Full wwPDB EM Validation Report

Jun 19, 2026 – 06:43 am BST

PDB ID	:	8BTK / pdb_00008btk
EMDB ID	:	EMD-16232
Title	:	Structure of the TRAP complex with the Sec translocon and a translating ribosome
Authors	:	Jaskolowski, M.; Jomaa, A.; Gamerdinger, M.; Shrestha, S.; Leibundgut, M.; Deuerling, E.; Ban, N.
Deposited on	:	2022-11-29
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

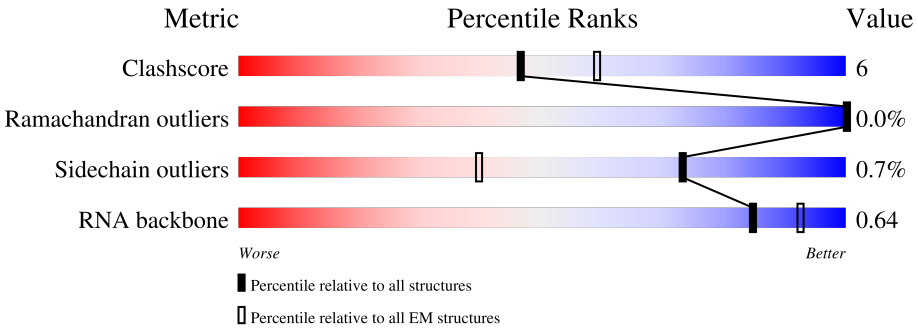
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

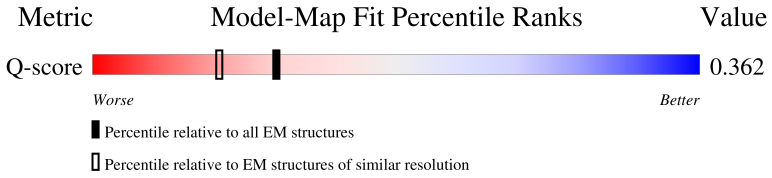
1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B5	4808	52% 23% 22%
2	B7	120	81% 18%
3	B8	158	59% 34% 5%

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Mol	Chain	Length	Quality of chain
4	BA	257	77% 22%
5	BB	403	82% 16%
6	BC	413	77% 11% 12%
7	BD	297	85% 14%
8	BE	291	5% 69% 14% 16%
9	BF	247	75% 17% 9%
10	BG	266	79% 9% 12%
11	BH	192	82% 17%
12	BI	214	81% 18%
13	BJ	178	85% 11%
14	BK	29	7% 100%
15	BL	211	85% 13%
16	BM	218	52% 11% 37%
17	BN	204	83% 16%
18	BO	203	90% 8%
19	BP	184	70% 17% 14%
20	BQ	188	82% 17%
21	BR	196	5% 78% 14% 8%
22	BS	176	84% 16%
23	BT	160	81% 18%
24	BU	128	68% 9% 23%
25	BV	140	82% 17%
26	BW	157	31% 66% 11% 23%
27	BX	156	67% 9% 24%
28	BY	145	83% 9% 8%

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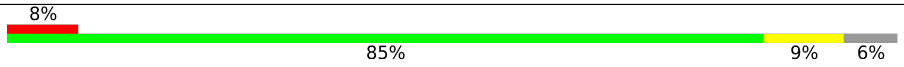
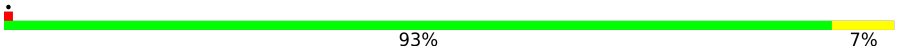
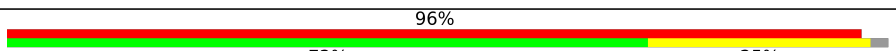
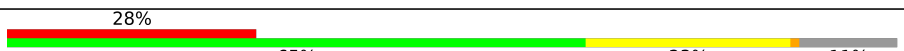
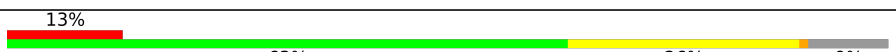
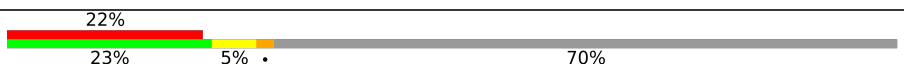
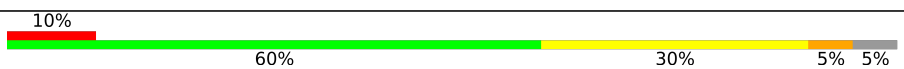
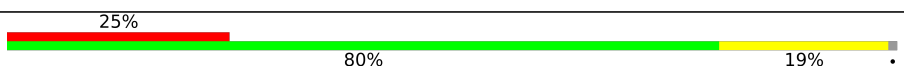
Mol	Chain	Length	Quality of chain
29	BZ	136	
30	Ba	148	
31	Bb	245	
32	Bc	115	
33	Bd	125	
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	106	
44	Bp	92	
45	Br	137	
46	Bs	318	
47	Bt	165	
48	Bv	217	
49	SX	476	
50	SY	68	
51	SZ	96	
52	A2	1870	
53	AA	84	

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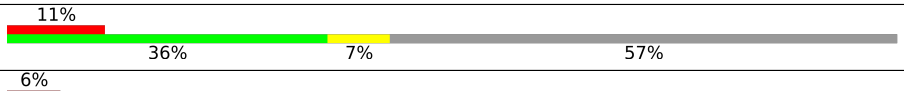
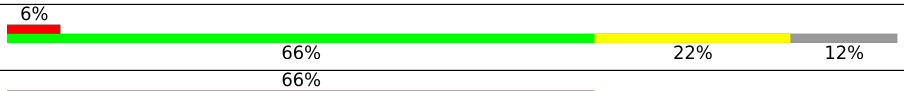
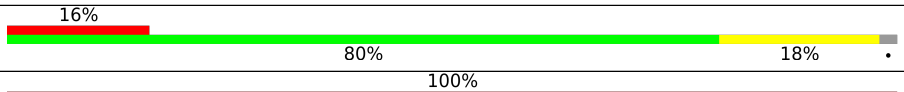
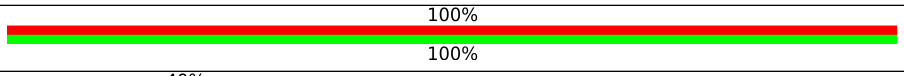
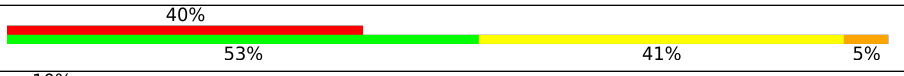
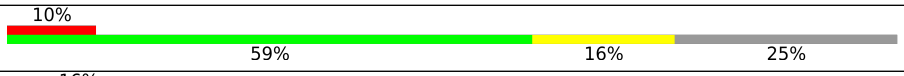
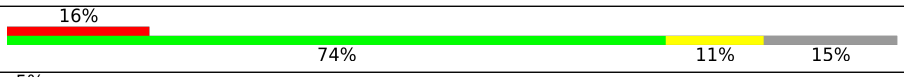
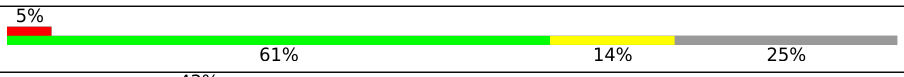
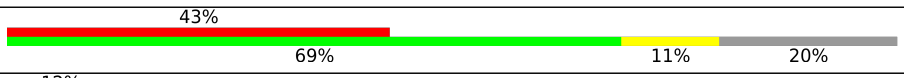
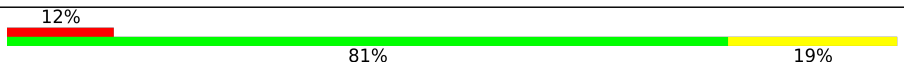
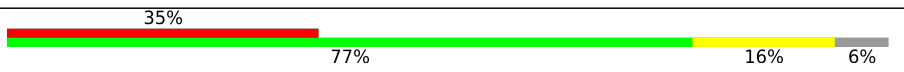
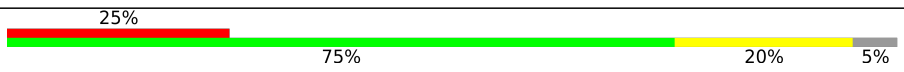
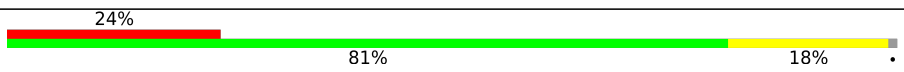
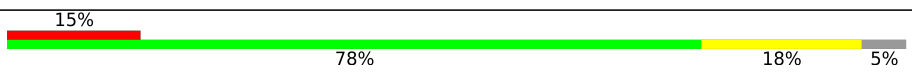
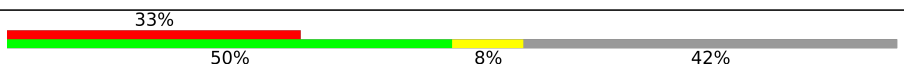
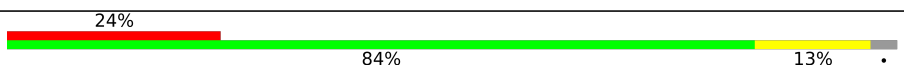
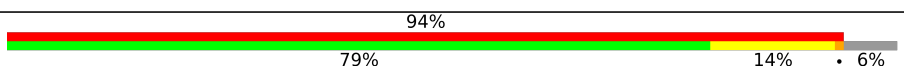
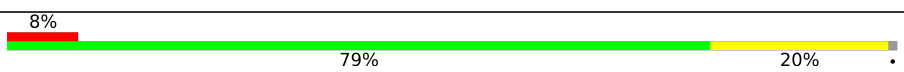
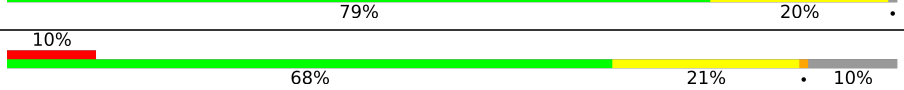
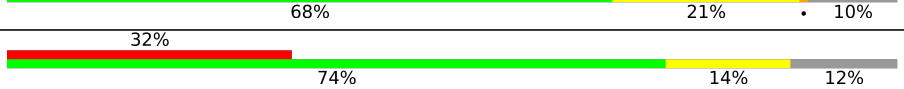
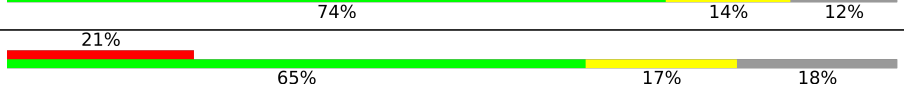
Mol	Chain	Length	Quality of chain
54	AB	69	
55	AC	156	
56	AD	133	
57	AE	115	
58	AF	317	
59	AG	56	
60	AH	4	
61	AT	75	
62	AZ	295	
63	Aa	264	
64	Ab	293	
65	Ac	281	
66	Ad	263	
67	Ae	204	
68	Af	249	
69	Ag	432	
70	Ah	208	
71	Ai	194	
72	Aj	165	
73	Ak	158	
74	Al	132	
75	Am	151	
76	An	151	
77	Ao	145	
78	Ap	172	

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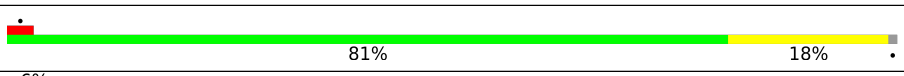
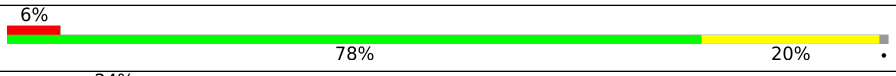
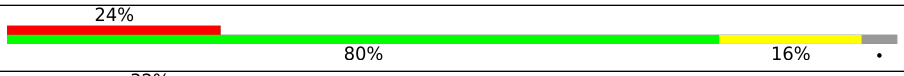
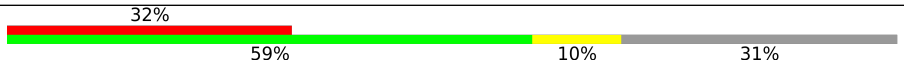
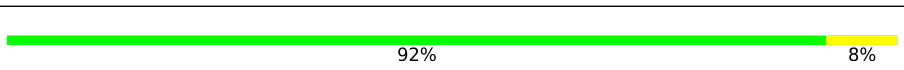
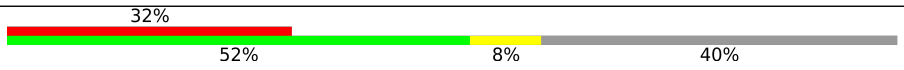
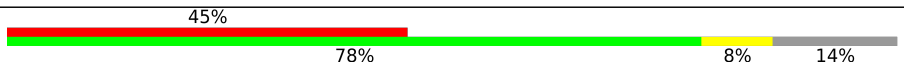
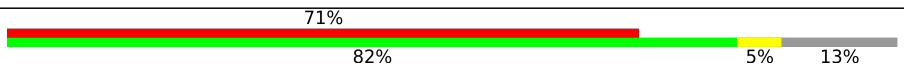
Mol	Chain	Length	Quality of chain
79	Aq	135	
80	Ar	152	
81	As	145	
82	At	119	
83	Au	83	
84	Av	130	
85	Aw	143	
86	Ax	130	
87	Ay	124	
88	Az	25	
89	TA	286	
90	TB	183	
91	TC	185	
92	TD	173	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 233722 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	B5	3764	80772	36003	14762	26243	3764	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B7	119	2538	1131	451	837	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B8	156	3319	1481	585	1097	156	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BA	253	1940	1214	396	324	6	0	0

- Molecule 5 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BB	398	3206	2042	605	546	13	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 7 is a protein called Ribosomal_L18_c domain-containing protein.

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 9 is a protein called uL30,60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BG	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	86	ALA	VAL	conflict	UNP G1STW0
BG	191	GLY	CYS	conflict	UNP G1STW0

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

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

- Molecule 12 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 13 is a protein called Ribosomal protein L11.

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

- Molecule 14 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	BK	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 15 is a protein called L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	210	Total	C	N	O	S	0	0
			1701	1065	354	278	4		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 16 is a protein called Ribosomal protein L14.

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

- Molecule 17 is a protein called Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	174	LEU	ILE	conflict	UNP A0A0N8ETI8
BO	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 19 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 20 is a protein called eL18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	1	MET	THR	conflict	UNP G1TTY7

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Chain	Residue	Modelled	Actual	Comment	Reference
BS	18	PRO	-	insertion	UNP G1TTY7
BS	19	THR	-	insertion	UNP G1TTY7
BS	20	PRO	SER	conflict	UNP G1TTY7
BS	49	SER	LEU	conflict	UNP G1TTY7
BS	50	GLN	GLU	conflict	UNP G1TTY7
BS	95	ARG	HIS	conflict	UNP G1TTY7
BS	101	THR	ILE	conflict	UNP G1TTY7
BS	102	THR	MET	conflict	UNP G1TTY7
BS	104	GLY	SER	conflict	UNP G1TTY7
BS	138	ARG	PRO	conflict	UNP G1TTY7
BS	168	SER	TYR	conflict	UNP G1TTY7

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	conflict	UNP G1TSG1
BU	36	ALA	GLU	conflict	UNP G1TSG1
BU	39	PHE	SER	conflict	UNP G1TSG1
BU	54	GLY	ARG	conflict	UNP G1TSG1
BU	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 25 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 27 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 28 is a protein called Ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 32 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 33 is a protein called Ribosomal protein L31.

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

- Molecule 34 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bj	88	Total	C	N	O	S	0	0
			721	443	160	113	5		

- Molecule 40 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 41 is a protein called eL39.

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

- Molecule 42 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 44 is a protein called eL43.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Br	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	103	ARG	HIS	conflict	UNP G1U7L1

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 47 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 48 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bv	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 49 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SX	425	Total	C	N	O	S	0	0
			3317	2186	534	576	21		

- Molecule 50 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SY	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 51 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SZ	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A2	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 53 is a protein called 40S ribosomal protein S27.

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

- Molecule 54 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 55 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 56 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AD	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 57 is a protein called eS26.

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

- Molecule 58 is a protein called RACK1.

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

- Molecule 59 is a protein called uS14.

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

- Molecule 60 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AH	4	Total	C	N	O	P	0	0
			66	28	11	23	4		

- Molecule 61 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AT	75	Total	C	N	O	P	0	0
			1597	713	279	530	75		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 63 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 64 is a protein called Ribosomal_S5_C domain-containing protein,40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	2	ALA	VAL	conflict	UNP A0A5F9D8I1
Ab	36	ARG	CYS	conflict	UNP A0A5F9D8I1
Ab	38	ARG	GLY	conflict	UNP A0A5F9D8I1
Ab	39	GLY	LYS	conflict	UNP A0A5F9D8I1
Ab	40	ARG	ALA	conflict	UNP A0A5F9D8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	42	ARG	ASP	conflict	UNP A0A5F9D8I1
Ab	73	MET	VAL	conflict	UNP G1TUT9
Ab	119	GLY	ALA	conflict	UNP G1TUT9
Ab	194	ARG	HIS	conflict	UNP G1TUT9
Ab	215	MET	LEU	conflict	UNP G1TUT9
Ab	227	ARG	TRP	conflict	UNP G1TUT9
Ab	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 65 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 66 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 67 is a protein called Ribosomal protein S5.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 70 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 71 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 72 is a protein called Ribosomal protein eS10.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 74 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 75 is a protein called uS15.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	136	Total	C	N	O	S	0	0
			1017	622	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	5F0	ASP	conflict	UNP G1U472

- Molecule 77 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 78 is a protein called uS9.

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

- Molecule 79 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 80 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 81 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	conflict	UNP G1TN62
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 82 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	At	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 83 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Au	3	ASN	SER	conflict	UNP G1TM82
Au	4	ASP	ASN	conflict	UNP G1TM82
Au	33	GLN	PRO	conflict	UNP G1TM82
Au	50	PHE	SER	conflict	UNP G1TM82

- Molecule 84 is a protein called Ribosomal protein S15a.

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

- Molecule 85 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 86 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 87 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 88 is a protein called 60S ribosomal protein L41.

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

- Molecule 89 is a protein called Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	TA	172	Total	C	N	O	S	0	0
			1372	888	219	261	4		

- Molecule 90 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	TB	161	Total	C	N	O	S	0	0
			1254	807	210	235	2		

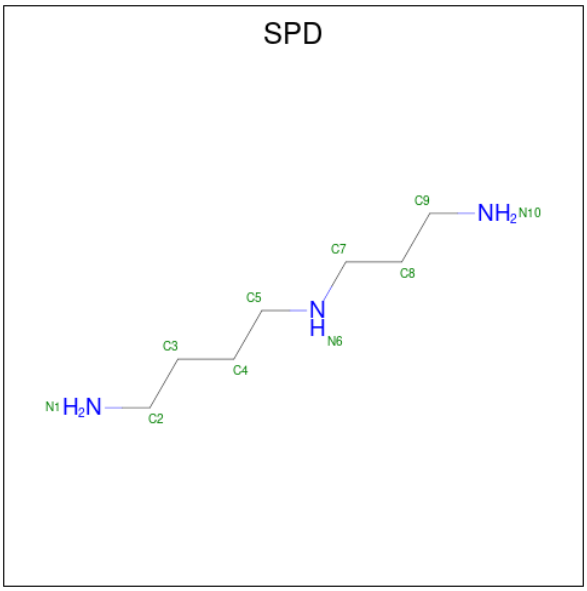
- Molecule 91 is a protein called Signal sequence receptor subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	TC	160	Total	C	N	O	S	0	0
			1295	853	212	227	3		

- Molecule 92 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	TD	150	Total	C	N	O	S	0	0
			1185	755	199	228	3		

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
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93	B5	1	Total C N 10 7 3	0
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93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0

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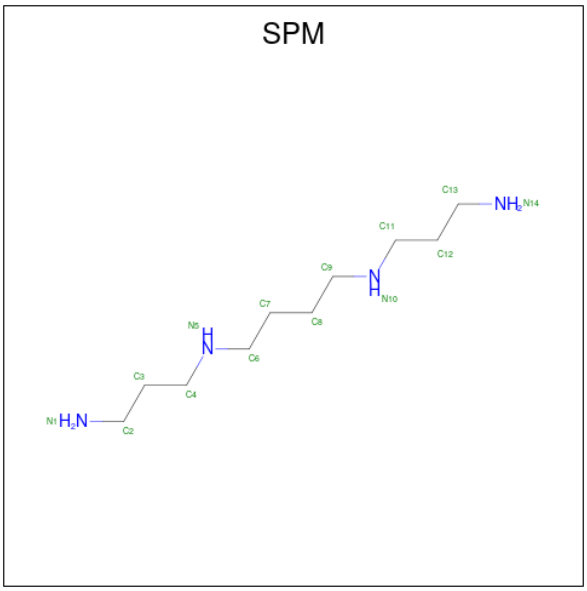
Mol	Chain	Residues	Atoms	AltConf
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	B5	1	Total C N 10 7 3	0
93	BN	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0
93	A2	1	Total C N 10 7 3	0

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



Mol	Chain	Residues	Atoms	AltConf
94	B5	1	Total C N 14 10 4	0
94	B5	1	Total C N 14 10 4	0
94	A2	1	Total C N 14 10 4	0

- Molecule 95 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
95	B5	510	Total Mg 510 510	0
95	B7	15	Total Mg 15 15	0
95	B8	16	Total Mg 16 16	0
95	BA	4	Total Mg 4 4	0
95	BB	3	Total Mg 3 3	0
95	BC	1	Total Mg 1 1	0
95	BH	1	Total Mg 1 1	0
95	BI	2	Total Mg 2 2	0
95	BL	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
95	BN	1	Total Mg 1 1	0
95	BP	1	Total Mg 1 1	0
95	BQ	2	Total Mg 2 2	0
95	BR	1	Total Mg 1 1	0
95	BT	2	Total Mg 2 2	0
95	BV	1	Total Mg 1 1	0
95	Ba	1	Total Mg 1 1	0
95	Bb	1	Total Mg 1 1	0
95	Be	2	Total Mg 2 2	0
95	Bf	1	Total Mg 1 1	0
95	Bj	1	Total Mg 1 1	0
95	Bl	1	Total Mg 1 1	0
95	Bo	1	Total Mg 1 1	0
95	A2	167	Total Mg 167 167	0
95	AH	1	Total Mg 1 1	0
95	AT	7	Total Mg 7 7	0
95	Ad	1	Total Mg 1 1	0
95	Ae	1	Total Mg 1 1	0
95	Ak	1	Total Mg 1 1	0
95	An	1	Total Mg 1 1	0
95	Ar	1	Total Mg 1 1	0

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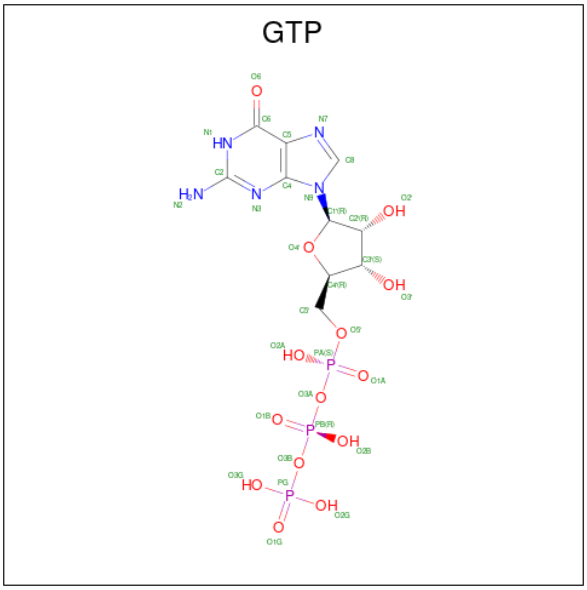
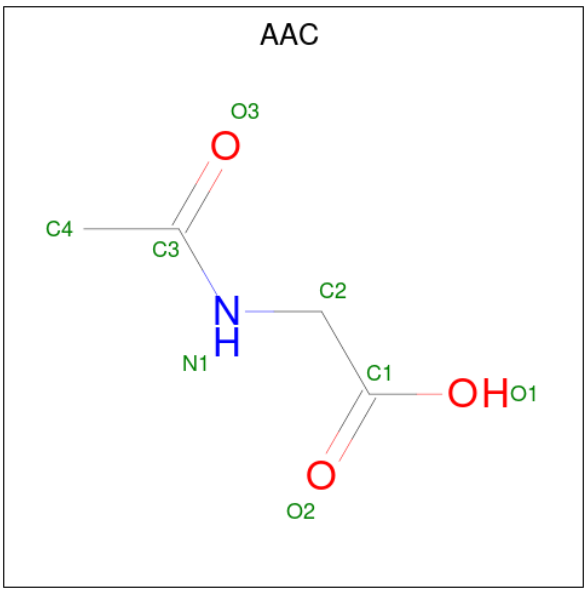
Mol	Chain	Residues	Atoms		AltConf
95	As	1	Total	Mg	0
			1	1	

- Molecule 96 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
96	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 97 is ACETYLAMINO-ACETIC ACID (CCD ID: AAC) (formula: $C_4H_7NO_3$).



Mol	Chain	Residues	Atoms				AltConf
97	BD	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 98 is ZINC ION (CCD ID: ZN) (formula: Zn).

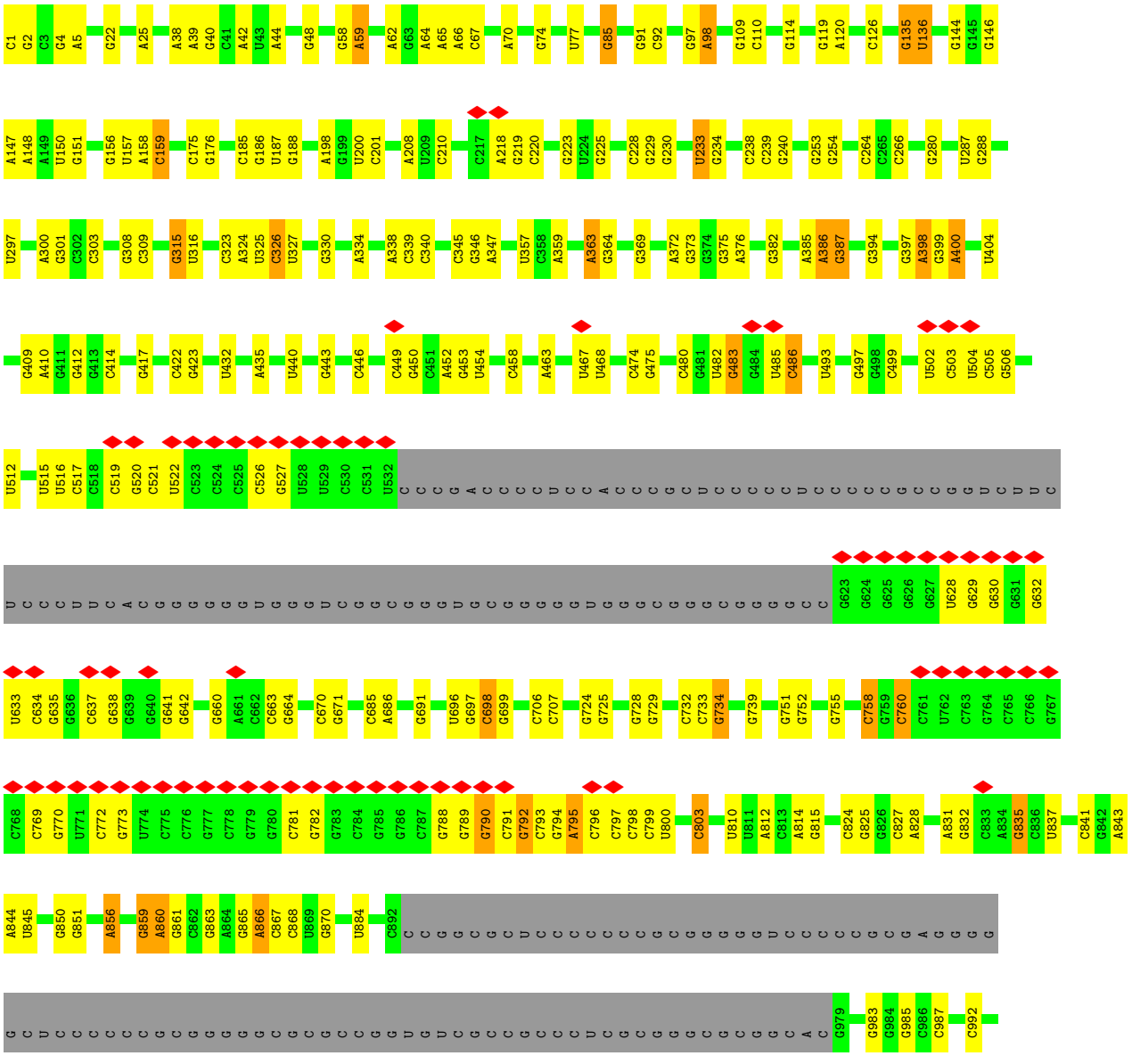
Mol	Chain	Residues	Atoms		AltConf
98	Bg	1	Total	Zn	0
			1	1	
98	Bj	1	Total	Zn	0
			1	1	
98	Bm	1	Total	Zn	0
			1	1	
98	Bo	1	Total	Zn	0
			1	1	
98	Bp	1	Total	Zn	0
			1	1	
98	AC	1	Total	Zn	0
			1	1	
98	AE	1	Total	Zn	0
			1	1	
98	AG	1	Total	Zn	0
			1	1	

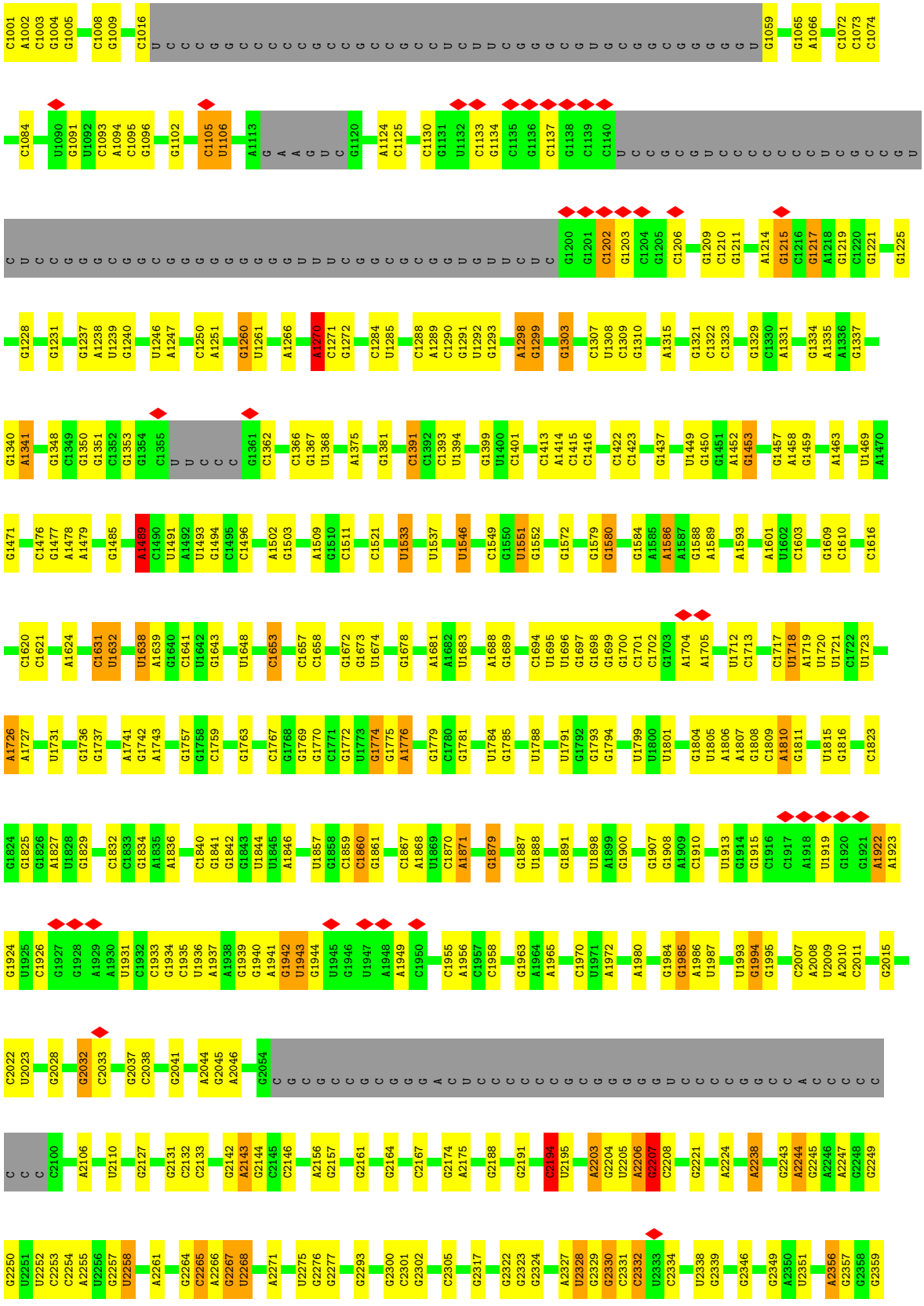
3 Residue-property plots (i)

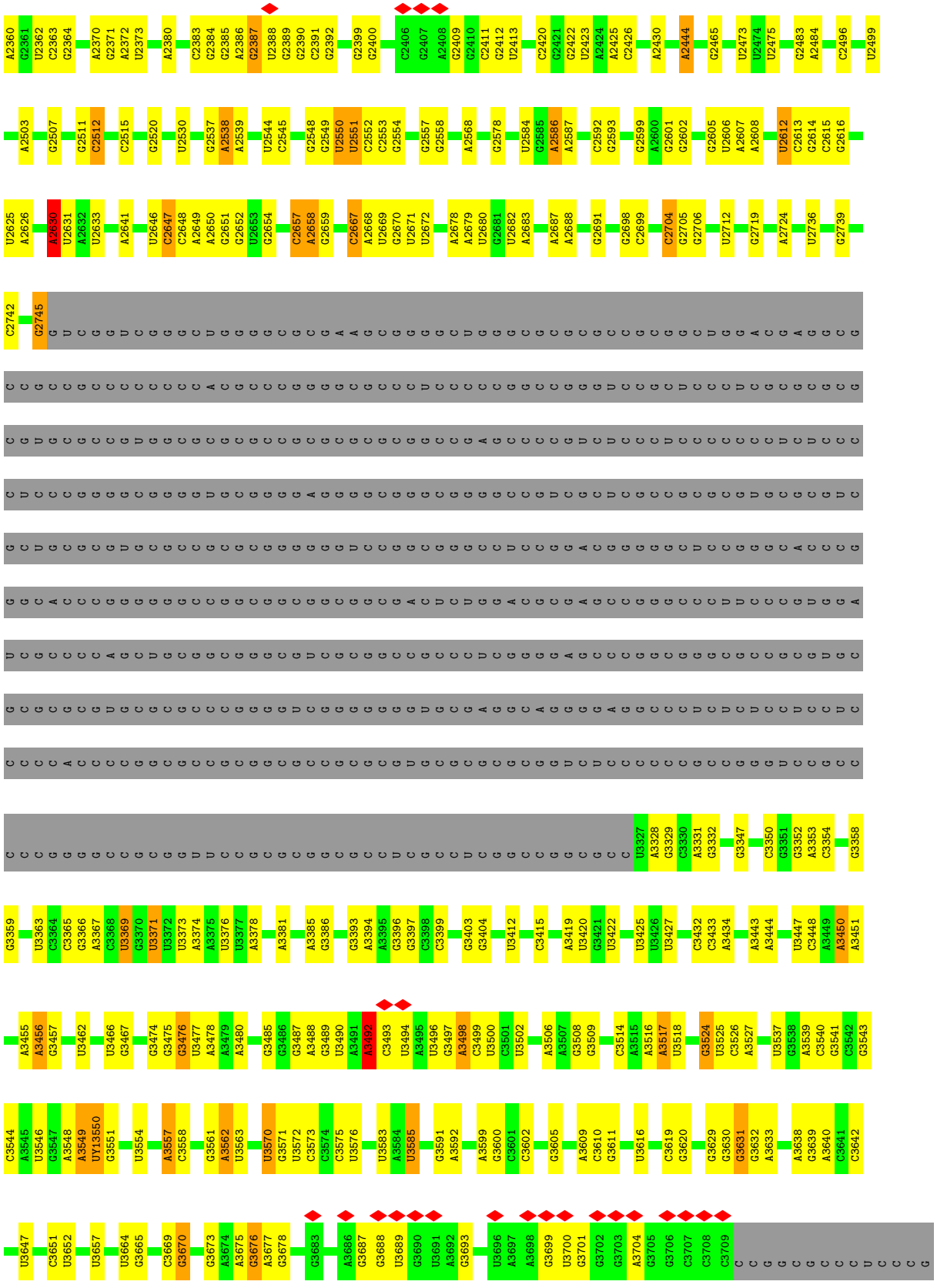
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

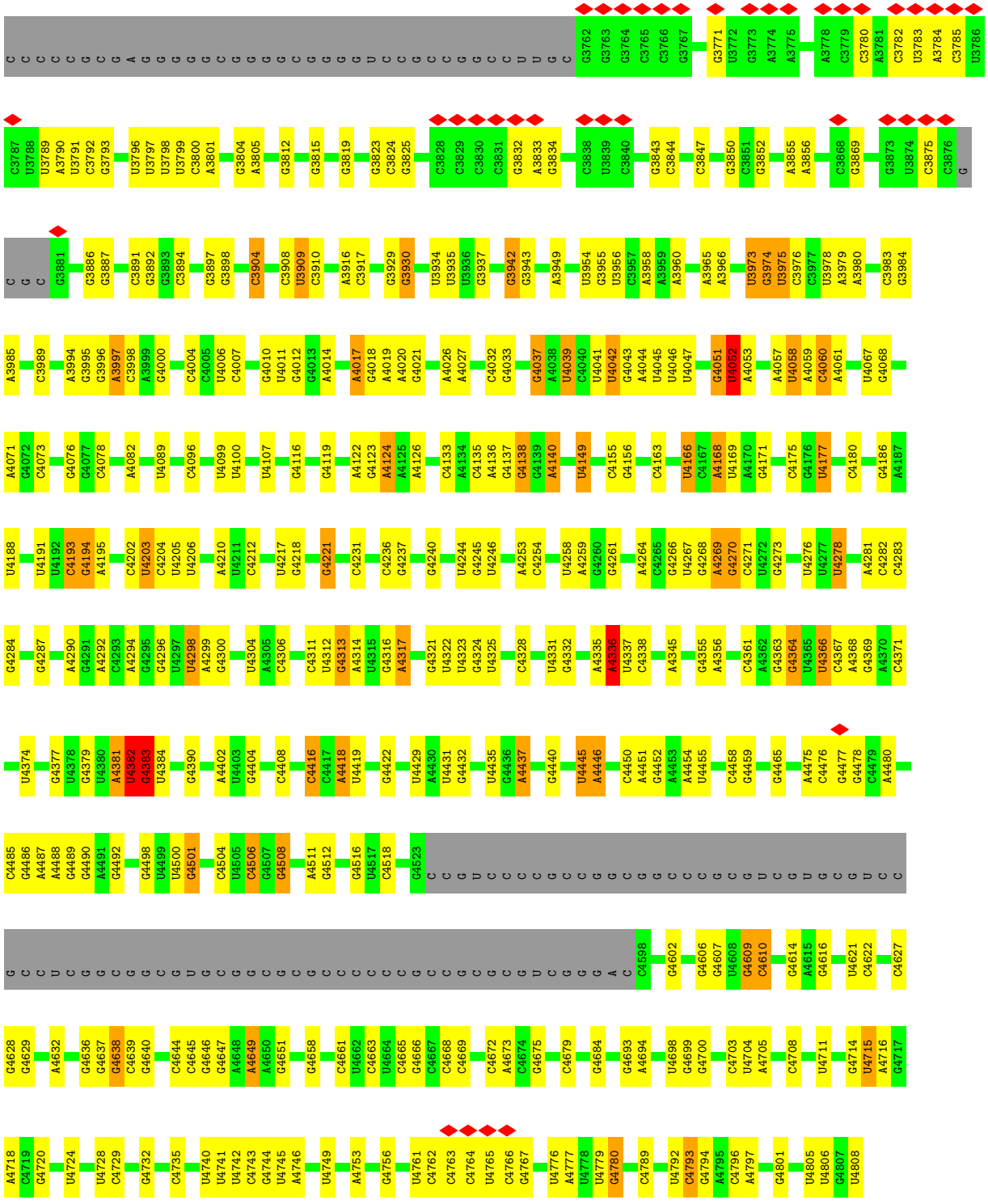
- Molecule 1: 28S rRNA

Chain B5:



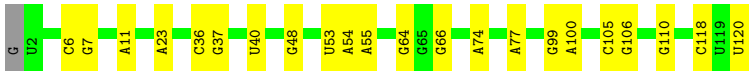






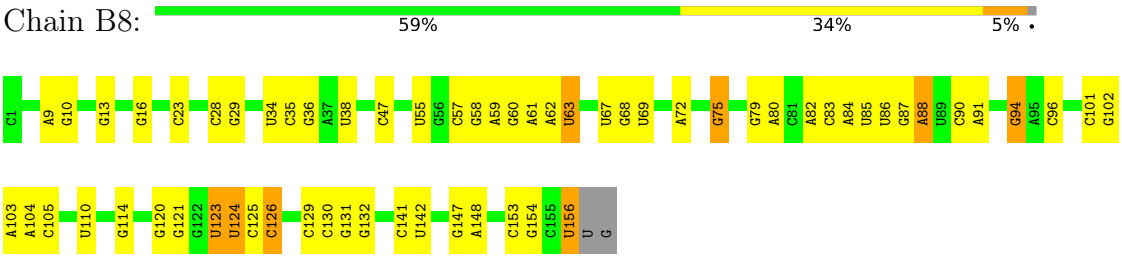
• Molecule 2: 5S rRNA

Chain B7:



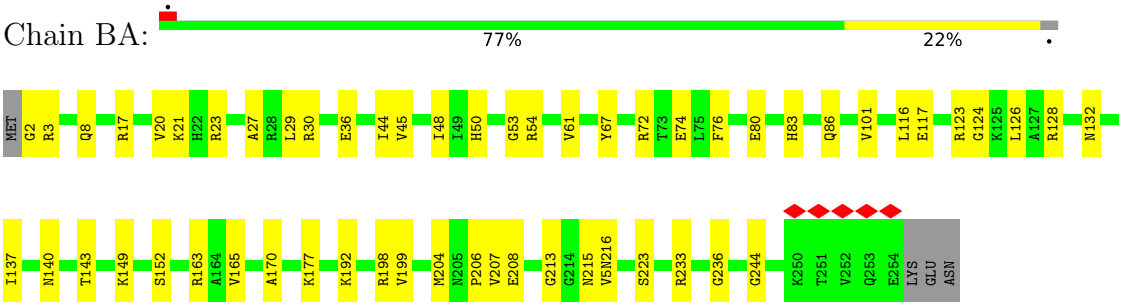
• Molecule 3: 5.8S rRNA

Chain B8:



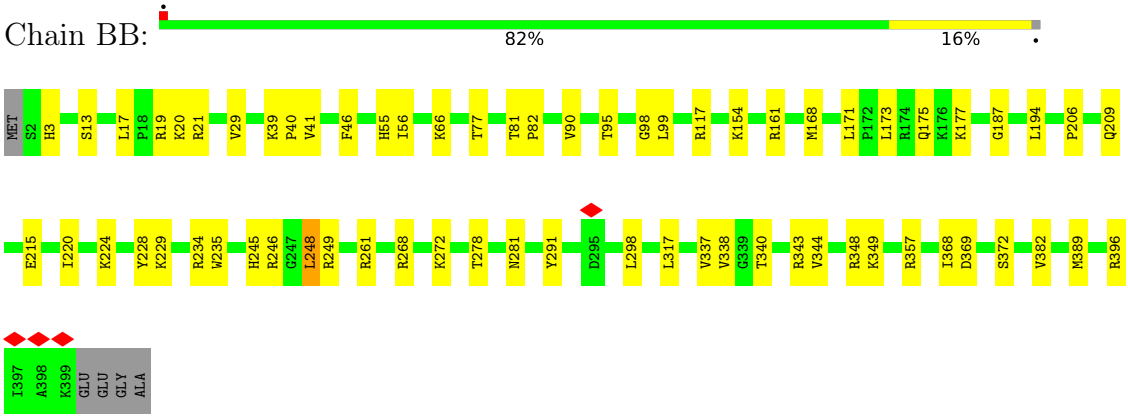
• Molecule 4: 60S ribosomal protein L8

Chain BA:



