45	BA	468	A2M	1	0
45	BA	166	A2M	1	0
1	AA	4423	PSU	2	0
45	BA	1850	MA6	3	0
45	BA	512	A2M	1	0
1	AA	4457	PSU	2	0
1	AA	4227	OMU	1	0
45	BA	296	PSU	1	0
45	BA	1643	PSU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	4636	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 290 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	M7G	BA	1933	-	24,26,31	4.92	20 (83%)	34,39,49	1.79	9 (26%)

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
82	M7G	BA	1933	-	-	1/7/25/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BA	1933	M7G	C8-N7	10.42	1.51	1.33
82	BA	1933	M7G	C2'-C3'	-10.37	1.24	1.53
82	BA	1933	M7G	C2-N3	6.55	1.49	1.33
82	BA	1933	M7G	O4'-C4'	-6.34	1.30	1.45
82	BA	1933	M7G	C4-N3	6.12	1.48	1.34
82	BA	1933	M7G	C2-N2	5.64	1.47	1.34
82	BA	1933	M7G	C3'-C4'	5.49	1.67	1.53
82	BA	1933	M7G	C8-N9	5.47	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BA	1933	M7G	C1'-N9	-5.08	1.32	1.47
82	BA	1933	M7G	C5-N7	5.04	1.45	1.39
82	BA	1933	M7G	O4'-C1'	4.22	1.52	1.42
82	BA	1933	M7G	C5-C6	3.76	1.53	1.43
82	BA	1933	M7G	C2-N1	3.69	1.46	1.37
82	BA	1933	M7G	C6-N1	3.43	1.45	1.38
82	BA	1933	M7G	O2'-C2'	3.17	1.50	1.43
82	BA	1933	M7G	C4-N9	2.94	1.45	1.38
82	BA	1933	M7G	O6-C6	-2.29	1.19	1.23
82	BA	1933	M7G	O3'-C3'	2.22	1.48	1.43
82	BA	1933	M7G	C2'-C1'	2.18	1.60	1.53
82	BA	1933	M7G	C5-C4	2.15	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	BA	1933	M7G	C2-N3-C4	4.39	120.11	112.30
82	BA	1933	M7G	C5-C4-N3	-4.26	119.99	128.15
82	BA	1933	M7G	C5-C6-N1	3.81	119.75	111.79
82	BA	1933	M7G	O6-C6-C5	-3.12	121.03	128.06
82	BA	1933	M7G	C2-N1-C6	-2.71	120.15	125.10
82	BA	1933	M7G	C3'-C2'-C1'	2.29	105.78	101.43
82	BA	1933	M7G	N9-C8-N7	-2.18	106.83	112.21
82	BA	1933	M7G	C2'-C3'-C4'	2.17	106.86	102.64
82	BA	1933	M7G	C5-C4-N9	2.02	110.31	105.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

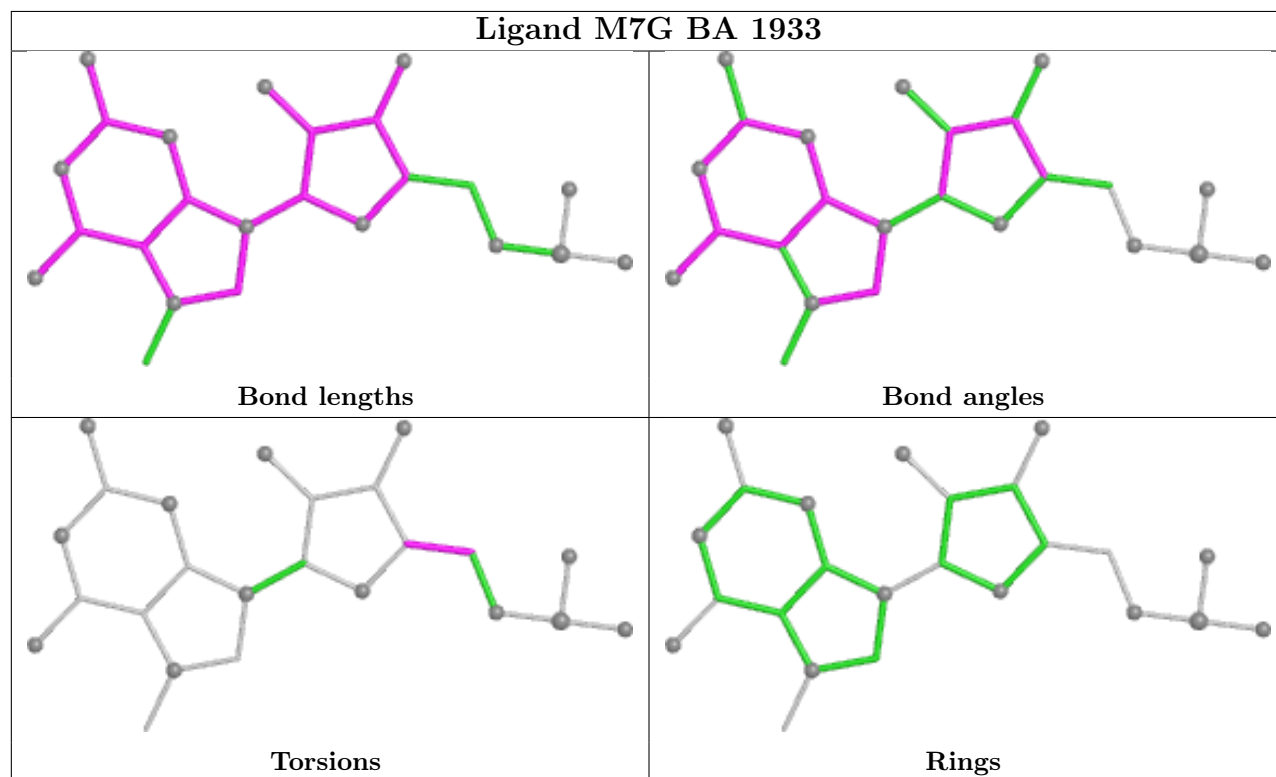
Mol	Chain	Res	Type	Atoms
82	BA	1933	M7G	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

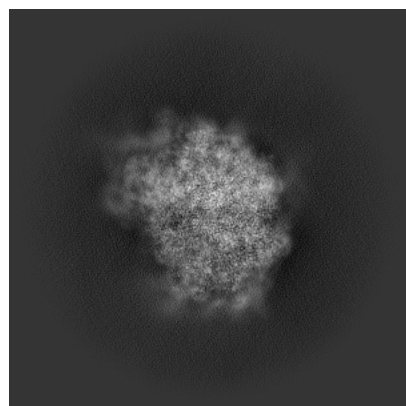
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66301. These allow visual inspection of the internal detail of the map and identification of artifacts.

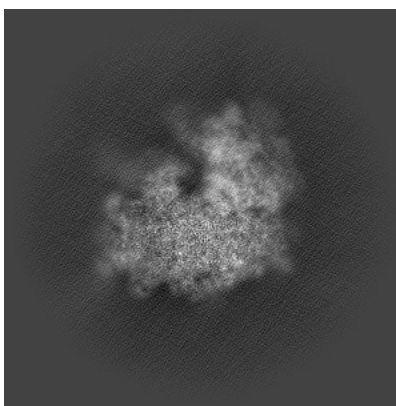
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

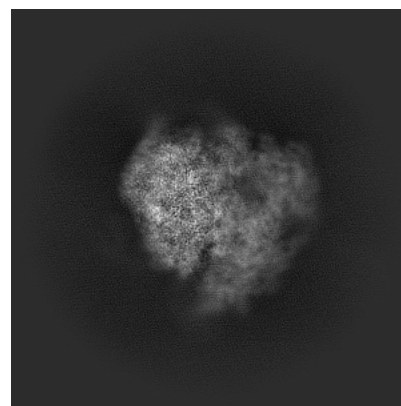
6.1.1 Primary map



X

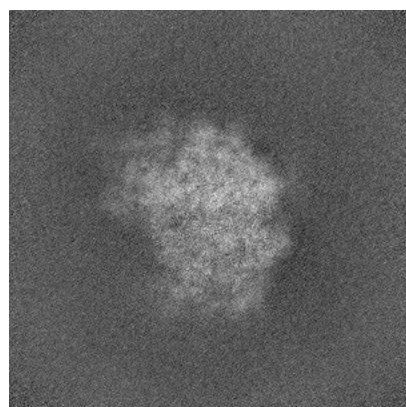


Y

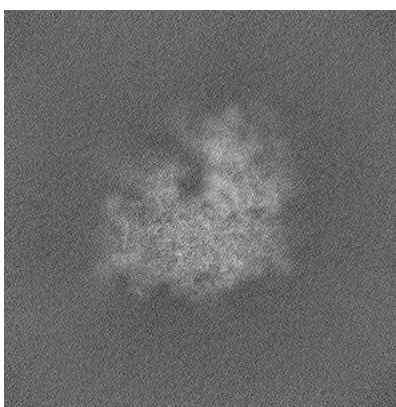


Z

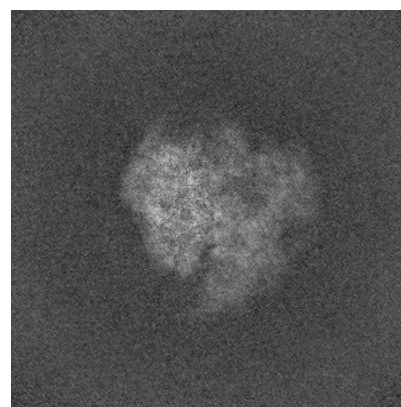
6.1.2 Raw map



X



Y

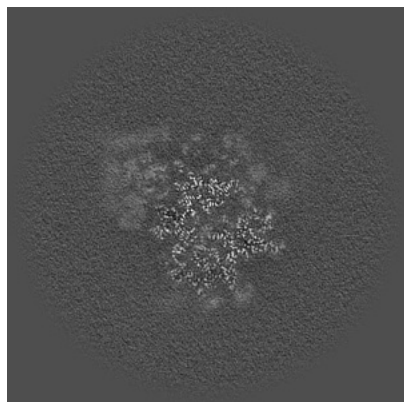


Z

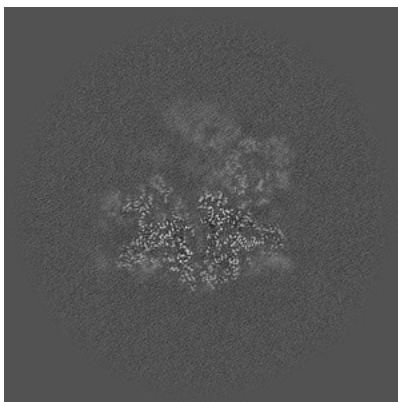
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