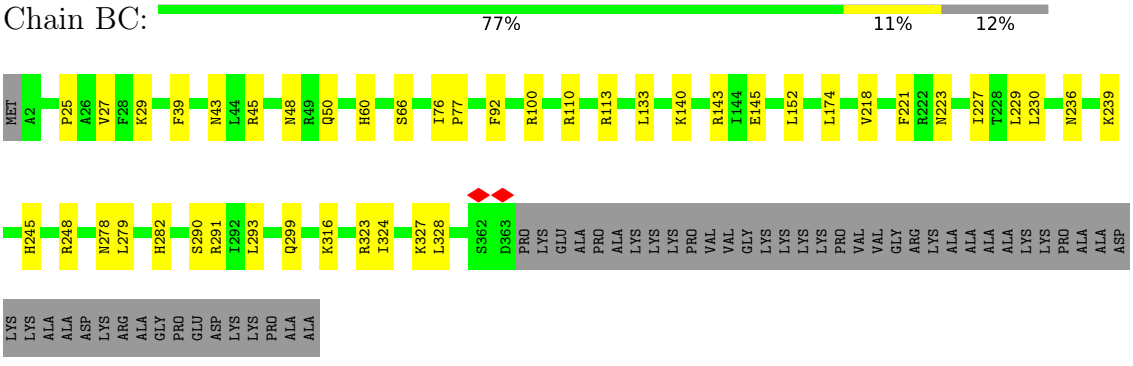
• Molecule 5: Ribosomal protein L3

Chain BB:



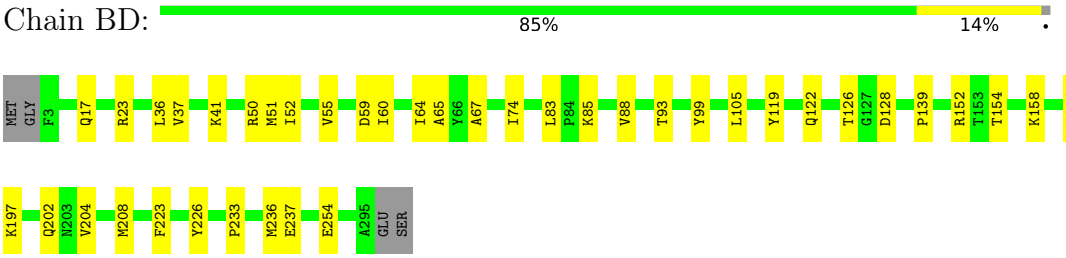
• Molecule 6: 60S ribosomal protein L4

Chain BC:



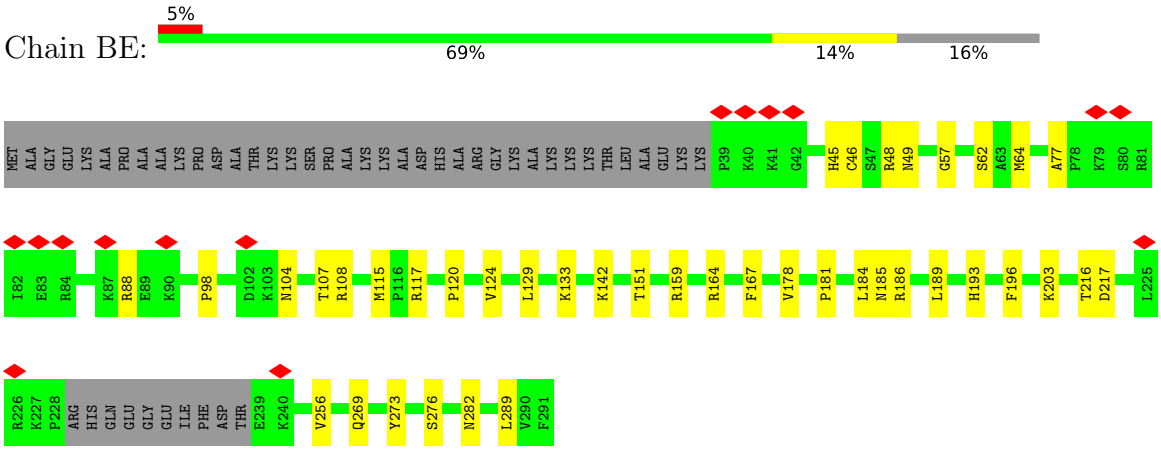
• Molecule 7: Ribosomal_L18_c domain-containing protein

Chain BD:



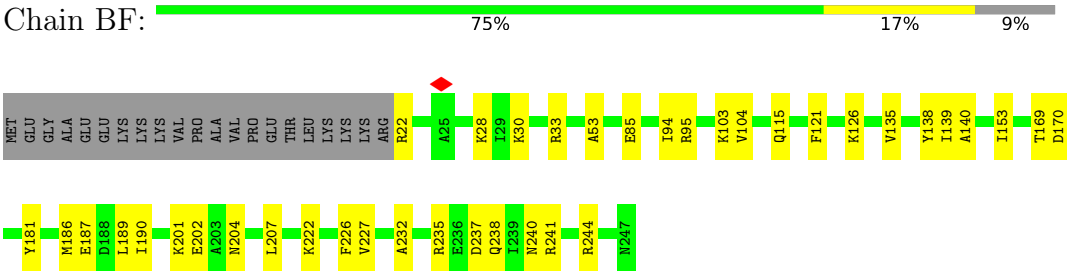
• Molecule 8: 60S ribosomal protein L6

Chain BE:



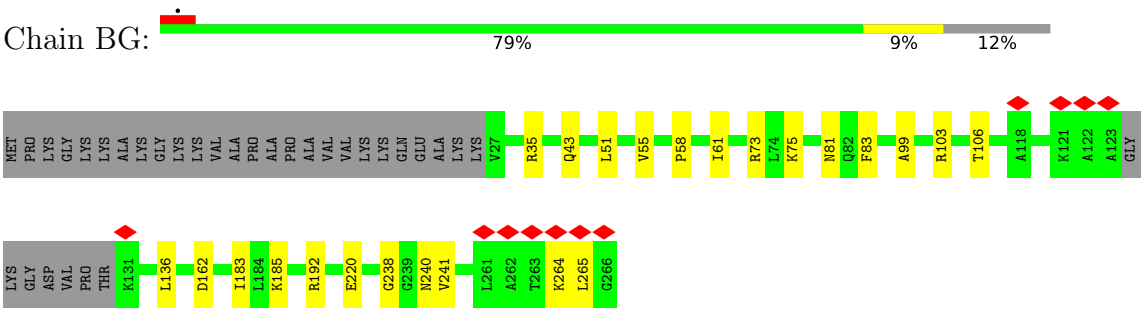
• Molecule 9: uL30,60S ribosomal protein L7

Chain BF:



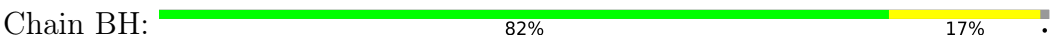
• Molecule 10: 60S ribosomal protein L7a

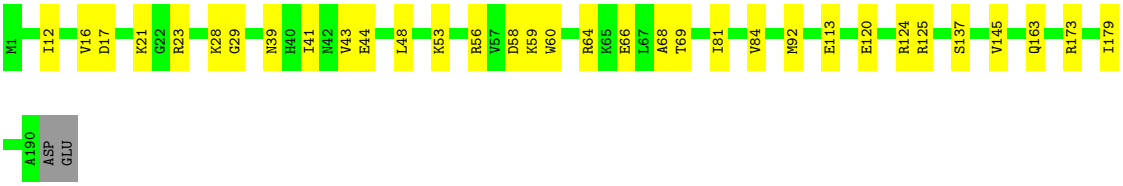
Chain BG:



• Molecule 11: 60S ribosomal protein L9

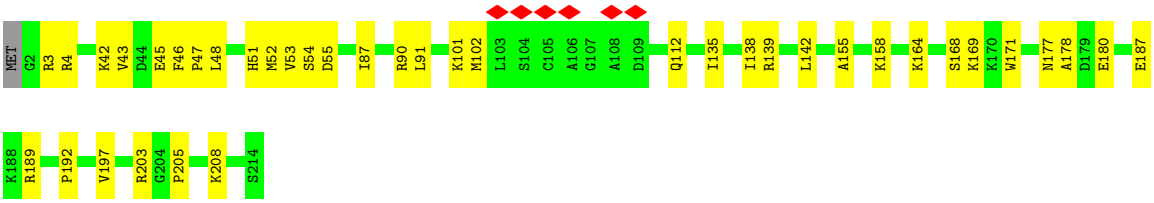
Chain BH:





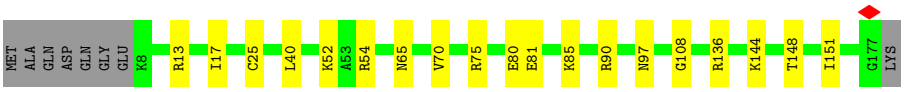
• Molecule 12: Ribosomal protein L10

Chain BI:



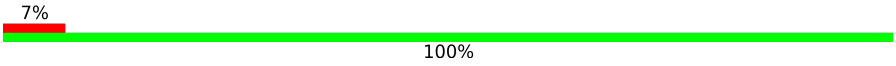
• Molecule 13: Ribosomal protein L11

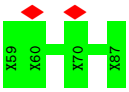
Chain BJ:



• Molecule 14: Nascent chain

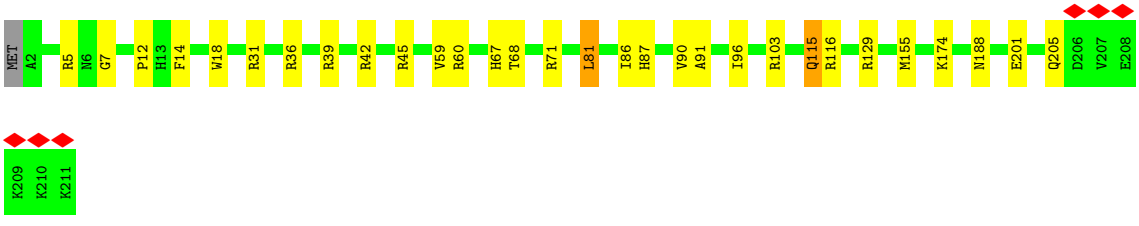
Chain BK:





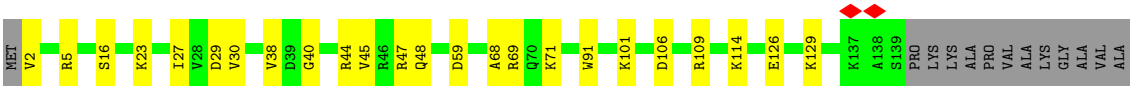
• Molecule 15: L13

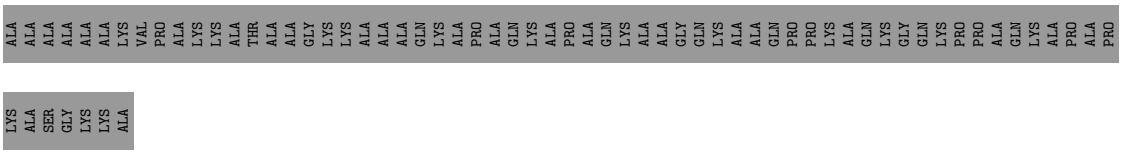
Chain BL:



• Molecule 16: Ribosomal protein L14

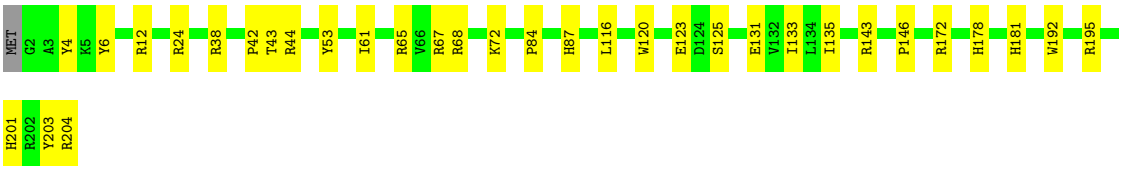
Chain BM:





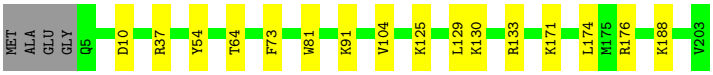
• Molecule 17: Ribosomal protein L15

Chain BN:



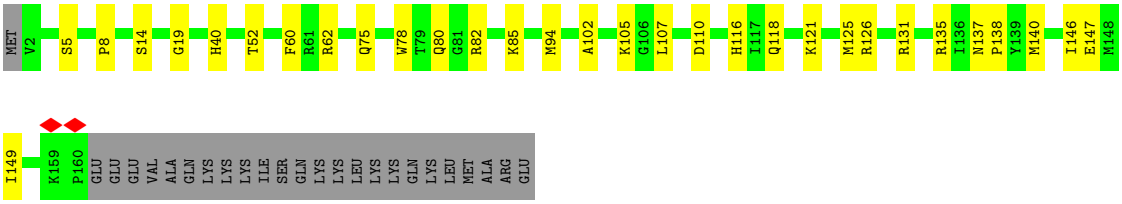
• Molecule 18: 60S ribosomal protein L13a

Chain BO:



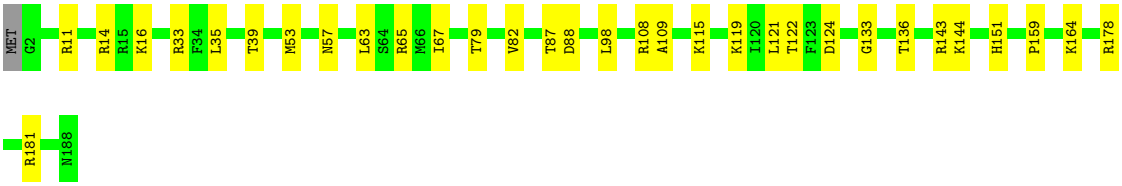
• Molecule 19: uL22

Chain BP:



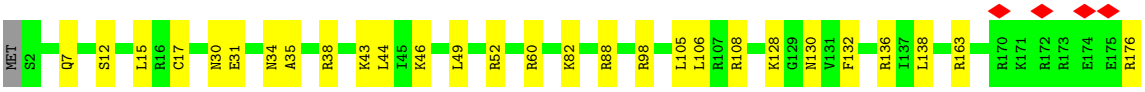
• Molecule 20: eL18

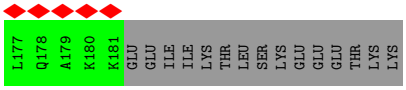
Chain BQ:



• Molecule 21: 60S ribosomal protein L19

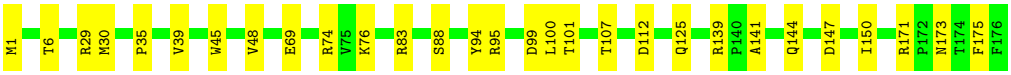
Chain BR:





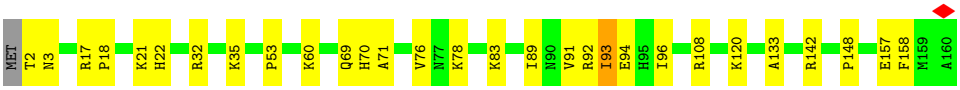
• Molecule 22: 60S ribosomal protein L18a

Chain BS:



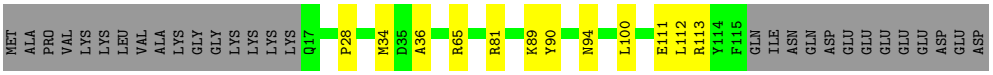
• Molecule 23: 60S ribosomal protein L21

Chain BT:



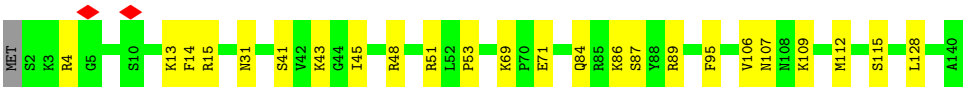
• Molecule 24: 60S ribosomal protein L22

Chain BU:



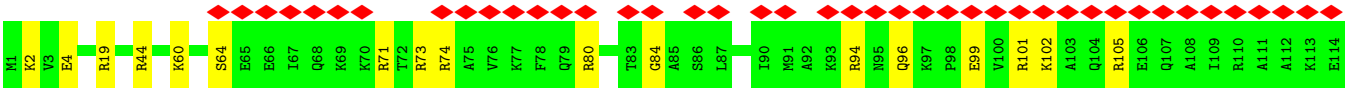
• Molecule 25: Ribosomal protein L23

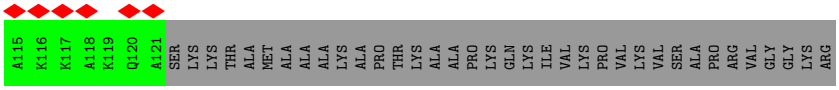
Chain BV:



• Molecule 26: Ribosomal protein L24

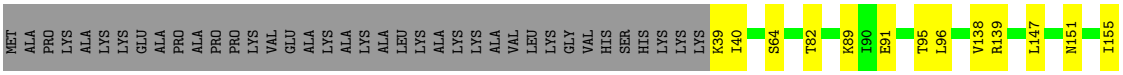
Chain BW:





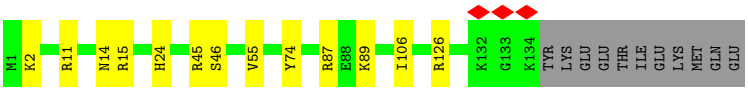
• Molecule 27: Ribosomal_L23eN domain-containing protein

Chain BX:



• Molecule 28: Ribosomal protein L26

Chain BY:



• Molecule 29: 60S ribosomal protein L27

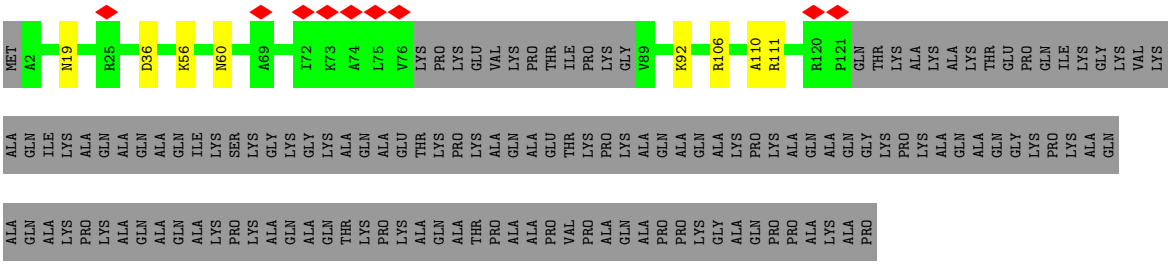
Chain BZ:

• Molecule 30: 60S ribosomal protein L27a

Chain Ba:

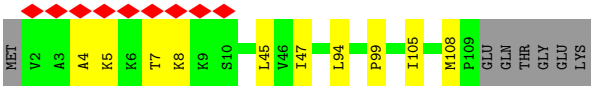
• Molecule 31: 60S ribosomal protein L29

Chain Bb:



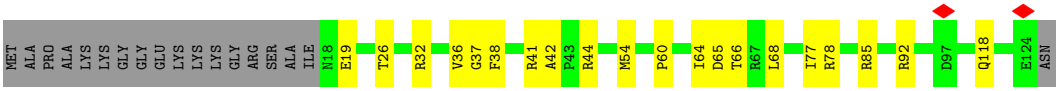
• Molecule 32: eL30

Chain Bc:



• Molecule 33: Ribosomal protein L31

Chain Bd:

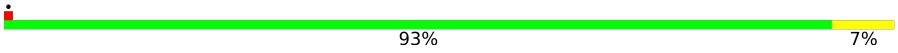


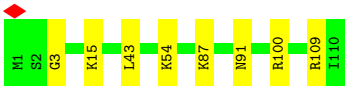
• Molecule 34: eL32

Chain Be:

• Molecule 35: 60S ribosomal protein L35a

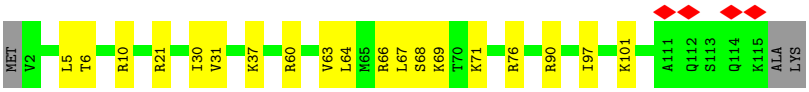
Chain Bf:





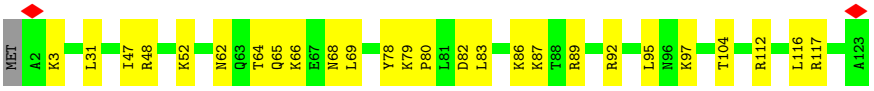
• Molecule 36: 60S ribosomal protein L34

Chain Bg:



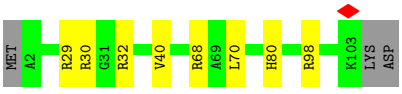
• Molecule 37: 60S ribosomal protein L35

Chain Bh:



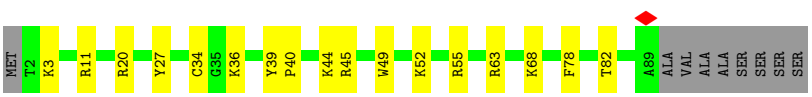
• Molecule 38: 60S ribosomal protein L36

Chain Bi:



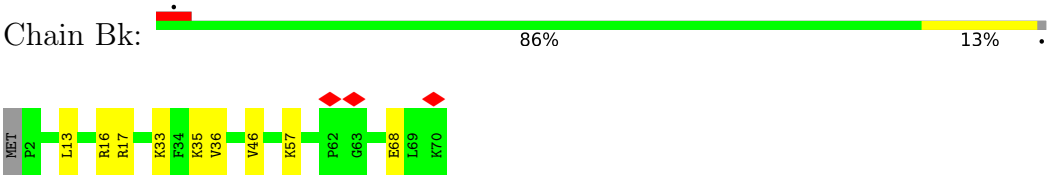
• Molecule 39: Ribosomal protein L37

Chain Bj:



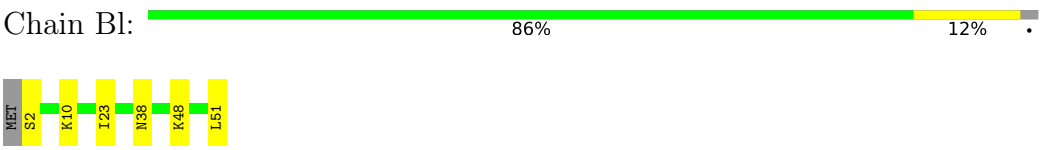
• Molecule 40: eL38

Chain Bk:



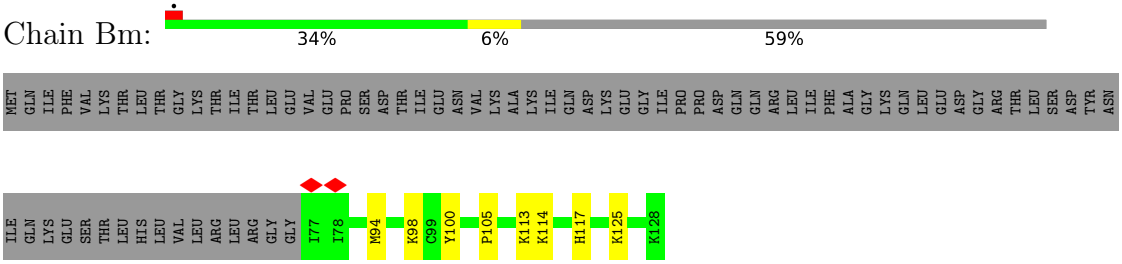
• Molecule 41: eL39

Chain Bl:



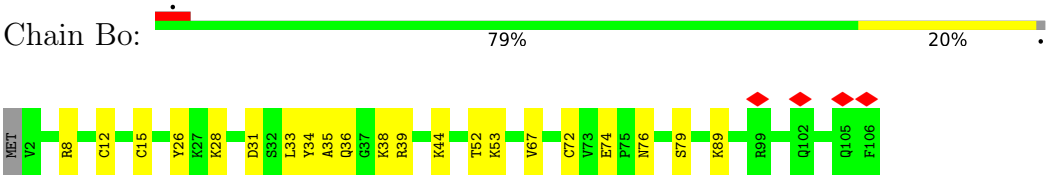
• Molecule 42: Ubiquitin

Chain Bm:



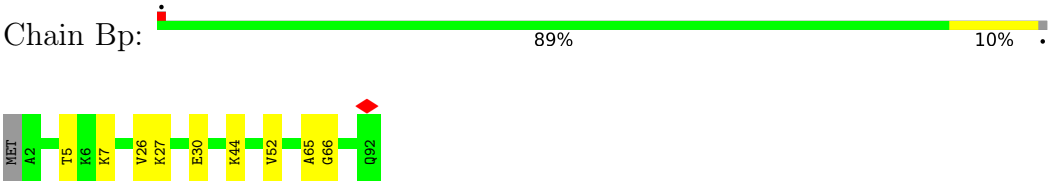
• Molecule 43: eL42

Chain Bo:



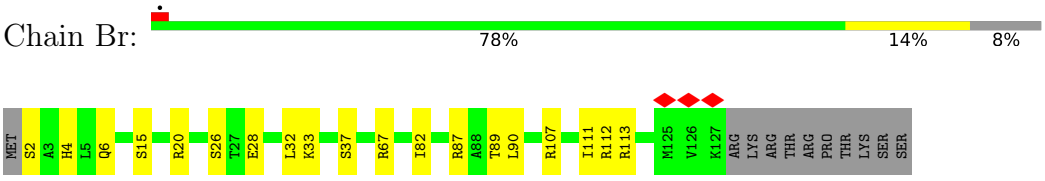
• Molecule 44: eL43

Chain Bp:



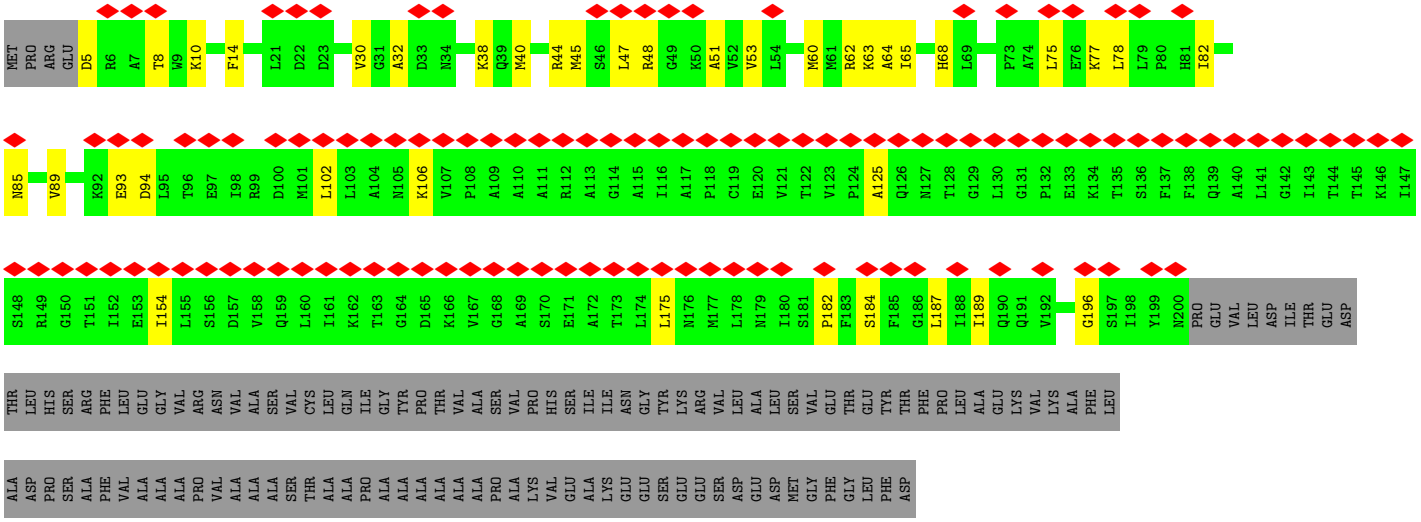
• Molecule 45: 60S ribosomal protein L28

Chain Br:



• Molecule 46: 60S acidic ribosomal protein P0

Chain Bs:

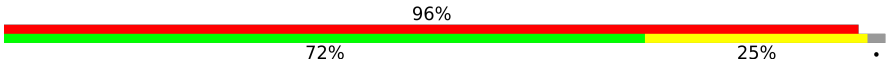


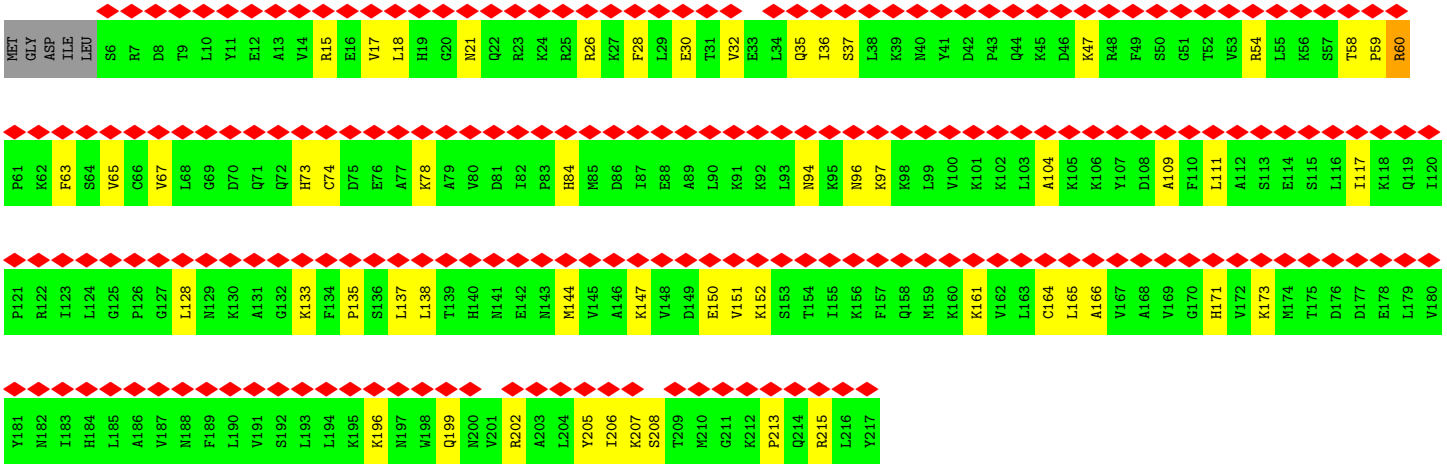
• Molecule 47: Ribosomal protein L12

Chain Bt:

• Molecule 48: Ribosomal protein uL1

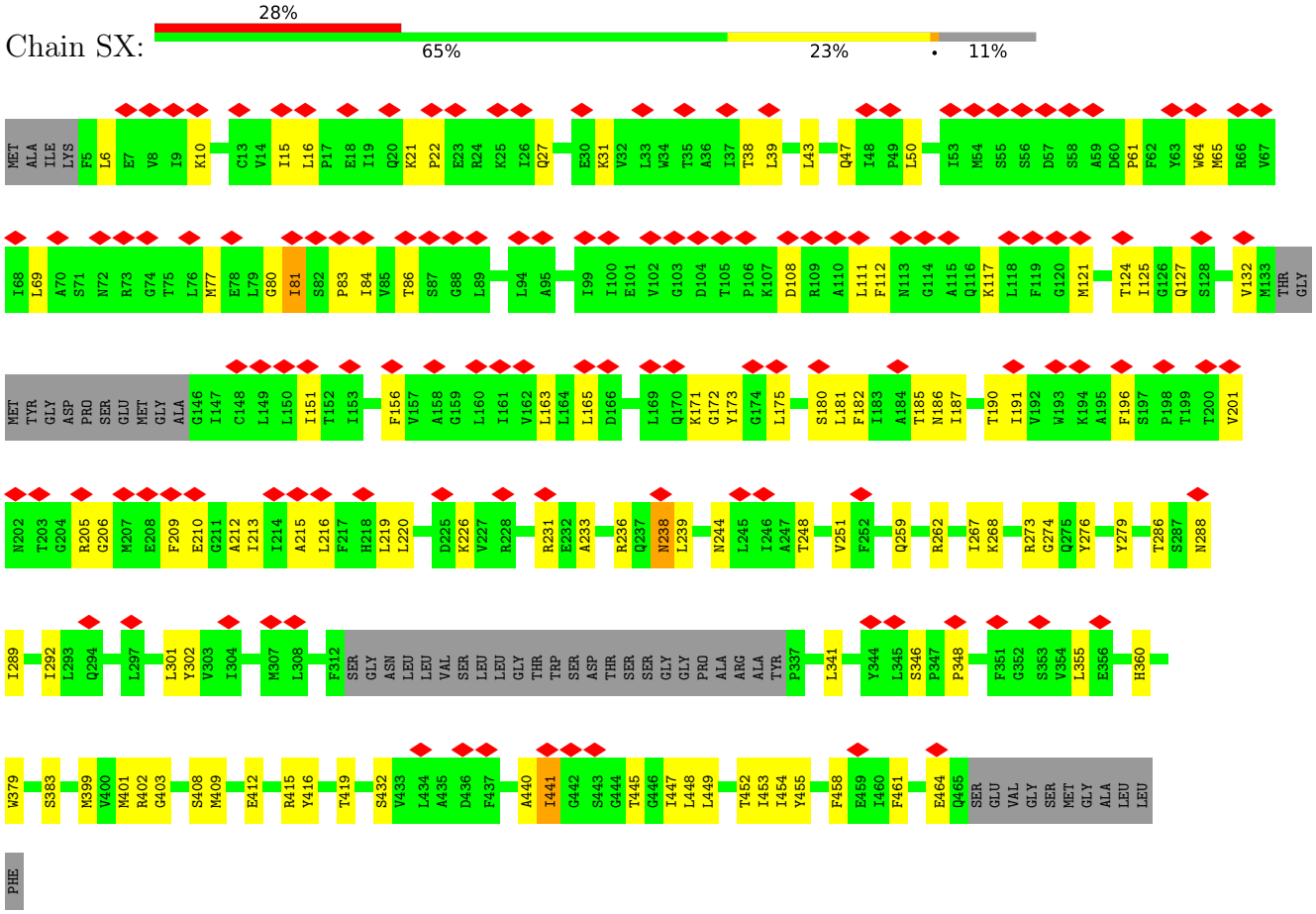
Chain Bv:





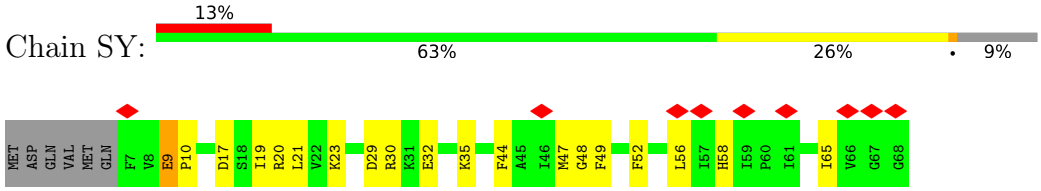
• Molecule 49: Protein transport protein Sec61 subunit alpha isoform 1

Chain SX:



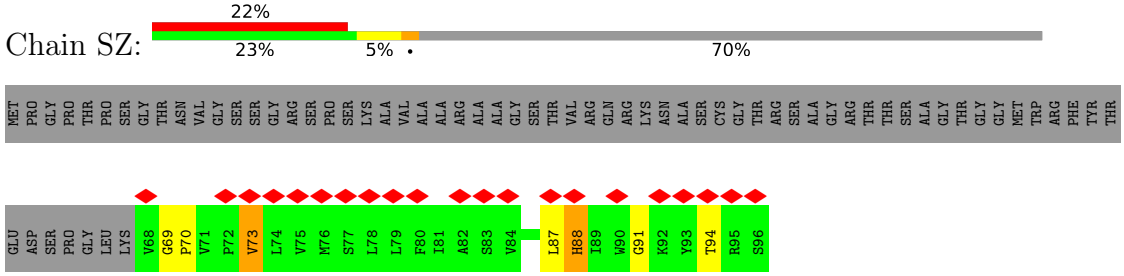
• Molecule 50: Protein transport protein Sec61 subunit gamma

Chain SY:



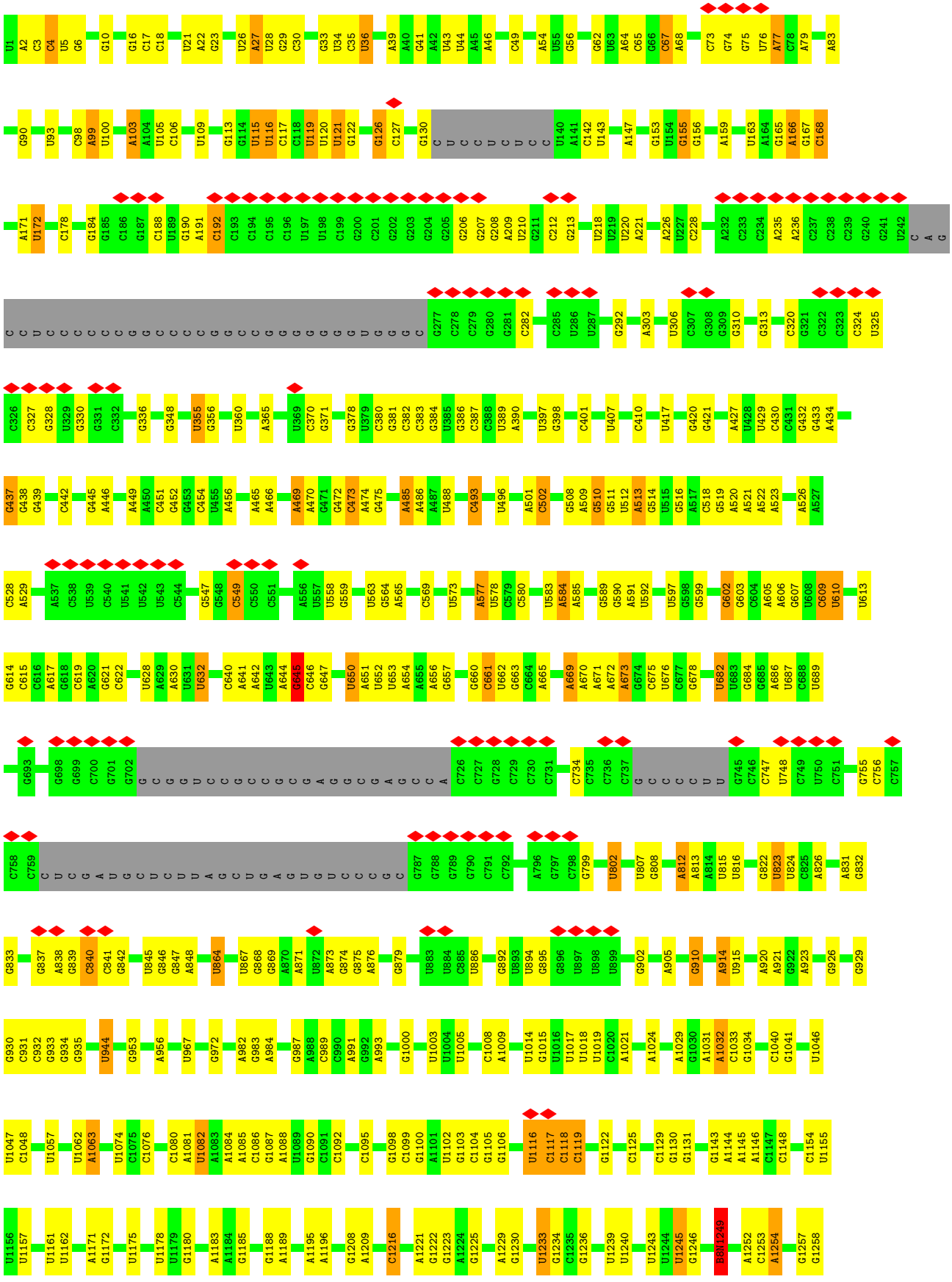
• Molecule 51: Protein transport protein Sec61 subunit beta

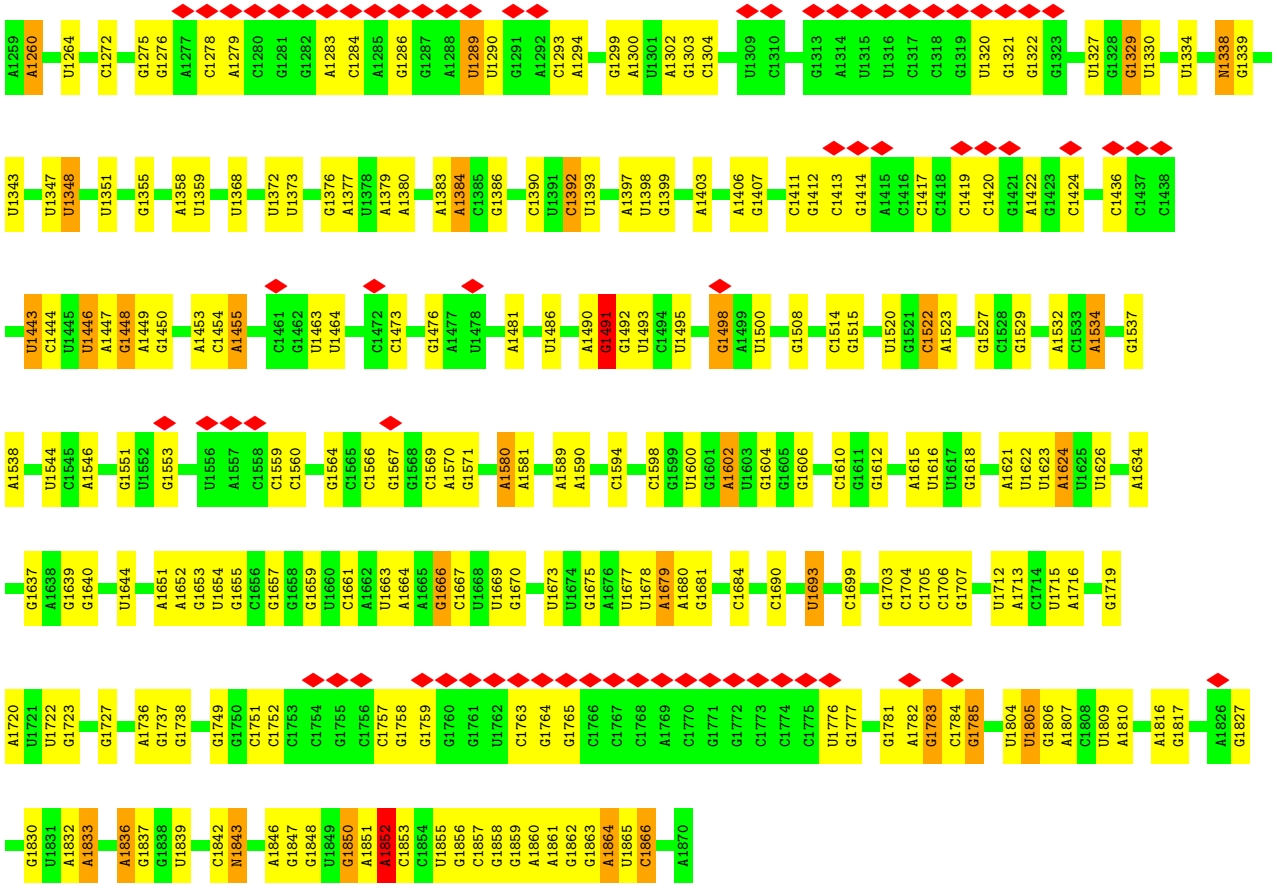
Chain SZ:



• Molecule 52: 18S rRNA

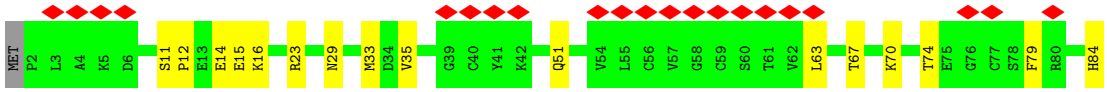
Chain A2:





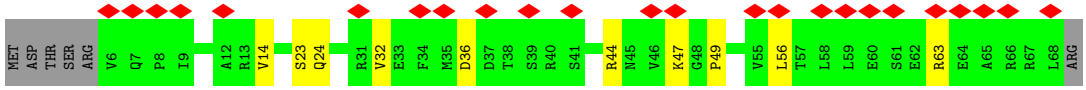
• Molecule 53: 40S ribosomal protein S27

Chain AA:



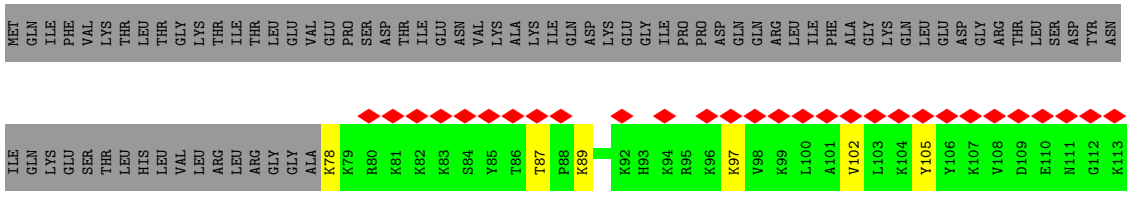
• Molecule 54: Ribosomal protein S28

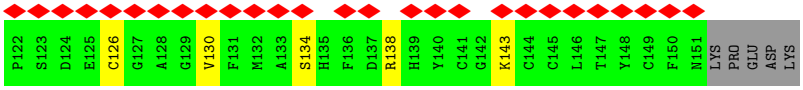
Chain AB:



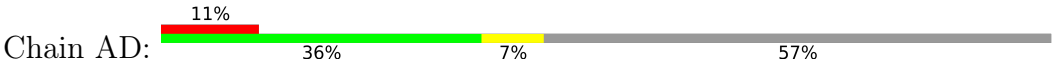
• Molecule 55: Ribosomal protein S27a

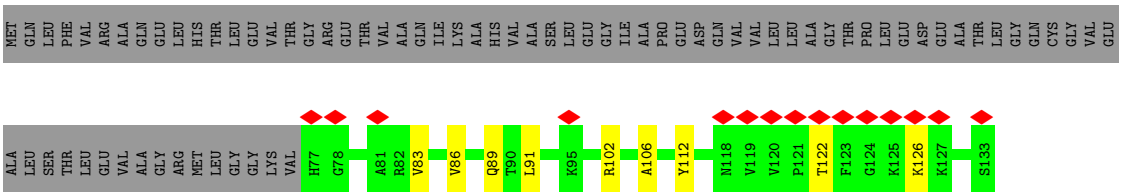
Chain AC:



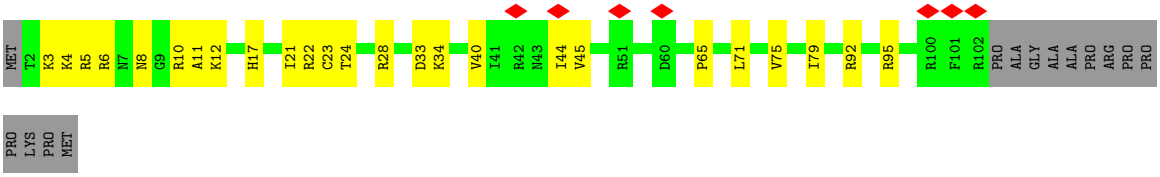


• Molecule 56: 40S ribosomal protein S30

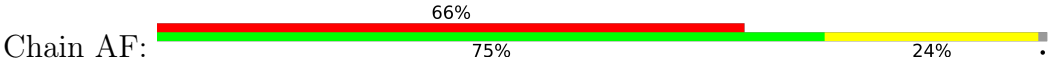


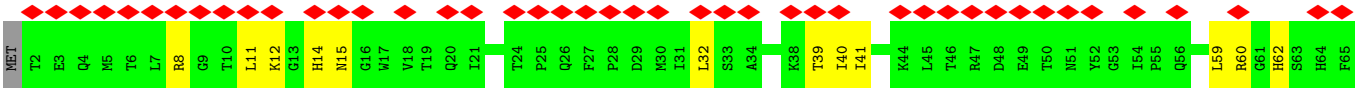


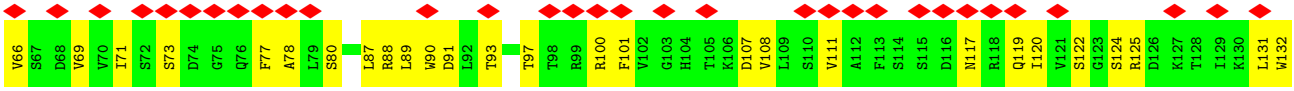
• Molecule 57: eS26

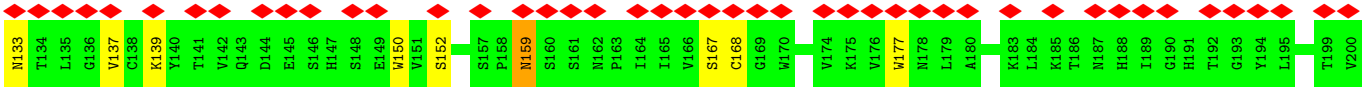


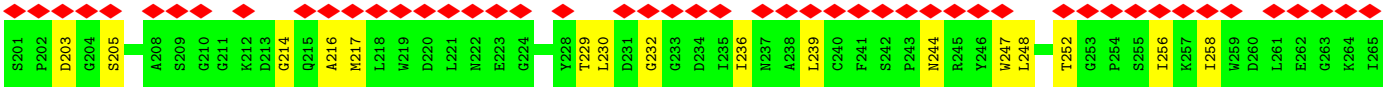
• Molecule 58: RACK1

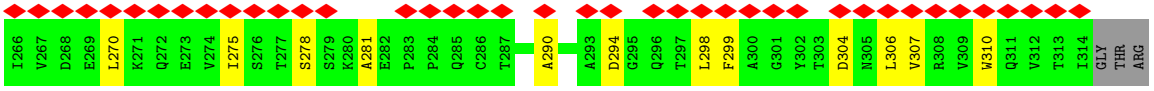




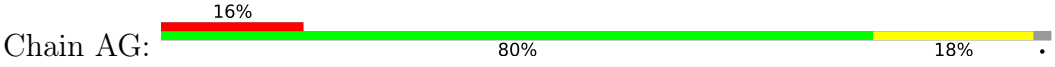


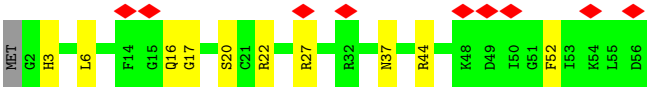




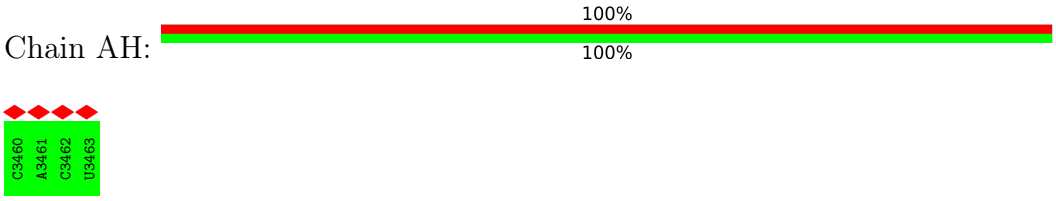


• Molecule 59: uS14

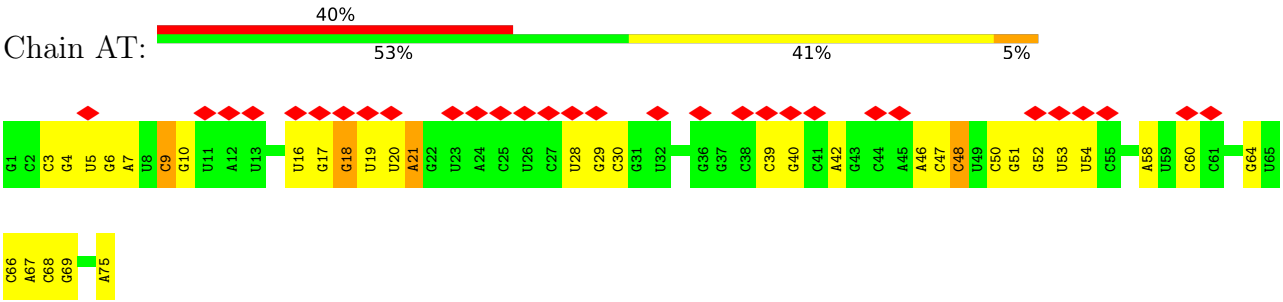




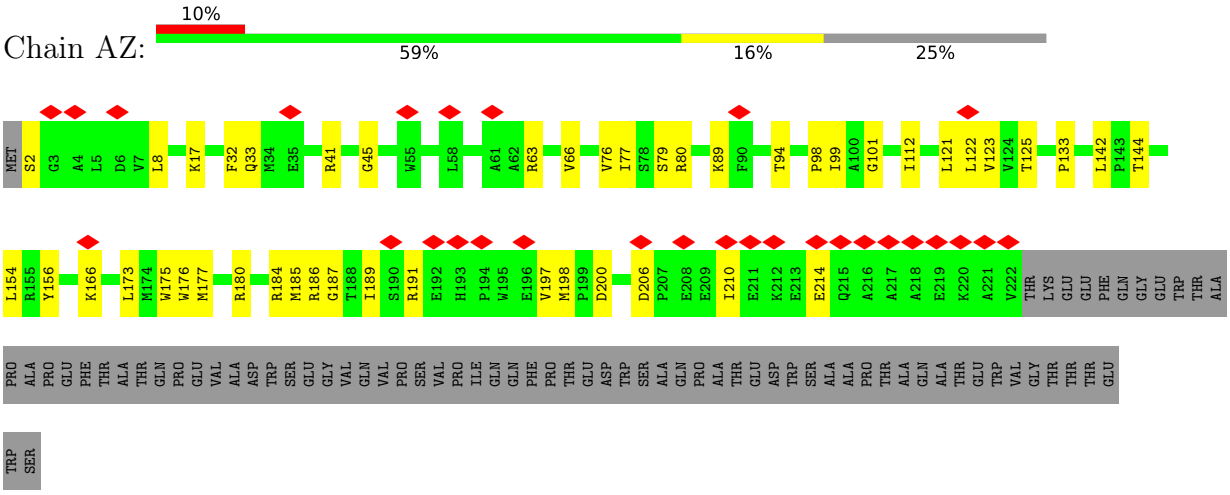
• Molecule 60: mRNA



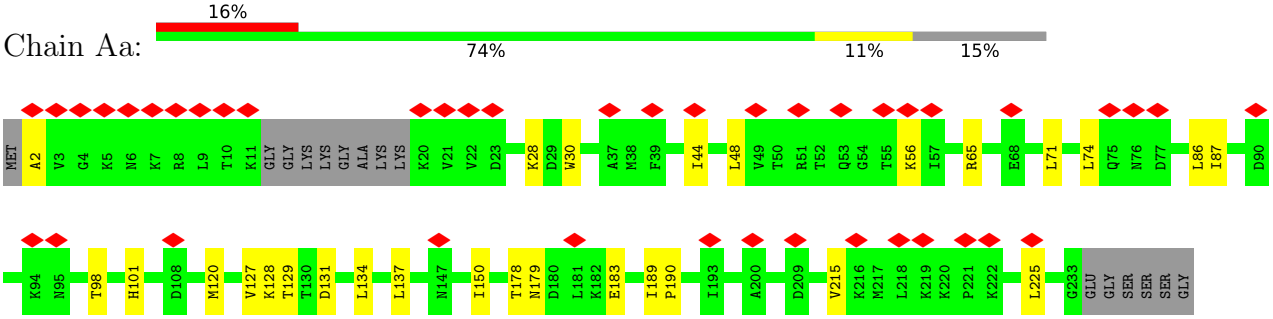
• Molecule 61: P-site tRNA



• Molecule 62: 40S ribosomal protein SA

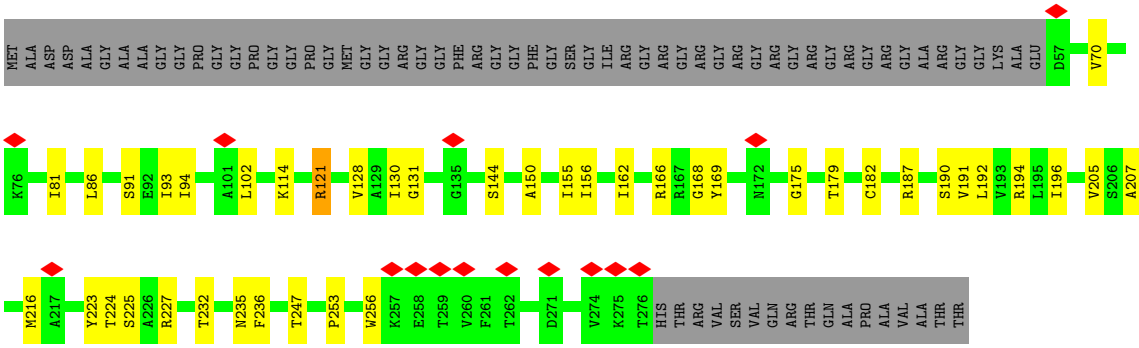


• Molecule 63: 40S ribosomal protein S3a



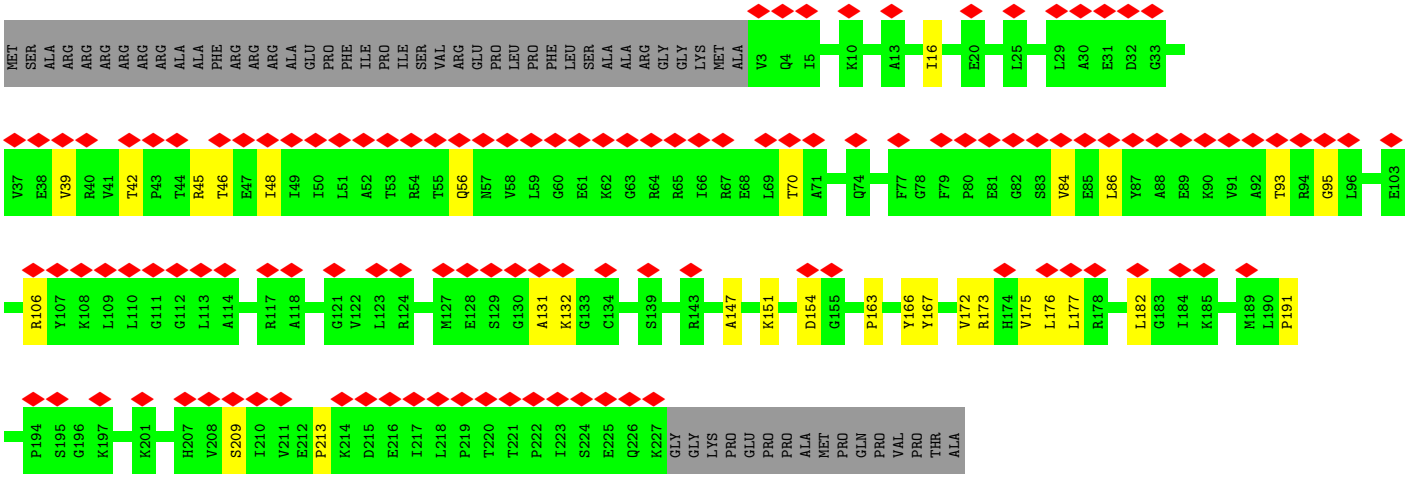
• Molecule 64: Ribosomal_S5_C domain-containing protein,40S ribosomal protein S2

Chain Ab:



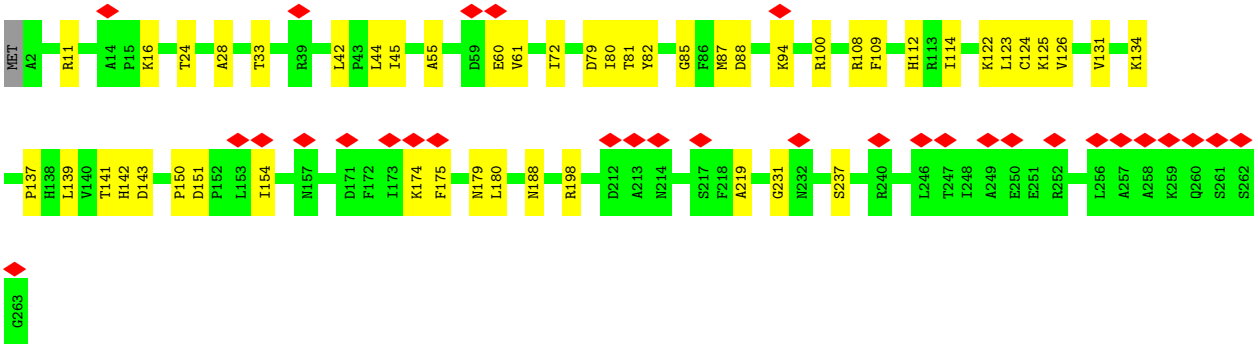
• Molecule 65: 40S ribosomal protein S3

Chain Ac:



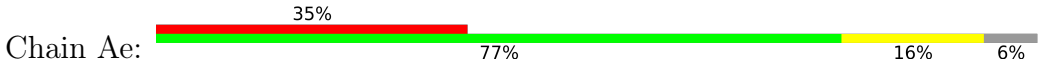
• Molecule 66: 40S ribosomal protein S4

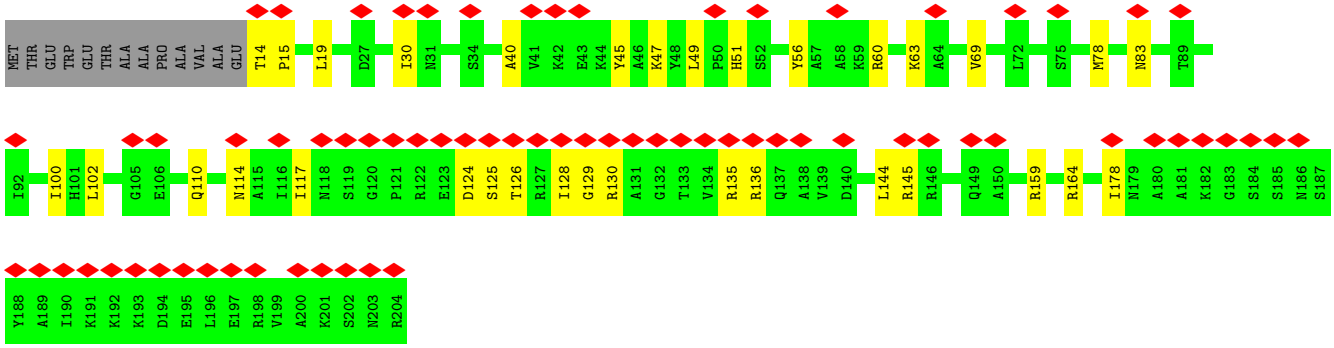
Chain Ad:



• Molecule 67: Ribosomal protein S5

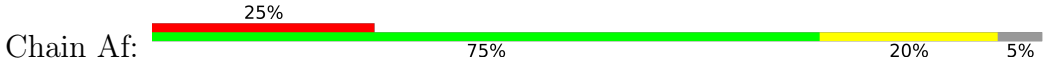
Chain Ae:

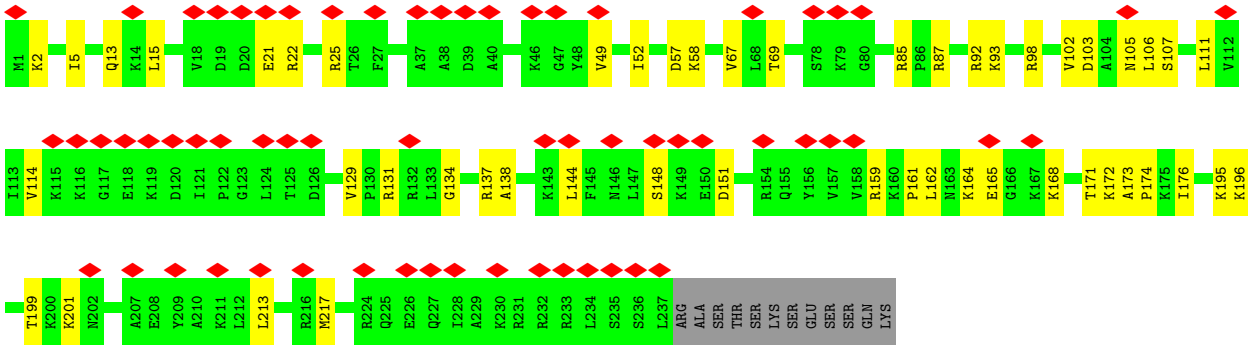




• Molecule 68: 40S ribosomal protein S6

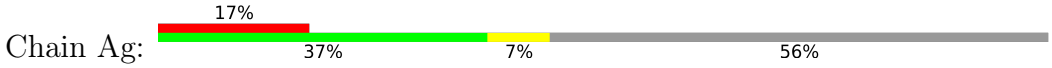
Chain Af:

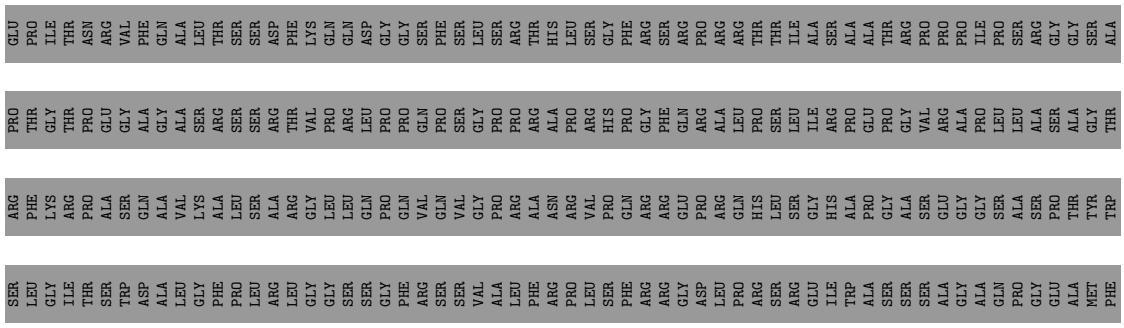


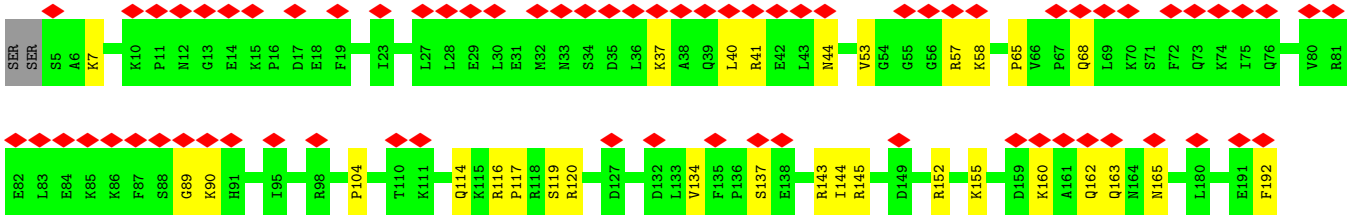


• Molecule 69: 40S ribosomal protein S7

Chain Ag:

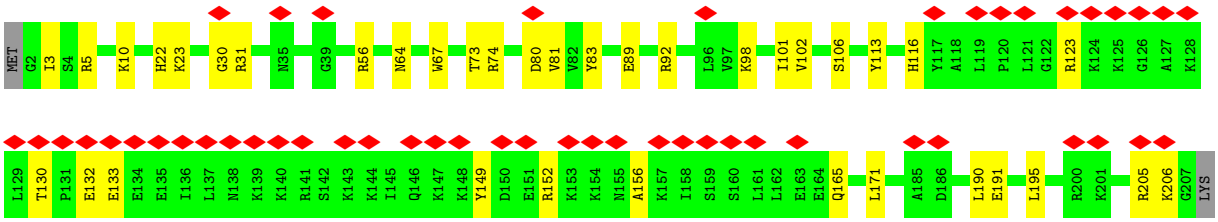






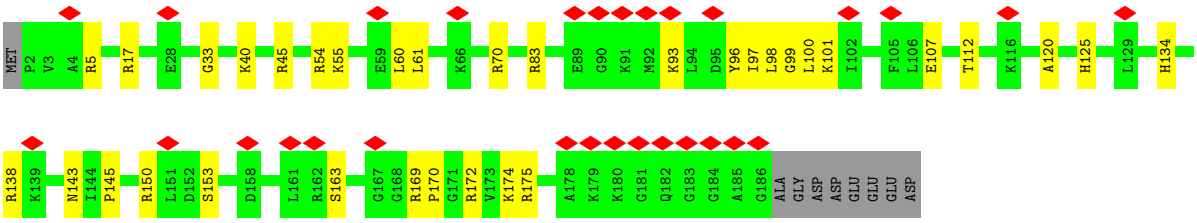
• Molecule 70: 40S ribosomal protein S8

Chain Ah:



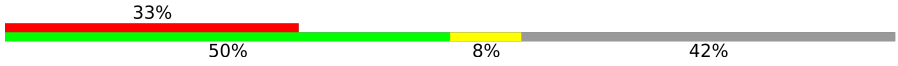
• Molecule 71: Ribosomal protein S9 (Predicted)

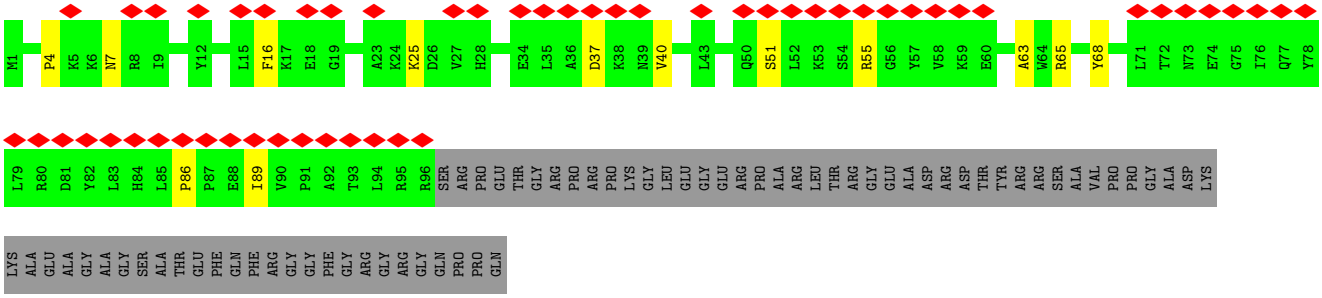
Chain Ai:



• Molecule 72: Ribosomal protein eS10

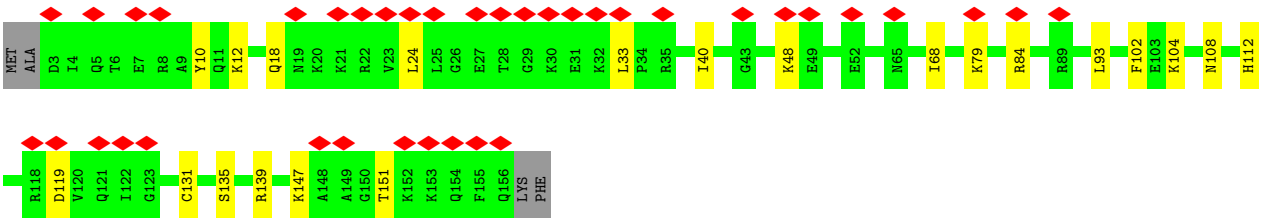
Chain Aj:





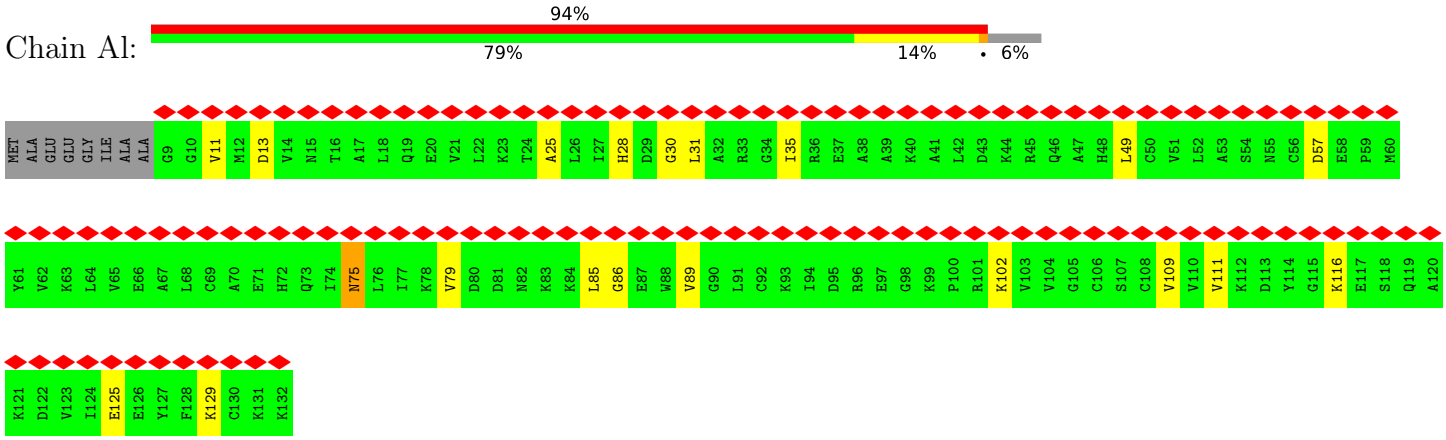
• Molecule 73: 40S ribosomal protein S11

Chain Ak:



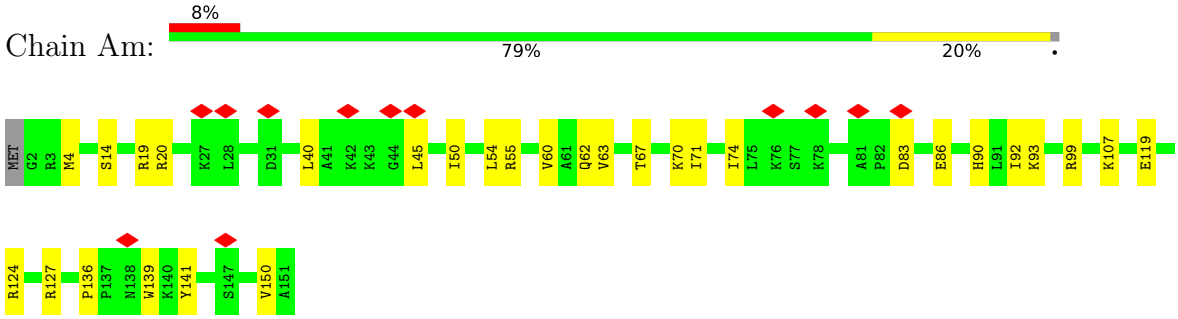
• Molecule 74: 40S ribosomal protein S12

Chain Al:



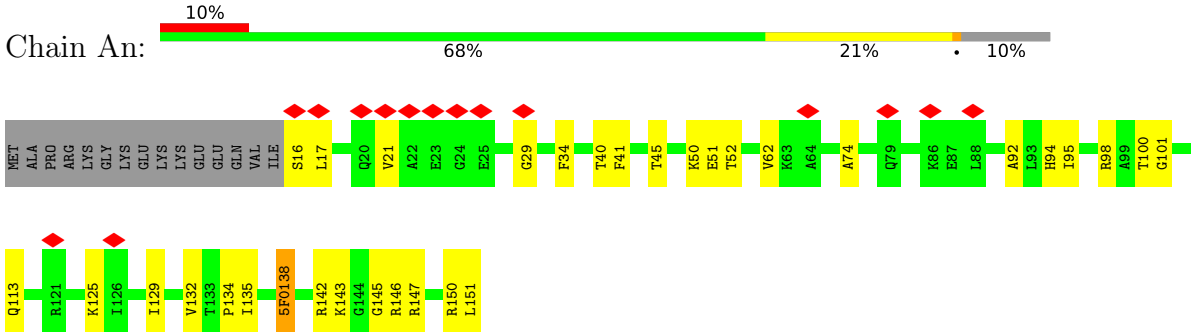
• Molecule 75: uS15

Chain Am:



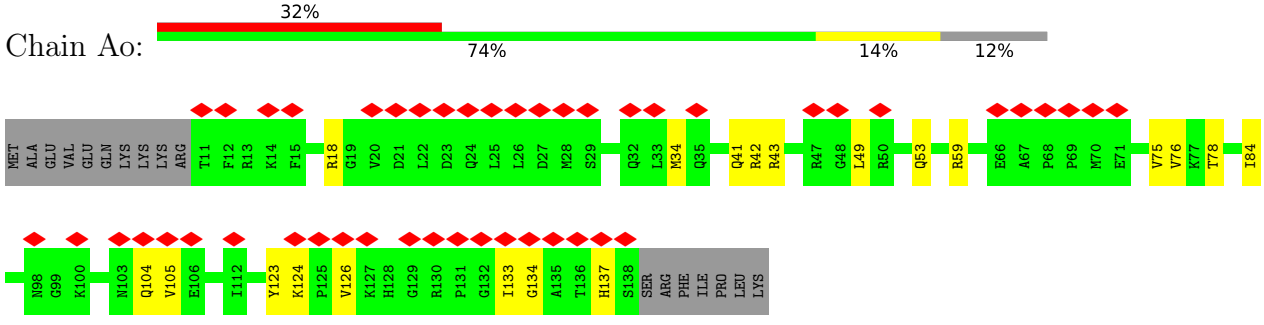
• Molecule 76: 40S ribosomal protein S14

Chain An:

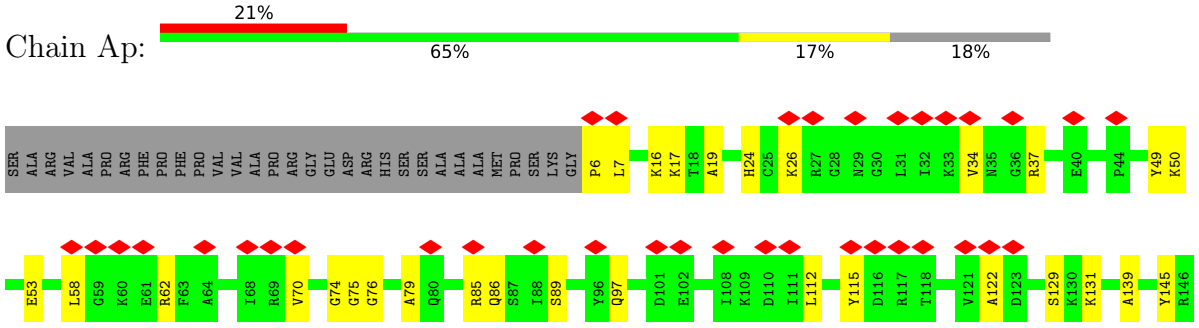


• Molecule 77: 40S ribosomal protein uS19

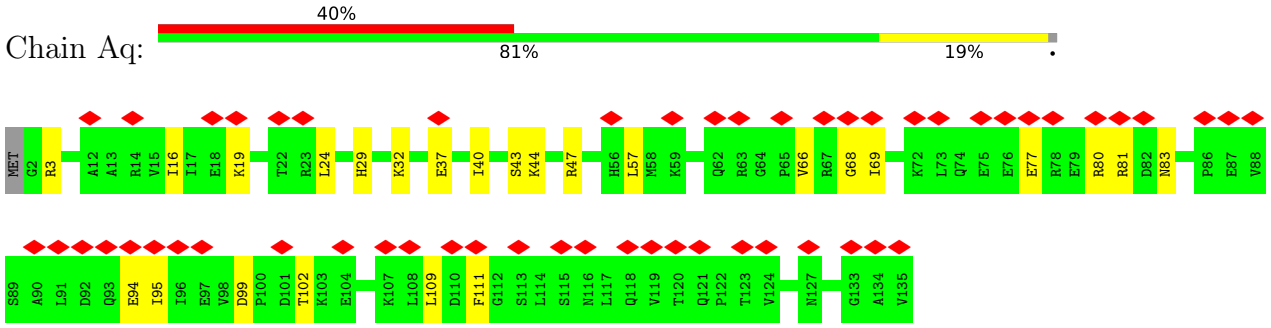
Chain Ao:



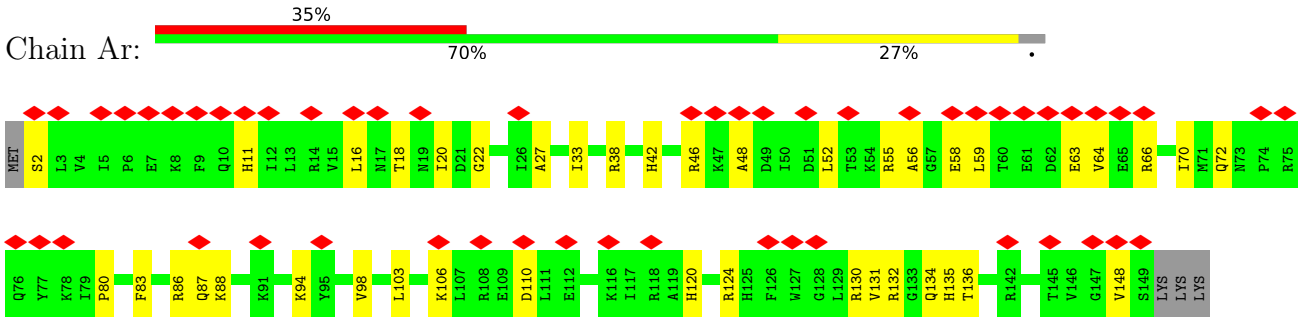
• Molecule 78: uS9



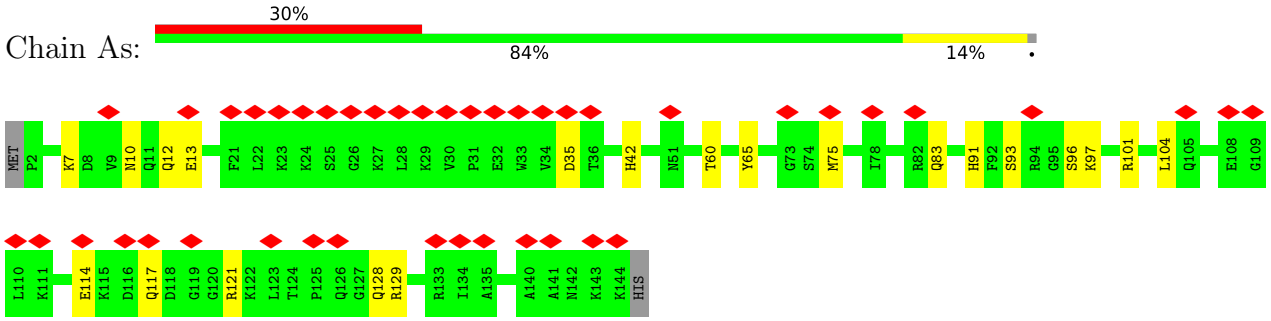
• Molecule 79: 40S ribosomal protein eS17



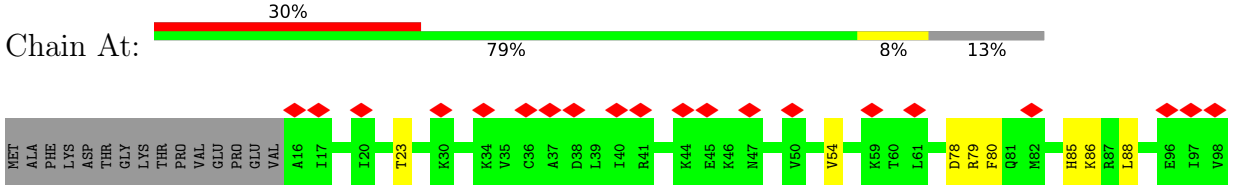
• Molecule 80: 40S ribosomal protein S18

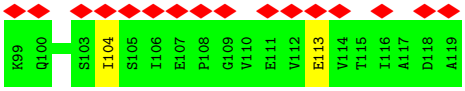


• Molecule 81: 40S ribosomal protein S19



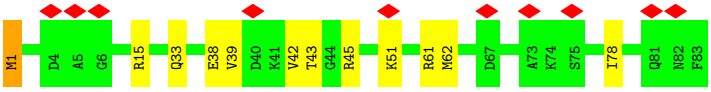
• Molecule 82: 40S ribosomal protein uS10





• Molecule 83: 40S ribosomal protein S21

Chain Au:

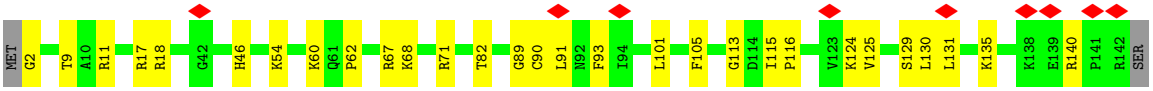


• Molecule 84: Ribosomal protein S15a

Chain Av:

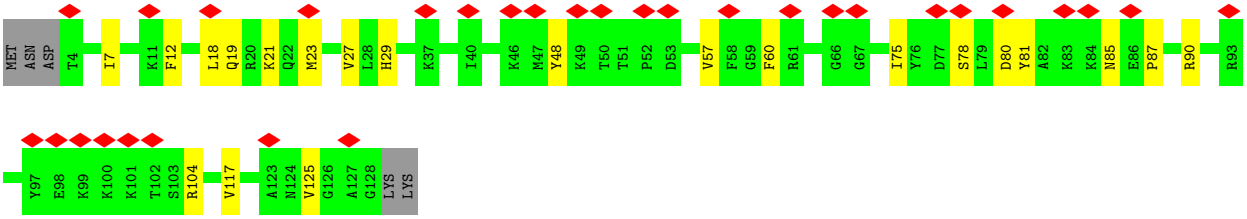
• Molecule 85: 40S ribosomal protein S23

Chain Aw:



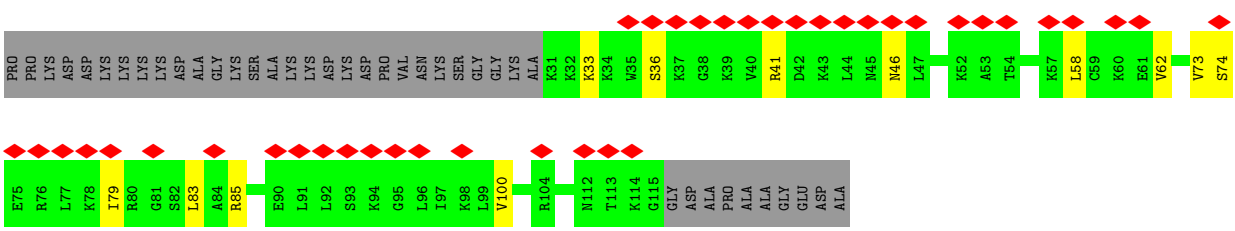
• Molecule 86: 40S ribosomal protein S24

Chain Ax:



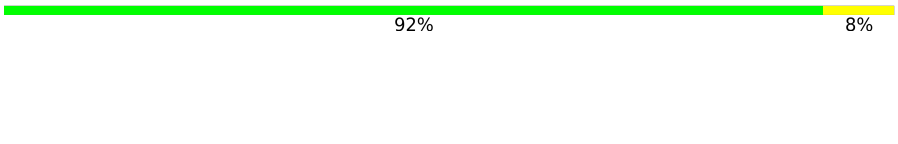
• Molecule 87: 40S ribosomal protein S25

Chain Ay:



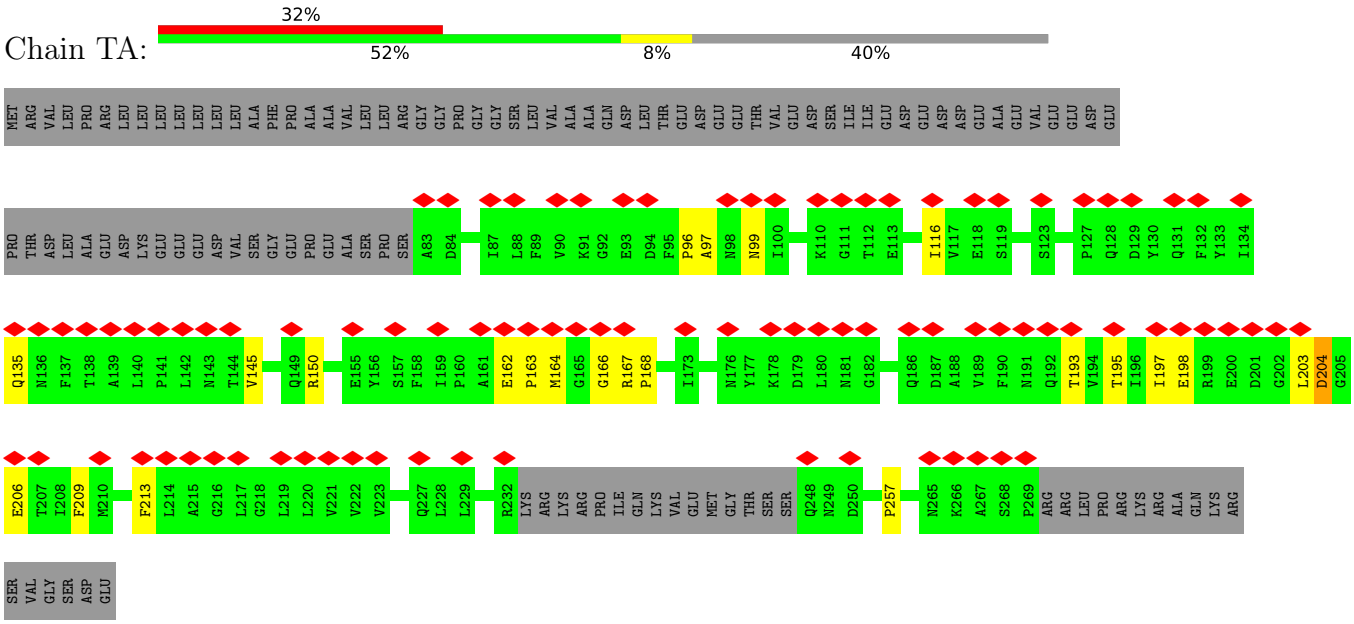
• Molecule 88: 60S ribosomal protein L41

Chain Az:



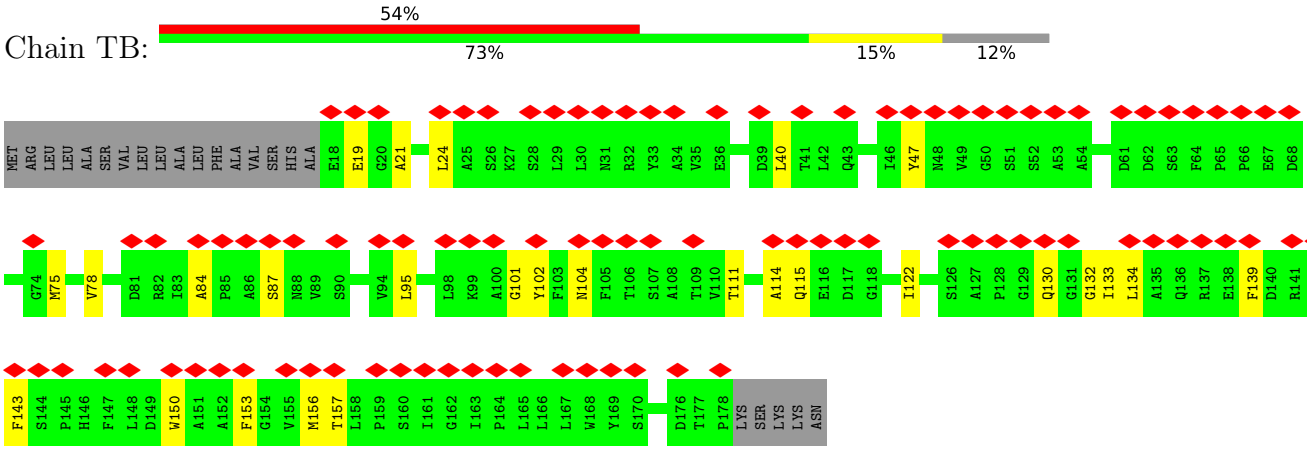
• Molecule 89: Translocon-associated protein subunit alpha

Chain TA:



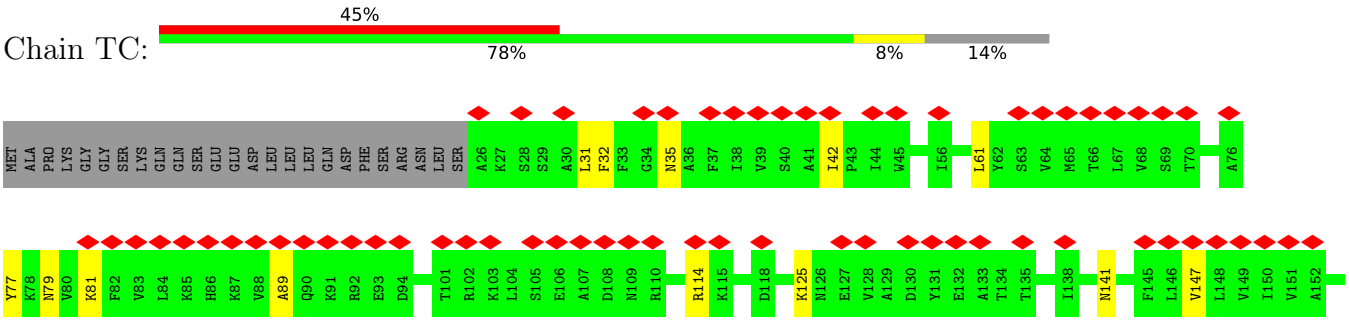
• Molecule 90: Translocon-associated protein subunit beta

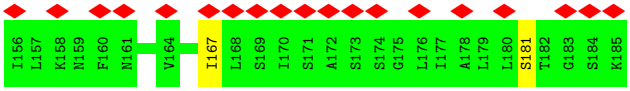
Chain TB:



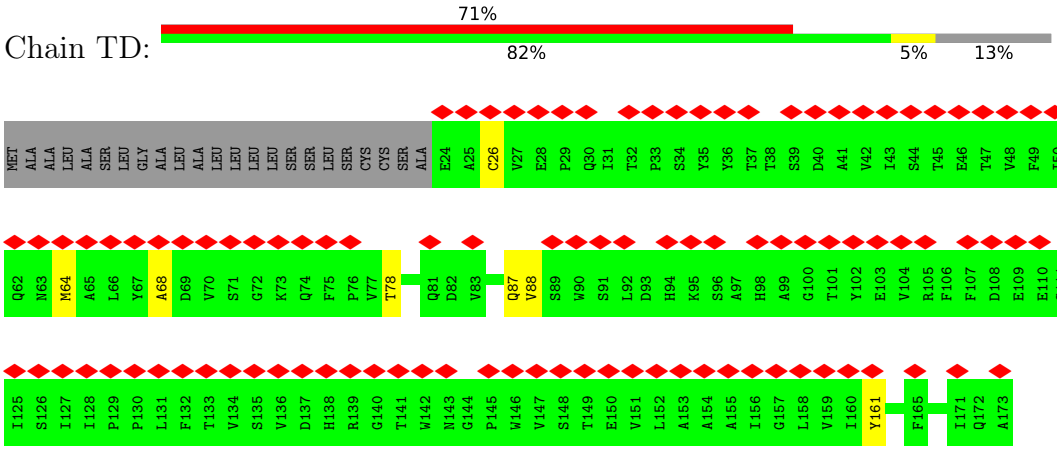
• Molecule 91: Signal sequence receptor subunit 3

Chain TC:





• Molecule 92: Translocon-associated protein subunit delta



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 5F0, AAC, OMC, V5N, UR3, MG, B8N, 6MZ, SPD, GTP, SPM, AYA, MA6, SAC, NMM, M3L, A2M, 5MU, 4AC, AME, PSU, UY1, HIC, 1MA, 5MC, HY3, MLZ, G7M, OMU, ZN

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	B5	0.10	2/87403 (0.0%)	0.11	0/136359
2	B7	0.05	0/2835	0.08	0/4418
3	B8	0.06	0/3635	0.13	0/5661
4	BA	0.08	0/1965	0.22	0/2633
5	BB	0.07	0/3261	0.19	0/4364
6	BC	0.07	0/2932	0.19	0/3939
7	BD	0.06	0/2437	0.19	0/3264
8	BE	0.08	0/1998	0.20	0/2673
9	BF	0.07	0/1922	0.19	0/2563
10	BG	0.07	0/1908	0.18	0/2566
11	BH	0.06	0/1535	0.19	0/2063
12	BI	0.08	0/1756	0.21	0/2346
13	BJ	0.06	0/1385	0.19	0/1852
15	BL	0.07	0/1732	0.20	0/2316
16	BM	0.06	0/1158	0.18	0/1547
17	BN	0.07	0/1746	0.19	0/2338
18	BO	0.06	0/1662	0.18	0/2222
19	BP	0.07	0/1317	0.21	0/1768
20	BQ	0.07	0/1539	0.20	0/2054
21	BR	0.05	0/1524	0.16	0/2013
22	BS	0.08	0/1497	0.19	0/2008
23	BT	0.07	0/1326	0.20	0/1770
24	BU	0.06	0/820	0.19	0/1100
25	BV	0.08	0/1048	0.20	0/1402
26	BW	0.06	0/1006	0.19	0/1334
27	BX	0.07	0/984	0.19	0/1323
28	BY	0.06	0/1132	0.21	0/1504
29	BZ	0.07	0/1130	0.17	0/1507
30	Ba	0.07	0/1179	0.21	0/1572
31	Bb	0.08	0/884	0.20	0/1169
32	Bc	0.06	0/847	0.17	0/1134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Bd	0.08	0/903	0.20	0/1216
34	Be	0.06	0/1088	0.20	0/1451
35	Bf	0.08	0/903	0.19	0/1208
36	Bg	0.06	0/916	0.19	0/1220
37	Bh	0.05	0/1021	0.16	0/1348
38	Bi	0.07	0/841	0.21	0/1112
39	Bj	0.07	0/736	0.21	0/973
40	Bk	0.06	0/575	0.17	0/761
41	Bl	0.06	0/459	0.18	0/608
42	Bm	0.06	0/426	0.20	0/564
43	Bo	0.08	0/866	0.21	0/1141
44	Bp	0.06	0/718	0.20	0/953
45	Br	0.07	0/1020	0.20	0/1366
46	Bs	0.08	0/1530	0.20	0/2064
47	Bt	0.07	0/1193	0.21	0/1609
48	Bv	0.08	0/1735	0.25	0/2328
49	SX	0.09	0/3388	0.24	0/4590
50	SY	0.09	0/504	0.24	0/673
51	SZ	0.10	0/236	0.23	0/321
52	A2	0.13	3/40342 (0.0%)	0.11	0/62877
53	AA	0.06	0/665	0.20	0/891
54	AB	0.05	0/497	0.18	0/666
55	AC	0.07	0/622	0.22	0/822
56	AD	0.06	0/462	0.20	0/607
57	AE	0.07	0/828	0.20	0/1109
58	AF	0.07	0/2493	0.21	0/3394
59	AG	0.06	0/470	0.19	0/623
60	AH	0.04	0/72	0.10	0/110
61	AT	0.04	0/1714	0.09	0/2668
62	AZ	0.07	0/1771	0.19	0/2406
63	Aa	0.07	0/1841	0.21	0/2459
64	Ab	0.07	0/1742	0.20	0/2354
65	Ac	0.07	0/1779	0.19	0/2395
66	Ad	0.07	0/2118	0.20	0/2849
67	Ae	0.08	0/1531	0.25	0/2059
68	Af	0.07	0/1946	0.19	0/2590
69	Ag	0.06	0/1552	0.18	0/2079
70	Ah	0.06	0/1715	0.19	0/2287
71	Ai	0.06	0/1550	0.18	0/2069
72	Aj	0.07	0/834	0.20	0/1125
73	Ak	0.07	0/1284	0.20	0/1717
74	Al	0.07	0/968	0.22	0/1296
75	Am	0.07	0/1232	0.19	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	An	0.07	0/1020	0.19	0/1366
77	Ao	0.07	0/1069	0.19	0/1429
78	Ap	0.08	0/1142	0.24	0/1528
79	Aq	0.06	0/1094	0.18	0/1469
80	Ar	0.07	0/1226	0.19	0/1643
81	As	0.06	0/1119	0.18	0/1498
82	At	0.06	0/831	0.19	0/1115
83	Au	0.05	0/636	0.17	0/852
84	Av	0.07	0/1051	0.19	0/1406
85	Aw	0.06	0/1107	0.20	0/1475
86	Ax	0.06	0/1032	0.18	0/1371
87	Ay	0.07	0/691	0.21	0/922
88	Az	0.05	0/240	0.14	0/305
89	TA	0.09	0/1404	0.22	0/1910
90	TB	0.07	0/1287	0.20	0/1753
91	TC	0.06	0/1324	0.16	0/1791
92	TD	0.06	0/1214	0.21	0/1656
All	All	0.09	5/244076 (0.0%)	0.15	0/356885

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

Mol	Chain	#Chirality outliers	#Planarity outliers
43	Bo	0	1
76	An	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1327	OMU	O3'-P	5.08	1.61	1.56
1	B5	4269	A2M	O3'-P	5.08	1.61	1.56
52	A2	159	A2M	O3'-P	5.07	1.61	1.56
52	A2	1679	A2M	O3'-P	5.04	1.61	1.56
1	B5	3562	A2M	O3'-P	5.02	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	An	138	5F0	Mainchain,Peptide
43	Bo	53	MLZ	Mainchain