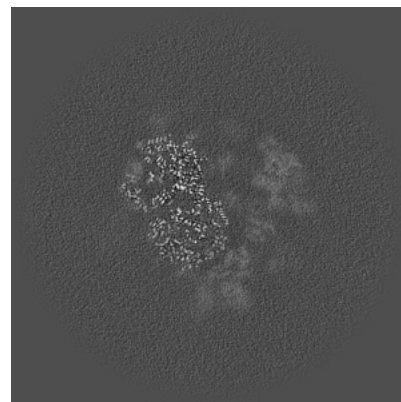
6.2.1 Primary map



X Index: 320

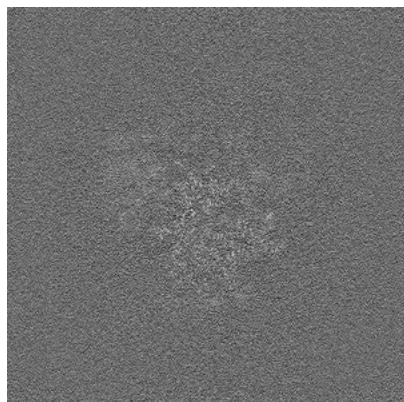


Y Index: 320

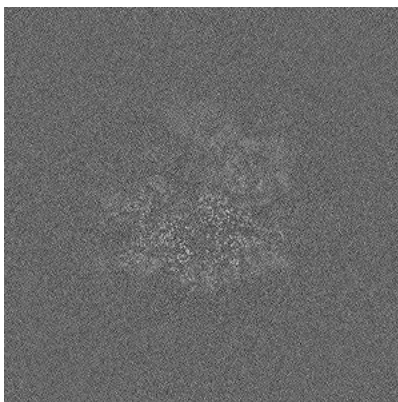


Z Index: 320

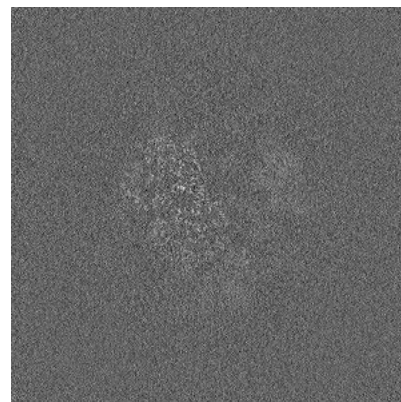
6.2.2 Raw map



X Index: 320



Y Index: 320

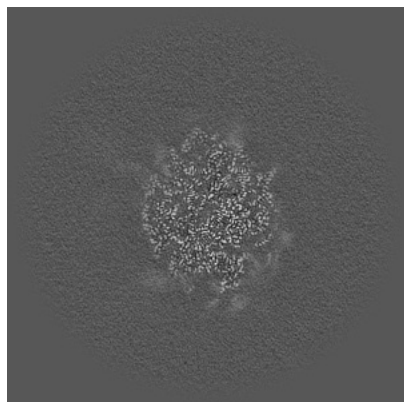


Z Index: 320

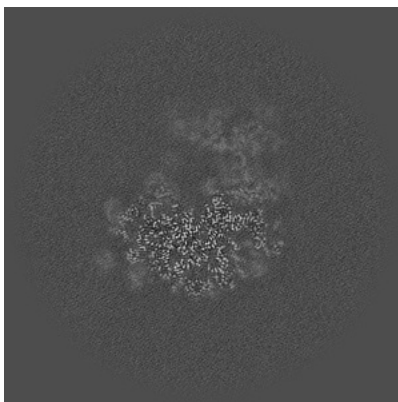
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

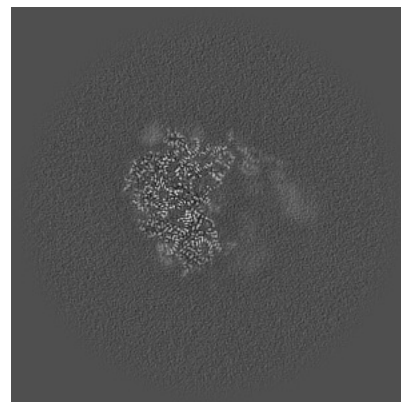
6.3.1 Primary map



X Index: 287

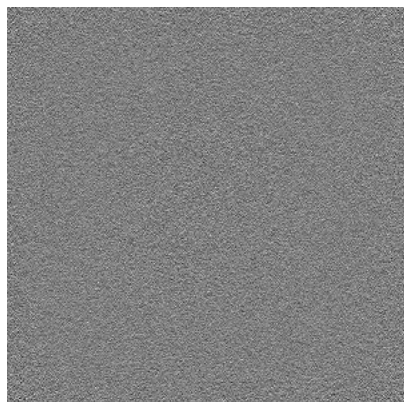


Y Index: 338

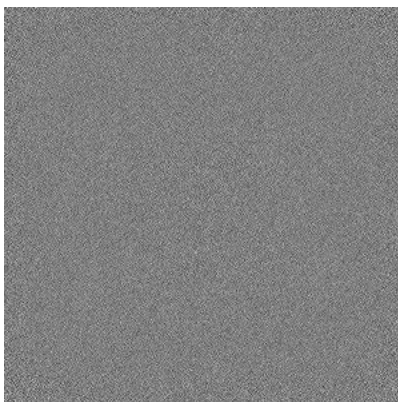


Z Index: 283

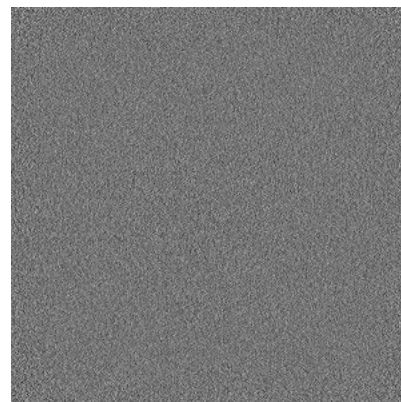
6.3.2 Raw map



X Index: 0



Y Index: 0

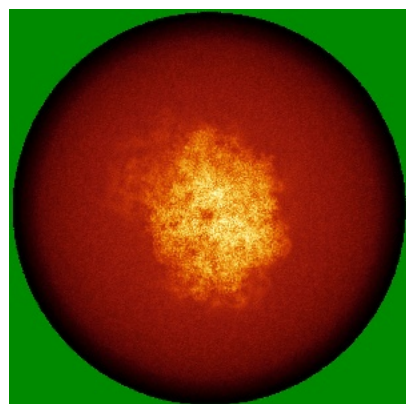


Z Index: 0

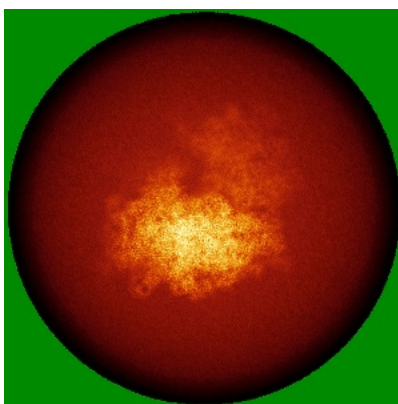
The images above show the largest variance slices of the map in three orthogonal directions.

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

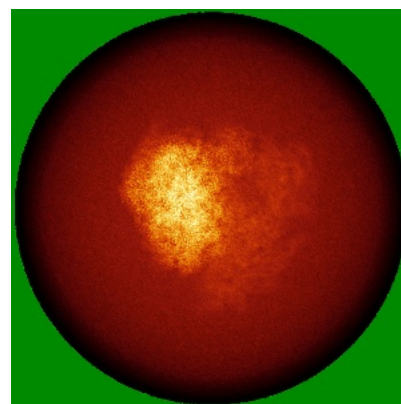
6.4.1 Primary map



X

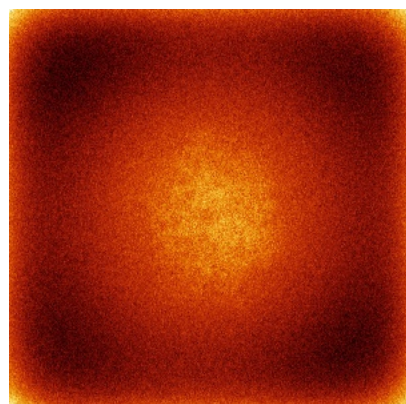


Y

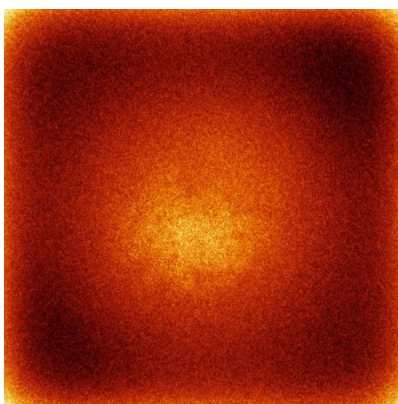


Z

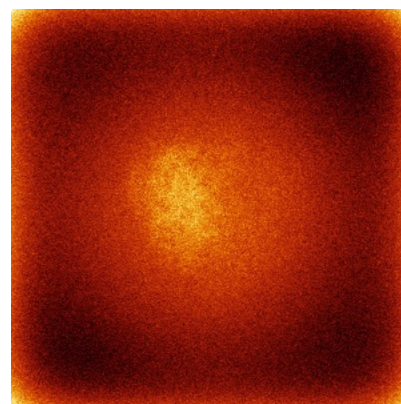
6.4.2 Raw map



X



Y

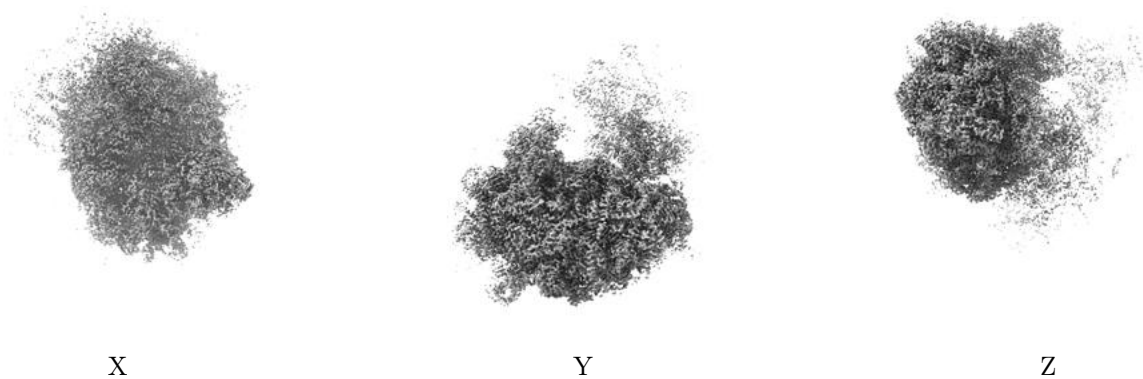


Z

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

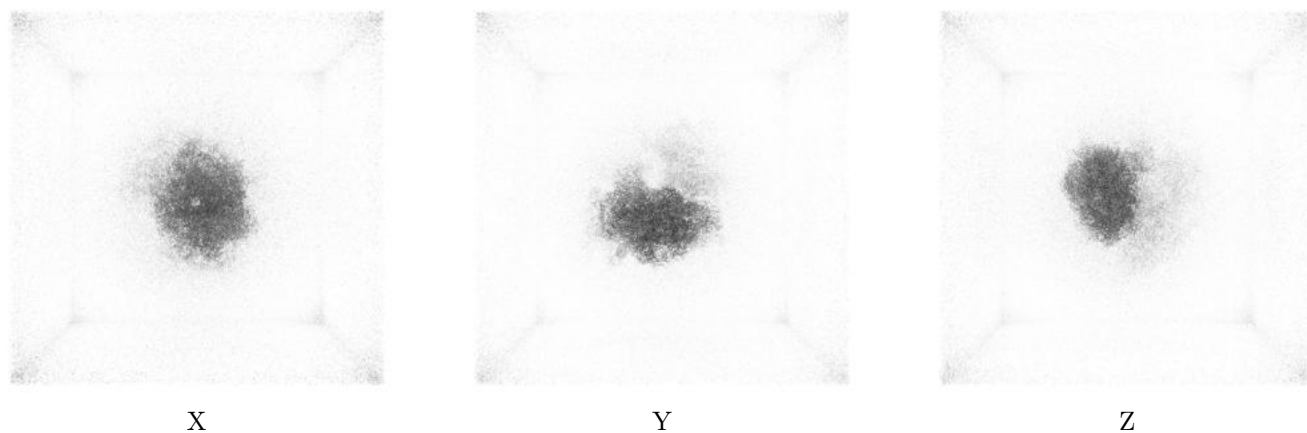
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

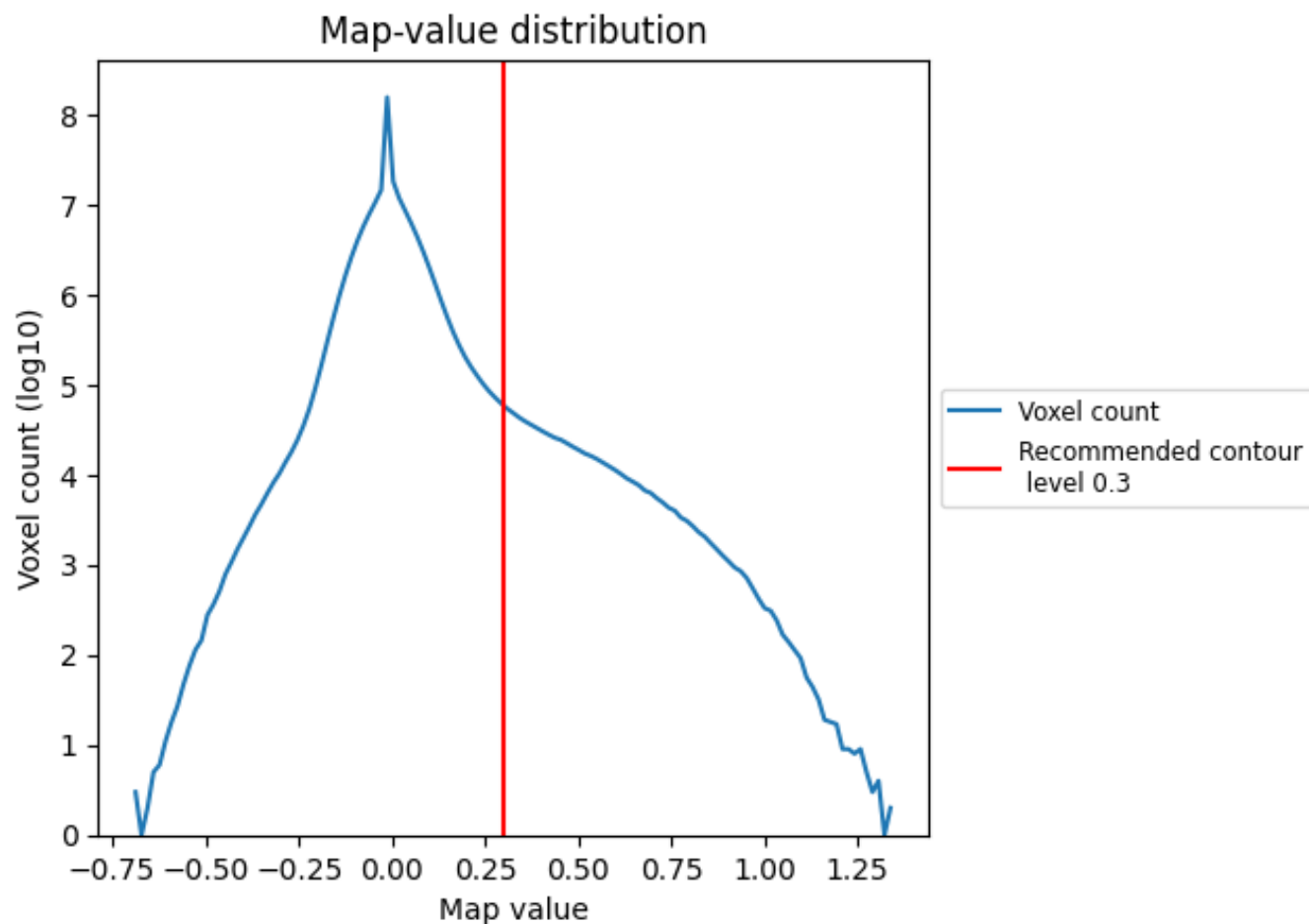
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