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	B5	80772	0	40880	726	0
2	B7	2538	0	1284	12	0
3	B8	3319	0	1684	39	0
4	BA	1940	0	2029	43	0
5	BB	3206	0	3352	50	0
6	BC	2886	0	3057	30	0
7	BD	2391	0	2424	30	0
8	BE	1960	0	2153	29	0
9	BF	1886	0	2008	28	0
10	BG	1877	0	2023	15	0
11	BH	1516	0	1597	21	0
12	BI	1717	0	1764	25	0
13	BJ	1362	0	1399	13	0
14	BK	145	0	33	0	0
15	BL	1701	0	1820	24	0
16	BM	1137	0	1211	19	0
17	BN	1701	0	1749	26	0
18	BO	1630	0	1778	13	0
19	BP	1289	0	1329	20	0
20	BQ	1515	0	1634	21	0
21	BR	1508	0	1664	20	0
22	BS	1457	0	1492	18	0
23	BT	1298	0	1366	26	0
24	BU	806	0	827	7	0
25	BV	1034	0	1097	21	0
26	BW	991	0	1048	16	0
27	BX	967	0	1040	10	0
28	BY	1115	0	1205	12	0
29	BZ	1107	0	1182	20	0
30	Ba	1163	0	1202	22	0
31	Bb	881	0	957	7	0
32	Bc	836	0	888	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Bd	888	0	930	11	0
34	Be	1070	0	1165	15	0
35	Bf	884	0	924	7	0
36	Bg	906	0	998	14	0
37	Bh	1013	0	1147	24	0
38	Bi	830	0	916	6	0
39	Bj	721	0	755	17	0
40	Bk	569	0	637	6	0
41	Bl	447	0	479	5	0
42	Bm	432	0	470	7	0
43	Bo	863	0	929	13	0
44	Bp	708	0	756	7	0
45	Br	1014	0	1083	14	0
46	Bs	1507	0	1564	25	0
47	Bt	1178	0	1235	28	0
48	Bv	1707	0	1815	34	0
49	SX	3317	0	3447	76	0
50	SY	494	0	527	12	0
51	SZ	229	0	245	6	0
52	A2	37833	0	19167	377	0
53	AA	651	0	672	10	0
54	AB	495	0	523	7	0
55	AC	610	0	634	12	0
56	AD	457	0	502	11	0
57	AE	814	0	863	19	0
58	AF	2436	0	2393	49	0
59	AG	459	0	448	9	0
60	AH	66	0	33	0	0
61	AT	1597	0	811	23	0
62	AZ	1743	0	1748	28	0
63	Aa	1815	0	1908	21	0
64	Ab	1706	0	1796	29	0
65	Ac	1751	0	1846	19	0
66	Ad	2076	0	2177	29	0
67	Ae	1509	0	1563	27	0
68	Af	1923	0	2089	39	0
69	Ag	1529	0	1627	20	0
70	Ah	1686	0	1772	27	0
71	Ai	1525	0	1640	23	0
72	Aj	810	0	836	8	0
73	Ak	1262	0	1335	14	0
74	Al	958	0	993	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	Am	1208	0	1294	21	0
76	An	1017	0	1035	23	0
77	Ao	1048	0	1093	14	0
78	Ap	1124	0	1193	21	0
79	Aq	1080	0	1135	17	0
80	Ar	1217	0	1279	27	0
81	As	1113	0	1145	17	0
82	At	821	0	883	7	0
83	Au	640	0	633	9	0
84	Av	1034	0	1080	18	0
85	Aw	1099	0	1162	21	0
86	Ax	1015	0	1086	14	0
87	Ay	683	0	761	11	0
88	Az	239	0	289	2	0
89	TA	1372	0	1332	17	0
90	TB	1254	0	1230	17	0
91	TC	1295	0	1340	9	0
92	TD	1185	0	1148	6	0
93	A2	80	0	152	9	0
93	B5	210	0	399	13	0
93	BN	10	0	19	0	0
94	A2	14	0	26	1	0
94	B5	28	0	52	3	0
95	A2	167	0	0	0	0
95	AH	1	0	0	0	0
95	AT	7	0	0	0	0
95	Ad	1	0	0	0	0
95	Ae	1	0	0	0	0
95	Ak	1	0	0	0	0
95	An	1	0	0	0	0
95	Ar	1	0	0	0	0
95	As	1	0	0	0	0
95	B5	510	0	0	0	0
95	B7	15	0	0	0	0
95	B8	16	0	0	0	0
95	BA	4	0	0	0	0
95	BB	3	0	0	0	0
95	BC	1	0	0	0	0
95	BH	1	0	0	0	0
95	BI	2	0	0	0	0
95	BL	1	0	0	0	0
95	BN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	BP	1	0	0	0	0
95	BQ	2	0	0	0	0
95	BR	1	0	0	0	0
95	BT	2	0	0	0	0
95	BV	1	0	0	0	0
95	Ba	1	0	0	0	0
95	Bb	1	0	0	0	0
95	Be	2	0	0	0	0
95	Bf	1	0	0	0	0
95	Bj	1	0	0	0	0
95	Bl	1	0	0	0	0
95	Bo	1	0	0	0	0
96	B7	32	0	11	0	0
97	BD	7	0	6	0	0
98	AC	1	0	0	0	0
98	AE	1	0	0	0	0
98	AG	1	0	0	0	0
98	Bg	1	0	0	0	0
98	Bj	1	0	0	0	0
98	Bm	1	0	0	0	0
98	Bo	1	0	0	0	0
98	Bp	1	0	0	0	0
All	All	233722	0	176357	2204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2204) 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)
52:A2:1092:C:HO2'	84:Av:2:VAL:N	1.66	0.94
1:B5:2277:G:H5'	49:SX:403:GLY:HA2	1.70	0.74
1:B5:4361:C:H5"	5:BB:357:ARG:HE	1.53	0.73
52:A2:929:G:H1	52:A2:1014:U:H3	1.36	0.73
52:A2:1397:A:O2'	52:A2:1399:G:N7	2.21	0.73
1:B5:4292:A:N7	4:BA:215:ASN:ND2	2.38	0.72
1:B5:3673:G:N2	1:B5:3800:C:O2	2.22	0.72
1:B5:40:G:N2	1:B5:4126:A:N7	2.38	0.71
1:B5:1415:C:H5"	20:BQ:144:LYS:HG2	1.74	0.70
52:A2:1491:OMG:HM22	52:A2:1492:G:H5'	1.74	0.70
1:B5:2205:U:H2'	1:B5:2206:A2M:H8	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:2704:OMC:HM22	1:B5:2705:G:H5'	1.73	0.69
19:BP:126:ARG:HG3	19:BP:140:MET:HE1	1.74	0.69
76:An:98:ARG:HB3	76:An:132:VAL:HG23	1.74	0.69
52:A2:165:G:H2'	52:A2:166:A2M:H8	1.74	0.69
1:B5:2143:A:N7	6:BC:143:ARG:NH1	2.41	0.69
1:B5:4366:OMU:HM22	1:B5:4367:C:H5'	1.75	0.69
52:A2:1143:G:OP1	64:Ab:187:ARG:NH1	2.26	0.69
1:B5:3540:OMC:HM22	1:B5:3541:G:H5'	1.74	0.69
1:B5:3909:U:H5'	1:B5:3910:C:H5"	1.75	0.69
52:A2:153:G:N3	68:Af:13:GLN:NE2	2.41	0.69
1:B5:3373:U:OP2	1:B5:3378:A:N6	2.25	0.68
48:Bv:74:CYS:SG	48:Bv:78:LYS:NZ	2.67	0.68
1:B5:4416:C:O2'	25:BV:15:ARG:NH2	2.27	0.68
1:B5:1341:A:HO2'	1:B5:1422:C:HO2'	1.42	0.68
1:B5:1260:OMG:HM22	1:B5:1261:U:H5'	1.76	0.68
38:Bi:98:ARG:O	48:Bv:215:ARG:NH2	2.25	0.68
52:A2:1216:C:H42	52:A2:1221:A:H61	1.42	0.68
1:B5:2400:G:H1	1:B5:2413:U:H3	1.41	0.67
49:SX:251:VAL:HB	49:SX:448:LEU:HD21	1.74	0.67
52:A2:1080:C:O2'	52:A2:1183:A:N1	2.27	0.67
13:BJ:144:LYS:O	13:BJ:148:THR:OG1	2.13	0.67
21:BR:98:ARG:NH2	21:BR:132:PHE:O	2.26	0.67
1:B5:223:G:N3	6:BC:223:ASN:ND2	2.42	0.67
49:SX:117:LYS:HG2	49:SX:163:LEU:HD22	1.76	0.67
70:Ah:101:ILE:HD12	70:Ah:190:LEU:HD11	1.77	0.67
75:Am:4:MET:SD	75:Am:124:ARG:NH2	2.67	0.67
52:A2:847:G:N7	66:Ad:108:ARG:NH2	2.43	0.67
3:B8:88:A:OP2	37:Bh:3:LYS:NZ	2.28	0.66
49:SX:27:GLN:HB2	49:SX:31:LYS:HG3	1.76	0.66
76:An:101:GLY:HA3	76:An:134:PRO:HG2	1.76	0.66
1:B5:3557:A2M:HM'2	1:B5:3558:C:H5'	1.77	0.66
8:BE:115:MET:O	45:Br:87:ARG:NH1	2.29	0.66
52:A2:1031:A:H2'	52:A2:1032:A2M:H8	1.77	0.66
52:A2:1392:OMC:HM22	52:A2:1393:U:H5'	1.76	0.66
1:B5:2688:A:H61	1:B5:3575:C:H42	1.44	0.66
66:Ad:125:LYS:H	66:Ad:142:HIS:HD2	1.43	0.66
76:An:34:PHE:HB3	76:An:41:PHE:HB2	1.77	0.66
1:B5:4364:OMG:H5"	25:BV:15:ARG:HB2	1.78	0.66
71:Ai:170:PRO:O	71:Ai:175:ARG:NH1	2.28	0.66
25:BV:69:LYS:HG2	25:BV:71:GLU:HG2	1.78	0.66
62:AZ:8:LEU:HD11	83:Au:39:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BD:83:LEU:HB3	7:BD:88:VAL:HB	1.77	0.65
9:BF:104:VAL:HG13	9:BF:135:VAL:HG12	1.77	0.65
49:SX:10:LYS:HB3	49:SX:111:LEU:HD13	1.78	0.65
58:AF:78:ALA:HB3	58:AF:90:TRP:HB2	1.78	0.65
26:BW:80:ARG:NH2	68:Af:129:VAL:O	2.29	0.65
69:Ag:144:ILE:HG21	69:Ag:152:ARG:HH21	1.62	0.65
43:Bo:34:TYR:O	43:Bo:39:ARG:NH1	2.30	0.65
89:TA:167:ARG:HG2	89:TA:168:PRO:HD2	1.79	0.65
1:B5:2250:G:N2	41:Bl:51:LEU:OXT	2.29	0.65
52:A2:1486:U:OP1	65:Ac:151:LYS:NZ	2.30	0.65
74:Al:79:VAL:HG21	74:Al:85:LEU:HD13	1.79	0.65
27:BX:147:LEU:O	27:BX:151:ASN:ND2	2.30	0.65
52:A2:920:A:O2'	93:A2:1906:SPD:N1	2.30	0.65
1:B5:4666:G:N2	1:B5:4666:G:OP2	2.29	0.65
58:AF:11:LEU:HB2	58:AF:307:VAL:HB	1.79	0.65
69:Ag:143:ARG:HB2	69:Ag:155:LYS:HB2	1.77	0.64
49:SX:210:GLU:HA	49:SX:239:LEU:HD13	1.80	0.64
33:Bd:64:ILE:HG23	33:Bd:68:LEU:HD23	1.77	0.64
52:A2:905:A:O2'	73:Ak:48:LYS:NZ	2.31	0.64
83:Au:43:THR:OG1	83:Au:45:ARG:NH1	2.30	0.64
53:AA:84:HIS:OXT	75:Am:19:ARG:NH1	2.29	0.64
1:B5:308:G:OP2	1:B5:308:G:N2	2.27	0.64
1:B5:1237:G:OP2	1:B5:1237:G:N2	2.26	0.64
93:B5:4923:SPD:H101	18:BO:91:LYS:HD3	1.62	0.64
1:B5:1844:U:H3	1:B5:2010:A:H61	1.45	0.64
52:A2:875:G:N3	69:Ag:114:GLN:NE2	2.43	0.64
1:B5:1809:C:H2'	1:B5:1810:A2M:H8	1.80	0.64
1:B5:2444:A:N6	1:B5:2587:A:OP2	2.30	0.64
58:AF:119:GLN:HB3	58:AF:131:LEU:HD11	1.80	0.64
1:B5:4271:C:OP1	5:BB:246:ARG:NH1	2.30	0.64
7:BD:41:LYS:NZ	23:BT:32:ARG:O	2.30	0.64
43:Bo:36:GLN:OE1	43:Bo:39:ARG:NH2	2.31	0.64
59:AG:3:HIS:HB3	59:AG:6:LEU:HB2	1.80	0.64
1:B5:4508:G:OP2	18:BO:37:ARG:NH1	2.30	0.63
58:AF:244:ASN:ND2	58:AF:294:ASP:O	2.30	0.63
49:SX:210:GLU:HG3	49:SX:239:LEU:HD22	1.79	0.63
66:Ad:112:HIS:NE2	66:Ad:237:SER:O	2.31	0.63
63:Aa:28:LYS:HB3	63:Aa:48:LEU:HD11	1.81	0.63
81:As:104:LEU:HD13	81:As:121:ARG:HD3	1.80	0.63
1:B5:330:G:N7	93:B5:4906:SPD:N10	2.45	0.63
58:AF:87:LEU:HB2	58:AF:101:PHE:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BN:53:TYR:HB2	17:BN:133:ILE:HD13	1.81	0.63
51:SZ:70:PRO:HB2	51:SZ:73:VAL:HB	1.79	0.63
52:A2:437:OMG:HM22	52:A2:438:G:H5'	1.80	0.63
1:B5:228:C:O2'	28:BY:14:ASN:ND2	2.31	0.63
46:Bs:32:ALA:O	46:Bs:85:ASN:ND2	2.32	0.63
52:A2:926:G:H1	52:A2:1018:U:H3	1.47	0.63
52:A2:1383:A:H2'	52:A2:1384:A2M:H8	1.78	0.63
75:Am:136:PRO:HG2	75:Am:139:TRP:HB2	1.79	0.63
77:Ao:18:ARG:NH1	80:Ar:88:LYS:O	2.31	0.63
1:B5:4304:U:OP2	5:BB:246:ARG:NH2	2.32	0.63
1:B5:4636:G:O2'	1:B5:4666:G:N7	2.32	0.63
1:B5:1810:A2M:HM'2	1:B5:1811:G:H5'	1.80	0.62
1:B5:3561:G:H2'	1:B5:3562:A2M:H8	1.81	0.62
24:BU:100:LEU:HD13	24:BU:112:LEU:HD23	1.81	0.62
46:Bs:47:LEU:HB3	46:Bs:51:ALA:HB3	1.79	0.62
52:A2:1157:U:O4	64:Ab:194:ARG:NH1	2.32	0.62
1:B5:1757:G:N2	1:B5:1757:G:OP2	2.32	0.62
58:AF:217:MET:HG2	58:AF:229:THR:HG22	1.81	0.62
1:B5:835:G:OP1	16:BM:23:LYS:NZ	2.31	0.62
1:B5:3699:G:N2	48:Bv:164:CYS:SG	2.73	0.62
5:BB:95:THR:OG1	5:BB:98:GLY:O	2.17	0.62
8:BE:49:ASN:HD21	8:BE:57:GLY:HA3	1.64	0.62
52:A2:65:C:N4	68:Af:134:GLY:O	2.31	0.62
1:B5:1391:C:O2'	31:Bb:106:ARG:NH2	2.32	0.62
1:B5:3497:G:O2'	1:B5:3499:C:N4	2.32	0.62
10:BG:58:PRO:HD2	10:BG:61:ILE:HD12	1.81	0.62
67:Ae:56:TYR:HB3	67:Ae:63:LYS:HA	1.81	0.62
1:B5:4366:OMU:OP2	1:B5:4416:C:N4	2.33	0.62
52:A2:1594:C:H1'	81:As:12:GLN:HE22	1.64	0.62
1:B5:198:A:OP2	28:BY:126:ARG:NH2	2.32	0.62
1:B5:1130:C:H42	1:B5:1209:G:H1	1.46	0.62
5:BB:261:ARG:HB2	18:BO:64:THR:HG21	1.81	0.62
1:B5:3619:OMC:HM22	1:B5:3620:G:H5'	1.81	0.62
1:B5:1503:G:OP1	93:B5:4915:SPD:N10	2.32	0.62
1:B5:1653:C:O2'	9:BF:176:ARG:NH2	2.33	0.62
52:A2:953:G:H21	76:An:52:THR:HG21	1.65	0.62
68:Af:162:LEU:HD11	68:Af:172:LYS:HB2	1.80	0.62
46:Bs:65:ILE:HG23	46:Bs:75:LEU:HB3	1.82	0.62
68:Af:85:ARG:O	68:Af:87:ARG:NH1	2.33	0.62
1:B5:1299:G:OP1	20:BQ:108:ARG:NH2	2.28	0.61
1:B5:2106:A:OP1	45:Br:107:ARG:NH2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BA:36:GLU:OE1	4:BA:163:ARG:NH1	2.31	0.61
22:BS:173:ASN:ND2	22:BS:175:PHE:O	2.33	0.61
59:AG:22:ARG:HH11	65:Ac:16:ILE:HG21	1.62	0.61
69:Ag:162:GLN:OE1	69:Ag:165:ASN:ND2	2.33	0.61
1:B5:2548:G:O6	21:BR:46:LYS:NZ	2.32	0.61
4:BA:117:GLU:HG2	4:BA:124:GLY:H	1.65	0.61
52:A2:1076:C:OP1	75:Am:107:LYS:NZ	2.33	0.61
1:B5:1846:A:H4'	9:BF:222:LYS:HE3	1.81	0.61
52:A2:1293:C:N3	55:AC:138:ARG:NH2	2.48	0.61
64:Ab:81:ILE:HG23	64:Ab:86:LEU:HB2	1.82	0.61
85:Aw:71:ARG:NH1	85:Aw:82:THR:OG1	2.33	0.61
1:B5:4018:G:N2	1:B5:4018:G:OP2	2.30	0.61
52:A2:1355:G:N2	52:A2:1358:A:OP2	2.32	0.61
58:AF:120:ILE:HB	58:AF:132:TRP:HB2	1.82	0.61
1:B5:2194:OMC:HM22	1:B5:2195:U:H5'	1.83	0.61
1:B5:3455:A:H2'	1:B5:3456:A2M:H8	1.81	0.61
1:B5:3518:U:OP1	1:B5:4296:G:O2'	2.16	0.61
1:B5:4383:OMG:HM22	1:B5:4384:U:H5'	1.83	0.61
3:B8:47:C:H1'	3:B8:61:A:H2'	1.82	0.61
11:BH:23:ARG:HE	11:BH:39:ASN:HA	1.65	0.61
52:A2:1180:G:N2	52:A2:1183:A:OP2	2.32	0.61
86:Ax:57:VAL:HB	86:Ax:60:PHE:HE1	1.64	0.61
1:B5:3420:U:OP2	4:BA:198:ARG:NH2	2.33	0.61
1:B5:1910:C:N4	1:B5:1940:G:OP2	2.34	0.61
1:B5:4122:A:O2'	30:Ba:42:ARG:NH1	2.34	0.61
47:Bt:63:THR:HB	47:Bt:70:GLN:HB2	1.82	0.61
49:SX:6:LEU:HD22	49:SX:10:LYS:HE3	1.81	0.61
52:A2:35:C:H2'	52:A2:36:PSU:H6	1.66	0.61
1:B5:364:G:O6	39:Bj:55:ARG:NH2	2.33	0.61
37:Bh:65:GLN:HE21	89:TA:257:PRO:HD3	1.66	0.61
69:Ag:7:LYS:NZ	69:Ag:40:LEU:O	2.33	0.61
74:Al:79:VAL:HG11	74:Al:85:LEU:HB2	1.82	0.61
22:BS:147:ASP:HB3	22:BS:150:ILE:HB	1.82	0.60
47:Bt:119:ARG:HB3	47:Bt:121:LEU:HD13	1.82	0.60
62:AZ:41:ARG:HE	62:AZ:45:GLY:HA2	1.66	0.60
1:B5:1137:C:H42	1:B5:1203:G:H1	1.47	0.60
1:B5:4379:G:OP2	93:B5:4916:SPD:N1	2.34	0.60
2:B7:55:A:O2'	13:BJ:151:ILE:O	2.16	0.60
63:Aa:71:LEU:HD11	63:Aa:189:ILE:HG23	1.83	0.60
67:Ae:49:LEU:HD12	78:Ap:50:LYS:HG2	1.82	0.60
1:B5:4268:G:O2'	1:B5:4271:C:OP2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:4779:U:OP2	5:BB:396:ARG:NH2	2.33	0.60
62:AZ:177:MET:SD	62:AZ:180:ARG:NH2	2.74	0.60
1:B5:2391:C:O2'	91:TC:114:ARG:NH1	2.34	0.60
1:B5:2658:A2M:HM'2	1:B5:2659:G:H5'	1.83	0.60
37:Bh:80:PRO:HD2	37:Bh:83:LEU:HD12	1.84	0.60
52:A2:1399:G:O2'	58:AF:88:ARG:NH2	2.33	0.60
3:B8:102:G:OP1	39:Bj:20:ARG:NH1	2.35	0.60
52:A2:381:G:OP1	70:Ah:31:ARG:NE	2.33	0.60
52:A2:1551:G:H3'	52:A2:1580:A:H61	1.66	0.60
53:AA:11:SER:OG	53:AA:14:GLU:OE1	2.18	0.60
1:B5:4287:G:N2	1:B5:4290:A:OP2	2.30	0.60
3:B8:123:U:O2	3:B8:126:C:N4	2.34	0.60
52:A2:75:G:O2'	52:A2:77:A:OP1	2.19	0.60
1:B5:85:G:N2	1:B5:98:A:OP2	2.35	0.60
1:B5:1394:U:H3'	9:BF:30:LYS:HE3	1.84	0.60
1:B5:2247:A:N1	1:B5:2630:A2M:N6	2.48	0.60
1:B5:4744:G:N2	1:B5:4780:G:O2'	2.34	0.60
52:A2:49:C:H2'	52:A2:473:C:H41	1.67	0.60
52:A2:1264:U:O2	59:AG:16:GLN:NE2	2.34	0.60
48:Bv:67:VAL:HG12	48:Bv:84:HIS:HD2	1.66	0.60
49:SX:412:GLU:OE1	49:SX:415:ARG:NH1	2.35	0.60
52:A2:1131:G:N2	52:A2:1131:G:OP2	2.35	0.60
52:A2:1600:U:OP2	87:Ay:46:ASN:ND2	2.34	0.60
59:AG:44:ARG:NH1	82:At:78:ASP:OD2	2.34	0.60
62:AZ:94:THR:HG23	62:AZ:186:ARG:HH12	1.66	0.60
24:BU:28:PRO:HB2	24:BU:34:MET:HG2	1.83	0.60
57:AE:44:ILE:HD12	57:AE:65:PRO:HG2	1.83	0.60
1:B5:2300:G:OP1	17:BN:65:ARG:NH2	2.35	0.60
1:B5:2360:A:O2'	36:Bg:66:ARG:NH1	2.35	0.60
52:A2:126:G:O6	68:Af:196:LYS:NZ	2.29	0.60
52:A2:1566:C:OP2	81:As:101:ARG:NH1	2.35	0.60
1:B5:856:A:H1'	1:B5:2015:G:H5"	1.84	0.59
52:A2:228:C:H42	52:A2:902:G:H1'	1.66	0.59
52:A2:381:G:OP1	70:Ah:56:ARG:NH2	2.35	0.59
52:A2:1569:C:OP1	81:As:96:SER:OG	2.19	0.59
84:Av:14:ILE:HD11	84:Av:27:ILE:HD11	1.83	0.59
1:B5:3930:G:H5'	4:BA:233:ARG:HB2	1.84	0.59
58:AF:133:ASN:HB3	58:AF:139:LYS:HE3	1.83	0.59
1:B5:3541:G:OP2	1:B5:3541:G:N2	2.31	0.59
1:B5:4416:C:O2'	1:B5:4418:A:OP2	2.20	0.59
1:B5:1776:A:OP1	23:BT:108:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1390:C:OP1	79:Aq:43:SER:OG	2.20	0.59
70:Ah:89:GLU:OE1	70:Ah:92:ARG:NH2	2.36	0.59
7:BD:65:ALA:HB2	7:BD:74:ILE:HD13	1.84	0.59
12:BI:101:LYS:NZ	12:BI:102:MET:O	2.35	0.59
46:Bs:48:ARG:HD3	47:Bt:123:ARG:HG2	1.85	0.59
52:A2:1034:G:N1	52:A2:1081:A:O2'	2.31	0.59
1:B5:4684:G:N1	35:Bf:3:GLY:O	2.32	0.59
20:BQ:16:LYS:O	20:BQ:33:ARG:NH2	2.29	0.59
52:A2:665:A:O2'	52:A2:671:A:N1	2.33	0.59
66:Ad:79:ASP:HB3	66:Ad:82:TYR:HB2	1.85	0.59
1:B5:2250:G:N2	1:B5:2250:G:OP2	2.33	0.59
1:B5:2362:U:O2'	1:B5:2373:U:O2	2.21	0.59
52:A2:442:C:O2'	68:Af:92:ARG:NH2	2.35	0.59
52:A2:1018:U:OP1	75:Am:62:GLN:NE2	2.34	0.59
4:BA:27:ALA:O	4:BA:128:ARG:NH1	2.36	0.59
66:Ad:11:ARG:HA	66:Ad:28:ALA:HB2	1.83	0.59
12:BI:54:SER:HB2	12:BI:135:ILE:HD11	1.83	0.59
52:A2:434:A:H5"	70:Ah:22:HIS:HB3	1.85	0.59
1:B5:1915:G:N3	47:Bt:138:SER:OG	2.36	0.58
1:B5:2332:C:O2'	1:B5:2334:C:N4	2.36	0.58
3:B8:60:G:O6	37:Bh:62:ASN:ND2	2.32	0.58
1:B5:1805:U:OP1	12:BI:4:ARG:NH1	2.34	0.58
1:B5:3404:G:OP2	1:B5:3404:G:N2	2.34	0.58
1:B5:4218:G:O2'	42:Bm:100:TYR:O	2.21	0.58
1:B5:4745:U:H4'	1:B5:4746:A:H5'	1.85	0.58
26:BW:73:ARG:NH1	52:A2:1781:G:OP2	2.36	0.58
52:A2:360:U:OP2	85:Aw:18:ARG:NH1	2.35	0.58
1:B5:4202:OMC:HM22	1:B5:4203:PSU:H5"	1.84	0.58
26:BW:2:LYS:NZ	26:BW:4:GLU:OE2	2.35	0.58
33:Bd:38:PHE:HB3	33:Bd:78:ARG:HG2	1.84	0.58
37:Bh:64:THR:O	37:Bh:68:ASN:ND2	2.32	0.58
52:A2:4:C:H4'	64:Ab:207:ALA:HB2	1.85	0.58
26:BW:96:GLN:O	26:BW:101:ARG:NH2	2.36	0.58
32:Bc:5:LYS:NZ	52:A2:930:G:OP1	2.35	0.58
1:B5:2712:U:O2'	1:B5:2724:A:N7	2.33	0.58
1:B5:3819:G:H1	1:B5:3904:C:H42	1.52	0.58
8:BE:189:LEU:HD21	8:BE:256:VAL:HG21	1.84	0.58
52:A2:521:A:O2'	52:A2:826:A:N3	2.36	0.58
1:B5:4163:C:N4	1:B5:4168:A:O2'	2.37	0.58
1:B5:4708:C:O2'	19:BP:75:GLN:NE2	2.36	0.58
40:Bk:13:LEU:HD23	40:Bk:16:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AZ:89:LYS:NZ	79:Aq:83:ASN:OD1	2.36	0.58
69:Ag:144:ILE:HB	84:Av:52:ILE:HB	1.84	0.58
80:Ar:22:GLY:HA2	80:Ar:56:ALA:HB3	1.84	0.58
1:B5:1423:C:OP1	30:Ba:132:ARG:NH2	2.35	0.58
1:B5:1804:G:N2	1:B5:1807:A:OP2	2.29	0.58
1:B5:2028:G:H1	1:B5:2038:C:H41	1.52	0.58
1:B5:3783:U:H2'	1:B5:3784:A:H8	1.69	0.58
1:B5:4282:OMC:HM22	1:B5:4283:C:H5'	1.86	0.58
1:B5:4367:C:OP1	25:BV:48:ARG:NH1	2.34	0.58
6:BC:39:PHE:O	6:BC:43:ASN:ND2	2.35	0.58
52:A2:577:A2M:HM'2	52:A2:578:U:H5'	1.85	0.58
52:A2:1087:G:OP2	57:AE:12:LYS:NZ	2.37	0.58
52:A2:1529:G:O2'	52:A2:1667:C:OP1	2.20	0.58
54:AB:47:LYS:NZ	67:Ae:125:SER:O	2.35	0.58
59:AG:52:PHE:HB3	82:At:80:PHE:HB3	1.86	0.58
59:AG:22:ARG:HH21	59:AG:37:ASN:HB2	1.68	0.58
62:AZ:176:TRP:HE1	62:AZ:197:VAL:HG23	1.69	0.58
74:Al:89:VAL:HG11	74:Al:109:VAL:HG11	1.86	0.58
1:B5:2363:C:H2'	1:B5:2364:G:H8	1.68	0.58
1:B5:3701:G:H1'	48:Bv:166:ALA:HB3	1.86	0.58
70:Ah:67:TRP:NE1	70:Ah:191:GLU:OE2	2.36	0.58
1:B5:230:G:OP1	28:BY:15:ARG:NH1	2.36	0.58
1:B5:3422:U:O2'	1:B5:3549:A:N3	2.37	0.58
1:B5:3978:U:O4	43:Bo:8:ARG:NH2	2.36	0.58
49:SX:187:ILE:HB	49:SX:447:ILE:HG12	1.86	0.58
49:SX:231:ARG:NH2	89:TA:162:GLU:OE2	2.36	0.58
52:A2:165:G:N2	52:A2:165:G:OP2	2.37	0.58
52:A2:1704:OMC:HM22	52:A2:1705:C:H5'	1.85	0.58
1:B5:1624:A:N3	1:B5:1791:U:O2'	2.33	0.57
57:AE:23:CYS:O	76:An:142:ARG:NH1	2.37	0.57
1:B5:4073:C:OP1	23:BT:70:HIS:NE2	2.37	0.57
2:B7:23:A:N3	2:B7:118:C:O2'	2.37	0.57
58:AF:133:ASN:HD21	58:AF:137:VAL:HB	1.69	0.57
76:An:95:ILE:HB	76:An:129:ILE:HG12	1.86	0.57
1:B5:2161:G:N2	1:B5:2164:G:OP2	2.33	0.57
1:B5:4794:G:N2	33:Bd:118:GLN:OE1	2.37	0.57
12:BI:87:ILE:HG12	12:BI:138:ILE:HG12	1.85	0.57
25:BV:13:LYS:HD2	25:BV:128:LEU:HD21	1.86	0.57
52:A2:382:C:OP2	70:Ah:31:ARG:NH2	2.38	0.57
1:B5:399:G:H2'	1:B5:400:A2M:H8	1.87	0.57
1:B5:480:C:OP1	45:Br:67:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:483:G:O2'	1:B5:486:C:OP2	2.22	0.57
18:BO:10:ASP:OD2	18:BO:37:ARG:NH2	2.36	0.57
48:Bv:32:VAL:HA	48:Bv:208:SER:HA	1.86	0.57
53:AA:33:MET:HB2	53:AA:79:PHE:HB2	1.86	0.57
1:B5:1935:C:H42	1:B5:1939:G:H22	1.52	0.57
1:B5:3476:OMG:HM22	1:B5:3477:U:H5'	1.86	0.57
58:AF:256:ILE:HB	58:AF:270:LEU:HB2	1.85	0.57
68:Af:98:ARG:NH2	68:Af:103:ASP:OD1	2.38	0.57
71:Ai:170:PRO:HB3	71:Ai:174:LYS:HE3	1.87	0.57
1:B5:48:G:OP1	17:BN:192:TRP:NE1	2.38	0.57
1:B5:1399:G:OP2	1:B5:1399:G:N2	2.37	0.57
1:B5:2499:U:H5"	29:BZ:38:TYR:HB3	1.87	0.57
6:BC:327:LYS:NZ	9:BF:169:THR:O	2.37	0.57
52:A2:914:A:N6	69:Ag:119:SER:O	2.37	0.57
49:SX:180:SER:HB2	49:SX:453:ILE:HD13	1.86	0.57
80:Ar:98:VAL:HG11	80:Ar:106:LYS:HG3	1.86	0.57
1:B5:458:C:OP2	8:BE:117:ARG:NH1	2.38	0.57
1:B5:2473:U:O4	24:BU:89:LYS:NZ	2.35	0.57
19:BP:102:ALA:HB1	19:BP:107:LEU:HB2	1.85	0.57
52:A2:510:OMG:HM22	52:A2:511:G:H5'	1.87	0.57
4:BA:116:LEU:HB3	4:BA:126:LEU:HB2	1.87	0.57
52:A2:99:A2M:HM'2	52:A2:100:U:H5'	1.87	0.57
52:A2:292:G:N2	73:Ak:40:ILE:O	2.34	0.57
52:A2:589:G:OP2	52:A2:589:G:N2	2.36	0.57
68:Af:103:ASP:OD2	68:Af:105:ASN:ND2	2.36	0.57
73:Ak:104:LYS:O	85:Aw:11:ARG:NH2	2.37	0.57
1:B5:1449:U:H2'	1:B5:1450:G:H8	1.70	0.56
1:B5:3843:G:H4'	1:B5:3844:C:H5'	1.87	0.56
1:B5:4061:A:OP1	23:BT:69:GLN:NE2	2.37	0.56
1:B5:4422:G:OP1	5:BB:281:ASN:ND2	2.37	0.56
1:B5:4764:C:O2'	1:B5:4767:G:N3	2.34	0.56
94:B5:4911:SPM:H22	20:BQ:11:ARG:HB3	1.87	0.56
11:BH:113:GLU:HG2	11:BH:125:ARG:HG2	1.86	0.56
66:Ad:45:ILE:HA	66:Ad:61:VAL:HG11	1.86	0.56
1:B5:2739:G:OP1	21:BR:136:ARG:NH1	2.38	0.56
66:Ad:143:ASP:OD1	66:Ad:143:ASP:N	2.39	0.56
1:B5:1217:G:H4'	8:BE:77:ALA:HB2	1.86	0.56
1:B5:1910:C:O3'	46:Bs:38:LYS:NZ	2.38	0.56
45:Br:90:LEU:HD22	45:Br:111:ILE:HG23	1.86	0.56
48:Bv:21:ASN:HB2	48:Bv:26:ARG:HD3	1.87	0.56
64:Ab:187:ARG:HD2	64:Ab:192:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ae:100:ILE:HA	67:Ae:178:ILE:HD11	1.88	0.56
79:Aq:77:GLU:OE2	79:Aq:81:ARG:NH2	2.38	0.56
80:Ar:16:LEU:HD21	80:Ar:72:GLN:HE21	1.70	0.56
80:Ar:20:ILE:HD11	80:Ar:33:ILE:HG13	1.87	0.56
86:Ax:21:LYS:HB2	86:Ax:75:ILE:HB	1.87	0.56
86:Ax:87:PRO:HD2	86:Ax:90:ARG:HD2	1.87	0.56
1:B5:2484:A:OP1	36:Bg:21:ARG:NH2	2.37	0.56
1:B5:3450:A2M:HM'2	1:B5:3451:A:H5'	1.87	0.56
1:B5:4336:A2M:HM'2	1:B5:4337:U:H5'	1.86	0.56
48:Bv:128:LEU:HD13	48:Bv:135:PRO:HD3	1.88	0.56
49:SX:267:ILE:HG13	49:SX:279:TYR:HB2	1.87	0.56
52:A2:508:G:OP2	86:Ax:104:ARG:NH2	2.38	0.56
78:Ap:37:ARG:HG2	81:As:7:LYS:HB3	1.87	0.56
1:B5:3415:C:OP1	4:BA:132:ASN:ND2	2.37	0.56
31:Bb:56:LYS:O	31:Bb:60:ASN:ND2	2.30	0.56
58:AF:80:SER:OG	58:AF:90:TRP:NE1	2.34	0.56
65:Ac:42:THR:OG1	65:Ac:45:ARG:O	2.21	0.56
4:BA:53:GLY:O	4:BA:192:LYS:NZ	2.39	0.56
9:BF:121:PHE:O	9:BF:204:ASN:ND2	2.39	0.56
19:BP:118:GLN:NE2	19:BP:147:GLU:OE2	2.38	0.56
46:Bs:102:LEU:HD11	46:Bs:187:LEU:HD12	1.88	0.56
52:A2:1329:OMG:HM22	52:A2:1330:U:H5'	1.88	0.56
61:AT:47:C:O2'	61:AT:58:A:O2'	2.21	0.56
1:B5:369:G:N2	1:B5:372:A:OP2	2.31	0.56
1:B5:859:G:O2'	1:B5:2106:A:N6	2.39	0.56
9:BF:126:LYS:HB2	23:BT:133:ALA:HB3	1.88	0.56
49:SX:38:THR:HG22	49:SX:165:LEU:HD22	1.87	0.56
58:AF:40:ILE:HB	58:AF:59:LEU:HB2	1.87	0.56
1:B5:2245:G:O2'	36:Bg:10:ARG:O	2.24	0.56
1:B5:2257:G:H2'	1:B5:2258:OMU:H6	1.88	0.56
52:A2:1347:U:H2'	52:A2:1348:PSU:H6	1.70	0.56
52:A2:1624:A:OP2	93:A2:1903:SPD:N1	2.38	0.56
71:Ai:93:LYS:HB2	71:Ai:96:TYR:HD2	1.71	0.56
78:Ap:129:SER:O	78:Ap:131:LYS:NZ	2.39	0.56
80:Ar:46:ARG:HG2	81:As:35:ASP:HB2	1.86	0.56
1:B5:3371:PSU:HN3	1:B5:3381:A:H61	1.53	0.56
29:BZ:25:ILE:HA	29:BZ:43:VAL:HG12	1.88	0.56
52:A2:1804:U:H2'	52:A2:1805:OMU:H6	1.87	0.56
1:B5:1980:A:N7	1:B5:4180:C:O2'	2.39	0.56
5:BB:19:ARG:HB2	5:BB:234:ARG:HH21	1.70	0.56
27:BX:82:THR:HG22	27:BX:155:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Aj:51:SER:OG	72:Aj:55:ARG:NH1	2.38	0.56
80:Ar:38:ARG:O	80:Ar:42:HIS:ND1	2.35	0.56
1:B5:1:C:H42	3:B8:156:U:H3	1.51	0.55
1:B5:280:G:OP2	17:BN:44:ARG:NH2	2.38	0.55
68:Af:5:ILE:HG12	68:Af:111:LEU:HB2	1.88	0.55
1:B5:264:C:O2	37:Bh:112:ARG:NH2	2.40	0.55
1:B5:2146:C:O2'	1:B5:2175:A:N1	2.36	0.55
5:BB:215:GLU:OE2	5:BB:349:LYS:NZ	2.36	0.55
10:BG:103:ARG:NH2	10:BG:192:ARG:O	2.40	0.55
30:Ba:71:PRO:HG2	30:Ba:108:TYR:HA	1.87	0.55
35:Bf:43:LEU:O	35:Bf:109:ARG:NH1	2.35	0.55
43:Bo:26:TYR:HB3	43:Bo:67:VAL:HB	1.88	0.55
52:A2:1446:PSU:O2	52:A2:1447:A:N6	2.39	0.55
52:A2:1663:U:O4	52:A2:1664:A:N6	2.39	0.55
56:AD:83:VAL:HG11	85:Aw:91:LEU:HB3	1.87	0.55
1:B5:4679:C:OP1	8:BE:159:ARG:NH1	2.39	0.55
49:SX:289:ILE:HA	49:SX:292:ILE:HD12	1.88	0.55
52:A2:1148:C:OP1	57:AE:6:ARG:NH1	2.39	0.55
52:A2:1842:C:H2'	52:A2:1843:4AC:H6	1.87	0.55
61:AT:18:G:OP1	61:AT:58:A:N6	2.34	0.55
71:Ai:138:ARG:NH1	71:Ai:153:SER:OG	2.37	0.55
74:Al:25:ALA:O	74:Al:30:GLY:N	2.35	0.55
77:Ao:59:ARG:HH11	77:Ao:76:VAL:HG13	1.71	0.55
21:BR:15:LEU:HD13	21:BR:52:ARG:HB2	1.89	0.55
40:Bk:57:LYS:NZ	40:Bk:68:GLU:OE2	2.37	0.55
52:A2:1125:C:H5"	63:Aa:150:ILE:HG12	1.88	0.55
64:Ab:121:ARG:NH1	64:Ab:121:ARG:O	2.40	0.55
87:Ay:58:LEU:HD12	87:Ay:62:VAL:HG21	1.88	0.55
1:B5:432:U:O2	93:B5:4923:SPD:N6	2.40	0.55
48:Bv:111:LEU:HD21	48:Bv:151:VAL:HG21	1.89	0.55
52:A2:1500:U:H4'	65:Ac:176:LEU:HD13	1.88	0.55
70:Ah:73:THR:O	70:Ah:74:ARG:NH1	2.34	0.55
1:B5:4166:PSU:O2	1:B5:4221:G:N2	2.40	0.55
1:B5:4632:A:OP1	18:BO:188:LYS:NZ	2.39	0.55
1:B5:4663:C:O2	1:B5:4665:C:N4	2.39	0.55
6:BC:218:VAL:HA	6:BC:229:LEU:HG	1.89	0.55
12:BI:177:ASN:HB2	12:BI:180:GLU:HG2	1.89	0.55
29:BZ:36:ARG:NH1	29:BZ:38:TYR:OH	2.37	0.55
29:BZ:92:ASP:HB3	29:BZ:95:VAL:HG12	1.87	0.55
50:SY:49:PHE:HA	50:SY:52:PHE:HD2	1.71	0.55
52:A2:1021:A:N7	75:Am:70:LYS:NZ	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1254:A:OP2	52:A2:1527:G:N2	2.36	0.55
52:A2:1544:U:H5"	78:Ap:37:ARG:HH12	1.72	0.55
73:Ak:119:ASP:O	73:Ak:147:LYS:NZ	2.32	0.55
1:B5:992:C:OP1	1:B5:1106:U:O2'	2.24	0.55
3:B8:141:C:OP1	17:BN:38:ARG:NH1	2.39	0.55
4:BA:30:ARG:HG3	4:BA:76:PHE:HZ	1.72	0.55
25:BV:31:ASN:ND2	25:BV:115:SER:OG	2.39	0.55
47:Bt:10:ILE:HG12	47:Bt:65:GLN:HG2	1.88	0.55
52:A2:381:G:N1	52:A2:384:G:OP2	2.34	0.55
52:A2:1417:C:OP1	81:As:129:ARG:NH1	2.39	0.55
62:AZ:76:VAL:HG12	62:AZ:123:VAL:HB	1.89	0.55
69:Ag:57:ARG:NH2	69:Ag:89:GLY:O	2.39	0.55
71:Ai:107:GLU:HA	71:Ai:112:THR:HG21	1.88	0.55
78:Ap:34:VAL:HG22	78:Ap:70:VAL:HB	1.88	0.55
90:TB:104:ASN:HA	90:TB:130:GLN:HA	1.89	0.55
10:BG:73:ARG:NH1	10:BG:241:VAL:O	2.38	0.55
20:BQ:151:HIS:ND1	20:BQ:164:LYS:O	2.40	0.55
46:Bs:125:ALA:HA	46:Bs:154:ILE:HB	1.87	0.55
47:Bt:65:GLN:NE2	47:Bt:70:GLN:OE1	2.40	0.55
48:Bv:94:ASN:OD1	48:Bv:97:LYS:NZ	2.34	0.55
52:A2:1300:A:O2'	52:A2:1302:A:OP1	2.23	0.55
1:B5:1924:G:H1'	1:B5:1942:G:H2'	1.88	0.55
1:B5:2007:C:OP1	35:Bf:15:LYS:NZ	2.37	0.55
46:Bs:77:LYS:HE2	46:Bs:196:GLY:HA2	1.89	0.55
55:AC:116:ARG:NH1	55:AC:120:GLU:OE2	2.39	0.55
65:Ac:106:ARG:HG3	65:Ac:175:VAL:HB	1.89	0.55
47:Bt:80:LEU:HD13	47:Bt:112:ILE:HG23	1.88	0.55
52:A2:380:C:O2	70:Ah:5:ARG:NE	2.40	0.55
52:A2:1240:U:H5"	77:Ao:124:LYS:HD3	1.89	0.55
1:B5:1717:C:H2'	1:B5:1718:PSU:H6	1.72	0.54
4:BA:101:VAL:HG22	4:BA:165:VAL:HG22	1.87	0.54
13:BJ:17:ILE:HD12	13:BJ:80:GLU:HG2	1.88	0.54
49:SX:276:TYR:OH	49:SX:402:ARG:NH1	2.37	0.54
52:A2:493:C:N4	52:A2:508:G:OP2	2.36	0.54
63:Aa:189:ILE:HB	63:Aa:190:PRO:HD3	1.89	0.54
1:B5:758:C:O2'	1:B5:760:C:N4	2.35	0.54
1:B5:2652:G:O2'	1:B5:4390:G:OP1	2.23	0.54
61:AT:21:A:H61	61:AT:46:A:H2'	1.72	0.54
1:B5:432:U:H1'	93:B5:4923:SPD:HN6	1.72	0.54
1:B5:1741:A:H5"	1:B5:1742:G:H5'	1.89	0.54
10:BG:99:ALA:HB1	10:BG:136:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BZ:95:VAL:HG13	29:BZ:96:VAL:HG23	1.89	0.54
49:SX:15:ILE:HG22	49:SX:16:LEU:HG	1.89	0.54
49:SX:39:LEU:HD21	49:SX:181:LEU:HB3	1.89	0.54
52:A2:1095:C:O2	84:Av:16:ASN:ND2	2.40	0.54
3:B8:123:U:H4'	3:B8:124:U:H5'	1.90	0.54
8:BE:120:PRO:O	45:Br:112:ARG:NH1	2.37	0.54
37:Bh:66:LYS:NZ	37:Bh:82:ASP:OD2	2.40	0.54
49:SX:236:ARG:HG2	49:SX:239:LEU:HB2	1.88	0.54
52:A2:1338:4AC:H2'	52:A2:1339:G:C8	2.43	0.54
67:Ae:102:LEU:HD21	87:Ay:100:VAL:HG21	1.88	0.54
90:TB:101:GLY:O	90:TB:133:ILE:N	2.39	0.54
1:B5:865:G:N7	9:BF:28:LYS:NZ	2.44	0.54
7:BD:55:VAL:HG13	7:BD:60:ILE:HG12	1.89	0.54
13:BJ:81:GLU:OE2	13:BJ:85:LYS:NZ	2.41	0.54
52:A2:1522:C:OP2	80:Ar:136:THR:OG1	2.25	0.54
78:Ap:58:LEU:HB3	78:Ap:62:ARG:HD2	1.90	0.54
79:Aq:44:LYS:HG3	79:Aq:47:ARG:HH21	1.73	0.54
81:As:60:THR:HG23	81:As:75:MET:HE2	1.89	0.54
1:B5:1334:G:N2	1:B5:1337:G:OP2	2.32	0.54
1:B5:2022:C:OP2	20:BQ:14:ARG:NH2	2.41	0.54
6:BC:133:LEU:HD13	45:Br:6:GLN:HE21	1.73	0.54
61:AT:48:5MC:HN41	61:AT:64:G:H1	1.55	0.54
92:TD:26:CYS:HB2	92:TD:64:MET:HE1	1.90	0.54
1:B5:347:A:O2'	6:BC:50:GLN:NE2	2.39	0.54
32:Bc:47:ILE:HD12	32:Bc:94:LEU:HD11	1.90	0.54
65:Ac:177:LEU:HD13	65:Ac:182:LEU:HD13	1.89	0.54
1:B5:3353:A:O2'	1:B5:4404:G:O2'	2.24	0.54
3:B8:72:A:H61	3:B8:79:G:H1	1.56	0.54
18:BO:125:LYS:HG2	18:BO:129:LEU:HD12	1.89	0.54
1:B5:435:A:O2'	34:Be:26:ASP:OD2	2.23	0.54
1:B5:3456:A2M:HM'2	1:B5:3457:G:H5'	1.89	0.54
49:SX:191:ILE:HD11	49:SX:447:ILE:HD13	1.90	0.54
52:A2:30:C:O2'	52:A2:597:U:OP1	2.26	0.54
52:A2:64:A:H2	52:A2:83:A:H62	1.54	0.54
52:A2:1019:U:O2'	75:Am:86:GLU:OE2	2.25	0.54
52:A2:1752:C:O2	52:A2:1785:G:N2	2.41	0.54
55:AC:102:VAL:HG21	74:Al:35:ILE:HG21	1.89	0.54
58:AF:88:ARG:HH12	58:AF:100:ARG:HH21	1.56	0.54
71:Ai:120:ALA:O	71:Ai:125:HIS:ND1	2.38	0.54
1:B5:1485:G:O2'	39:Bj:45:ARG:NH2	2.37	0.54
4:BA:30:ARG:NH1	4:BA:36:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SX:236:ARG:HD3	49:SX:239:LEU:HD12	1.89	0.54
52:A2:1032:A2M:HM'2	52:A2:1033:C:H5'	1.90	0.54
53:AA:15:GLU:O	53:AA:23:ARG:NE	2.39	0.54
58:AF:167:SER:OG	58:AF:177:TRP:NE1	2.32	0.54
74:Al:49:LEU:HB3	74:Al:111:VAL:HB	1.90	0.54
1:B5:1437:G:N7	15:BL:188:ASN:ND2	2.55	0.53
1:B5:3642:C:O2'	1:B5:3942:OMG:N2	2.38	0.53
1:B5:3651:C:OP1	4:BA:2:GLY:N	2.41	0.53
1:B5:4480:A:H61	1:B5:4704:U:H3	1.56	0.53
8:BE:181:PRO:HD2	8:BE:184:LEU:HD12	1.90	0.53
47:Bt:154:ASP:HB3	47:Bt:159:ALA:HB3	1.89	0.53
48:Bv:73:HIS:ND1	48:Bv:144:MET:SD	2.77	0.53
52:A2:1498:G:N7	72:Aj:25:LYS:NZ	2.42	0.53
53:AA:16:LYS:HA	53:AA:23:ARG:HH21	1.73	0.53
1:B5:58:G:H4'	1:B5:59:A:H4'	1.90	0.53
1:B5:1937:A:N3	1:B5:1958:C:O2'	2.40	0.53
1:B5:2317:G:H22	1:B5:2346:G:H5"	1.72	0.53
1:B5:3386:G:O2'	1:B5:3425:U:OP1	2.22	0.53
32:Bc:8:LYS:NZ	52:A2:1009:A:OP2	2.38	0.53
49:SX:50:LEU:HD12	51:SZ:88:HIS:HB2	1.90	0.53
49:SX:212:ALA:HB3	49:SX:215:ALA:HB3	1.89	0.53
52:A2:1144:A:H5'	64:Ab:190:SER:HB3	1.90	0.53
58:AF:247:TRP:HB3	58:AF:258:ILE:HD11	1.91	0.53
1:B5:707:C:O2	8:BE:133:LYS:NZ	2.39	0.53
1:B5:2602:G:H1'	1:B5:2607:A:H2	1.73	0.53
1:B5:4273:G:OP2	1:B5:4273:G:N2	2.39	0.53
3:B8:121:G:H1	3:B8:129:C:H42	1.57	0.53
6:BC:293:LEU:O	6:BC:299:GLN:NE2	2.40	0.53
7:BD:152:ARG:HG3	7:BD:154:THR:HG23	1.90	0.53
8:BE:104:ASN:OD1	8:BE:108:ARG:NH2	2.41	0.53
22:BS:99:ASP:OD1	22:BS:100:LEU:N	2.41	0.53
74:Al:75:ASN:N	74:Al:75:ASN:OD1	2.41	0.53
85:Aw:93:PHE:O	85:Aw:140:ARG:NH1	2.41	0.53
1:B5:1211:G:O6	31:Bb:111:ARG:NH2	2.35	0.53
1:B5:4138:OMG:HM21	1:B5:4140:A:H2'	1.90	0.53
1:B5:4610:C:N4	22:BS:171:ARG:O	2.40	0.53
48:Bv:65:VAL:HG22	48:Bv:109:ALA:HB3	1.90	0.53
52:A2:126:G:OP2	68:Af:195:LYS:NZ	2.40	0.53
52:A2:127:C:O2	66:Ad:134:LYS:NZ	2.41	0.53
52:A2:1602:A:OP2	52:A2:1637:G:N2	2.36	0.53
1:B5:632:G:H5"	1:B5:633:U:H5'	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1225:G:H5'	6:BC:323:ARG:HB2	1.90	0.53
1:B5:1414:A:OP1	20:BQ:65:ARG:NH2	2.41	0.53
1:B5:2323:G:H2'	1:B5:2324:G:H8	1.74	0.53
1:B5:4011:U:N3	7:BD:17:GLN:O	2.41	0.53
49:SX:206:GLY:HA3	49:SX:209:PHE:HE1	1.73	0.53
52:A2:512:U:O2'	52:A2:577:A2M:N1	2.42	0.53
52:A2:1260:A:N6	52:A2:1520:U:OP1	2.30	0.53
89:TA:168:PRO:HA	89:TA:195:THR:HA	1.89	0.53
1:B5:835:G:OP1	16:BM:44:ARG:NH1	2.42	0.53
1:B5:1341:A:N1	1:B5:1453:G:O2'	2.41	0.53
1:B5:4311:C:O2	5:BB:268:ARG:NH2	2.40	0.53
48:Bv:15:ARG:HH21	48:Bv:18:LEU:HD23	1.74	0.53
62:AZ:33:GLN:HB3	62:AZ:154:LEU:HD12	1.91	0.53
65:Ac:70:THR:HG22	65:Ac:86:LEU:HD13	1.90	0.53
1:B5:1284:OMC:OP1	30:Ba:6:ARG:NH2	2.41	0.53
1:B5:1621:C:O2'	1:B5:1643:G:OP1	2.23	0.53
1:B5:2330:G:N2	3:B8:125:C:N3	2.55	0.53
1:B5:2363:C:H1'	1:B5:2483:G:H21	1.74	0.53
1:B5:4052:OMU:HM22	1:B5:4053:A:H5'	1.91	0.53
1:B5:4379:G:OP1	93:B5:4916:SPD:N10	2.42	0.53
19:BP:138:PRO:HB3	19:BP:140:MET:HE3	1.91	0.53
48:Bv:207:LYS:HB3	48:Bv:213:PRO:HA	1.91	0.53
52:A2:142:C:N4	52:A2:330:G:OP1	2.39	0.53
69:Ag:44:ASN:O	69:Ag:68:GLN:NE2	2.42	0.53
70:Ah:130:THR:OG1	70:Ah:132:GLU:OE1	2.26	0.53
1:B5:1284:OMC:HM22	1:B5:1285:U:H5'	1.89	0.53
77:Ao:34:MET:HB3	77:Ao:42:ARG:HG3	1.90	0.53
86:Ax:7:ILE:HG22	86:Ax:27:VAL:HG22	1.91	0.53
1:B5:238:C:OP2	28:BY:45:ARG:NH2	2.41	0.53
1:B5:375:G:OP2	39:Bj:52:LYS:NZ	2.39	0.53
1:B5:1772:G:OP1	23:BT:120:LYS:NZ	2.39	0.53
1:B5:2267:OMG:HM22	1:B5:2268:U:H5"	1.91	0.53
1:B5:2549:G:H3'	1:B5:2550:U:H4'	1.89	0.53
7:BD:37:VAL:HB	7:BD:67:ALA:HB2	1.90	0.53
8:BE:167:PHE:HA	8:BE:178:VAL:HG12	1.91	0.53
29:BZ:12:LEU:HB2	29:BZ:81:MET:HB3	1.90	0.53
52:A2:62:G:H1'	52:A2:172:OMU:HM23	1.91	0.53
52:A2:656:A:H4'	52:A2:657:G:H3'	1.90	0.53
52:A2:1859:G:N7	76:An:146:ARG:NH2	2.57	0.53
71:Ai:60:LEU:HD22	71:Ai:70:ARG:HA	1.91	0.53
82:At:23:THR:HB	82:At:113:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:2142:G:H5'	45:Br:15:SER:HB2	1.91	0.52
52:A2:513:A2M:HM'2	52:A2:514:G:H5'	1.91	0.52
62:AZ:144:THR:OG1	62:AZ:156:TYR:O	2.22	0.52
70:Ah:3:ILE:O	70:Ah:30:GLY:N	2.40	0.52
75:Am:99:ARG:NH2	75:Am:119:GLU:OE2	2.41	0.52
89:TA:168:PRO:HB3	89:TA:195:THR:HG22	1.90	0.52
1:B5:2032:G:H4'	1:B5:2033:C:H3'	1.92	0.52
1:B5:2221:G:N2	1:B5:2224:A:OP2	2.43	0.52
1:B5:3450:A2M:H8	1:B5:3450:A2M:O5'	2.10	0.52
1:B5:3676:OMG:HM22	1:B5:3677:A:H5'	1.91	0.52
3:B8:67:U:H2'	3:B8:68:G:H8	1.74	0.52
3:B8:153:C:OP1	10:BG:185:LYS:NZ	2.41	0.52
52:A2:421:G:O2'	52:A2:661:C:N3	2.41	0.52
1:B5:2275:U:H5"	49:SX:273:ARG:HB2	1.91	0.52
1:B5:4732:G:H22	1:B5:4797:A:H2	1.56	0.52
3:B8:96:C:H5"	37:Bh:66:LYS:HG2	1.91	0.52
7:BD:93:THR:O	7:BD:158:LYS:NZ	2.41	0.52
9:BF:237:ASP:O	9:BF:240:ASN:ND2	2.38	0.52
24:BU:111:GLU:OE2	24:BU:113:ARG:NE	2.38	0.52
38:Bi:70:LEU:HD21	38:Bi:80:HIS:HE1	1.73	0.52
58:AF:107:ASP:HB2	58:AF:125:ARG:HH11	1.75	0.52
62:AZ:17:LYS:HB3	62:AZ:173:LEU:HD11	1.91	0.52
63:Aa:129:THR:OG1	63:Aa:131:ASP:OD1	2.26	0.52
65:Ac:131:ALA:HA	65:Ac:191:PRO:HD3	1.91	0.52
68:Af:49:VAL:HG23	68:Af:114:VAL:HB	1.91	0.52
1:B5:1340:G:HO2'	1:B5:1423:C:HO2'	1.55	0.52
12:BI:55:ASP:OD2	12:BI:164:LYS:NZ	2.42	0.52
36:Bg:5:LEU:HD21	36:Bg:30:ILE:HG22	1.90	0.52
49:SX:83:PRO:HD3	49:SX:127:GLN:HE22	1.75	0.52
52:A2:564:G:O6	71:Ai:172:ARG:NH2	2.38	0.52
56:AD:86:VAL:HA	56:AD:89:GLN:HE21	1.75	0.52
57:AE:45:VAL:HA	76:An:113:GLN:HE22	1.74	0.52
1:B5:4068:G:N2	1:B5:4071:A:OP2	2.36	0.52
15:BL:42:ARG:HG3	15:BL:45:ARG:HH21	1.73	0.52
19:BP:8:PRO:HG3	19:BP:149:ILE:HD13	1.91	0.52
30:Ba:13:GLY:O	34:Be:39:ARG:NE	2.39	0.52
33:Bd:19:GLU:OE1	33:Bd:92:ARG:NH1	2.43	0.52
52:A2:1567:G:N2	52:A2:1570:A:OP2	2.39	0.52
80:Ar:80:PRO:HG2	80:Ar:83:PHE:HB2	1.91	0.52
1:B5:85:G:O2'	1:B5:97:G:O6	2.25	0.52
1:B5:1726:A:N3	1:B5:3956:U:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:2647:OMC:HM22	1:B5:2648:C:H5'	1.90	0.52
1:B5:4060:C:O2'	31:Bb:36:ASP:OD1	2.22	0.52
3:B8:63:U:O2'	37:Bh:52:LYS:NZ	2.40	0.52
52:A2:355:OMU:HM22	52:A2:356:G:H5'	1.90	0.52
52:A2:869:G:OP2	52:A2:869:G:N2	2.39	0.52
52:A2:1861:A:N7	57:AE:34:LYS:NZ	2.57	0.52
58:AF:69:VAL:HA	58:AF:80:SER:HA	1.91	0.52
64:Ab:169:TYR:OH	64:Ab:175:GLY:O	2.26	0.52
75:Am:124:ARG:HG2	75:Am:127:ARG:HH12	1.74	0.52
1:B5:1270:A2M:OP2	1:B5:4191:U:O2'	2.27	0.52
57:AE:11:ALA:HB3	57:AE:33:ASP:HB2	1.91	0.52
61:AT:7:A:O2'	61:AT:48:5MC:O4'	2.28	0.52
68:Af:2:LYS:HB3	68:Af:15:LEU:HD11	1.91	0.52
1:B5:2363:C:H2'	1:B5:2364:G:C8	2.45	0.52
3:B8:13:G:O2'	19:BP:121:LYS:O	2.26	0.52
47:Bt:13:VAL:HB	47:Bt:62:LEU:HB2	1.90	0.52
49:SX:205:ARG:HD3	89:TA:166:GLY:C	2.35	0.52
52:A2:121:OMU:HM22	52:A2:122:G:H5'	1.92	0.52
52:A2:166:A2M:HM'2	52:A2:167:G:H5'	1.91	0.52
52:A2:1448:OMG:HM22	52:A2:1449:A:H5'	1.92	0.52
63:Aa:137:LEU:HG	63:Aa:215:VAL:HG22	1.92	0.52
1:B5:44:A:H5"	94:B5:4914:SPM:H71	1.91	0.52
1:B5:1546:U:OP2	1:B5:2699:C:O2'	2.23	0.52
1:B5:2465:G:O6	24:BU:81:ARG:NH2	2.43	0.52
1:B5:4780:G:N1	5:BB:389:MET:O	2.38	0.52
3:B8:38:U:O2'	37:Bh:86:LYS:NZ	2.31	0.52
36:Bg:64:LEU:HD23	36:Bg:67:LEU:HD12	1.91	0.52
49:SX:182:PHE:O	49:SX:186:ASN:ND2	2.37	0.52
49:SX:238:ASN:HD21	89:TA:163:PRO:HB2	1.74	0.52
52:A2:1338:4AC:H2'	52:A2:1339:G:H8	1.75	0.52
64:Ab:102:LEU:HD22	64:Ab:130:ILE:HG12	1.91	0.52
64:Ab:191:VAL:HG11	64:Ab:236:PHE:HA	1.92	0.52
1:B5:66:A:O2'	1:B5:326:C:O2	2.27	0.52
1:B5:4278:PSU:OP2	1:B5:4300:G:N1	2.43	0.52
3:B8:75:OMG:OP2	28:BY:74:TYR:OH	2.25	0.52
7:BD:41:LYS:HE2	23:BT:93:ILE:HG21	1.92	0.52
29:BZ:22:LYS:NZ	29:BZ:129:TRP:O	2.37	0.52
68:Af:57:ASP:HA	68:Af:106:LEU:HA	1.91	0.52
75:Am:40:LEU:HD12	75:Am:50:ILE:HG23	1.92	0.52
1:B5:3812:G:O6	4:BA:72:ARG:NH2	2.40	0.51
2:B7:6:C:H4'	7:BD:52:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BQ:119:LYS:HE3	20:BQ:121:LEU:HD21	1.92	0.51
21:BR:44:LEU:HD22	21:BR:49:LEU:HD12	1.90	0.51
39:Bj:27:TYR:HA	39:Bj:34:CYS:HA	1.93	0.51
46:Bs:10:LYS:HG3	46:Bs:60:MET:HE1	1.92	0.51
47:Bt:80:LEU:HD23	47:Bt:83:LYS:HD2	1.92	0.51
52:A2:1018:U:H5'	75:Am:55:ARG:HE	1.75	0.51
52:A2:1443:OMU:HM22	52:A2:1444:C:H5'	1.92	0.51
52:A2:1598:C:OP2	87:Ay:85:ARG:NH2	2.43	0.51
52:A2:1652:A:H1'	67:Ae:83:ASN:HD22	1.75	0.51
52:A2:1865:U:H5'	57:AE:79:ILE:HD11	1.92	0.51
62:AZ:184:ARG:HD3	62:AZ:191:ARG:HG2	1.91	0.51
85:Aw:67:ARG:HG3	85:Aw:115:ILE:HG12	1.93	0.51
1:B5:3669:C:H1'	17:BN:125:SER:HB3	1.91	0.51
1:B5:4638:G:N2	1:B5:4661:C:O2	2.43	0.51
49:SX:64:TRP:HZ2	49:SX:346:SER:HA	1.74	0.51
49:SX:355:LEU:HD23	49:SX:355:LEU:H	1.74	0.51
52:A2:1143:G:N2	52:A2:1146:A:OP2	2.35	0.51
66:Ad:124:CYS:HB3	66:Ad:141:THR:HB	1.91	0.51
1:B5:253:G:H2'	1:B5:254:G:H8	1.74	0.51
1:B5:788:G:H2'	1:B5:789:G:H8	1.75	0.51
1:B5:1341:A:O2'	1:B5:1422:C:O2'	2.18	0.51
1:B5:1631:C:H41	1:B5:4124:A:H5"	1.75	0.51
1:B5:2370:A:OP1	21:BR:38:ARG:NH2	2.33	0.51
46:Bs:62:ARG:NH2	46:Bs:82:ILE:O	2.43	0.51
52:A2:642:A:OP1	71:Ai:40:LYS:NZ	2.40	0.51
52:A2:1289:OMU:OP2	55:AC:97:LYS:NZ	2.42	0.51
54:AB:32:VAL:HG11	54:AB:56:LEU:HD12	1.93	0.51
62:AZ:77:ILE:HG13	62:AZ:99:ILE:HB	1.92	0.51
63:Aa:179:ASN:ND2	63:Aa:183:GLU:OE1	2.39	0.51
87:Ay:74:SER:OG	87:Ay:79:ILE:O	2.28	0.51
90:TB:134:LEU:HD23	90:TB:139:PHE:HD1	1.75	0.51
91:TC:147:VAL:HG21	92:TD:161:TYR:HB2	1.91	0.51
1:B5:1915:G:N2	47:Bt:138:SER:O	2.42	0.51
1:B5:2249:G:N7	41:Bl:2:SER:N	2.58	0.51
1:B5:4368:A:H4'	5:BB:13:SER:HB2	1.93	0.51
15:BL:129:ARG:NH1	37:Bh:116:LEU:O	2.38	0.51
17:BN:181:HIS:O	17:BN:195:ARG:NH2	2.37	0.51
48:Bv:63:PHE:O	48:Bv:152:LYS:NZ	2.43	0.51
49:SX:108:ASP:O	49:SX:112:PHE:N	2.42	0.51
52:A2:120:U:H2'	52:A2:121:OMU:H6	1.92	0.51
52:A2:599:G:O2'	52:A2:606:A:N1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AT:29:G:H4'	80:Ar:148:VAL:HG11	1.93	0.51
84:Av:45:GLY:O	84:Av:68:ARG:NH2	2.43	0.51
1:B5:136:U:O4	37:Bh:79:LYS:NZ	2.34	0.51
1:B5:308:G:O6	17:BN:12:ARG:NH1	2.44	0.51
1:B5:4264:A:OP1	1:B5:4266:G:O2'	2.28	0.51
23:BT:18:PRO:HG2	23:BT:21:LYS:HB2	1.93	0.51
52:A2:1571:G:N7	81:As:97:LYS:NZ	2.57	0.51