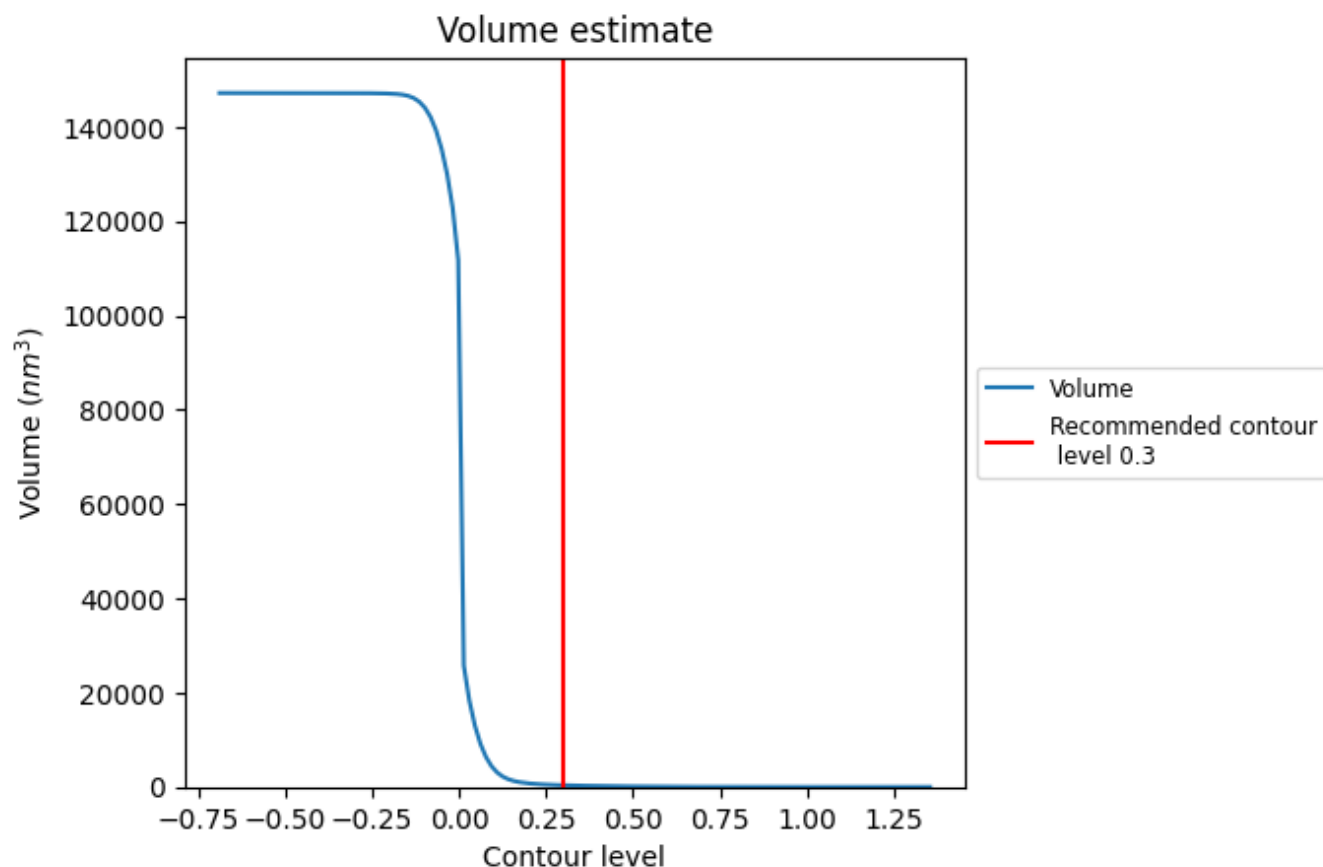
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

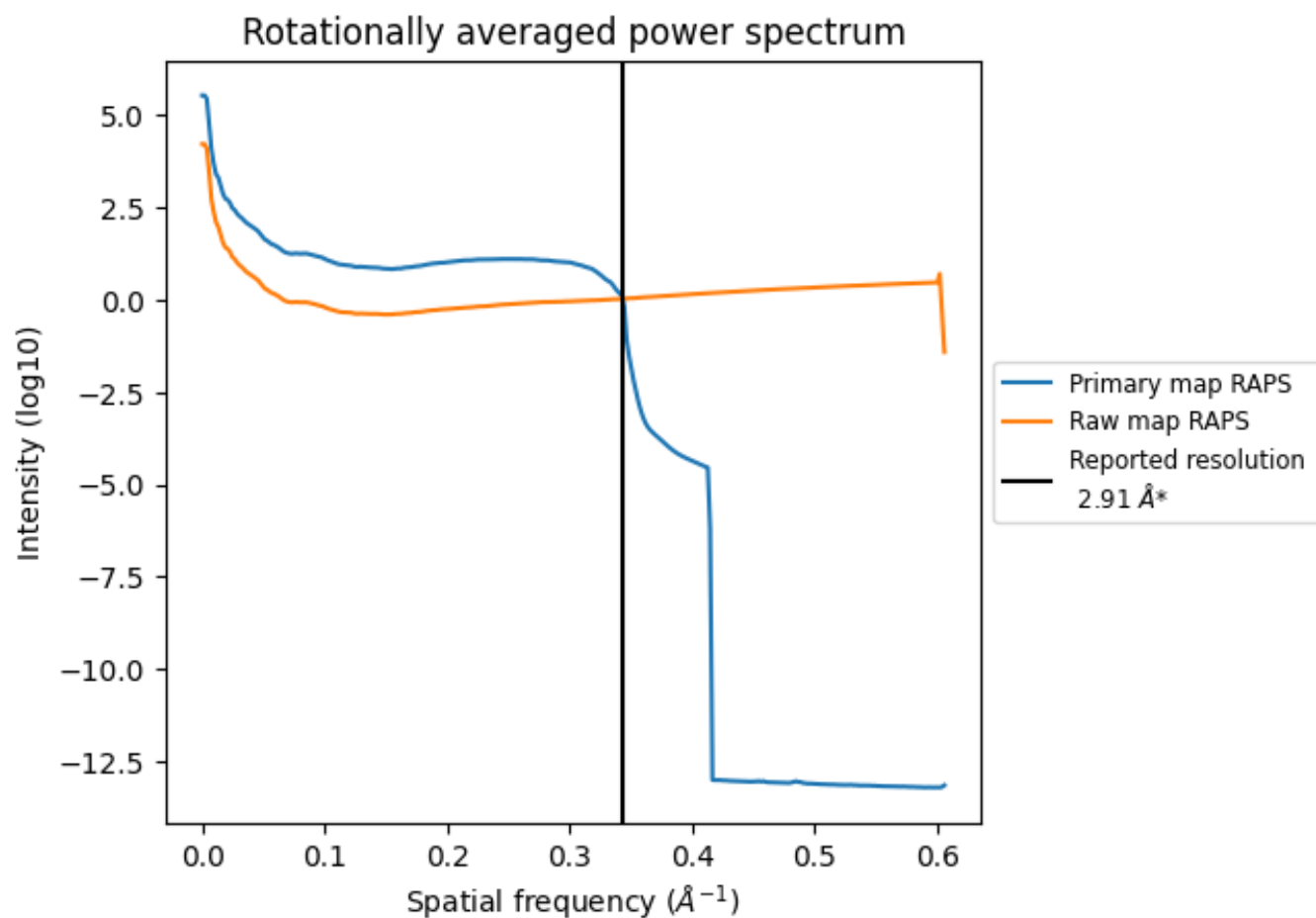
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 322 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 ⓘ