52:A2:1758:G:H1	52:A2:1776:U:H3	1.59	0.51
58:AF:77:PHE:HB3	58:AF:89:LEU:HD11	1.93	0.51
68:Af:148:SER:N	68:Af:151:ASP:OD2	2.43	0.51
69:Ag:37:LYS:HE3	69:Ag:41:ARG:HE	1.76	0.51
75:Am:86:GLU:O	75:Am:90:HIS:ND1	2.38	0.51
82:At:86:LYS:HE2	82:At:88:LEU:HD21	1.93	0.51
1:B5:1476:C:OP1	6:BC:100:ARG:NH2	2.44	0.51
1:B5:3353:A:HO2'	1:B5:4404:G:HO2'	1.58	0.51
25:BV:69:LYS:NZ	25:BV:71:GLU:OE2	2.34	0.51
52:A2:27:A2M:HM'2	52:A2:28:U:H5'	1.92	0.51
52:A2:1289:OMU:HM22	52:A2:1290:U:H5'	1.91	0.51
52:A2:1551:G:N2	52:A2:1560:C:O2	2.38	0.51
66:Ad:44:LEU:HD21	66:Ad:72:ILE:HD11	1.93	0.51
84:Av:90:GLN:HE22	84:Av:117:ARG:HE	1.58	0.51
1:B5:338:A:OP1	15:BL:31:ARG:NH2	2.39	0.51
1:B5:1125:C:H5	8:BE:62:SER:HB2	1.76	0.51
1:B5:1348:G:H1	1:B5:1368:U:H3	1.58	0.51
1:B5:1551:U:O2'	19:BP:135:ARG:NH1	2.42	0.51
1:B5:1825:G:H1	1:B5:1832:C:H42	1.59	0.51
1:B5:3996:G:OP1	13:BJ:97:ASN:ND2	2.43	0.51
3:B8:102:G:OP2	3:B8:104:A:O2'	2.27	0.51
15:BL:81:LEU:HD12	15:BL:86:ILE:HB	1.93	0.51
47:Bt:32:ILE:HB	47:Bt:35:LEU:HD11	1.92	0.51
66:Ad:131:VAL:HA	66:Ad:137:PRO:HA	1.93	0.51
76:An:40:THR:HG21	76:An:74:ALA:HB2	1.92	0.51
1:B5:4231:C:O2'	42:Bm:114:LYS:NZ	2.43	0.51
1:B5:4437:A:O2'	11:BH:68:ALA:O	2.27	0.51
68:Af:67:VAL:HG12	68:Af:69:THR:HG22	1.93	0.51
1:B5:74:G:H5"	15:BL:59:VAL:HB	1.92	0.51
1:B5:373:G:OP2	39:Bj:36:LYS:NZ	2.42	0.51
1:B5:2293:G:OP1	4:BA:17:ARG:NH1	2.44	0.51
1:B5:4501:G:H3'	8:BE:282:ASN:HD21	1.76	0.51
9:BF:135:VAL:HG23	9:BF:139:ILE:HD13	1.93	0.51
15:BL:91:ALA:HB1	15:BL:96:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Bd:54:MET:HE3	33:Bd:60:PRO:HA	1.92	0.51
52:A2:1856:G:OP2	76:An:147:ARG:NH2	2.37	0.51
80:Ar:124:ARG:NE	80:Ar:130:ARG:O	2.33	0.51
1:B5:1016:C:O2'	1:B5:1059:G:O4'	2.29	0.51
1:B5:1416:C:OP1	20:BQ:144:LYS:NZ	2.44	0.51
1:B5:2422:G:N2	1:B5:2425:A:OP2	2.28	0.51
2:B7:105:C:OP2	12:BI:203:ARG:NH1	2.37	0.51
9:BF:153:ILE:HD12	9:BF:190:ILE:HG12	1.93	0.51
13:BJ:90:ARG:NH2	13:BJ:108:GLY:O	2.43	0.51
58:AF:111:VAL:HG23	58:AF:122:SER:HB3	1.93	0.51
62:AZ:198:MET:HG2	62:AZ:200:ASP:H	1.76	0.51
67:Ae:47:LYS:NZ	78:Ap:115:TYR:O	2.44	0.51
1:B5:755:G:H1	1:B5:800:U:H3	1.59	0.50
1:B5:1674:U:H5'	93:B5:4918:SPD:H41	1.93	0.50
1:B5:3562:A2M:HM'2	1:B5:3563:U:H5'	1.93	0.50
17:BN:116:LEU:HD22	17:BN:135:ILE:HD11	1.93	0.50
52:A2:43:U:OP2	52:A2:486:A:N6	2.28	0.50
52:A2:501:A:H4'	93:A2:1907:SPD:H52	1.92	0.50
52:A2:1299:G:H4'	77:Ao:78:THR:HA	1.93	0.50
74:Al:11:VAL:HG13	74:Al:13:ASP:H	1.76	0.50
1:B5:135:G:N2	37:Bh:95:LEU:O	2.31	0.50
1:B5:4071:A:H1'	7:BD:36:LEU:HD23	1.93	0.50
1:B5:4602:G:OP1	11:BH:21:LYS:NZ	2.42	0.50
4:BA:29:LEU:O	4:BA:123:ARG:NE	2.34	0.50
7:BD:37:VAL:HG12	7:BD:50:ARG:HD3	1.94	0.50
52:A2:1859:G:OP1	57:AE:17:HIS:NE2	2.37	0.50
75:Am:54:LEU:HB3	75:Am:60:VAL:HB	1.91	0.50
80:Ar:59:LEU:HD23	80:Ar:64:VAL:HG22	1.94	0.50
1:B5:2538:A:OP1	40:Bk:35:LYS:NZ	2.36	0.50
1:B5:4366:OMU:OP1	25:BV:51:ARG:NH1	2.44	0.50
5:BB:66:LYS:HB2	25:BV:14:PHE:HE2	1.77	0.50
21:BR:98:ARG:NH2	21:BR:130:ASN:OD1	2.40	0.50
29:BZ:136:PHE:OXT	36:Bg:90:ARG:NH2	2.44	0.50
52:A2:953:G:OP1	63:Aa:56:LYS:NZ	2.44	0.50
52:A2:1651:A:H5"	78:Ap:139:ALA:HB2	1.92	0.50
52:A2:1680:A:H2'	67:Ae:60:ARG:HD2	1.91	0.50
64:Ab:168:GLY:N	64:Ab:179:THR:O	2.36	0.50
66:Ad:100:ARG:HB2	66:Ad:114:ILE:HD13	1.94	0.50
79:Aq:29:HIS:HA	79:Aq:32:LYS:HE2	1.93	0.50
1:B5:2276:G:OP1	49:SX:268:LYS:NZ	2.44	0.50
1:B5:2649:A:O2'	93:B5:4915:SPD:N1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:3908:C:H5	10:BG:73:ARG:HH12	1.58	0.50
2:B7:48:G:OP1	7:BD:226:TYR:OH	2.29	0.50
17:BN:201:HIS:O	17:BN:204:ARG:NH1	2.42	0.50
52:A2:191:A:H62	52:A2:208:G:H21	1.58	0.50
52:A2:1015:G:N2	53:AA:51:GLN:OE1	2.45	0.50
58:AF:203:ASP:OD1	58:AF:205:SER:OG	2.29	0.50
90:TB:75:MET:HE2	92:TD:87:GLN:HB3	1.92	0.50
1:B5:1271:C:H2'	1:B5:1272:G:C8	2.47	0.50
1:B5:3432:C:O2'	1:B5:3506:A:N3	2.43	0.50
42:Bm:94:MET:HG2	42:Bm:105:PRO:HA	1.93	0.50
52:A2:26:U:H2'	52:A2:27:A2M:H8	1.94	0.50
84:Av:70:ASN:ND2	84:Av:130:PHE:OXT	2.42	0.50
85:Aw:131:LEU:HD11	85:Aw:135:LYS:HE3	1.93	0.50
1:B5:793:C:N3	1:B5:794:G:N1	2.60	0.50
1:B5:2625:U:OP2	41:Bl:10:LYS:NZ	2.41	0.50
20:BQ:178:ARG:N	30:Ba:51:GLY:HA2	2.27	0.50
26:BW:74:ARG:NH2	52:A2:1783:G:O6	2.44	0.50
52:A2:168:C:OP1	68:Af:131:ARG:NH2	2.44	0.50
52:A2:682:PSU:H4'	85:Aw:9:THR:HG22	1.92	0.50
76:An:92:ALA:HA	76:An:125:LYS:HB2	1.93	0.50
89:TA:150:ARG:HD2	90:TB:122:ILE:HB	1.93	0.50
1:B5:158:A:H5"	1:B5:159:C:H2'	1.94	0.50
1:B5:866:A:H8	9:BF:22:ARG:HD3	1.75	0.50
1:B5:1673:G:N2	1:B5:1674:U:O4	2.36	0.50
1:B5:1779:G:OP2	9:BF:201:LYS:NZ	2.44	0.50
1:B5:2599:G:O6	29:BZ:51:ARG:NH2	2.35	0.50
1:B5:2602:G:O2'	1:B5:2605:G:N2	2.43	0.50
1:B5:4057:A:H2'	1:B5:4058:PSU:H6	1.77	0.50
1:B5:4254:C:H5"	25:BV:43:LYS:HD3	1.92	0.50
9:BF:189:LEU:HD21	9:BF:207:LEU:HD21	1.94	0.50
44:Bp:7:LYS:O	44:Bp:27:LYS:NZ	2.40	0.50
52:A2:518:OMC:HM22	52:A2:519:G:H5'	1.93	0.50
1:B5:1648:U:OP1	20:BQ:143:ARG:NH2	2.45	0.50
6:BC:230:LEU:HD21	6:BC:236:ASN:H	1.76	0.50
49:SX:185:THR:HG22	50:SY:47:MET:HG3	1.94	0.50
52:A2:1675:G:OP1	67:Ae:51:HIS:NE2	2.33	0.50
69:Ag:117:PRO:HB2	69:Ag:120:ARG:HD3	1.93	0.50
70:Ah:22:HIS:ND1	70:Ah:23:LYS:O	2.40	0.50
83:Au:15:ARG:NH1	83:Au:33:GLN:OE1	2.44	0.50
90:TB:157:THR:HG22	91:TC:42:ILE:HD13	1.94	0.50
1:B5:1463:A:OP1	6:BC:110:ARG:NH1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1827:A:N6	1:B5:3605:G:O2'	2.43	0.50
1:B5:2011:C:H5"	9:BF:115:GLN:HE21	1.77	0.50
1:B5:4269:A2M:H5"	1:B5:4270:G:H5'	1.93	0.50
1:B5:4506:C:OP2	18:BO:171:LYS:NZ	2.36	0.50
12:BI:171:TRP:HB2	12:BI:178:ALA:HA	1.92	0.50
26:BW:94:ARG:NH1	68:Af:144:LEU:O	2.45	0.50
52:A2:90:G:OP2	93:A2:1904:SPD:N10	2.45	0.50
52:A2:1008:C:H2'	52:A2:1009:A:C8	2.47	0.50
52:A2:1245:PSU:H5"	55:AC:78:LYS:HD2	1.93	0.50
1:B5:1394:U:O2'	9:BF:33:ARG:NE	2.45	0.49
1:B5:2568:A:N6	21:BR:88:ARG:O	2.44	0.49
11:BH:41:ILE:HG22	11:BH:43:VAL:HG13	1.94	0.49
13:BJ:13:ARG:O	13:BJ:136:ARG:NH1	2.45	0.49
15:BL:7:GLY:O	30:Ba:49:HIS:NE2	2.45	0.49
52:A2:98:C:OP2	52:A2:427:A:O2'	2.29	0.49
58:AF:14:HIS:HE1	58:AF:41:ILE:HB	1.76	0.49
63:Aa:2:ALA:N	76:An:62:VAL:O	2.45	0.49
66:Ad:180:LEU:N	66:Ad:231:GLY:O	2.45	0.49
78:Ap:53:GLU:OE1	78:Ap:85:ARG:NH2	2.41	0.49
1:B5:2745:G:OP2	1:B5:3328:A:N6	2.34	0.49
1:B5:3631:OMG:HM22	1:B5:3632:G:H5'	1.95	0.49
1:B5:4699:G:H2'	1:B5:4700:G:C8	2.47	0.49
3:B8:94:G:H21	39:Bj:82:THR:HB	1.77	0.49
8:BE:151:THR:OG1	8:BE:203:LYS:NZ	2.40	0.49
11:BH:92:MET:HE2	11:BH:179:ILE:HG22	1.95	0.49
47:Bt:108:GLU:HA	47:Bt:111:ASN:HD21	1.77	0.49
47:Bt:133:LEU:HD11	47:Bt:151:ILE:HG13	1.94	0.49
49:SX:21:LYS:HB3	49:SX:171:LYS:HB3	1.94	0.49
52:A2:54:A:H3'	52:A2:452:G:H22	1.78	0.49
58:AF:91:ASP:OD2	58:AF:93:THR:OG1	2.24	0.49
1:B5:239:C:OP1	28:BY:46:SER:OG	2.30	0.49
1:B5:1763:G:H5"	23:BT:35:LYS:HE3	1.93	0.49
29:BZ:76:ASN:OD1	29:BZ:77:TYR:N	2.45	0.49
33:Bd:42:ALA:HB3	33:Bd:77:ILE:HG13	1.93	0.49
52:A2:522:A:OP1	71:Ai:45:ARG:NH1	2.40	0.49
58:AF:87:LEU:HD21	58:AF:108:VAL:HG11	1.95	0.49
58:AF:214:GLY:HA2	58:AF:236:ILE:HG13	1.94	0.49
71:Ai:54:ARG:NH1	71:Ai:98:LEU:O	2.45	0.49
80:Ar:63:GLU:HG2	80:Ar:66:ARG:HH22	1.77	0.49
1:B5:440:U:O2'	35:Bf:91:ASN:O	2.27	0.49
9:BF:235:ARG:HB2	9:BF:238:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BH:48:LEU:HD11	11:BH:56:ARG:HH11	1.77	0.49
33:Bd:26:THR:OG1	33:Bd:85:ARG:NH1	2.36	0.49
34:Be:78:LEU:HB3	45:Br:20:ARG:HD3	1.94	0.49
52:A2:371:G:O2'	70:Ah:10:LYS:NZ	2.45	0.49
52:A2:1448:OMG:OP1	82:At:85:HIS:ND1	2.46	0.49
72:Aj:4:PRO:HB2	72:Aj:7:ASN:HD22	1.77	0.49
84:Av:101:PHE:HA	84:Av:113:HIS:CE1	2.48	0.49
85:Aw:46:HIS:HB3	85:Aw:101:LEU:HD11	1.94	0.49
1:B5:1610:C:O2	1:B5:4136:A:O2'	2.31	0.49
1:B5:2601:G:O2'	1:B5:2608:A:N3	2.35	0.49
1:B5:4017:A:OP1	1:B5:4018:G:N2	2.45	0.49
2:B7:40:U:O2	13:BJ:75:ARG:NE	2.35	0.49
6:BC:60:HIS:HA	6:BC:92:PHE:HE1	1.76	0.49
8:BE:164:ARG:O	8:BE:185:ASN:ND2	2.46	0.49
27:BX:64:SER:HB2	37:Bh:69:LEU:HD13	1.94	0.49
52:A2:17:C:O2'	52:A2:1195:A:N1	2.40	0.49
64:Ab:253:PRO:HA	64:Ab:256:TRP:CE2	2.47	0.49
90:TB:19:GLU:O	90:TB:115:GLN:NE2	2.46	0.49
1:B5:2551:U:O3'	21:BR:43:LYS:NZ	2.39	0.49
1:B5:3393:G:N7	4:BA:152:SER:OG	2.43	0.49
1:B5:4500:U:OP1	35:Bf:100:ARG:NH2	2.37	0.49
11:BH:44:GLU:OE2	16:BM:2:VAL:N	2.45	0.49
34:Be:70:LEU:HD11	34:Be:76:LYS:HB3	1.94	0.49
47:Bt:147:HIS:HD2	47:Bt:149:HIS:HB2	1.76	0.49
52:A2:10:G:H21	64:Ab:114:LYS:HA	1.77	0.49
52:A2:28:U:H2'	52:A2:29:G:H8	1.78	0.49
52:A2:523:A:H5"	71:Ai:145:PRO:HD2	1.94	0.49
52:A2:619:C:H41	85:Aw:67:ARG:HH22	1.61	0.49
52:A2:1278:C:H42	52:A2:1321:G:H1	1.60	0.49
1:B5:1697:G:H2'	1:B5:1698:G:C8	2.48	0.49
1:B5:1736:G:OP1	9:BF:103:LYS:NZ	2.45	0.49
1:B5:1984:G:O6	1:B5:3602:C:O2'	2.29	0.49
1:B5:2252:U:H4'	1:B5:2271:A:H4'	1.95	0.49
1:B5:4313:G:H5'	5:BB:20:LYS:HB3	1.94	0.49
1:B5:4649:A:H4'	5:BB:95:THR:HG22	1.95	0.49
6:BC:60:HIS:NE2	6:BC:100:ARG:HD3	2.28	0.49
15:BL:201:GLU:O	15:BL:205:GLN:N	2.45	0.49
52:A2:689:U:OP1	69:Ag:116:ARG:NH2	2.46	0.49
70:Ah:81:VAL:HG22	70:Ah:102:VAL:HG12	1.95	0.49
9:BF:53:ALA:HB2	9:BF:187:GLU:HG3	1.94	0.49
15:BL:12:PRO:HB2	15:BL:14:PHE:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:445:G:H4'	93:A2:1904:SPD:H91	1.95	0.49
58:AF:39:THR:HG22	58:AF:60:ARG:HG2	1.94	0.49
73:Ak:18:GLN:HG2	73:Ak:33:LEU:HD21	1.93	0.49
1:B5:1994:G:O5'	18:BO:130:LYS:NZ	2.45	0.49
1:B5:2110:U:OP1	45:Br:37:SER:OG	2.27	0.49
19:BP:19:GLY:N	19:BP:146:ILE:O	2.44	0.49
25:BV:13:LYS:HB3	25:BV:128:LEU:HD11	1.94	0.49
34:Be:65:LYS:O	34:Be:75:ARG:NH2	2.45	0.49
48:Bv:60:ARG:HD3	48:Bv:173:LYS:HB2	1.95	0.49
49:SX:248:THR:HG23	49:SX:441:ILE:HG23	1.95	0.49
52:A2:1846:A:H2'	52:A2:1847:G:C8	2.48	0.49
61:AT:42:A:H4'	87:Ay:33:LYS:HE3	1.93	0.49
63:Aa:86:LEU:HB3	63:Aa:98:THR:HB	1.94	0.49
1:B5:1308:U:OP2	15:BL:36:ARG:NH2	2.44	0.49
1:B5:2667:OMC:HM22	1:B5:2668:A:H5'	1.95	0.49
1:B5:4316:G:H2'	1:B5:4317:A2M:H8	1.95	0.49
6:BC:239:LYS:O	6:BC:248:ARG:NH1	2.39	0.49
12:BI:53:VAL:HG11	23:BT:158:PHE:HZ	1.78	0.49
52:A2:469:A2M:HM'2	52:A2:470:A:H5'	1.95	0.49
52:A2:1286:G:H1	74:Al:57:ASP:HB2	1.78	0.49
68:Af:102:VAL:HG13	68:Af:106:LEU:HD12	1.95	0.49
1:B5:699:G:OP1	34:Be:5:ARG:NH2	2.46	0.48
1:B5:1381:G:N2	1:B5:1413:C:OP2	2.39	0.48
1:B5:1942:G:N2	1:B5:1943:U:O4	2.42	0.48
1:B5:4186:G:O3'	12:BI:112:GLN:NE2	2.46	0.48
4:BA:137:ILE:HD11	4:BA:149:LYS:HB2	1.93	0.48
16:BM:126:GLU:HA	16:BM:129:LYS:HE2	1.95	0.48
20:BQ:122:THR:OG1	20:BQ:124:ASP:OD1	2.23	0.48
46:Bs:45:MET:HG3	46:Bs:48:ARG:HH21	1.77	0.48
49:SX:61:PRO:HB2	49:SX:64:TRP:HB2	1.95	0.48
52:A2:630:A:O2'	52:A2:632:U:OP1	2.31	0.48
52:A2:1522:C:H5'	77:Ao:126:VAL:HB	1.95	0.48
55:AC:118:ARG:NH1	55:AC:134:SER:OG	2.45	0.48
56:AD:102:ARG:HD3	56:AD:106:ALA:HB1	1.94	0.48
57:AE:23:CYS:HB3	57:AE:28:ARG:H	1.78	0.48
90:TB:150:TRP:HA	90:TB:153:PHE:HB3	1.95	0.48
1:B5:423:G:N2	19:BP:118:GLN:OE1	2.41	0.48
1:B5:1008:C:H2'	1:B5:1009:G:H8	1.78	0.48
1:B5:1093:C:H2'	1:B5:1094:A:C8	2.48	0.48
1:B5:1315:A:N1	3:B8:28:C:O2'	2.47	0.48
1:B5:3498:A:O2'	52:A2:1850:G:N3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:3792:C:H2’	1:B5:3793:G:C8	2.47	0.48
10:BG:83:PHE:HA	10:BG:183:ILE:HD13	1.95	0.48
21:BR:12:SER:OG	21:BR:17:CYS:O	2.24	0.48
52:A2:1618:G:N1	52:A2:1621:A:OP2	2.46	0.48
64:Ab:91:SER:HB3	64:Ab:156:ILE:HG23	1.95	0.48
1:B5:4323:U:H2’	1:B5:4324:G:C8	2.48	0.48
3:B8:57:C:OP2	39:Bj:68:LYS:NZ	2.45	0.48
16:BM:29:ASP:OD1	16:BM:30:VAL:N	2.45	0.48
26:BW:80:ARG:NH1	52:A2:167:G:O2’	2.47	0.48
48:Bv:138:LEU:HD21	48:Bv:147:LYS:HG2	1.96	0.48
52:A2:1373:U:OP1	52:A2:1386:G:N2	2.33	0.48
1:B5:345:C:H2’	1:B5:346:G:C8	2.48	0.48
1:B5:1641:C:OP1	31:Bb:19:ASN:ND2	2.45	0.48
1:B5:2207:OMG:HM22	1:B5:2208:OMC:H5”	1.94	0.48
1:B5:2323:G:H2’	1:B5:2324:G:C8	2.48	0.48
1:B5:3780:C:O2’	48:Bv:207:LYS:NZ	2.41	0.48
1:B5:4194:G:H5”	1:B5:4195:A:H5”	1.94	0.48
1:B5:4511:A:N6	11:BH:60:TRP:O	2.38	0.48
4:BA:140:ASN:ND2	4:BA:143:THR:OG1	2.46	0.48
16:BM:40:GLY:HA3	16:BM:45:VAL:HB	1.94	0.48
49:SX:220:LEU:O	49:SX:226:LYS:NZ	2.45	0.48
52:A2:1776:U:H2’	52:A2:1777:G:C8	2.48	0.48
78:Ap:76:GLY:H	78:Ap:79:ALA:HB3	1.78	0.48
1:B5:521:C:O2’	15:BL:115:GLN:OE1	2.29	0.48
1:B5:696:U:H5’	8:BE:124:VAL:HG21	1.95	0.48
1:B5:1210:C:H2’	1:B5:1211:G:H8	1.76	0.48
1:B5:3965:A:H5”	23:BT:2:THR:HG22	1.94	0.48
1:B5:3975:U:H4’	43:Bo:89:LYS:HE2	1.96	0.48
1:B5:4698:U:H2’	1:B5:4699:G:C8	2.48	0.48
49:SX:379:TRP:NE1	49:SX:383:SER:OG	2.47	0.48
52:A2:17:C:H2’	52:A2:18:C:C6	2.48	0.48
52:A2:119:PSU:O4	66:Ad:33:THR:OG1	2.26	0.48
52:A2:1099:C:H2’	52:A2:1100:G:C8	2.49	0.48
52:A2:1805:OMU:HM22	52:A2:1806:G:H5’	1.94	0.48
63:Aa:28:LYS:NZ	76:An:51:GLU:OE1	2.42	0.48
5:BB:41:VAL:HA	5:BB:187:GLY:HA3	1.95	0.48
23:BT:94:GLU:OE1	23:BT:94:GLU:N	2.44	0.48
37:Bh:86:LYS:O	37:Bh:92:ARG:NH1	2.37	0.48
38:Bi:29:ARG:HA	38:Bi:32:ARG:HH21	1.79	0.48
52:A2:617:A:H1’	56:AD:86:VAL:HG23	1.94	0.48
52:A2:864:PSU:O2’	84:Av:78:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ae:129:GLY:HA3	67:Ae:135:ARG:HH22	1.78	0.48
1:B5:1458:A:H4'	1:B5:1459:G:H5'	1.95	0.48
1:B5:1678:G:N3	1:B5:1681:A:N6	2.61	0.48
1:B5:2167:C:O2'	34:Be:98:GLU:OE2	2.29	0.48
1:B5:2265:OMC:HM22	1:B5:2266:A:H5'	1.95	0.48
5:BB:224:LYS:HE3	5:BB:340:THR:HG22	1.96	0.48
7:BD:128:ASP:O	7:BD:164:LYS:NZ	2.44	0.48
25:BV:87:SER:HB3	26:BW:19:ARG:HH21	1.78	0.48
42:Bm:113:LYS:HG2	42:Bm:117:HIS:HE1	1.79	0.48
48:Bv:104:ALA:O	48:Bv:133:LYS:NZ	2.45	0.48
49:SX:22:PRO:HB3	51:SZ:69:GLY:HA2	1.95	0.48
52:A2:609:C:H2'	52:A2:610:PSU:H6	1.79	0.48
52:A2:646:C:H2'	52:A2:647:G:H8	1.78	0.48
52:A2:1017:U:H5"	75:Am:14:SER:HB3	1.95	0.48
52:A2:1473:C:O2'	58:AF:15:ASN:ND2	2.47	0.48
66:Ad:151:ASP:HB3	66:Ad:154:ILE:HG13	1.95	0.48
1:B5:2261:A:H5"	19:BP:125:MET:HE1	1.95	0.48
1:B5:2678:A:O2'	5:BB:228:TYR:O	2.32	0.48
1:B5:3432:C:H2'	1:B5:3478:A:H61	1.78	0.48
11:BH:137:SER:HB2	11:BH:145:VAL:HG23	1.95	0.48
18:BO:81:TRP:HB2	18:BO:104:VAL:HG21	1.96	0.48
49:SX:441:ILE:HG22	49:SX:447:ILE:HD12	1.94	0.48
52:A2:1284:C:H41	74:Al:102:LYS:HE2	1.79	0.48
56:AD:91:LEU:HD23	56:AD:91:LEU:H	1.79	0.48
64:Ab:128:VAL:HG11	64:Ab:155:ILE:HG12	1.95	0.48
67:Ae:40:ALA:HB1	67:Ae:45:TYR:CG	2.48	0.48
89:TA:135:GLN:HB2	89:TA:164:MET:HE1	1.96	0.48
1:B5:70:A:OP2	30:Ba:64:LYS:NZ	2.37	0.48
1:B5:1335:A:N7	93:B5:4903:SPD:N10	2.62	0.48
1:B5:2127:G:OP1	30:Ba:7:LYS:NZ	2.40	0.48
17:BN:120:TRP:HE1	17:BN:123:GLU:HB3	1.79	0.48
52:A2:989:C:H1'	63:Aa:120:MET:HE3	1.95	0.48
52:A2:1088:A:OP1	57:AE:3:LYS:NZ	2.42	0.48
52:A2:1764:G:H2'	52:A2:1765:G:C8	2.49	0.48
1:B5:385:A:H4'	1:B5:386:A:H5'	1.96	0.48
1:B5:2131:G:O2'	1:B5:2133:C:O5'	2.30	0.48
1:B5:4445:U:H1'	1:B5:4446:A:H5"	1.96	0.48
12:BI:48:LEU:HB2	12:BI:142:LEU:HD23	1.96	0.48
19:BP:5:SER:OG	19:BP:116:HIS:NE2	2.46	0.48
39:Bj:20:ARG:NH1	39:Bj:39:TYR:OH	2.43	0.48
50:SY:65:ILE:HG23	51:SZ:88:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:116:OMU:HM22	52:A2:117:C:H5'	1.96	0.48
52:A2:191:A:H3'	52:A2:192:C:H5"	1.96	0.48
62:AZ:63:ARG:HH21	83:Au:38:GLU:HA	1.78	0.48
74:Al:125:GLU:OE1	74:Al:129:LYS:NZ	2.47	0.48
1:B5:2146:C:OP1	34:Be:107:ASN:ND2	2.47	0.47
5:BB:317:LEU:HD22	5:BB:382:VAL:HG13	1.94	0.47
11:BH:16:VAL:HG21	11:BH:81:ILE:HG23	1.95	0.47
25:BV:84:GLN:NE2	25:BV:86:LYS:O	2.46	0.47
46:Bs:68:HIS:HB3	46:Bs:75:LEU:HD22	1.95	0.47
52:A2:1666:G:P	81:As:91:HIS:HE2	2.35	0.47
1:B5:404:U:O3'	28:BY:87:ARG:NH2	2.45	0.47
1:B5:706:C:OP1	8:BE:142:LYS:NZ	2.42	0.47
1:B5:3798:U:H2'	1:B5:3799:U:C6	2.49	0.47
1:B5:3998:C:H42	13:BJ:25:CYS:HB3	1.77	0.47
1:B5:4485:C:H42	1:B5:4699:G:H1	1.62	0.47
6:BC:45:ARG:O	6:BC:48:ASN:ND2	2.46	0.47
9:BF:181:TYR:CZ	9:BF:202:GLU:HG2	2.50	0.47
46:Bs:53:VAL:HG13	46:Bs:89:VAL:HG22	1.96	0.47
47:Bt:125:LEU:HD12	47:Bt:164:ALA:HB3	1.95	0.47
52:A2:1104:C:H2'	52:A2:1105:G:C8	2.49	0.47
52:A2:1236:G:O2'	77:Ao:134:GLY:O	2.29	0.47
91:TC:77:TYR:HE1	91:TC:141:ASN:HB2	1.79	0.47
1:B5:40:G:N7	93:B5:4907:SPD:N1	2.60	0.47
1:B5:186:G:N2	1:B5:186:G:OP2	2.48	0.47
1:B5:4204:C:H2'	1:B5:4205:U:C6	2.49	0.47
4:BA:3:ARG:HG2	4:BA:207:VAL:HG22	1.97	0.47
13:BJ:52:LYS:HB3	13:BJ:65:ASN:HA	1.95	0.47
15:BL:116:ARG:NH2	15:BL:155:MET:O	2.39	0.47
18:BO:130:LYS:HB2	18:BO:133:ARG:HG2	1.95	0.47
20:BQ:133:GLY:O	20:BQ:136:THR:OG1	2.29	0.47
62:AZ:214:GLU:HG2	79:Aq:80:ARG:HH12	1.79	0.47
64:Ab:131:GLY:HA3	64:Ab:216:MET:HB3	1.96	0.47
1:B5:1834:G:O2'	1:B5:1846:A:N3	2.43	0.47
1:B5:1868:A:C8	1:B5:1871:A:H1'	2.50	0.47
1:B5:2243:G:H21	36:Bg:6:THR:HG22	1.80	0.47
1:B5:2301:C:O2'	1:B5:3403:G:N3	2.47	0.47
1:B5:3352:G:OP1	1:B5:3354:C:N4	2.48	0.47
1:B5:3942:OMG:HM22	1:B5:3943:G:H5'	1.96	0.47
1:B5:4043:G:H2'	1:B5:4044:A:H8	1.78	0.47
1:B5:4693:G:H2'	1:B5:4694:A:C8	2.49	0.47
3:B8:36:G:C5	37:Bh:89:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BD:59:ASP:OD1	7:BD:60:ILE:N	2.47	0.47
36:Bg:68:SER:OG	36:Bg:71:LYS:NZ	2.39	0.47
49:SX:132:VAL:HG12	49:SX:151:ILE:HD12	1.96	0.47
52:A2:1453:A:O2'	52:A2:1476:G:N2	2.48	0.47
52:A2:1610:C:OP2	80:Ar:134:GLN:NE2	2.47	0.47
52:A2:1855:U:OP1	76:An:150:ARG:NH2	2.47	0.47
76:An:29:GLY:O	76:An:94:HIS:N	2.35	0.47
78:Ap:24:HIS:HE1	78:Ap:26:LYS:HD3	1.80	0.47
1:B5:38:A:H5"	30:Ba:35:ALA:HB2	1.97	0.47
1:B5:1888:U:OP1	11:BH:64:ARG:NH1	2.48	0.47
1:B5:2687:A:N6	1:B5:3571:G:O2'	2.47	0.47
1:B5:4004:C:OP2	13:BJ:54:ARG:NH1	2.47	0.47
6:BC:76:ILE:HD12	6:BC:77:PRO:HD2	1.97	0.47
16:BM:5:ARG:NE	16:BM:59:ASP:OD1	2.48	0.47
16:BM:47:ARG:NH2	16:BM:68:ALA:O	2.43	0.47
46:Bs:48:ARG:HH11	47:Bt:123:ARG:HG2	1.79	0.47
48:Bv:59:PRO:HG2	48:Bv:63:PHE:HE1	1.79	0.47
52:A2:190:G:O2'	52:A2:209:A:N6	2.47	0.47
52:A2:1758:G:H2'	52:A2:1759:G:H8	1.79	0.47
70:Ah:83:TYR:HB3	70:Ah:101:ILE:HB	1.97	0.47
1:B5:1005:G:OP1	23:BT:142:ARG:NH1	2.38	0.47
1:B5:3664:U:H2'	1:B5:3665:G:C8	2.49	0.47
7:BD:122:GLN:NE2	7:BD:126:THR:OG1	2.44	0.47
15:BL:87:HIS:HB3	15:BL:90:VAL:HG23	1.96	0.47
43:Bo:12:CYS:HB3	43:Bo:15:CYS:HB2	1.95	0.47
49:SX:267:ILE:HG22	49:SX:399:MET:HE3	1.97	0.47
52:A2:621:G:O4'	93:A2:1902:SPD:N1	2.48	0.47
52:A2:1639:G:H4'	87:Ay:36:SER:HB3	1.96	0.47
66:Ad:55:ALA:HB1	66:Ad:60:GLU:HB2	1.96	0.47
67:Ae:110:GLN:HE21	67:Ae:114:ASN:HD21	1.63	0.47
1:B5:4668:C:H5"	16:BM:114:LYS:HD2	1.97	0.47
4:BA:45:VAL:HG22	4:BA:61:VAL:HG22	1.96	0.47
19:BP:52:THR:HG23	19:BP:85:LYS:HG3	1.96	0.47
33:Bd:37:GLY:O	33:Bd:41:ARG:HG3	2.15	0.47
34:Be:37:LYS:HD2	34:Be:38:PRO:HD2	1.96	0.47
49:SX:286:THR:C	49:SX:288:ASN:H	2.21	0.47
52:A2:430:C:O2'	52:A2:812:A:N1	2.47	0.47
52:A2:1757:C:H2'	52:A2:1758:G:C8	2.49	0.47
58:AF:32:LEU:HB2	58:AF:71:ILE:HD11	1.97	0.47
58:AF:73:SER:OG	58:AF:117:ASN:OD1	2.28	0.47
58:AF:107:ASP:HB2	58:AF:125:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Ab:232:THR:HG22	64:Ab:235:ASN:H	1.80	0.47
90:TB:21:ALA:HB3	90:TB:114:ALA:HA	1.96	0.47
91:TC:79:ASN:HB2	91:TC:181:SER:HB2	1.97	0.47
1:B5:327:U:O2'	38:Bi:30:ARG:NH1	2.47	0.47
1:B5:1788:U:H3'	15:BL:5:ARG:NH2	2.30	0.47
16:BM:27:ILE:HD13	16:BM:38:VAL:HG12	1.97	0.47
49:SX:268:LYS:HD2	49:SX:276:TYR:CZ	2.49	0.47
52:A2:1546:A:H4'	78:Ap:74:GLY:HA2	1.97	0.47
52:A2:1706:C:H2'	52:A2:1707:G:C8	2.49	0.47
52:A2:1843:4AC:O7	88:Az:4:LYS:NZ	2.47	0.47
66:Ad:100:ARG:HH12	66:Ad:122:LYS:HA	1.79	0.47
90:TB:111:THR:HG22	90:TB:122:ILE:HG12	1.97	0.47
1:B5:156:G:N2	1:B5:157:U:O4	2.48	0.47
1:B5:2420:C:OP1	29:BZ:111:ARG:NH1	2.48	0.47
1:B5:4450:C:H2'	1:B5:4451:A:C8	2.49	0.47
6:BC:278:ASN:OD1	6:BC:279:LEU:N	2.48	0.47
7:BD:197:LYS:HB3	7:BD:202:GLN:HB2	1.96	0.47
8:BE:193:HIS:HB3	8:BE:196:PHE:HD2	1.80	0.47
19:BP:131:ARG:HG3	19:BP:137:ASN:ND2	2.30	0.47
26:BW:60:LYS:O	26:BW:64:SER:OG	2.31	0.47
52:A2:1098:G:H4'	62:AZ:32:PHE:CD1	2.50	0.47
52:A2:1653:G:H1	52:A2:1673:U:H3	1.63	0.47
58:AF:150:TRP:NE1	79:Aq:37:GLU:OE1	2.47	0.47
62:AZ:189:ILE:HG22	62:AZ:191:ARG:H	1.79	0.47
66:Ad:87:MET:HE2	66:Ad:123:LEU:HB2	1.97	0.47
78:Ap:86:GLN:HE22	78:Ap:122:ALA:HB2	1.78	0.47
87:Ay:79:ILE:HB	87:Ay:83:LEU:HD23	1.97	0.47
1:B5:2364:G:H5'	1:B5:2483:G:H1'	1.96	0.47
1:B5:3480:A:HO2'	4:BA:223:SER:HG	1.62	0.47
1:B5:4331:U:H2'	1:B5:4332:G:H8	1.80	0.47
12:BI:51:HIS:HD2	12:BI:168:SER:HB2	1.80	0.47
32:Bc:4:ALA:O	32:Bc:7:THR:OG1	2.29	0.47
52:A2:126:G:H8	68:Af:199:THR:HG21	1.79	0.47
52:A2:1564:G:OP1	81:As:121:ARG:NH1	2.44	0.47
58:AF:12:LYS:HG2	58:AF:306:LEU:HD22	1.97	0.47
58:AF:290:ALA:HB3	58:AF:299:PHE:HB2	1.97	0.47
65:Ac:93:THR:HG22	65:Ac:95:GLY:H	1.80	0.47
1:B5:1696:U:H2'	1:B5:1697:G:C8	2.50	0.46
1:B5:4672:C:H42	1:B5:4673:A:H62	1.61	0.46
3:B8:58:G:N7	39:Bj:63:ARG:NH2	2.54	0.46
6:BC:29:LYS:O	6:BC:282:HIS:NE2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BX:89:LYS:HB3	27:BX:95:THR:HB	1.97	0.46
27:BX:91:GLU:OE2	49:SX:415:ARG:NH2	2.32	0.46
34:Be:104:SER:O	34:Be:108:ARG:HG3	2.15	0.46
43:Bo:28:LYS:NZ	43:Bo:31:ASP:OD1	2.46	0.46
52:A2:686:A:H5"	84:Av:31:SER:HB3	1.96	0.46
56:AD:112:TYR:CG	71:Ai:33:GLY:HA3	2.49	0.46
70:Ah:106:SER:HB3	70:Ah:171:LEU:HG	1.97	0.46
75:Am:93:LYS:HA	75:Am:150:VAL:HG21	1.98	0.46
1:B5:1134:G:H1	1:B5:1206:C:H42	1.61	0.46
1:B5:2615:C:O3'	40:Bk:17:ARG:NH2	2.48	0.46
1:B5:3886:G:H2'	1:B5:3887:G:H8	1.80	0.46
1:B5:3958:A:N1	23:BT:3:ASN:ND2	2.54	0.46
1:B5:3974:OMG:H5"	1:B5:3975:U:O4'	2.15	0.46
1:B5:4609:G:H5"	16:BM:91:TRP:CE2	2.51	0.46
4:BA:116:LEU:N	4:BA:126:LEU:O	2.48	0.46
6:BC:25:PRO:HB2	6:BC:27:VAL:HG12	1.97	0.46
53:AA:12:PRO:HB3	69:Ag:192:PHE:CG	2.50	0.46
55:AC:126:CYS:HB3	55:AC:143:LYS:HD3	1.97	0.46
1:B5:62:A:N3	1:B5:77:U:O2'	2.43	0.46
1:B5:443:G:H5"	35:Bf:54:LYS:HB3	1.98	0.46
1:B5:526:C:H2'	1:B5:527:G:C8	2.51	0.46
1:B5:1737:G:O2'	23:BT:60:LYS:NZ	2.48	0.46
1:B5:1919:U:H5	47:Bt:92:ARG:HH22	1.62	0.46
1:B5:2359:G:OP2	36:Bg:37:LYS:NZ	2.45	0.46
1:B5:2646:U:H2'	1:B5:2647:OMC:H6	1.80	0.46
1:B5:4328:C:O2'	5:BB:99:LEU:O	2.20	0.46
2:B7:77:A:H62	2:B7:99:G:H21	1.62	0.46
3:B8:9:A:H2'	3:B8:10:G:H8	1.80	0.46
3:B8:101:C:O2'	39:Bj:20:ARG:O	2.26	0.46
47:Bt:137:GLN:HB3	47:Bt:148:PRO:HG2	1.97	0.46
52:A2:398:G:OP2	73:Ak:108:ASN:ND2	2.49	0.46
52:A2:944:U:O2'	76:An:135:ILE:O	2.33	0.46
52:A2:1085:A:OP1	52:A2:1859:G:O2'	2.27	0.46
52:A2:1209:A:O2'	52:A2:1836:A:N7	2.46	0.46
52:A2:1234:G:N3	52:A2:1253:C:O2'	2.44	0.46
52:A2:1678:U:O4	52:A2:1679:A2M:N6	2.49	0.46
56:AD:122:THR:HG21	56:AD:126:LYS:HG2	1.96	0.46
70:Ah:113:TYR:OH	70:Ah:156:ALA:O	2.32	0.46
83:Au:38:GLU:OE2	83:Au:51:LYS:NZ	2.48	0.46
1:B5:74:G:O6	15:BL:103:ARG:NH2	2.47	0.46
1:B5:3455:A:OP2	38:Bi:68:ARG:NH2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:147:G:H2'	3:B8:148:A:H8	1.79	0.46
12:BI:46:PHE:HB2	12:BI:139:ARG:HH11	1.81	0.46
21:BR:31:GLU:HA	21:BR:34:ASN:HD21	1.81	0.46
47:Bt:18:THR:OG1	47:Bt:21:GLU:O	2.27	0.46
48:Bv:117:ILE:HD13	48:Bv:137:LEU:HD21	1.97	0.46
50:SY:17:ASP:OD1	50:SY:20:ARG:NH2	2.49	0.46
52:A2:1222:G:H2'	52:A2:1223:G:C8	2.51	0.46
69:Ag:65:PRO:HD2	69:Ag:68:GLN:HE21	1.80	0.46
73:Ak:84:ARG:O	73:Ak:112:HIS:ND1	2.48	0.46
77:Ao:123:TYR:OH	80:Ar:124:ARG:NH1	2.48	0.46
89:TA:96:PRO:HG2	89:TA:99:ASN:HB2	1.97	0.46
89:TA:97:ALA:HB3	89:TA:198:GLU:HA	1.97	0.46
1:B5:382:G:N1	1:B5:385:A:OP2	2.47	0.46
1:B5:1688:A:H2'	1:B5:1689:G:C8	2.51	0.46
5:BB:55:HIS:NE2	5:BB:369:ASP:OD2	2.48	0.46
7:BD:204:VAL:HB	7:BD:236:MET:HE1	1.98	0.46
10:BG:51:LEU:O	10:BG:55:VAL:HG23	2.16	0.46
21:BR:163:ARG:HA	52:A2:874:G:H5'	1.96	0.46
49:SX:43:LEU:HB3	50:SY:58:HIS:NE2	2.30	0.46
49:SX:401:MET:HG3	49:SX:409:MET:HE1	1.97	0.46
49:SX:408:SER:O	49:SX:412:GLU:HG2	2.16	0.46
52:A2:383:C:H2'	52:A2:384:G:C8	2.50	0.46
53:AA:67:THR:OG1	53:AA:70:LYS:O	2.34	0.46
55:AC:102:VAL:HA	55:AC:105:TYR:HD2	1.80	0.46
72:Aj:16:PHE:HE2	72:Aj:89:ILE:HG22	1.81	0.46
1:B5:25:A:N3	1:B5:339:C:O2'	2.43	0.46
1:B5:387:G:OP2	28:BY:89:LYS:NZ	2.46	0.46
1:B5:1093:C:H2'	1:B5:1094:A:H8	1.81	0.46
1:B5:1298:A:N1	1:B5:1329:G:O2'	2.46	0.46
1:B5:1697:G:H2'	1:B5:1698:G:H8	1.81	0.46
1:B5:2557:G:H2'	1:B5:2558:G:H8	1.80	0.46
1:B5:2706:G:O2'	21:BR:82:LYS:O	2.25	0.46
5:BB:291:TYR:HB3	5:BB:298:LEU:HD11	1.96	0.46
46:Bs:85:ASN:OD1	46:Bs:85:ASN:N	2.43	0.46
52:A2:65:C:C6	68:Af:174:PRO:HB3	2.51	0.46
52:A2:67:C:N4	68:Af:168:LYS:O	2.49	0.46
52:A2:171:A:OP2	68:Af:137:ARG:NH2	2.42	0.46
68:Af:159:ARG:HB3	68:Af:171:THR:HB	1.97	0.46
1:B5:287:U:H2'	1:B5:288:G:C8	2.51	0.46
3:B8:82:A:OP1	3:B8:86:U:O2'	2.32	0.46
52:A2:1249:B8N:O2'	78:Ap:145:TYR:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AF:108:VAL:HA	58:AF:124:SER:HA	1.98	0.46
64:Ab:70:VAL:HG21	64:Ab:93:ILE:HG23	1.97	0.46
80:Ar:124:ARG:HB2	80:Ar:131:VAL:HG12	1.98	0.46
1:B5:781:C:H2'	1:B5:782:G:C8	2.50	0.46
1:B5:1922:A:H1'	1:B5:1949:A:H4'	1.98	0.46
1:B5:2204:G:O2'	1:B5:3591:G:O6	2.26	0.46
1:B5:3897:G:H2'	1:B5:3898:G:H8	1.80	0.46
1:B5:4089:U:O2'	43:Bo:31:ASP:OD1	2.31	0.46
22:BS:29:ARG:HB2	23:BT:148:PRO:HB2	1.98	0.46
30:Ba:103:VAL:HB	30:Ba:108:TYR:HB2	1.98	0.46
48:Bv:37:SER:HB2	48:Bv:202:ARG:HB2	1.96	0.46
49:SX:454:ILE:O	49:SX:458:PHE:N	2.46	0.46
52:A2:1172:G:O2'	52:A2:1188:G:O6	2.29	0.46
52:A2:1534:A:OP2	67:Ae:164:ARG:NH1	2.48	0.46
52:A2:1758:G:H2'	52:A2:1759:G:C8	2.51	0.46
58:AF:62:HIS:HD2	58:AF:66:VAL:HG22	1.81	0.46
1:B5:1699:G:H2'	1:B5:1700:G:H8	1.81	0.46
1:B5:1907:G:H2'	1:B5:1908:G:C8	2.50	0.46
1:B5:2371:G:H4'	1:B5:2626:A:H4'	1.97	0.46
1:B5:3488:A:H2'	1:B5:3489:G:H8	1.81	0.46
1:B5:3997:A:H5"	13:BJ:108:GLY:HA3	1.97	0.46
10:BG:75:LYS:HG2	10:BG:240:ASN:HB2	1.98	0.46
12:BI:42:LYS:HB2	12:BI:45:GLU:HG3	1.97	0.46
46:Bs:93:GLU:HG2	46:Bs:94:ASP:H	1.80	0.46
52:A2:378:G:H5'	70:Ah:98:LYS:HB3	1.98	0.46
52:A2:602:OMG:HM22	52:A2:603:G:H5'	1.97	0.46
52:A2:1118:C:O2'	52:A2:1119:C:O4'	2.34	0.46
52:A2:1508:G:N2	55:AC:87:THR:O	2.26	0.46
1:B5:417:G:H1'	3:B8:16:G:N2	2.30	0.46
1:B5:752:G:H1	1:B5:803:C:H42	1.63	0.46
1:B5:1489:A2M:N3	39:Bj:11:ARG:HB2	2.31	0.46
1:B5:1784:U:H2'	1:B5:1785:G:C8	2.51	0.46
1:B5:3800:C:H2'	1:B5:3801:A:C8	2.51	0.46
1:B5:4805:U:H2'	1:B5:4806:U:C6	2.51	0.46
3:B8:120:G:H1	3:B8:130:C:H42	1.64	0.46
6:BC:66:SER:HA	6:BC:77:PRO:HA	1.97	0.46
8:BE:45:HIS:ND1	8:BE:46:CYS:O	2.49	0.46
8:BE:98:PRO:HA	8:BE:107:THR:HA	1.97	0.46
48:Bv:196:LYS:HG2	48:Bv:199:GLN:HB2	1.98	0.46
52:A2:984:A:OP1	52:A2:1074:U:O2'	2.31	0.46
55:AC:126:CYS:HB2	55:AC:130:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AT:47:C:C2	61:AT:58:A:H1'	2.51	0.46
64:Ab:94:ILE:HG21	64:Ab:162:ILE:HD12	1.98	0.46
80:Ar:18:THR:HG21	80:Ar:33:ILE:HA	1.98	0.46
1:B5:1493:U:H2'	1:B5:1494:G:H8	1.80	0.45
1:B5:3419:A:O2'	4:BA:236:GLY:N	2.50	0.45
1:B5:3894:C:OP1	29:BZ:59:LYS:NZ	2.32	0.45
1:B5:4041:U:H2'	1:B5:4042:PSU:H6	1.81	0.45
1:B5:4714:G:O2'	1:B5:4716:A:N6	2.46	0.45
6:BC:316:LYS:HB2	6:BC:324:ILE:HG13	1.97	0.45
11:BH:41:ILE:HD13	11:BH:69:THR:HB	1.98	0.45
26:BW:94:ARG:HH12	68:Af:144:LEU:HD12	1.80	0.45
29:BZ:9:LYS:HB3	29:BZ:25:ILE:HD12	1.97	0.45
73:Ak:68:ILE:HD13	73:Ak:131:CYS:HB3	1.97	0.45
85:Aw:124:LYS:HG2	85:Aw:129:SER:HA	1.97	0.45
1:B5:208:A:H2	1:B5:233:U:H5"	1.81	0.45
1:B5:3805:A:N1	1:B5:3917:C:N4	2.65	0.45
1:B5:4271:C:H5"	5:BB:245:HIC:HB2	1.97	0.45
27:BX:39:LYS:HB3	27:BX:40:ILE:H	1.55	0.45
30:Ba:14:HIS:O	30:Ba:16:SER:N	2.50	0.45
44:Bp:26:VAL:HG22	44:Bp:30:GLU:HG2	1.98	0.45
52:A2:35:C:H5"	52:A2:580:C:H5"	1.97	0.45
52:A2:646:C:H2'	52:A2:647:G:C8	2.51	0.45
52:A2:657:G:H5'	52:A2:663:G:N2	2.30	0.45
52:A2:935:G:H22	52:A2:1009:A:H2	1.64	0.45
52:A2:1590:A:N3	52:A2:1654:U:O2'	2.44	0.45
57:AE:3:LYS:NZ	57:AE:8:ASN:OD1	2.49	0.45
67:Ae:19:LEU:HD21	67:Ae:69:VAL:HG11	1.97	0.45
1:B5:733:C:H4'	16:BM:69:ARG:HH21	1.81	0.45
1:B5:1806:A:N3	1:B5:4149:PSU:O2'	2.42	0.45
1:B5:3488:A:H2'	1:B5:3489:G:C8	2.51	0.45
1:B5:3856:A:H1'	10:BG:35:ARG:HB2	1.99	0.45
1:B5:4051:G:O5'	23:BT:83:LYS:NZ	2.49	0.45
20:BQ:88:ASP:HB2	20:BQ:109:ALA:HB2	1.98	0.45
49:SX:302:TYR:CE1	49:SX:341:LEU:HD22	2.52	0.45
52:A2:1615:A:OP2	77:Ao:42:ARG:NH2	2.35	0.45
58:AF:40:ILE:O	58:AF:59:LEU:N	2.43	0.45
1:B5:150:U:N3	10:BG:162:ASP:O	2.43	0.45
1:B5:1772:G:N2	1:B5:1774:G:O4'	2.49	0.45
1:B5:1879:G:H22	1:B5:4180:C:H5"	1.80	0.45
5:BB:19:ARG:HB2	5:BB:234:ARG:NH2	2.32	0.45
6:BC:140:LYS:HE3	6:BC:245:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BR:30:ASN:O	21:BR:34:ASN:ND2	2.50	0.45
45:Br:26:SER:OG	45:Br:28:GLU:OE1	2.28	0.45
48:Bv:54:ARG:HH22	48:Bv:150:GLU:HB3	1.82	0.45
52:A2:1657:G:H1	52:A2:1669:U:H3	1.64	0.45
61:AT:39:C:H2'	61:AT:40:G:H8	1.80	0.45
75:Am:20:ARG:HH21	84:Av:56:HIS:HB3	1.82	0.45
1:B5:114:G:N2	1:B5:158:A:H61	2.15	0.45
1:B5:734:G:OP2	16:BM:71:LYS:NZ	2.47	0.45
1:B5:2252:U:H2'	1:B5:2252:U:O2	2.16	0.45
1:B5:4669:C:H5"	8:BE:269:GLN:HG2	1.99	0.45
5:BB:248:LEU:HD12	5:BB:249:ARG:HG3	1.97	0.45
6:BC:221:PHE:HB3	6:BC:227:ILE:HG21	1.98	0.45
10:BG:265:LEU:HD23	10:BG:265:LEU:H	1.81	0.45
46:Bs:53:VAL:HG22	46:Bs:89:VAL:HG13	1.99	0.45
52:A2:417:U:O2'	52:A2:653:U:O2'	2.25	0.45
52:A2:1014:U:OP1	52:A2:1130:G:O2'	2.34	0.45
58:AF:88:ARG:HH11	58:AF:97:THR:HG21	1.82	0.45
72:Aj:63:ALA:HB3	72:Aj:68:TYR:HE2	1.81	0.45
1:B5:1603:C:OP1	93:B5:4919:SPD:N10	2.47	0.45
1:B5:4431:U:H2'	1:B5:4432:G:C8	2.52	0.45
1:B5:4637:G:N2	1:B5:4661:C:O2	2.28	0.45
8:BE:273:TYR:OH	16:BM:106:ASP:OD2	2.31	0.45
11:BH:44:GLU:HB3	11:BH:58:ASP:HB2	1.99	0.45
36:Bg:60:ARG:HB2	36:Bg:63:VAL:HG23	1.97	0.45
49:SX:238:ASN:OD1	49:SX:238:ASN:N	2.49	0.45
50:SY:44:PHE:O	50:SY:48:GLY:N	2.47	0.45
52:A2:220:U:H2'	52:A2:221:A:C8	2.51	0.45
52:A2:1670:G:OP1	82:At:79:ARG:NH2	2.46	0.45
74:Al:31:LEU:HD11	74:Al:109:VAL:HB	1.97	0.45
1:B5:1298:A:N6	1:B5:1458:A:O4'	2.50	0.45
1:B5:3403:G:OP1	17:BN:72:LYS:NZ	2.46	0.45
1:B5:4135:C:H2'	1:B5:4136:A:H8	1.81	0.45
1:B5:4516:G:OP1	18:BO:176:ARG:NH1	2.45	0.45
9:BF:226:PHE:N	9:BF:232:ALA:O	2.50	0.45
10:BG:81:ASN:ND2	10:BG:238:GLY:HA3	2.32	0.45
26:BW:71:ARG:NH1	52:A2:1782:A:H5'	2.32	0.45
50:SY:19:ILE:HG22	50:SY:23:LYS:HE3	1.98	0.45
52:A2:894:U:H2'	52:A2:895:G:H8	1.82	0.45
63:Aa:179:ASN:HB3	63:Aa:183:GLU:HB2	1.97	0.45
67:Ae:164:ARG:HE	87:Ay:41:ARG:HH11	1.65	0.45
68:Af:52:ILE:HD13	68:Af:102:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Ah:116:HIS:O	70:Ah:152:ARG:NH2	2.50	0.45
73:Ak:147:LYS:HD2	73:Ak:151:THR:HG21	1.99	0.45
1:B5:521:C:H2'	1:B5:522:U:C6	2.51	0.45
1:B5:3448:C:H42	1:B5:3467:G:HO2'	1.62	0.45
1:B5:4796:C:H2'	1:B5:4797:A:C8	2.52	0.45
6:BC:290:SER:HB3	45:Br:4:HIS:HE1	1.82	0.45
7:BD:208:MET:HE3	7:BD:233:PRO:HG3	1.98	0.45
9:BF:94:ILE:HD13	9:BF:140:ALA:HB2	1.99	0.45
52:A2:558:U:H2'	52:A2:559:G:C8	2.52	0.45
52:A2:1090:G:H4'	94:A2:1909:SPM:H111	1.98	0.45
52:A2:1229:A:H2'	52:A2:1230:G:C8	2.52	0.45
54:AB:49:PRO:HG2	67:Ae:144:LEU:HD23	1.99	0.45
56:AD:83:VAL:HG21	85:Aw:91:LEU:HD23	1.97	0.45
66:Ad:85:GLY:N	66:Ad:88:ASP:OD2	2.41	0.45
75:Am:92:ILE:HG23	75:Am:141:TYR:HE1	1.82	0.45
1:B5:788:G:H2'	1:B5:789:G:C8	2.51	0.45
1:B5:863:G:O2'	8:BE:88:ARG:NH1	2.49	0.45
1:B5:2302:G:N2	1:B5:2305:C:OP2	2.44	0.45
1:B5:3585:PSU:O2'	1:B5:4718:A:N3	2.50	0.45
1:B5:4627:C:H2'	1:B5:4628:G:C8	2.52	0.45
6:BC:143:ARG:HE	6:BC:145:GLU:CD	2.24	0.45
52:A2:1727:G:H1	52:A2:1809:U:H3	1.64	0.45
58:AF:232:GLY:HA3	58:AF:252:THR:HG21	1.98	0.45
61:AT:50:C:H2'	61:AT:51:G:C8	2.51	0.45
73:Ak:135:SER:O	73:Ak:139:ARG:NH1	2.46	0.45
79:Aq:94:GLU:HG2	79:Aq:95:ILE:HG13	1.98	0.45
92:TD:68:ALA:HB3	92:TD:88:VAL:HG21	1.99	0.45
1:B5:1:C:H2'	1:B5:2:G:H8	1.81	0.45
1:B5:1202:C:N4	1:B5:1203:G:O6	2.49	0.45
1:B5:4331:U:H2'	1:B5:4332:G:C8	2.52	0.45
1:B5:4720:G:OP2	1:B5:4720:G:N2	2.40	0.45
5:BB:90:VAL:HG13	5:BB:161:ARG:HB2	1.99	0.45
9:BF:227:VAL:HA	22:BS:39:VAL:HG22	1.99	0.45
26:BW:74:ARG:HH21	52:A2:1751:C:N4	2.14	0.45
37:Bh:87:LYS:NZ	39:Bj:78:PHE:O	2.37	0.45
43:Bo:44:LYS:HE2	43:Bo:52:THR:HB	1.98	0.45
52:A2:519:G:H2'	52:A2:520:A:H8	1.82	0.45
52:A2:1684:C:H5'	67:Ae:130:ARG:HD2	1.99	0.45
61:AT:5:U:H2'	61:AT:6:G:C8	2.52	0.45
73:Ak:84:ARG:HB3	73:Ak:112:HIS:CE1	2.52	0.45
1:B5:1727:A:O2'	1:B5:3955:G:O2'	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1815:U:H2'	1:B5:1816:G:C8	2.52	0.44
1:B5:1860:C:H42	16:BM:16:SER:HB2	1.82	0.44
1:B5:4254:C:OP1	25:BV:43:LYS:NZ	2.39	0.44
1:B5:4283:C:H2'	1:B5:4284:G:C8	2.51	0.44
20:BQ:63:LEU:N	20:BQ:87:THR:O	2.50	0.44
46:Bs:106:LYS:HB3	46:Bs:184:SER:HB3	1.99	0.44
48:Bv:36:ILE:HD11	48:Bv:165:LEU:HD12	1.98	0.44
49:SX:248:THR:OG1	49:SX:440:ALA:O	2.34	0.44
52:A2:22:A:H2'	52:A2:23:G:C8	2.51	0.44
52:A2:682:PSU:O2'	52:A2:1161:U:OP1	2.35	0.44
61:AT:66:C:H2'	61:AT:67:A:C8	2.52	0.44
65:Ac:39:VAL:HG22	65:Ac:48:ILE:HG22	1.98	0.44
68:Af:138:ALA:HA	68:Af:176:ILE:HD11	1.99	0.44
85:Aw:90:CYS:HB3	85:Aw:130:LEU:HD11	1.99	0.44
1:B5:410:A:O2'	1:B5:414:C:O2'	2.32	0.44
1:B5:697:G:N2	1:B5:698:C:O2	2.50	0.44
1:B5:1321:G:H4'	1:B5:1322:C:H3'	1.98	0.44
1:B5:1353:G:O6	1:B5:1362:C:N4	2.51	0.44
1:B5:1496:C:H5"	4:BA:21:LYS:HG2	1.99	0.44
1:B5:1985:G:O2'	1:B5:1986:A:N7	2.48	0.44
1:B5:2386:A:O2'	1:B5:2387:G:O4'	2.33	0.44
1:B5:4175:C:N3	12:BI:158:LYS:NZ	2.65	0.44
12:BI:51:HIS:CD2	12:BI:168:SER:HB2	2.52	0.44
22:BS:76:LYS:NZ	22:BS:100:LEU:O	2.42	0.44
52:A2:5:U:H2'	52:A2:6:G:H8	1.81	0.44
52:A2:35:C:H2'	52:A2:36:PSU:C6	2.50	0.44
52:A2:813:A:H5"	66:Ad:16:LYS:HD2	1.99	0.44
52:A2:1413:C:H2'	52:A2:1414:G:H8	1.81	0.44
67:Ae:30:ILE:HG23	67:Ae:117:ILE:HD11	1.98	0.44
71:Ai:99:GLY:O	71:Ai:101:LYS:NZ	2.43	0.44
84:Av:27:ILE:HB	84:Av:61:ILE:HB	1.99	0.44
1:B5:253:G:H2'	1:B5:254:G:C8	2.52	0.44
1:B5:1215:G:H5"	31:Bb:110:ALA:HB1	1.99	0.44
1:B5:1270:A2M:HM'2	1:B5:1271:C:H5'	1.98	0.44
1:B5:1493:U:H2'	1:B5:1494:G:C8	2.52	0.44
1:B5:3677:A:H2'	1:B5:3678:G:C8	2.52	0.44
1:B5:4135:C:H2'	1:B5:4136:A:C8	2.53	0.44
5:BB:56:ILE:HG22	5:BB:368:ILE:HA	1.99	0.44
20:BQ:67:ILE:HG12	20:BQ:98:LEU:HD11	2.00	0.44
21:BR:176:ARG:HH12	52:A2:910:G:H5'	1.82	0.44
30:Ba:36:GLY:HA3	30:Ba:40:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:1508:G:C6	55:AC:89:LYS:HB2	2.53	0.44
63:Aa:30:TRP:CE2	63:Aa:48:LEU:HD13	2.52	0.44
65:Ac:213:PRO:HG3	79:Aq:19:LYS:HB3	2.00	0.44
67:Ae:164:ARG:HB3	87:Ay:41:ARG:HH12	1.81	0.44
69:Ag:160:LYS:HA	69:Ag:163:GLN:HB2	1.97	0.44
81:As:10:ASN:HB3	81:As:13:GLU:HG2	2.00	0.44
86:Ax:12:PHE:HD1	86:Ax:23:MET:HB3	1.81	0.44
91:TC:31:LEU:O	91:TC:35:ASN:ND2	2.38	0.44
1:B5:728:G:H2'	1:B5:729:G:H8	1.82	0.44
1:B5:751:G:H2'	1:B5:752:G:H8	1.82	0.44
1:B5:2651:G:O3'	21:BR:60:ARG:NH1	2.51	0.44
1:B5:3412:U:OP1	4:BA:54:ARG:NH2	2.39	0.44
1:B5:3527:A:O2'	52:A2:1720:A:N1	2.39	0.44
1:B5:4177:PSU:OP2	12:BI:3:ARG:NH1	2.40	0.44
1:B5:4381:A:H3'	1:B5:4382:PSU:H4'	1.99	0.44
4:BA:48:ILE:HD13	44:Bp:65:ALA:HB2	1.99	0.44
19:BP:40:HIS:NE2	19:BP:110:ASP:O	2.47	0.44
52:A2:115:U:O2'	52:A2:382:C:O2	2.27	0.44
52:A2:420:G:N2	52:A2:662:U:O2	2.51	0.44
1:B5:841:C:OP2	9:BF:241:ARG:NH1	2.51	0.44
1:B5:1509:A:OP1	44:Bp:5:THR:OG1	2.27	0.44
1:B5:1842:G:OP1	35:Bf:87:LYS:NZ	2.38	0.44
1:B5:2188:G:N7	30:Ba:9:ARG:NH2	2.65	0.44
1:B5:4699:G:H2'	1:B5:4700:G:H8	1.83	0.44
2:B7:74:A:N1	2:B7:100:A:H5"	2.32	0.44
12:BI:47:PRO:HB2	12:BI:142:LEU:HD21	1.99	0.44
40:Bk:33:LYS:HG2	40:Bk:46:VAL:HG22	1.99	0.44
41:Bl:23:ILE:HG23	41:Bl:38:ASN:HB2	1.99	0.44
52:A2:156:G:OP1	68:Af:2:LYS:NZ	2.40	0.44
52:A2:528:C:H2'	52:A2:529:A:C8	2.52	0.44
52:A2:807:U:H2'	52:A2:808:G:C8	2.53	0.44
52:A2:1706:C:O2	52:A2:1852:MA6:O2'	2.32	0.44
52:A2:1865:U:H3'	57:AE:5:ARG:HH21	1.82	0.44
53:AA:35:VAL:HG21	53:AA:63:LEU:HD13	1.98	0.44
54:AB:36:ASP:OD1	54:AB:36:ASP:N	2.51	0.44
57:AE:24:THR:HG21	57:AE:71:LEU:HD22	1.98	0.44
62:AZ:187:GLY:HA2	83:Au:45:ARG:HE	1.82	0.44
69:Ag:104:PRO:HD3	69:Ag:116:ARG:HD3	1.99	0.44
75:Am:63:VAL:HG21	75:Am:71:ILE:HD11	1.99	0.44
79:Aq:109:LEU:HG	79:Aq:111:PHE:HD2	1.83	0.44
81:As:65:TYR:HE1	81:As:128:GLN:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ax:18:LEU:O	86:Ax:85:ASN:ND2	2.49	0.44
1:B5:345:C:H2'	1:B5:346:G:H8	1.83	0.44
1:B5:3492:A2M:N6	52:A2:1827:G:OP2	2.51	0.44
1:B5:3675:A:H2'	1:B5:3676:OMG:H8	1.83	0.44
1:B5:3989:C:OP2	1:B5:4010:G:N1	2.48	0.44
1:B5:4367:C:OP1	25:BV:48:ARG:HD2	2.17	0.44
5:BB:77:THR:HG21	5:BB:337:VAL:HG22	1.99	0.44
25:BV:45:ILE:HG21	25:BV:53:PRO:HB3	1.99	0.44
46:Bs:30:VAL:HG12	46:Bs:189:ILE:HG12	1.99	0.44
58:AF:278:SER:HB2	58:AF:281:ALA:HB3	1.99	0.44
61:AT:50:C:H2'	61:AT:51:G:H8	1.83	0.44
90:TB:102:TYR:HA	90:TB:132:GLY:HA2	2.00	0.44
1:B5:1471:G:O2'	15:BL:18:TRP:NE1	2.49	0.44
1:B5:3664:U:H2'	1:B5:3665:G:H8	1.83	0.44
1:B5:4138:OMG:N3	1:B5:4193:5MC:HM52	2.33	0.44
2:B7:6:C:O2'	7:BD:50:ARG:NH2	2.51	0.44
12:BI:192:PRO:HA	12:BI:197:VAL:HG12	2.00	0.44
22:BS:69:GLU:HG2	22:BS:101:THR:HG22	2.00	0.44
45:Br:82:ILE:HG22	45:Br:89:THR:HG22	2.00	0.44
48:Bv:94:ASN:O	48:Bv:97:LYS:NZ	2.42	0.44