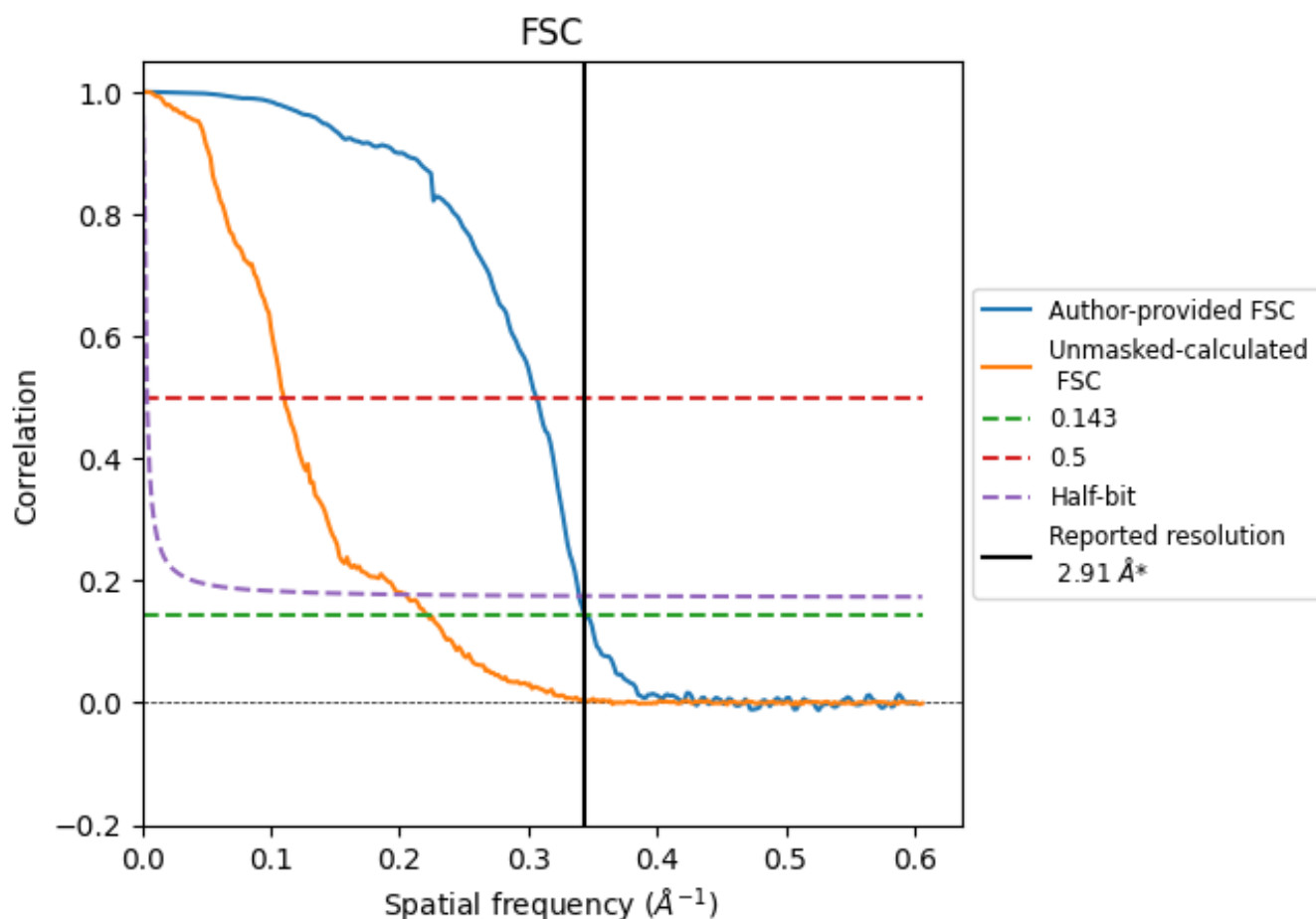


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

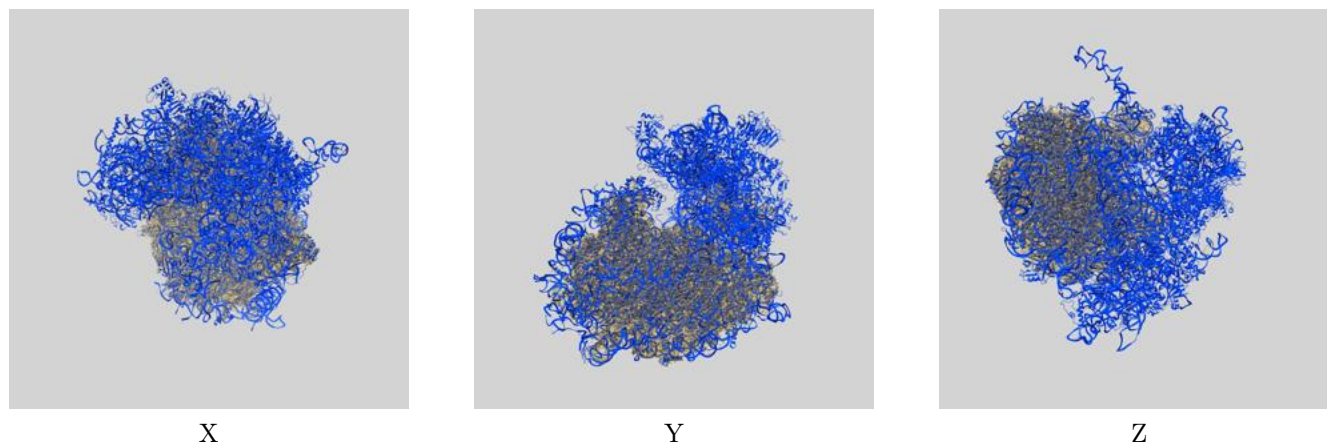
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.27	2.95
Unmasked-calculated*	4.51	9.08	4.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

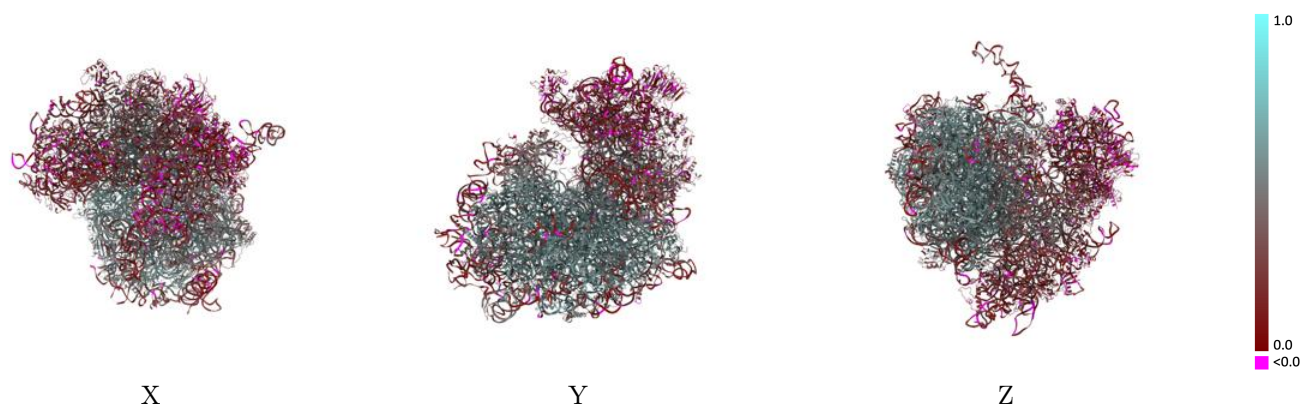
This section contains information regarding the fit between EMDB map EMD-66301 and PDB model 9WW7. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



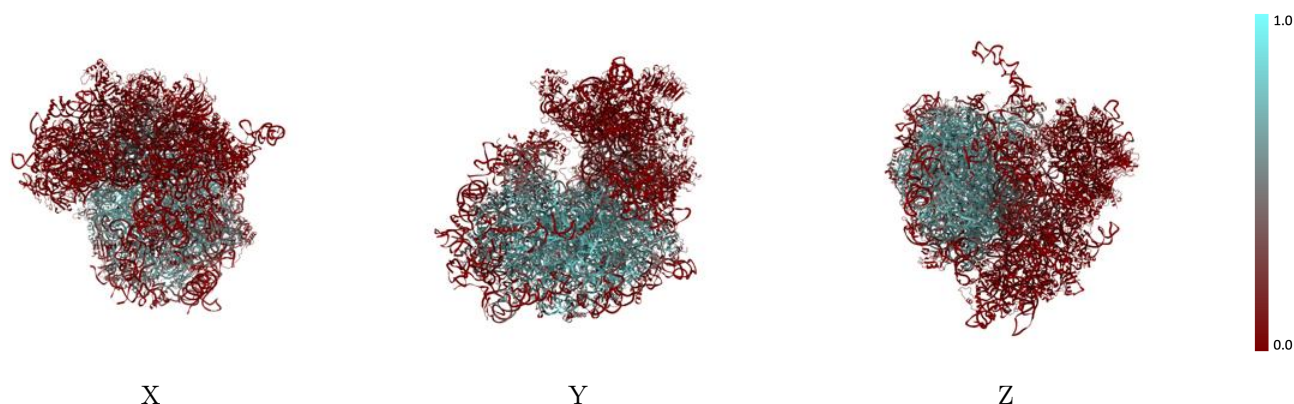
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



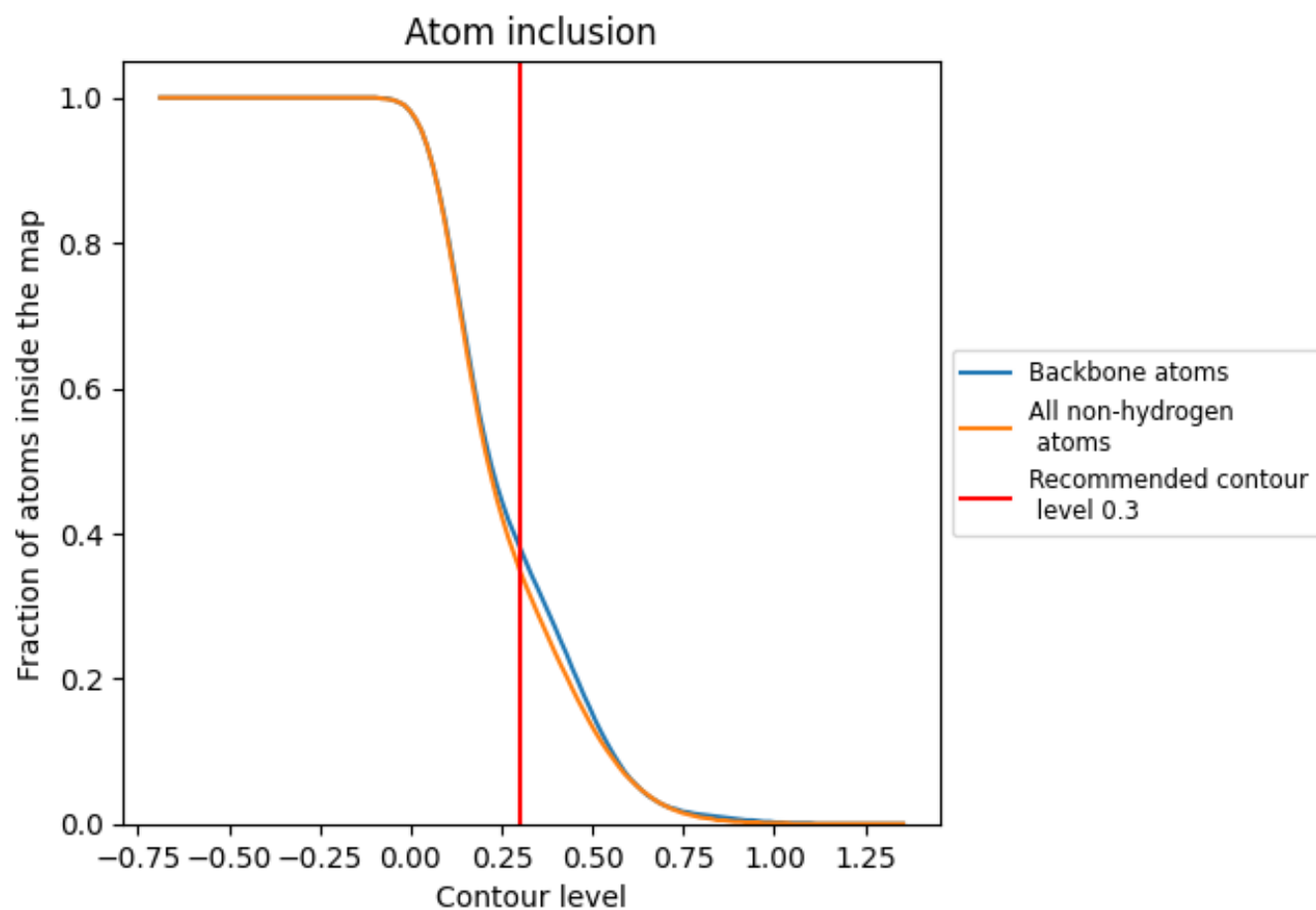
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 35% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3500	 0.4050
AA	 0.5290	 0.4560
AB	 0.5150	 0.4980
AC	 0.6540	 0.5310
AD	 0.7060	 0.6100
AE	 0.5740	 0.5720
AF	 0.6530	 0.5810
AG	 0.2980	 0.4600
AH	 0.3690	 0.4870
AI	 0.6350	 0.5800
AJ	 0.4530	 0.5090
AK	 0.2880	 0.5000
AL	 0.0500	 0.3800
AM	 0.0860	 0.3880
AN	 0.5030	 0.5390
AO	 0.4190	 0.5340
AP	 0.7480	 0.6170
AQ	 0.5970	 0.5750
AR	 0.6450	 0.5920
AS	 0.7020	 0.6080
AT	 0.4360	 0.5200
AU	 0.5250	 0.5680
AV	 0.5450	 0.5720
AW	 0.0250	 0.3420
AX	 0.5910	 0.5900
AY	 0.4860	 0.5770
AZ	 0.5740	 0.5770
Aa	 0.5690	 0.5580
Ab	 0.4560	 0.5380
Ac	 0.6770	 0.5980
Ad	 0.2950	 0.4740
Ae	 0.4140	 0.5000
Af	 0.5570	 0.5520
Ag	 0.6590	 0.5980
Ah	 0.6780	 0.6090



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Chain	Atom inclusion	Q-score
Ai	 0.6190	 0.5820
Aj	 0.5450	 0.5620
Ak	 0.3810	 0.5160
Al	 0.7220	 0.6120
Am	 0.2160	 0.4710
An	 0.5700	 0.5840
Ao	 0.0030	 0.1970
Aq	 0.4520	 0.5440
Ar	 0.6210	 0.5950
As	 0.6000	 0.5750
BA	 0.0690	 0.2600
BB	 0.0020	 0.2720
BC	 0.0060	 0.2830
BD	 0.0110	 0.3310
BE	 0.0010	 0.2190
BF	 0.0010	 0.1610
BG	 0.0050	 0.2550
BH	 0.0050	 0.2590
BI	 0.0000	 0.0910
BJ	 0.0260	 0.3470
BK	 0.0010	 0.2050
BL	 0.0000	 0.1990
BM	 0.0020	 0.2220
BN	 0.0000	 0.1700
BO	 0.0010	 0.2030
BP	 0.0060	 0.3140
BQ	 0.0170	 0.3550
BR	 0.0080	 0.2740
BS	 0.0000	 0.1510
BT	 0.0070	 0.1380
BU	 0.0000	 0.1460
BV	 0.0130	 0.2820
BW	 0.0000	 0.1840
BX	 0.0030	 0.1950
BY	 0.0000	 0.1210
BZ	 0.0500	 0.3990
Ba	 0.0100	 0.3140
Bb	 0.0310	 0.4230
Bc	 0.0000	 0.1510
Bd	 0.0020	 0.1470
Be	 0.0050	 0.3070
Bf	 0.0000	 0.2130

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Chain	Atom inclusion	Q-score
Bg	 0.0020	 0.0760
Bh	 0.0000	 0.1790