49:SX:187:ILE:HD13	49:SX:447:ILE:HA	2.00	0.44
58:AF:120:ILE:N	58:AF:132:TRP:O	2.45	0.44
63:Aa:128:LYS:HA	63:Aa:134:LEU:HA	1.99	0.44
64:Ab:256:TRP:CG	84:Av:68:ARG:HD2	2.53	0.44
67:Ae:126:THR:HG23	67:Ae:128:ILE:HG13	2.00	0.44
68:Af:213:LEU:HG	68:Af:217:MET:HE2	1.99	0.44
81:As:83:GLN:HB2	81:As:93:SER:HB2	2.00	0.44
1:B5:229:G:H5"	28:BY:11:ARG:HG3	2.00	0.44
1:B5:733:C:H4'	16:BM:69:ARG:NH2	2.33	0.44
1:B5:1303:G:H4'	17:BN:203:TYR:HB2	1.98	0.44
1:B5:1620:C:O2'	94:B5:4911:SPM:N1	2.50	0.44
1:B5:1891:G:N2	1:B5:1970:C:O2	2.42	0.44
1:B5:1907:G:H2'	1:B5:1908:G:H8	1.82	0.44
1:B5:1933:C:H2'	1:B5:1934:G:H8	1.83	0.44
1:B5:4171:G:OP1	42:Bm:100:TYR:OH	2.27	0.44
1:B5:4675:G:C5	8:BE:186:ARG:HD3	2.53	0.44
3:B8:90:C:O2'	28:BY:24:HIS:ND1	2.36	0.44
6:BC:110:ARG:O	6:BC:113:ARG:NH1	2.38	0.44
12:BI:187:GLU:HG3	12:BI:189:ARG:HG3	2.00	0.44
21:BR:7:GLN:NE2	21:BR:35:ALA:O	2.44	0.44
29:BZ:107:LYS:HE2	29:BZ:111:ARG:HH21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:645:OMG:HM22	52:A2:646:C:H5'	1.99	0.44
52:A2:1222:G:O2'	52:A2:1677:U:O2	2.36	0.44
63:Aa:28:LYS:HD2	63:Aa:48:LEU:HG	2.00	0.44
76:An:16:SER:OG	76:An:17:LEU:N	2.50	0.44
79:Aq:57:LEU:HD13	79:Aq:69:ILE:HD11	2.00	0.44
1:B5:660:G:O2'	6:BC:291:ARG:NH1	2.51	0.44
1:B5:2511:G:OP1	21:BR:128:LYS:NZ	2.50	0.44
1:B5:2682:U:O4	1:B5:2683:A:N6	2.51	0.44
1:B5:3783:U:H2'	1:B5:3784:A:C8	2.51	0.44
27:BX:151:ASN:ND2	50:SY:20:ARG:HD2	2.33	0.44
37:Bh:31:LEU:HB3	37:Bh:47:ILE:HG12	2.00	0.44
49:SX:61:PRO:HG2	49:SX:65:MET:HE2	1.99	0.44
49:SX:292:ILE:HD13	49:SX:449:LEU:HB3	2.00	0.44
51:SZ:91:GLY:HA2	51:SZ:94:THR:HG22	2.00	0.44
52:A2:1171:A:N1	52:A2:1189:A:H5"	2.33	0.44
56:AD:83:VAL:HG22	85:Aw:68:LYS:HE2	2.00	0.44
61:AT:16:U:O2'	61:AT:18:G:OP2	2.31	0.44
64:Ab:166:ARG:HB3	64:Ab:247:THR:HB	2.00	0.44
64:Ab:192:LEU:HB3	64:Ab:227:ARG:HG2	2.00	0.44
66:Ad:175:PHE:HE2	66:Ad:198:ARG:HD2	1.82	0.44
70:Ah:206:LYS:HE3	70:Ah:206:LYS:HB3	1.86	0.44
71:Ai:60:LEU:HB3	71:Ai:70:ARG:HG3	2.00	0.44
89:TA:203:LEU:O	89:TA:204:ASP:HB3	2.17	0.44
89:TA:209:PHE:O	89:TA:213:PHE:N	2.36	0.44
1:B5:22:G:OP1	39:Bj:44:LYS:N	2.36	0.43
1:B5:1004:G:H2'	1:B5:1005:G:C8	2.52	0.43
1:B5:1769:G:H2'	1:B5:1770:G:H8	1.83	0.43
1:B5:1840:C:H2'	1:B5:1841:G:H8	1.83	0.43
1:B5:2208:OMC:HM21	1:B5:2671:U:H2'	2.00	0.43
1:B5:2691:G:O2'	1:B5:3570:U:O4	2.31	0.43
1:B5:3478:A:H5"	4:BA:244:GLY:HA3	1.99	0.43
1:B5:3791:U:H2'	1:B5:3792:C:O4'	2.17	0.43
1:B5:4715:U:H1'	5:BB:343:ARG:HH12	1.81	0.43
17:BN:42:PRO:HG3	17:BN:61:ILE:HG13	2.00	0.43
25:BV:89:ARG:HB2	25:BV:95:PHE:CE2	2.53	0.43
48:Bv:47:LYS:HE2	48:Bv:161:LYS:HD2	1.99	0.43
52:A2:585:A:OP1	71:Ai:169:ARG:NH2	2.50	0.43
52:A2:840:C:H42	86:Ax:48:TYR:HA	1.81	0.43
67:Ae:124:ASP:OD1	67:Ae:125:SER:N	2.50	0.43
75:Am:40:LEU:HB3	75:Am:45:LEU:HD12	1.98	0.43
92:TD:112:TYR:CZ	92:TD:116:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:422:C:H2'	1:B5:423:G:C8	2.54	0.43
1:B5:1701:C:H2'	1:B5:1702:C:C6	2.53	0.43
1:B5:1718:PSU:H2'	1:B5:1719:A:C8	2.54	0.43
1:B5:1955:C:H2'	1:B5:1956:A:H8	1.82	0.43
1:B5:2426:C:OP2	36:Bg:76:ARG:NH1	2.48	0.43
1:B5:2592:C:H2'	1:B5:2593:G:C8	2.53	0.43
1:B5:3396:G:H2'	1:B5:3397:G:C8	2.54	0.43
1:B5:3796:U:H2'	1:B5:3797:U:C6	2.53	0.43
1:B5:3984:G:H2'	1:B5:3985:A:C8	2.54	0.43
4:BA:206:PRO:HG3	4:BA:213:GLY:HA3	2.00	0.43
5:BB:29:VAL:HG13	5:BB:348:ARG:HD3	1.99	0.43
7:BD:85:LYS:NZ	7:BD:254:GLU:OE2	2.38	0.43
7:BD:196:ARG:NH2	7:BD:237:GLU:OE2	2.46	0.43
46:Bs:30:VAL:HG21	46:Bs:187:LEU:HD13	1.99	0.43
47:Bt:133:LEU:HD22	47:Bt:152:ILE:HD12	2.00	0.43
52:A2:303:A:O2'	70:Ah:64:ASN:OD1	2.36	0.43
52:A2:1320:U:H2'	52:A2:1321:G:C8	2.53	0.43
52:A2:1397:A:H8	52:A2:1450:G:H22	1.66	0.43
52:A2:1514:C:H2'	52:A2:1515:G:C8	2.52	0.43
52:A2:1690:C:OP1	93:A2:1901:SPD:N1	2.51	0.43
78:Ap:19:ALA:HB2	78:Ap:75:GLY:HA3	1.99	0.43
1:B5:1008:C:H2'	1:B5:1009:G:C8	2.52	0.43
1:B5:1829:G:OP2	1:B5:1829:G:N2	2.38	0.43
1:B5:3374:A:C4	39:Bj:3:LYS:HB3	2.53	0.43
1:B5:4335:A:N1	1:B5:4367:C:O2'	2.52	0.43
1:B5:4776:U:H2'	1:B5:4777:A:H8	1.84	0.43
3:B8:67:U:H2'	3:B8:68:G:C8	2.52	0.43
4:BA:2:GLY:HA2	4:BA:207:VAL:HG23	1.99	0.43
6:BC:152:LEU:HD21	6:BC:174:LEU:HD13	1.99	0.43
17:BN:178:HIS:HA	17:BN:181:HIS:NE2	2.34	0.43
22:BS:74:ARG:O	22:BS:76:LYS:NZ	2.51	0.43
49:SX:196:PHE:HE1	49:SX:213:ILE:HD11	1.83	0.43
52:A2:90:G:OP1	52:A2:446:A:N6	2.51	0.43
58:AF:239:LEU:HD22	58:AF:248:LEU:HD11	2.00	0.43
62:AZ:77:ILE:HG21	62:AZ:133:PRO:HG3	1.99	0.43
67:Ae:14:THR:HB	67:Ae:15:PRO:HD3	2.00	0.43
71:Ai:134:HIS:ND1	71:Ai:163:SER:OG	2.46	0.43
1:B5:1:C:H2'	1:B5:2:G:C8	2.53	0.43
1:B5:315:G:C8	30:Ba:62:HIS:HB2	2.53	0.43
1:B5:827:C:H2'	1:B5:828:A:C8	2.54	0.43
1:B5:1639:A:OP1	30:Ba:47:LYS:NZ	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1943:U:H2'	1:B5:1944:G:C8	2.53	0.43
1:B5:2687:A:O2'	1:B5:4377:G:H4'	2.17	0.43
1:B5:3600:G:H22	1:B5:3632:G:H1'	1.83	0.43
1:B5:3983:C:OP1	1:B5:4073:C:O2'	2.35	0.43
3:B8:28:C:H2'	3:B8:29:G:H8	1.84	0.43
7:BD:223:PHE:HB3	7:BD:226:TYR:HB2	2.01	0.43
11:BH:12:ILE:HB	11:BH:53:LYS:HB2	2.01	0.43
22:BS:83:ARG:HG3	22:BS:125:GLN:HB2	2.01	0.43
34:Be:90:MET:HG3	45:Br:33:LYS:HA	2.00	0.43
52:A2:5:U:H2'	52:A2:6:G:C8	2.52	0.43
61:AT:9:C:O2'	61:AT:10:G:N7	2.51	0.43
64:Ab:194:ARG:HB3	64:Ab:225:SER:HB3	2.01	0.43
65:Ac:163:PRO:HA	65:Ac:166:TYR:CE2	2.53	0.43
66:Ad:94:LYS:NZ	86:Ax:19:GLN:HE21	2.16	0.43
66:Ad:174:LYS:O	66:Ad:179:ASN:ND2	2.51	0.43
71:Ai:83:ARG:HH21	71:Ai:150:ARG:NH1	2.17	0.43
1:B5:637:C:H2'	1:B5:638:G:C8	2.53	0.43
1:B5:2411:C:H2'	1:B5:2412:G:H8	1.83	0.43
1:B5:2584:U:H2'	4:BA:50:HIS:HD2	1.84	0.43
1:B5:4059:A:H4'	23:BT:71:ALA:HB3	2.00	0.43
6:BC:328:LEU:HB3	9:BF:186:MET:HG3	1.99	0.43
7:BD:119:TYR:OH	7:BD:139:PRO:O	2.35	0.43
19:BP:60:PHE:CE1	19:BP:82:ARG:HB2	2.53	0.43
21:BR:106:LEU:HD13	21:BR:138:LEU:HD21	2.00	0.43
26:BW:99:GLU:HA	26:BW:102:LYS:HZ3	1.82	0.43
52:A2:1866:C:O2'	57:AE:95:ARG:NH1	2.50	0.43
59:AG:17:GLY:O	59:AG:27:ARG:NH1	2.51	0.43
66:Ad:126:VAL:HG22	66:Ad:139:LEU:HD21	2.01	0.43
68:Af:58:LYS:HA	68:Af:107:SER:HB2	1.99	0.43
78:Ap:89:SER:HB3	78:Ap:112:LEU:HD13	1.99	0.43
80:Ar:27:ALA:HB2	80:Ar:52:LEU:HD22	2.00	0.43
80:Ar:86:ARG:NH1	80:Ar:110:ASP:OD2	2.48	0.43
1:B5:74:G:O3'	15:BL:71:ARG:NH2	2.52	0.43
1:B5:1250:C:H2'	1:B5:1251:A:C8	2.53	0.43
1:B5:2391:C:H2'	1:B5:2392:G:C8	2.54	0.43
1:B5:2411:C:H2'	1:B5:2412:G:C8	2.54	0.43
1:B5:3976:C:O2'	1:B5:3980:A:N1	2.45	0.43
1:B5:4006:U:H2'	1:B5:4007:C:C6	2.53	0.43
1:B5:4032:C:H2'	1:B5:4033:G:C8	2.54	0.43
1:B5:4431:U:H2'	1:B5:4432:G:H8	1.84	0.43
42:Bm:98:M3L:HM13	42:Bm:98:M3L:HD2	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Bs:65:ILE:HG12	46:Bs:75:LEU:HD23	2.00	0.43
48:Bv:73:HIS:HA	48:Bv:144:MET:HE1	2.01	0.43
49:SX:86:THR:HG21	49:SX:301:LEU:HD21	2.01	0.43
52:A2:155:G:H4'	68:Af:15:LEU:HD22	2.01	0.43
52:A2:389:U:H2'	52:A2:390:A:C8	2.54	0.43
52:A2:1351:U:H3	52:A2:1380:A:H61	1.66	0.43
52:A2:1809:U:H2'	52:A2:1810:A:C8	2.54	0.43
52:A2:1864:A:OP2	57:AE:4:LYS:NZ	2.50	0.43
63:Aa:65:ARG:HE	76:An:50:LYS:HD3	1.84	0.43
66:Ad:42:LEU:HB2	66:Ad:109:PHE:CD2	2.54	0.43
85:Aw:60:LYS:HG3	85:Aw:116:PRO:HG3	1.99	0.43
1:B5:62:A:OP1	17:BN:172:ARG:NH1	2.51	0.43
1:B5:398:A2M:H8	1:B5:398:A2M:O5'	2.18	0.43
1:B5:1533:U:OP2	1:B5:3369:PSU:O2'	2.32	0.43
1:B5:1638:PSU:H2'	1:B5:1639:A:C8	2.54	0.43
1:B5:3852:G:N2	10:BG:43:GLN:O	2.52	0.43
1:B5:4371:C:H5'	5:BB:338:VAL:HA	2.01	0.43
19:BP:78:TRP:CD1	19:BP:80:GLN:H	2.36	0.43
24:BU:90:TYR:O	24:BU:94:ASN:ND2	2.34	0.43
48:Bv:17:VAL:HG21	48:Bv:206:ILE:HG22	2.01	0.43
50:SY:9:GLU:HG2	50:SY:10:PRO:HD3	2.01	0.43
52:A2:845:U:H2'	52:A2:846:G:H8	1.84	0.43
52:A2:987:G:OP2	52:A2:989:C:N4	2.52	0.43
52:A2:1376:G:H2'	52:A2:1377:A:H8	1.83	0.43
52:A2:1455:A:O5'	79:Aq:3:ARG:NH1	2.42	0.43
63:Aa:48:LEU:O	76:An:51:GLU:HG3	2.18	0.43
76:An:151:LEU:H	76:An:151:LEU:HD23	1.83	0.43
77:Ao:75:VAL:HG21	77:Ao:104:GLN:HG2	2.01	0.43
1:B5:151:G:OP2	17:BN:4:TYR:OH	2.24	0.43
1:B5:474:C:H2'	1:B5:475:G:C8	2.54	0.43
1:B5:860:A:N6	8:BE:129:LEU:O	2.49	0.43
1:B5:2515:C:OP1	44:Bp:44:LYS:NZ	2.50	0.43
4:BA:30:ARG:HG2	4:BA:74:GLU:HG3	2.00	0.43
22:BS:6:THR:HA	22:BS:107:THR:HG21	2.01	0.43
52:A2:502:C:OP1	93:A2:1907:SPD:N6	2.52	0.43
52:A2:614:G:N1	52:A2:630:A:OP2	2.47	0.43
52:A2:1411:C:H2'	52:A2:1412:G:C8	2.53	0.43
59:AG:22:ARG:HH21	59:AG:37:ASN:HD22	1.66	0.43
61:AT:28:U:H2'	61:AT:29:G:C8	2.53	0.43
69:Ag:37:LYS:HE3	69:Ag:41:ARG:HH21	1.84	0.43
1:B5:175:C:H2'	1:B5:176:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:526:C:H2'	1:B5:527:G:H8	1.84	0.43
1:B5:1290:C:H2'	1:B5:1291:G:C8	2.53	0.43
1:B5:1972:A:OP1	22:BS:88:SER:OG	2.37	0.43
4:BA:83:HIS:CE1	4:BA:86:GLN:HB2	2.54	0.43
48:Bv:60:ARG:O	48:Bv:171:HIS:ND1	2.51	0.43
49:SX:191:ILE:HD11	49:SX:447:ILE:HG21	2.00	0.43
62:AZ:66:VAL:HG21	62:AZ:185:MET:HB2	2.01	0.43
62:AZ:76:VAL:HG23	62:AZ:98:PRO:HA	2.00	0.43
70:Ah:123:ARG:NH1	70:Ah:133:GLU:OE1	2.49	0.43
1:B5:1290:C:H2'	1:B5:1291:G:H8	1.84	0.43
1:B5:1712:U:H2'	1:B5:1713:C:C6	2.54	0.43
1:B5:2301:C:H5"	17:BN:67:ARG:HD2	2.01	0.43
49:SX:125:ILE:HG12	49:SX:156:PHE:HZ	1.83	0.43
52:A2:190:G:OP1	70:Ah:149:TYR:OH	2.32	0.43
52:A2:653:U:H2'	52:A2:654:A:C8	2.54	0.43
52:A2:1679:A2M:OP2	67:Ae:63:LYS:NZ	2.35	0.43
52:A2:1719:G:O2'	52:A2:1816:A:N6	2.51	0.43
65:Ac:209:SER:HB3	79:Aq:40:ILE:HB	2.01	0.43
68:Af:22:ARG:HG2	68:Af:25:ARG:HH22	1.84	0.43
68:Af:164:LYS:HG2	68:Af:165:GLU:H	1.84	0.43
68:Af:201:LYS:HE3	68:Af:201:LYS:HB3	1.82	0.43
80:Ar:46:ARG:HH22	80:Ar:52:LEU:HD11	1.84	0.43
84:Av:26:LEU:HD11	84:Av:60:LYS:HB3	2.00	0.43
1:B5:685:C:H2'	1:B5:686:A:C8	2.54	0.42
1:B5:795:A:H3'	1:B5:796:C:C6	2.53	0.42
1:B5:3517:A2M:HM'1	1:B5:4283:C:H1'	2.01	0.42
1:B5:4298:PSU:H2'	1:B5:4299:A:C8	2.54	0.42
1:B5:4458:C:H2'	1:B5:4459:G:H8	1.85	0.42
2:B7:11:A:N1	2:B7:66:G:O2'	2.47	0.42
11:BH:173:ARG:NH1	42:Bm:125:LYS:O	2.42	0.42
22:BS:1:MET:HE3	22:BS:35:PRO:HD3	2.00	0.42
22:BS:45:TRP:HA	22:BS:48:VAL:HG22	2.01	0.42
24:BU:36:ALA:HB3	24:BU:65:ARG:HH21	1.84	0.42
28:BY:55:VAL:HG12	28:BY:106:ILE:HG12	2.01	0.42
34:Be:124:ASN:OD1	34:Be:124:ASN:N	2.52	0.42
43:Bo:72:CYS:HB3	43:Bo:79:SER:H	1.84	0.42
52:A2:99:A2M:H62	52:A2:434:A:H1'	1.83	0.42
52:A2:454:C:O2'	68:Af:92:ARG:O	2.28	0.42
52:A2:1063:A:OP1	93:A2:1905:SPD:H52	2.18	0.42
52:A2:1454:C:O2	52:A2:1454:C:H2'	2.18	0.42
66:Ad:137:PRO:HG2	66:Ad:150:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Am:67:THR:HG21	75:Am:74:ILE:HD11	2.00	0.42
78:Ap:16:LYS:HD2	78:Ap:16:LYS:HA	1.77	0.42
1:B5:837:U:OP2	16:BM:48:GLN:NE2	2.52	0.42
1:B5:1549:C:O2'	1:B5:1552:G:H1'	2.20	0.42
1:B5:1572:G:H1'	1:B5:2356:A:N6	2.33	0.42
1:B5:3347:G:H1'	26:BW:44:ARG:HE	1.84	0.42
1:B5:3365:C:H2'	1:B5:3366:G:C8	2.54	0.42
1:B5:4026:A:OP2	7:BD:23:ARG:NH2	2.45	0.42
1:B5:4429:U:OP2	1:B5:4452:G:N1	2.34	0.42
1:B5:4724:U:OP1	5:BB:175:GLN:NE2	2.53	0.42
29:BZ:50:PRO:HD3	29:BZ:68:ILE:HG12	2.00	0.42
46:Bs:14:PHE:HE1	46:Bs:64:ALA:HA	1.84	0.42
52:A2:1532:A:H4'	52:A2:1606:G:H4'	2.00	0.42
52:A2:1860:A:P	57:AE:10:ARG:HH12	2.41	0.42
54:AB:44:ARG:HH12	54:AB:63:ARG:HB2	1.84	0.42
58:AF:8:ARG:HA	58:AF:8:ARG:HH11	1.84	0.42
59:AG:20:SER:OG	72:Aj:65:ARG:NH1	2.53	0.42
63:Aa:87:ILE:HG22	63:Aa:101:HIS:HB2	2.01	0.42
80:Ar:55:ARG:HB2	80:Ar:58:GLU:HG3	2.00	0.42
85:Aw:54:LYS:HE3	85:Aw:91:LEU:HG	2.00	0.42
86:Ax:29:HIS:O	86:Ax:29:HIS:ND1	2.52	0.42
1:B5:751:G:H2'	1:B5:752:G:C8	2.54	0.42
1:B5:1307:C:OP2	15:BL:39:ARG:NH2	2.46	0.42
1:B5:1584:G:N1	4:BA:208:GLU:OE1	2.45	0.42
1:B5:1601:A:O2'	39:Bj:49:TRP:O	2.32	0.42
1:B5:2383:C:H2'	1:B5:2384:G:C8	2.54	0.42
1:B5:2612:U:C2	36:Bg:69:LYS:HB2	2.54	0.42
1:B5:2613:C:H2'	1:B5:2614:G:H8	1.83	0.42
1:B5:4037:G:H5'	1:B5:4039:PSU:C6	2.54	0.42
1:B5:4314:A:O3'	5:BB:21:ARG:NH2	2.52	0.42
3:B8:90:C:H2'	3:B8:91:A:C8	2.54	0.42
7:BD:99:TYR:HE2	7:BD:164:LYS:HG3	1.84	0.42
17:BN:146:PRO:HB2	37:Bh:104:THR:HG23	2.01	0.42
30:Ba:100:ILE:HG13	30:Ba:123:ILE:HB	2.02	0.42
34:Be:67:LYS:HG2	34:Be:68:HIS:CD2	2.54	0.42
49:SX:121:MET:O	49:SX:124:THR:OG1	2.33	0.42
52:A2:235:A:H2'	52:A2:236:A:C8	2.54	0.42
52:A2:678:G:H21	52:A2:1029:A:H62	1.67	0.42
58:AF:298:LEU:HB3	58:AF:310:TRP:HB2	2.00	0.42
72:Aj:37:ASP:OD1	72:Aj:37:ASP:N	2.51	0.42
86:Ax:78:SER:OG	86:Ax:80:ASP:OD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:120:A:N1	1:B5:148:A:O2'	2.44	0.42
1:B5:1003:C:H2'	1:B5:1004:G:C8	2.54	0.42
1:B5:1672:G:N3	1:B5:3960:A:H2'	2.34	0.42
1:B5:2423:U:P	29:BZ:36:ARG:HH22	2.42	0.42
1:B5:3480:A:O2'	4:BA:223:SER:OG	2.30	0.42
1:B5:3670:G:OP1	17:BN:24:ARG:NE	2.44	0.42
1:B5:4371:C:OP1	5:BB:224:LYS:HG3	2.19	0.42
1:B5:4741:U:H2'	1:B5:4742:U:C6	2.54	0.42
7:BD:208:MET:HB2	7:BD:233:PRO:HG3	2.02	0.42
19:BP:14:SER:O	19:BP:105:LYS:NZ	2.49	0.42
29:BZ:121:ARG:O	29:BZ:124:THR:OG1	2.36	0.42
32:Bc:99:PRO:HG3	32:Bc:105:ILE:HG13	2.02	0.42
33:Bd:36:VAL:HG21	33:Bd:44:ARG:HD3	2.01	0.42
34:Be:82:VAL:HG13	34:Be:114:ARG:HG2	2.02	0.42
52:A2:39:A:H61	52:A2:516:G:H1'	1.84	0.42
52:A2:206:G:H2'	52:A2:207:G:H8	1.84	0.42
52:A2:1537:G:H2'	52:A2:1538:A:C8	2.54	0.42
52:A2:1616:U:OP2	77:Ao:43:ARG:NH1	2.52	0.42
52:A2:1737:G:H2'	52:A2:1738:G:C8	2.54	0.42
64:Ab:182:CYS:HB2	84:Av:95:PRO:HB2	2.02	0.42
86:Ax:23:MET:N	86:Ax:23:MET:SD	2.92	0.42
89:TA:116:ILE:HG12	89:TA:145:VAL:HG22	2.00	0.42
90:TB:84:ALA:O	90:TB:87:SER:OG	2.27	0.42
1:B5:1931:U:O2'	1:B5:1941:A:OP1	2.26	0.42
1:B5:2592:C:H2'	1:B5:2593:G:H8	1.84	0.42
1:B5:3797:U:H2'	1:B5:3798:U:C6	2.55	0.42
7:BD:64:ILE:HG12	7:BD:105:LEU:HD21	2.01	0.42
8:BE:289:LEU:HB2	16:BM:109:ARG:NH2	2.34	0.42
20:BQ:79:THR:HB	20:BQ:136:THR:HG22	2.01	0.42
29:BZ:90:PRO:O	29:BZ:117:LYS:NZ	2.48	0.42
46:Bs:5:ASP:HB2	46:Bs:8:THR:HG22	2.02	0.42
48:Bv:35:GLN:HB2	48:Bv:205:TYR:HB2	2.00	0.42
52:A2:932:C:H2'	52:A2:933:G:C8	2.54	0.42
52:A2:1294:A:N3	55:AC:138:ARG:NH1	2.68	0.42
52:A2:1598:C:H4'	52:A2:1604:G:C6	2.54	0.42
58:AF:60:ARG:HE	78:Ap:97:GLN:HE22	1.68	0.42
61:AT:28:U:H2'	61:AT:29:G:H8	1.85	0.42
62:AZ:122:LEU:HB2	62:AZ:142:LEU:HD21	2.02	0.42
65:Ac:132:LYS:HE3	65:Ac:191:PRO:HA	2.02	0.42
71:Ai:61:LEU:HA	71:Ai:70:ARG:HH12	1.83	0.42
79:Aq:66:VAL:HG12	79:Aq:68:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ax:80:ASP:OD1	86:Ax:81:TYR:N	2.52	0.42
91:TC:32:PHE:HZ	91:TC:81:LYS:HD2	1.83	0.42
1:B5:1335:A:H62	93:B5:4903:SPD:H102	1.68	0.42
1:B5:4261:G:H5"	5:BB:3:HIS:CE1	2.54	0.42
1:B5:4628:G:H2'	1:B5:4629:G:C8	2.55	0.42
5:BB:46:PHE:HE2	5:BB:81:THR:HB	1.85	0.42
5:BB:117:ARG:HA	5:BB:177:LYS:HD3	2.00	0.42
12:BI:169:LYS:NZ	23:BT:157:GLU:OE2	2.41	0.42
23:BT:53:PRO:HD3	23:BT:91:VAL:HG13	2.01	0.42
25:BV:107:ASN:HD21	25:BV:109:LYS:HB2	1.85	0.42
30:Ba:125:LYS:HG2	30:Ba:145:VAL:HB	2.01	0.42
33:Bd:65:ASP:OD1	33:Bd:66:THR:N	2.53	0.42
46:Bs:175:LEU:HD13	46:Bs:182:PRO:HG2	2.01	0.42
50:SY:29:ASP:OD1	50:SY:30:ARG:N	2.51	0.42
52:A2:622:C:OP1	85:Aw:113:GLY:N	2.47	0.42
52:A2:673:A:N6	52:A2:1162:U:O2'	2.53	0.42
52:A2:1707:G:H4'	88:Az:9:ARG:HH22	1.85	0.42
78:Ap:49:TYR:O	78:Ap:53:GLU:HG3	2.19	0.42
1:B5:641:G:H2'	1:B5:642:G:H8	1.85	0.42
1:B5:2238:A:O2'	1:B5:2650:A:OP2	2.38	0.42
1:B5:3331:A:H2'	1:B5:3332:G:C8	2.54	0.42
1:B5:4361:C:H5"	5:BB:357:ARG:NE	2.29	0.42
1:B5:4776:U:H2'	1:B5:4777:A:C8	2.54	0.42
49:SX:244:ASN:O	49:SX:248:THR:OG1	2.37	0.42
52:A2:22:A:H2'	52:A2:23:G:H8	1.84	0.42
52:A2:640:C:H2'	52:A2:641:A:C8	2.54	0.42
52:A2:1104:C:H2'	52:A2:1105:G:H8	1.84	0.42
52:A2:1612:G:O2'	80:Ar:87:GLN:O	2.36	0.42
52:A2:1659:G:OP2	52:A2:1661:C:N4	2.52	0.42
52:A2:1712:U:H2'	52:A2:1713:A:C8	2.55	0.42
62:AZ:125:THR:HG22	62:AZ:175:TRP:HE1	1.84	0.42
65:Ac:56:GLN:H	65:Ac:56:GLN:HG3	1.64	0.42
68:Af:93:LYS:HE2	68:Af:93:LYS:HB2	1.93	0.42
78:Ap:16:LYS:HG3	78:Ap:17:LYS:H	1.84	0.42
1:B5:300:A:H2'	1:B5:301:G:C8	2.55	0.42
1:B5:2203:A:H4'	1:B5:2204:G:H4'	2.02	0.42
5:BB:317:LEU:HB2	5:BB:372:SER:HB2	2.01	0.42
11:BH:29:GLY:HA3	11:BH:84:VAL:HB	2.01	0.42
15:BL:67:HIS:CD2	15:BL:68:THR:HG23	2.54	0.42
23:BT:92:ARG:HB3	23:BT:94:GLU:OE1	2.19	0.42
43:Bo:35:ALA:O	43:Bo:39:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Ab:196:ILE:HB	64:Ab:223:TYR:HB2	1.99	0.42
69:Ag:145:ARG:HE	84:Av:49:GLU:HB3	1.85	0.42
76:An:45:THR:HG22	76:An:52:THR:HG22	2.01	0.42
87:Ay:73:VAL:HG12	87:Ay:79:ILE:HD11	2.02	0.42
1:B5:1288:C:H2'	1:B5:1289:A:C8	2.53	0.42
1:B5:1586:A:N7	4:BA:199:VAL:HG21	2.35	0.42
1:B5:3897:G:H2'	1:B5:3898:G:C8	2.53	0.42
1:B5:4408:C:O2'	1:B5:4743:C:OP1	2.31	0.42
4:BA:20:VAL:HG12	4:BA:23:ARG:HD2	2.00	0.42
28:BY:2:LYS:HE3	28:BY:2:LYS:HB3	1.84	0.42
52:A2:106:C:OP1	52:A2:432:G:O2'	2.36	0.42
52:A2:807:U:H2'	52:A2:808:G:H8	1.85	0.42
52:A2:875:G:H2'	52:A2:876:A:C8	2.54	0.42
52:A2:1606:G:N2	52:A2:1634:A:N7	2.68	0.42
56:AD:83:VAL:HG12	85:Aw:89:GLY:HA2	2.02	0.42
58:AF:152:SER:HB2	58:AF:168:CYS:SG	2.60	0.42
62:AZ:79:SER:HA	62:AZ:101:GLY:HA2	2.02	0.42
67:Ae:78:MET:HB2	67:Ae:159:ARG:CZ	2.50	0.42
1:B5:223:G:H4'	1:B5:225:G:N7	2.34	0.42
1:B5:1759:C:H5'	7:BD:139:PRO:HB3	2.01	0.42
1:B5:1788:U:H3'	15:BL:5:ARG:HH22	1.84	0.42
1:B5:2203:A:N1	1:B5:3592:A:H5"	2.35	0.42
1:B5:2338:U:H2'	1:B5:2339:G:H8	1.85	0.42
9:BF:240:ASN:O	9:BF:244:ARG:HG2	2.20	0.42
43:Bo:33:LEU:HA	43:Bo:38:LYS:HG2	2.01	0.42
47:Bt:14:TYR:O	47:Bt:31:LYS:NZ	2.52	0.42
47:Bt:105:THR:HB	47:Bt:108:GLU:HG3	2.01	0.42
49:SX:187:ILE:O	49:SX:190:THR:OG1	2.33	0.42
49:SX:259:GLN:NE2	49:SX:452:THR:HG23	2.35	0.42
50:SY:32:GLU:CD	50:SY:35:LYS:HZ1	2.27	0.42
52:A2:39:A:OP2	71:Ai:5:ARG:NH1	2.53	0.42
52:A2:1129:C:H2'	52:A2:1130:G:C8	2.55	0.42
52:A2:1162:U:O4	85:Aw:2:GLY:N	2.53	0.42
52:A2:1833:6MZ:H8	52:A2:1833:6MZ:O5'	2.20	0.42
61:AT:68:C:H2'	61:AT:69:G:C8	2.55	0.42
61:AT:68:C:H2'	61:AT:69:G:H8	1.84	0.42
64:Ab:144:SER:HB3	64:Ab:150:ALA:HB2	2.02	0.42
74:Al:28:HIS:CE1	74:Al:116:LYS:HE3	2.55	0.42
1:B5:135:G:N7	37:Bh:97:LYS:HE3	2.34	0.41
1:B5:670:C:H2'	1:B5:671:G:C8	2.55	0.41
1:B5:1001:C:H2'	1:B5:1002:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:3539:A:O2'	52:A2:1817:G:O2'	2.34	0.41
1:B5:3700:U:H2'	1:B5:3701:G:C8	2.55	0.41
1:B5:4606:G:H2'	1:B5:4607:G:H8	1.85	0.41
3:B8:63:U:OP1	37:Bh:48:ARG:NH2	2.38	0.41
8:BE:216:THR:OG1	8:BE:217:ASP:N	2.53	0.41
9:BF:170:ASP:OD1	9:BF:171:ASN:N	2.53	0.41
12:BI:91:LEU:HD12	12:BI:135:ILE:HG23	2.02	0.41
15:BL:174:LYS:NZ	30:Ba:141:GLY:O	2.53	0.41
20:BQ:35:LEU:O	20:BQ:39:THR:OG1	2.30	0.41
26:BW:102:LYS:HG2	26:BW:105:ARG:NH2	2.35	0.41
49:SX:348:PRO:HB3	49:SX:360:HIS:CG	2.55	0.41
52:A2:16:G:H2'	52:A2:17:C:C6	2.55	0.41
52:A2:512:U:H2'	52:A2:513:A2M:H8	2.01	0.41
52:A2:583:U:H2'	52:A2:584:A:H5"	2.02	0.41
52:A2:1623:U:OP1	80:Ar:120:HIS:ND1	2.44	0.41
52:A2:1715:U:H2'	52:A2:1716:A:C8	2.55	0.41
52:A2:1806:G:H2'	52:A2:1807:A:C8	2.55	0.41
67:Ae:125:SER:O	67:Ae:136:ARG:NH2	2.48	0.41
73:Ak:93:LEU:HB3	73:Ak:102:PHE:HB3	2.02	0.41
75:Am:83:ASP:OD1	75:Am:83:ASP:N	2.53	0.41
80:Ar:48:ALA:HB2	80:Ar:70:ILE:HD12	2.02	0.41
90:TB:78:VAL:HB	92:TD:78:THR:HB	2.01	0.41
1:B5:1699:G:H2'	1:B5:1700:G:C8	2.55	0.41
1:B5:2387:G:H4'	1:B5:2389:G:N7	2.36	0.41
1:B5:3363:U:O2'	1:B5:3537:U:OP1	2.35	0.41
1:B5:3399:C:H4'	4:BA:8:GLN:HA	2.02	0.41
1:B5:3474:G:H2'	1:B5:3475:G:H8	1.84	0.41
1:B5:3524:OMG:HM22	1:B5:3525:U:H5'	2.02	0.41
1:B5:4047:U:OP1	23:BT:78:LYS:NZ	2.47	0.41
1:B5:4698:U:H2'	1:B5:4699:G:H8	1.85	0.41
11:BH:17:ASP:HB3	11:BH:28:LYS:HB3	2.03	0.41
17:BN:43:THR:OG1	17:BN:131:GLU:OE2	2.28	0.41
19:BP:94:MET:HE1	19:BP:146:ILE:HB	2.02	0.41
26:BW:84:GLY:HA2	68:Af:161:PRO:HD3	2.01	0.41
46:Bs:40:MET:HE1	46:Bs:187:LEU:HD11	2.02	0.41
51:SZ:87:LEU:O	51:SZ:91:GLY:N	2.53	0.41
52:A2:1048:C:H5"	76:An:143:LYS:HB2	2.01	0.41
71:Ai:97:ILE:HA	71:Ai:100:LEU:HD13	2.02	0.41
86:Ax:117:VAL:HG11	86:Ax:125:VAL:HG21	2.02	0.41
1:B5:2322:G:H2'	1:B5:2323:G:C8	2.55	0.41
1:B5:2679:A:H4'	5:BB:229:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:3954:U:H2'	1:B5:3955:G:H8	1.85	0.41
1:B5:4606:G:H2'	1:B5:4607:G:C8	2.55	0.41
5:BB:17:LEU:HD21	5:BB:235:TRP:HH2	1.85	0.41
23:BT:17:ARG:HB2	23:BT:22:HIS:CE1	2.56	0.41
45:Br:32:LEU:O	45:Br:113:ARG:NH1	2.48	0.41
49:SX:22:PRO:HD2	49:SX:172:GLY:HA2	2.01	0.41
52:A2:1221:A:O2'	67:Ae:145:ARG:NH1	2.42	0.41
52:A2:1334:U:OP1	65:Ac:147:ALA:N	2.53	0.41
65:Ac:163:PRO:O	65:Ac:167:TYR:HB2	2.20	0.41
68:Af:21:GLU:OE1	68:Af:25:ARG:NH2	2.53	0.41
74:Al:86:GLY:HA2	74:Al:89:VAL:HG22	2.02	0.41
90:TB:24:LEU:HB2	90:TB:47:TYR:HB2	2.03	0.41
90:TB:153:PHE:HA	90:TB:156:MET:HE2	2.02	0.41
1:B5:92:C:C2	30:Ba:55:LYS:HD3	2.56	0.41
1:B5:323:C:H2'	1:B5:324:A:C8	2.55	0.41
1:B5:1638:PSU:OP1	30:Ba:44:ASN:ND2	2.51	0.41
1:B5:2238:A:H1'	1:B5:2649:A:H1'	2.02	0.41
1:B5:2328:U:H2'	1:B5:2329:G:C8	2.55	0.41
1:B5:4032:C:H2'	1:B5:4033:G:H8	1.86	0.41
1:B5:4067:U:H2'	1:B5:4068:G:C8	2.55	0.41
1:B5:4253:A:O2'	25:BV:41:SER:OG	2.35	0.41
1:B5:4628:G:H2'	1:B5:4629:G:H8	1.86	0.41
1:B5:4735:C:OP1	33:Bd:32:ARG:NH1	2.52	0.41
3:B8:79:G:H2'	3:B8:80:A:C8	2.56	0.41
8:BE:48:ARG:HB2	8:BE:64:MET:HE1	2.02	0.41
8:BE:273:TYR:O	8:BE:276:SER:OG	2.38	0.41
27:BX:156:ILE:O	49:SX:416:TYR:OH	2.29	0.41
30:Ba:39:V5N:O2	30:Ba:40:HIS:N	2.50	0.41
52:A2:206:G:H2'	52:A2:207:G:C8	2.55	0.41
52:A2:485:A2M:O5'	52:A2:485:A2M:H8	2.20	0.41
52:A2:563:U:H2'	52:A2:564:G:C8	2.55	0.41
52:A2:824:U:N3	71:Ai:143:ASN:OD1	2.50	0.41
52:A2:1246:G:O2'	52:A2:1493:U:OP1	2.31	0.41
52:A2:1703:G:H2'	52:A2:1704:OMC:O4'	2.21	0.41
57:AE:22:ARG:NH2	76:An:145:GLY:O	2.54	0.41
61:AT:3:C:H2'	61:AT:4:G:C8	2.55	0.41
61:AT:51:G:H2'	61:AT:52:G:C8	2.54	0.41
70:Ah:80:ASP:OD1	70:Ah:81:VAL:N	2.53	0.41
80:Ar:132:ARG:HB2	80:Ar:134:GLN:NE2	2.35	0.41
1:B5:67:C:N4	1:B5:325:U:O3'	2.54	0.41
1:B5:790:G:O2'	1:B5:792:G:O4'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1105:C:C5	31:Bb:92:LYS:HD2	2.56	0.41
1:B5:1335:A:P	20:BQ:181:ARG:HH22	2.44	0.41
1:B5:1511:C:O2'	1:B5:2512:C:OP1	2.30	0.41
1:B5:3994:A:H2'	1:B5:3995:G:H8	1.86	0.41
1:B5:4337:U:H2'	1:B5:4338:C:C6	2.55	0.41
1:B5:4355:G:N7	25:BV:4:ARG:NH2	2.52	0.41
2:B7:36:C:H2'	2:B7:37:G:C8	2.55	0.41
4:BA:177:LYS:HG3	44:Bp:26:VAL:HG23	2.03	0.41
7:BD:51:MET:HA	7:BD:64:ILE:HD13	2.02	0.41
12:BI:205:PRO:HD2	12:BI:208:LYS:NZ	2.35	0.41
23:BT:93:ILE:HA	23:BT:96:ILE:HG12	2.02	0.41
32:Bc:45:LEU:HD21	32:Bc:108:MET:HE3	2.02	0.41
48:Bv:74:CYS:HB2	48:Bv:84:HIS:CE1	2.54	0.41
58:AF:216:ALA:HB3	58:AF:230:LEU:HB2	2.02	0.41
61:AT:30:C:OP1	77:Ao:137:HIS:N	2.53	0.41
69:Ag:134:VAL:O	69:Ag:137:SER:OG	2.26	0.41
89:TA:168:PRO:HB2	89:TA:193:THR:HG22	2.02	0.41
1:B5:519:C:H2'	1:B5:520:G:C8	2.55	0.41
1:B5:1350:G:H1	1:B5:1366:C:H42	1.68	0.41
1:B5:4155:C:H2'	1:B5:4156:G:C8	2.56	0.41
2:B7:105:C:H2'	2:B7:106:G:H8	1.85	0.41
3:B8:131:G:H2'	3:B8:132:G:H8	1.85	0.41
5:BB:82:PRO:HG3	5:BB:171:LEU:HD21	2.01	0.41
22:BS:95:ARG:NH2	22:BS:112:ASP:OD2	2.49	0.41
47:Bt:64:ILE:HA	47:Bt:69:ALA:HA	2.02	0.41
47:Bt:88:PRO:HA	47:Bt:89:PRO:HD3	1.94	0.41
52:A2:21:U:O2'	71:Ai:17:ARG:O	2.39	0.41
52:A2:547:G:H21	52:A2:549:C:H42	1.67	0.41
52:A2:1321:G:H2'	52:A2:1322:G:O4'	2.21	0.41
52:A2:1847:G:H2'	52:A2:1848:G:C8	2.56	0.41
58:AF:80:SER:HG	58:AF:90:TRP:HE1	1.61	0.41
79:Aq:16:ILE:HG22	79:Aq:24:LEU:HD11	2.02	0.41
1:B5:126:C:OP1	37:Bh:78:TYR:OH	2.39	0.41
1:B5:663:C:H2'	1:B5:664:G:C8	2.56	0.41
1:B5:769:C:H2'	1:B5:770:G:C8	2.56	0.41
1:B5:1292:U:H2'	1:B5:1293:G:C8	2.56	0.41
1:B5:2328:U:H2'	1:B5:2329:G:H8	1.86	0.41
1:B5:2654:G:N2	1:B5:2657:C:OP2	2.51	0.41
1:B5:3954:U:H2'	1:B5:3955:G:C8	2.55	0.41
1:B5:4281:A:H2'	1:B5:4282:OMC:H6	1.85	0.41
1:B5:4792:U:H3'	1:B5:4793:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Bo:74:GLU:HG3	43:Bo:76:ASN:H	1.86	0.41
49:SX:81:ILE:HG22	49:SX:84:ILE:HB	2.02	0.41
52:A2:675:C:H2'	52:A2:676:U:C6	2.55	0.41
52:A2:982:A:H2'	52:A2:983:G:C8	2.55	0.41
52:A2:1040:C:H2'	52:A2:1041:G:C8	2.56	0.41
58:AF:304:ASP:O	58:AF:306:LEU:HG	2.20	0.41
61:AT:3:C:H2'	61:AT:4:G:H8	1.84	0.41
65:Ac:172:VAL:O	65:Ac:173:ARG:NH1	2.40	0.41
69:Ag:58:LYS:HB2	69:Ag:90:LYS:HG2	2.02	0.41
1:B5:423:G:OP1	19:BP:62:ARG:NH1	2.47	0.41
1:B5:2244:A2M:HM'2	1:B5:2245:G:O5'	2.21	0.41
1:B5:3789:U:H2'	1:B5:3790:A:C8	2.55	0.41
1:B5:4052:OMU:OP2	20:BQ:159:PRO:HD2	2.21	0.41
1:B5:4205:U:H2'	1:B5:4206:U:C6	2.56	0.41
1:B5:4363:G:H2'	1:B5:4364:OMG:H8	1.86	0.41
1:B5:4450:C:H2'	1:B5:4451:A:H8	1.85	0.41
1:B5:4703:C:N4	1:B5:4704:U:O4	2.52	0.41
3:B8:141:C:H2'	3:B8:142:U:C6	2.56	0.41
11:BH:120:GLU:OE1	11:BH:124:ARG:NH2	2.43	0.41
29:BZ:48:ARG:HB3	29:BZ:69:LYS:HB3	2.01	0.41
34:Be:35:TRP:CZ2	34:Be:56:PRO:HD2	2.55	0.41
48:Bv:28:PHE:CZ	48:Bv:30:GLU:HG2	2.56	0.41
49:SX:173:TYR:CE2	49:SX:175:LEU:HB2	2.55	0.41
49:SX:268:LYS:HE3	49:SX:274:GLY:H	1.86	0.41
52:A2:496:U:H4'	66:Ad:24:THR:HG22	2.02	0.41
52:A2:1763:C:H2'	52:A2:1764:G:C8	2.55	0.41
52:A2:1857:C:H2'	52:A2:1858:G:C8	2.55	0.41
65:Ac:154:ASP:N	65:Ac:154:ASP:OD1	2.53	0.41
72:Aj:86:PRO:HD2	72:Aj:89:ILE:HD12	2.02	0.41
78:Ap:6:PRO:HB2	78:Ap:7:LEU:H	1.73	0.41
79:Aq:99:ASP:OD1	79:Aq:102:THR:N	2.48	0.41
81:As:42:HIS:HB2	81:As:83:GLN:HA	2.02	0.41
1:B5:303:C:OP2	17:BN:68:ARG:NH2	2.52	0.41
1:B5:357:U:O2	1:B5:359:A:N6	2.53	0.41
1:B5:629:G:H2'	1:B5:630:G:C8	2.56	0.41
1:B5:1793:G:N2	1:B5:4140:A:O4'	2.54	0.41
1:B5:1823:C:H4'	1:B5:2009:U:C4	2.56	0.41
1:B5:1867:C:H42	1:B5:1993:U:H1'	1.85	0.41
1:B5:2254:C:H2'	1:B5:2255:A:C8	2.56	0.41
1:B5:2736:U:O3'	70:Ah:205:ARG:NH1	2.54	0.41
1:B5:3433:OMC:H4'	1:B5:3434:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BB:39:LYS:HG2	5:BB:40:PRO:HD2	2.03	0.41
5:BB:175:GLN:HE21	5:BB:177:LYS:HB3	1.86	0.41
5:BB:206:PRO:HG2	5:BB:209:GLN:HG3	2.02	0.41
20:BQ:53:MET:HB3	20:BQ:57:ASN:HB2	2.02	0.41
23:BT:93:ILE:H	23:BT:93:ILE:HG13	1.60	0.41
25:BV:106:VAL:HG12	25:BV:112:MET:HA	2.02	0.41
36:Bg:97:ILE:HG22	36:Bg:101:LYS:HE3	2.03	0.41
49:SX:231:ARG:HA	89:TA:206:GLU:HG3	2.02	0.41
52:A2:212:C:H2'	52:A2:213:G:C8	2.56	0.41
52:A2:397:U:OP2	73:Ak:79:LYS:NZ	2.52	0.41
52:A2:485:A2M:HM'2	52:A2:486:A:C8	2.55	0.41
52:A2:660:G:H21	85:Aw:17:ARG:NH2	2.18	0.41
52:A2:1082:PSU:H5"	52:A2:1185:G:H4'	2.03	0.41
52:A2:1102:U:H2'	52:A2:1103:G:C8	2.55	0.41
54:AB:49:PRO:HA	67:Ae:60:ARG:HH21	1.86	0.41
62:AZ:80:ARG:HH22	62:AZ:166:LYS:HA	1.86	0.41
63:Aa:44:ILE:HD13	63:Aa:74:LEU:HD21	2.03	0.41
64:Ab:205:VAL:O	64:Ab:224:THR:OG1	2.30	0.41
66:Ad:188:ASN:ND2	66:Ad:219:ALA:O	2.54	0.41
70:Ah:165:GLN:HE22	70:Ah:195:LEU:HD11	1.86	0.41
80:Ar:11:HIS:O	80:Ar:22:GLY:N	2.40	0.41
89:TA:96:PRO:HA	89:TA:197:ILE:HG13	2.02	0.41
91:TC:61:LEU:HD11	91:TC:167:ILE:HG12	2.03	0.41
91:TC:89:ALA:O	91:TC:125:LYS:HE3	2.20	0.41
1:B5:1695:U:H2'	1:B5:1696:U:C6	2.55	0.41
1:B5:2249:G:O2'	41:Bl:48:LYS:NZ	2.47	0.41
1:B5:2384:G:H2'	1:B5:2385:G:H8	1.86	0.41
1:B5:2544:U:H2'	1:B5:2545:C:C6	2.56	0.41
1:B5:4020:A:H2'	1:B5:4021:G:C8	2.56	0.41
4:BA:80:GLU:HG3	44:Bp:66:GLY:HA2	2.02	0.41
5:BB:168:MET:HE1	5:BB:173:LEU:HD12	2.02	0.41
11:BH:59:LYS:HE2	11:BH:66:GLU:HB3	2.04	0.41
18:BO:54:TYR:OH	18:BO:73:PHE:O	2.33	0.41
22:BS:141:ALA:O	22:BS:144:GLN:HG2	2.21	0.41
29:BZ:87:VAL:HG12	29:BZ:89:ILE:HG13	2.03	0.41
49:SX:262:ARG:NH2	49:SX:455:TYR:OH	2.54	0.41
52:A2:98:C:H2'	52:A2:427:A:H4'	2.03	0.41
52:A2:103:A:H61	52:A2:356:G:H2'	1.86	0.41
52:A2:642:A:O2'	52:A2:646:C:OP1	2.39	0.41
62:AZ:33:GLN:NE2	83:Au:62:MET:O	2.54	0.41
62:AZ:210:ILE:HD13	79:Aq:81:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Ab:256:TRP:CD2	84:Av:68:ARG:HD2	2.56	0.41
73:Ak:10:TYR:CE2	73:Ak:12:LYS:HB3	2.56	0.41
1:B5:4:G:H2'	1:B5:5:A:C8	2.56	0.40
1:B5:2364:G:OP1	36:Bg:31:VAL:HG21	2.21	0.40
5:BB:154:LYS:HG3	5:BB:194:LEU:HD12	2.03	0.40
10:BG:264:LYS:HA	63:Aa:225:LEU:HD23	2.03	0.40
17:BN:6:TYR:CD2	38:Bi:40:VAL:HG13	2.56	0.40
18:BO:125:LYS:HE3	18:BO:125:LYS:HB3	1.97	0.40
22:BS:94:TYR:O	22:BS:139:ARG:NH2	2.54	0.40
49:SX:216:LEU:HD13	49:SX:233:ALA:HA	2.03	0.40
49:SX:419:THR:HG22	50:SY:21:LEU:HD22	2.03	0.40
52:A2:1105:G:H2'	52:A2:1106:G:C8	2.56	0.40
52:A2:1567:G:N7	81:As:101:ARG:NH2	2.68	0.40
53:AA:23:ARG:HH22	53:AA:29:ASN:HD21	1.69	0.40
58:AF:159:ASN:H	58:AF:159:ASN:HD22	1.69	0.40
77:Ao:41:GLN:HG3	77:Ao:84:ILE:HD13	2.03	0.40
83:Au:1:AME:HT23	83:Au:1:AME:HA	1.51	0.40
90:TB:102:TYR:HB3	90:TB:130:GLN:HE21	1.85	0.40
1:B5:175:C:H2'	1:B5:176:G:H8	1.86	0.40
1:B5:239:C:H2'	1:B5:240:G:C8	2.56	0.40
1:B5:300:A:H2'	1:B5:301:G:H8	1.85	0.40
1:B5:1004:G:H2'	1:B5:1005:G:H8	1.86	0.40
1:B5:1065:G:H2'	1:B5:1066:A:C8	2.56	0.40
1:B5:1210:C:H2'	1:B5:1211:G:C8	2.55	0.40
1:B5:2357:G:O2'	1:B5:2586:A:N6	2.55	0.40
1:B5:2507:G:H4'	1:B5:2520:G:H4'	2.03	0.40
1:B5:3487:G:H2'	1:B5:3488:A:H8	1.85	0.40
1:B5:3548:A:OP1	1:B5:3550:UY1:N1	2.54	0.40
1:B5:3815:G:N7	4:BA:67:TYR:OH	2.46	0.40
1:B5:3934:U:H2'	1:B5:3935:U:C6	2.56	0.40
1:B5:3973:OMU:HM21	1:B5:4082:A:H1'	2.03	0.40
1:B5:4312:U:O2'	5:BB:234:ARG:NH1	2.47	0.40
4:BA:80:GLU:HB2	4:BA:170:ALA:HA	2.03	0.40
4:BA:204:MET:HB3	4:BA:208:GLU:HG3	2.03	0.40
13:BJ:40:LEU:HD12	13:BJ:70:VAL:HG22	2.04	0.40
39:Bj:39:TYR:CG	39:Bj:40:PRO:HA	2.56	0.40
47:Bt:45:ASP:HB3	47:Bt:71:ILE:HD11	2.03	0.40
47:Bt:104:ILE:HB	47:Bt:143:VAL:HG22	2.02	0.40
49:SX:432:SER:HA	49:SX:445:THR:HG21	2.02	0.40
52:A2:432:G:H2'	52:A2:433:G:H8	1.87	0.40
52:A2:650:PSU:H2'	52:A2:651:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A2:832:G:H2'	52:A2:833:G:H8	1.87	0.40
52:A2:1116:U:H1'	52:A2:1117:C:H2'	2.04	0.40
52:A2:1693:PSU:O3'	57:AE:92:ARG:NH2	2.52	0.40
54:AB:23:SER:OG	54:AB:24:GLN:OE1	2.29	0.40
70:Ah:116:HIS:CG	70:Ah:152:ARG:HH21	2.39	0.40
84:Av:40:VAL:O	84:Av:44:HIS:ND1	2.48	0.40
90:TB:40:LEU:N	90:TB:95:LEU:O	2.42	0.40
1:B5:74:G:H5'	15:BL:60:ARG:O	2.22	0.40
1:B5:146:G:H2'	1:B5:147:A:H8	1.86	0.40
1:B5:363:A:N1	1:B5:376:A:H5"	2.37	0.40
1:B5:394:G:N2	1:B5:397:G:OP2	2.37	0.40
1:B5:1478:A:N3	1:B5:4135:C:O2'	2.51	0.40
1:B5:1984:G:O2'	1:B5:1985:G:H5"	2.21	0.40
1:B5:4046:U:H4'	23:BT:89:ILE:HG22	2.01	0.40
1:B5:4345:A:N1	1:B5:4356:A:H5"	2.37	0.40
1:B5:4432:G:H21	11:BH:163:GLN:HE22	1.68	0.40
1:B5:4616:G:OP1	16:BM:101:LYS:NZ	2.46	0.40
5:BB:234:ARG:HA	5:BB:272:LYS:HD2	2.03	0.40
17:BN:84:PRO:HA	17:BN:87:HIS:CG	2.57	0.40
17:BN:120:TRP:HZ2	17:BN:123:GLU:HG2	1.86	0.40
27:BX:95:THR:HA	27:BX:139:ARG:HA	2.02	0.40
27:BX:96:LEU:N	27:BX:138:VAL:O	2.41	0.40
52:A2:614:G:H1	52:A2:630:A:P	2.43	0.40
52:A2:1233:PSU:OP2	80:Ar:135:HIS:ND1	2.54	0.40
62:AZ:63:ARG:CZ	83:Au:78:ILE:HG23	2.51	0.40
77:Ao:49:LEU:HD22	77:Ao:53:GLN:HG2	2.03	0.40
1:B5:772:C:H2'	1:B5:773:G:C8	2.56	0.40
1:B5:2399:G:H2'	1:B5:2400:G:H8	1.86	0.40
1:B5:2616:G:H5'	40:Bk:17:ARG:HH21	1.87	0.40
1:B5:3526:C:H2'	1:B5:3527:A:C8	2.57	0.40
1:B5:4236:C:H2'	1:B5:4237:G:C8	2.57	0.40
5:BB:220:ILE:HG12	5:BB:278:THR:HG23	2.03	0.40
12:BI:52:MET:HE1	12:BI:155:ALA:HB3	2.02	0.40
15:BL:129:ARG:HH11	37:Bh:117:ARG:HD2	1.86	0.40
47:Bt:53:TRP:HD1	47:Bt:56:LEU:HB2	1.86	0.40
52:A2:456:A:O2'	52:A2:1736:A:N3	2.45	0.40
52:A2:613:U:H4'	56:AD:89:GLN:NE2	2.37	0.40
52:A2:1376:G:H2'	52:A2:1377:A:C8	2.57	0.40
66:Ad:80:ILE:HG13	66:Ad:81:THR:HG23	2.02	0.40
81:As:117:GLN:H	81:As:117:GLN:CD	2.30	0.40
1:B5:850:G:H2'	1:B5:851:G:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1095:C:H2'	1:B5:1096:G:C8	2.56	0.40
1:B5:1271:C:H5"	1:B5:4195:A:OP1	2.21	0.40
1:B5:1288:C:H2'	1:B5:1289:A:H8	1.85	0.40
1:B5:1723:U:P	12:BI:90:ARG:HH21	2.45	0.40
1:B5:2658:A2M:P	1:B5:2658:A2M:H8	2.62	0.40
1:B5:2742:C:P	21:BR:108:ARG:HH22	2.44	0.40
1:B5:3693:G:O2'	1:B5:3771:G:N2	2.54	0.40
1:B5:3782:C:H2'	1:B5:3783:U:C6	2.57	0.40
3:B8:153:C:H2'	3:B8:154:G:C8	2.57	0.40
9:BF:95:ARG:HD2	9:BF:138:TYR:HA	2.04	0.40
17:BN:143:ARG:NH1	37:Bh:95:LEU:HD23	2.37	0.40
22:BS:30:MET:HE2	22:BS:30:MET:HB3	1.91	0.40
48:Bv:59:PRO:HB2	48:Bv:171:HIS:CE1	2.56	0.40
49:SX:69:LEU:HB2	49:SX:80:GLY:HA2	2.03	0.40
52:A2:619:C:H41	85:Aw:67:ARG:NH2	2.19	0.40
52:A2:1278:C:H2'	52:A2:1279:A:H8	1.87	0.40
52:A2:1559:C:H2'	52:A2:1560:C:C6	2.57	0.40
64:Ab:102:LEU:HB3	64:Ab:130:ILE:HD11	2.02	0.40
68:Af:159:ARG:NE	68:Af:173:ALA:HB2	2.36	0.40
82:At:104:ILE:H	82:At:104:ILE:HG13	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
5	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
6	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
7	BD	291/297 (98%)	288 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BE	239/291 (82%)	236 (99%)	3 (1%)	0	100	100
9	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
10	BG	229/266 (86%)	229 (100%)	0	0	100	100
11	BH	188/192 (98%)	188 (100%)	0	0	100	100
12	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
13	BJ	168/178 (94%)	168 (100%)	0	0	100	100
15	BL	208/211 (99%)	206 (99%)	2 (1%)	0	100	100
16	BM	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
17	BN	201/204 (98%)	200 (100%)	1 (0%)	0	100	100
18	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
19	BP	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
20	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
21	BR	178/196 (91%)	178 (100%)	0	0	100	100
22	BS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	BV	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
26	BW	119/157 (76%)	119 (100%)	0	0	100	100
27	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
28	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
29	BZ	133/136 (98%)	133 (100%)	0	0	100	100
30	Ba	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	51
31	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
32	Bc	106/115 (92%)	106 (100%)	0	0	100	100
33	Bd	105/125 (84%)	105 (100%)	0	0	100	100
34	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
35	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
36	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
37	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
39	Bj	86/97 (89%)	86 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	Bk	67/70 (96%)	67 (100%)	0	0	100	100
41	Bl	48/51 (94%)	48 (100%)	0	0	100	100
42	Bm	49/128 (38%)	49 (100%)	0	0	100	100
43	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
44	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
45	Br	124/137 (90%)	124 (100%)	0	0	100	100
46	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
47	Bt	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
48	Bv	210/217 (97%)	205 (98%)	5 (2%)	0	100	100
49	SX	419/476 (88%)	404 (96%)	15 (4%)	0	100	100
50	SY	60/68 (88%)	60 (100%)	0	0	100	100
51	SZ	27/96 (28%)	27 (100%)	0	0	100	100
53	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
54	AB	61/69 (88%)	61 (100%)	0	0	100	100
55	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
56	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
57	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
58	AF	311/317 (98%)	307 (99%)	4 (1%)	0	100	100
59	AG	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
62	AZ	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
63	Aa	220/264 (83%)	219 (100%)	1 (0%)	0	100	100
64	Ab	218/293 (74%)	218 (100%)	0	0	100	100
65	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
66	Ad	260/263 (99%)	260 (100%)	0	0	100	100
67	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
68	Af	235/249 (94%)	235 (100%)	0	0	100	100
69	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
70	Ah	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
71	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
72	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
73	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
75	Am	148/151 (98%)	148 (100%)	0	0	100	100
76	An	133/151 (88%)	132 (99%)	1 (1%)	0	100	100
77	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
78	Ap	139/172 (81%)	138 (99%)	1 (1%)	0	100	100
79	Aq	132/135 (98%)	132 (100%)	0	0	100	100
80	Ar	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
81	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
82	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
83	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
84	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
85	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
86	Ax	123/130 (95%)	123 (100%)	0	0	100	100
87	Ay	83/124 (67%)	83 (100%)	0	0	100	100
88	Az	23/25 (92%)	23 (100%)	0	0	100	100
89	TA	168/286 (59%)	165 (98%)	3 (2%)	0	100	100
90	TB	159/183 (87%)	159 (100%)	0	0	100	100
91	TC	158/185 (85%)	158 (100%)	0	0	100	100
92	TD	148/173 (86%)	148 (100%)	0	0	100	100
All	All	13050/15304 (85%)	12903 (99%)	146 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	Ba	15	VAL

5.3.2 Protein sidechains (i)

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	BA	194/198 (98%)	193 (100%)	1 (0%)	81 80
5	BB	344/347 (99%)	342 (99%)	2 (1%)	78 79
6	BC	302/337 (90%)	302 (100%)	0	100 100
7	BD	247/250 (99%)	247 (100%)	0	100 100
8	BE	216/251 (86%)	216 (100%)	0	100 100
9	BF	197/215 (92%)	196 (100%)	1 (0%)	81 80
10	BG	199/223 (89%)	197 (99%)	2 (1%)	68 75
11	BH	169/171 (99%)	169 (100%)	0	100 100
12	BI	180/181 (99%)	179 (99%)	1 (1%)	78 79
13	BJ	143/149 (96%)	143 (100%)	0	100 100
15	BL	175/176 (99%)	173 (99%)	2 (1%)	65 74
16	BM	117/161 (73%)	117 (100%)	0	100 100
17	BN	171/172 (99%)	171 (100%)	0	100 100
18	BO	171/173 (99%)	170 (99%)	1 (1%)	78 79
19	BP	140/163 (86%)	140 (100%)	0	100 100
20	BQ	164/165 (99%)	162 (99%)	2 (1%)	63 73
21	BR	159/175 (91%)	158 (99%)	1 (1%)	78 79
22	BS	154/154 (100%)	154 (100%)	0	100 100
23	BT	139/140 (99%)	137 (99%)	2 (1%)	59 71
24	BU	88/113 (78%)	88 (100%)	0	100 100
25	BV	106/107 (99%)	106 (100%)	0	100 100
26	BW	100/126 (79%)	100 (100%)	0	100 100
27	BX	106/134 (79%)	106 (100%)	0	100 100
28	BY	124/135 (92%)	124 (100%)	0	100 100
29	BZ	117/118 (99%)	117 (100%)	0	100 100
30	Ba	118/119 (99%)	118 (100%)	0	100 100
31	Bb	87/183 (48%)	87 (100%)	0	100 100
32	Bc	92/98 (94%)	92 (100%)	0	100 100
33	Bd	98/110 (89%)	98 (100%)	0	100 100
34	Be	116/121 (96%)	116 (100%)	0	100 100
35	Bf	89/89 (100%)	89 (100%)	0	100 100
36	Bg	98/100 (98%)	98 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Bh	109/110 (99%)	109 (100%)	0	100	100
38	Bi	86/89 (97%)	86 (100%)	0	100	100
39	Bj	74/80 (92%)	74 (100%)	0	100	100
40	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	70
41	Bl	47/48 (98%)	47 (100%)	0	100	100
42	Bm	47/115 (41%)	47 (100%)	0	100	100
43	Bo	92/93 (99%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	71
45	Br	109/120 (91%)	109 (100%)	0	100	100
46	Bs	164/258 (64%)	161 (98%)	3 (2%)	51	69
47	Bt	128/137 (93%)	123 (96%)	5 (4%)	28	54
48	Bv	191/195 (98%)	188 (98%)	3 (2%)	55	70
49	SX	361/398 (91%)	352 (98%)	9 (2%)	42	63
50	SY	53/59 (90%)	51 (96%)	2 (4%)	29	55
51	SZ	26/74 (35%)	24 (92%)	2 (8%)	12	37
53	AA	75/76 (99%)	74 (99%)	1 (1%)	61	72
54	AB	56/62 (90%)	55 (98%)	1 (2%)	51	69
55	AC	67/140 (48%)	67 (100%)	0	100	100
56	AD	47/106 (44%)	47 (100%)	0	100	100
57	AE	88/98 (90%)	85 (97%)	3 (3%)	32	57
58	AF	272/275 (99%)	270 (99%)	2 (1%)	76	78
59	AG	48/49 (98%)	48 (100%)	0	100	100
62	AZ	182/243 (75%)	179 (98%)	3 (2%)	55	70
63	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	75
64	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	80
65	Ac	189/232 (82%)	187 (99%)	2 (1%)	65	74
66	Ad	224/225 (100%)	224 (100%)	0	100	100
67	Ae	161/170 (95%)	161 (100%)	0	100	100
68	Af	207/218 (95%)	207 (100%)	0	100	100
69	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	79
70	Ah	178/180 (99%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
71	Ai	161/168 (96%)	160 (99%)	1 (1%)	78 79
72	Aj	87/136 (64%)	86 (99%)	1 (1%)	65 74
73	Ak	139/142 (98%)	138 (99%)	1 (1%)	76 78
74	Al	104/108 (96%)	103 (99%)	1 (1%)	68 75
75	Am	130/131 (99%)	130 (100%)	0	100 100
76	An	105/118 (89%)	103 (98%)	2 (2%)	50 68
77	Ao	114/130 (88%)	112 (98%)	2 (2%)	51 69
78	Ap	117/140 (84%)	117 (100%)	0	100 100
79	Aq	120/121 (99%)	120 (100%)	0	100 100
80	Ar	127/131 (97%)	125 (98%)	2 (2%)	55 70
81	As	112/114 (98%)	111 (99%)	1 (1%)	70 76
82	At	94/107 (88%)	93 (99%)	1 (1%)	65 74
83	Au	67/67 (100%)	65 (97%)	2 (3%)	36 60
84	Av	112/113 (99%)	111 (99%)	1 (1%)	70 76
85	Aw	112/114 (98%)	110 (98%)	2 (2%)	51 69
86	Ax	107/112 (96%)	107 (100%)	0	100 100
87	Ay	75/102 (74%)	75 (100%)	0	100 100
88	Az	24/24 (100%)	24 (100%)	0	100 100
89	TA	151/249 (61%)	150 (99%)	1 (1%)	76 78
90	TB	134/152 (88%)	133 (99%)	1 (1%)	76 78
91	TC	142/164 (87%)	142 (100%)	0	100 100
92	TD	130/146 (89%)	130 (100%)	0	100 100
All	All	11361/12947 (88%)	11285 (99%)	76 (1%)	73 78

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	BA	44	ILE
5	BB	248	LEU
5	BB	344	VAL
9	BF	85	GLU
10	BG	106	THR
10	BG	220	GLU
12	BI	43	VAL

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Mol	Chain	Res	Type
15	BL	81	LEU
15	BL	115	GLN
18	BO	174	LEU
20	BQ	82	VAL
20	BQ	115	LYS
21	BR	105	LEU
23	BT	76	VAL
23	BT	93	ILE
40	Bk	36	VAL
44	Bp	52	VAL
46	Bs	44	ARG
46	Bs	63	LYS
46	Bs	78	LEU
47	Bt	12	VAL
47	Bt	15	LEU
47	Bt	35	LEU
47	Bt	73	VAL
47	Bt	74	VAL
48	Bv	58	THR
48	Bv	60	ARG
48	Bv	96	ASN
49	SX	47	GLN
49	SX	77	MET
49	SX	81	ILE
49	SX	201	VAL
49	SX	219	LEU
49	SX	238	ASN
49	SX	441	ILE
49	SX	461	PHE
49	SX	464	GLU
50	SY	9	GLU
50	SY	56	LEU
51	SZ	73	VAL
51	SZ	88	HIS
53	AA	74	THR
54	AB	14	VAL
57	AE	21	ILE
57	AE	40	VAL
57	AE	75	VAL
58	AF	159	ASN
58	AF	275	ILE
62	AZ	112	ILE

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Mol	Chain	Res	Type
62	AZ	121	LEU
62	AZ	206	ASP
63	Aa	127	VAL
63	Aa	178	THR
64	Ab	121	ARG
65	Ac	46	THR
65	Ac	84	VAL
69	Ag	53	VAL
71	Ai	55	LYS
72	Aj	40	VAL
73	Ak	24	LEU
74	Al	75	ASN
76	An	21	VAL
76	An	100	THR
77	Ao	105	VAL
77	Ao	133	ILE
80	Ar	94	LYS
80	Ar	103	LEU
81	As	114	GLU
82	At	54	VAL
83	Au	42	VAL
83	Au	61	ARG
84	Av	105	THR
85	Aw	105	PHE
85	Aw	125	VAL
89	TA	204	ASP
90	TB	143	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
4	BA	50	HIS
4	BA	83	HIS
4	BA	140	ASN
5	BB	167	GLN
5	BB	175	GLN
5	BB	184	GLN
5	BB	289	GLN
6	BC	48	ASN
6	BC	50	GLN
6	BC	61	GLN
6	BC	89	GLN

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Mol	Chain	Res	Type
6	BC	203	GLN
6	BC	212	ASN
6	BC	276	ASN
6	BC	329	ASN
7	BD	81	HIS
7	BD	122	GLN
7	BD	202	GLN
7	BD	275	GLN
7	BD	282	GLN
8	BE	131	HIS
8	BE	269	GLN
8	BE	282	ASN
9	BF	57	HIS
9	BF	115	GLN
9	BF	118	ASN
9	BF	199	HIS
9	BF	238	GLN
10	BG	38	ASN
10	BG	64	GLN
10	BG	81	ASN
10	BG	141	ASN
10	BG	236	HIS
11	BH	98	HIS
12	BI	59	GLN
12	BI	73	ASN
12	BI	163	GLN
13	BJ	71	HIS
13	BJ	97	ASN
13	BJ	104	ASN
16	BM	20	HIS
16	BM	33	GLN
16	BM	48	GLN
17	BN	158	HIS
18	BO	143	HIS
18	BO	173	GLN
18	BO	180	GLN
19	BP	75	GLN
19	BP	120	ASN
19	BP	137	ASN
21	BR	34	ASN
21	BR	39	GLN
21	BR	40	GLN

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Mol	Chain	Res	Type
21	BR	143	HIS
23	BT	131	GLN
24	BU	17	GLN
24	BU	38	ASN
24	BU	50	ASN
26	BW	120	GLN
27	BX	107	HIS
27	BX	111	GLN
28	BY	14	ASN
28	BY	56	GLN
30	Ba	34	ASN
33	Bd	79	ASN
33	Bd	116	ASN
34	Be	34	ASN
35	Bf	20	ASN
35	Bf	56	ASN
36	Bg	28	ASN
36	Bg	114	GLN
37	Bh	65	GLN
38	Bi	26	HIS
38	Bi	36	HIS
38	Bi	80	HIS
39	Bj	13	ASN
40	Bk	58	GLN
41	Bl	33	ASN
42	Bm	117	HIS
43	Bo	102	GLN
45	Br	4	HIS
45	Br	6	GLN
45	Br	30	ASN
46	Bs	68	HIS
46	Bs	191	GLN
47	Bt	65	GLN
48	Bv	96	ASN
49	SX	127	GLN
49	SX	397	GLN
49	SX	404	HIS
49	SX	414	ASN
50	SY	13	GLN
51	SZ	88	HIS
53	AA	29	ASN
53	AA	51	GLN

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Mol	Chain	Res	Type
56	AD	89	GLN
58	AF	62	HIS
58	AF	159	ASN
58	AF	188	HIS
58	AF	222	ASN
59	AG	37	ASN
62	AZ	113	GLN
63	Aa	40	ASN
63	Aa	76	ASN
63	Aa	101	HIS
63	Aa	118	GLN
63	Aa	208	HIS
64	Ab	115	GLN
65	Ac	145	GLN
66	Ad	98	ASN
66	Ad	142	HIS
66	Ad	157	ASN
67	Ae	65	GLN
67	Ae	118	ASN
67	Ae	137	GLN
68	Af	56	ASN
68	Af	177	GLN
69	Ag	68	GLN
69	Ag	91	HIS
70	Ah	7	ASN
70	Ah	146	GLN
70	Ah	167	GLN
72	Aj	50	GLN
72	Aj	77	GLN
74	Al	28	HIS
75	Am	36	GLN
76	An	113	GLN
78	Ap	24	HIS
78	Ap	86	GLN
78	Ap	97	GLN
78	Ap	114	GLN
80	Ar	72	GLN
81	As	12	GLN
83	Au	2	GLN
84	Av	90	GLN
84	Av	91	ASN
85	Aw	23	HIS

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Mol	Chain	Res	Type
85	Aw	46	HIS
85	Aw	92	ASN
86	Ax	19	GLN
86	Ax	85	ASN
87	Ay	112	ASN
90	TB	130	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3752/4808 (78%)	424 (11%)	2 (0%)
2	B7	118/120 (98%)	6 (5%)	0
3	B8	155/158 (98%)	20 (12%)	0
52	A2	1764/1870 (94%)	199 (11%)	0
60	AH	2/4 (50%)	0	0
61	AT	74/75 (98%)	8 (10%)	0
All	All	5865/7035 (83%)	657 (11%)	2 (0%)

All (657) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	59	A
1	B5	64	A
1	B5	65	A
1	B5	85	G
1	B5	91	G
1	B5	98	A
1	B5	109	G
1	B5	110	C
1	B5	119	G
1	B5	135	G
1	B5	136	U
1	B5	144	G
1	B5	159	C
1	B5	185	C
1	B5	187	U
1	B5	188	G
1	B5	200	U
1	B5	201	C

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Mol	Chain	Res	Type
1	B5	210	C
1	B5	218	A
1	B5	219	G
1	B5	220	C
1	B5	233	U
1	B5	234	G
1	B5	266	C
1	B5	297	U
1	B5	309	C
1	B5	315	G
1	B5	316	U
1	B5	326	C
1	B5	334	A
1	B5	340	C
1	B5	363	A
1	B5	386	A
1	B5	387	G
1	B5	409	G
1	B5	412	G
1	B5	446	C
1	B5	449	C
1	B5	450	G
1	B5	452	A
1	B5	453	G
1	B5	454	U
1	B5	463	A
1	B5	467	U
1	B5	468	U
1	B5	482	U
1	B5	483	G
1	B5	485	U
1	B5	486	C
1	B5	493	U
1	B5	497	G
1	B5	499	C
1	B5	502	U
1	B5	503	C
1	B5	504	U
1	B5	505	C
1	B5	506	G
1	B5	512	U
1	B5	515	U

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Mol	Chain	Res	Type
1	B5	516	U
1	B5	517	C
1	B5	628	U
1	B5	634	C
1	B5	635	G
1	B5	691	G
1	B5	698	C
1	B5	724	G
1	B5	725	G
1	B5	732	C
1	B5	734	G
1	B5	739	G
1	B5	758	C
1	B5	760	C
1	B5	790	G
1	B5	791	C
1	B5	792	G
1	B5	795	A
1	B5	797	C
1	B5	798	C
1	B5	799	C
1	B5	803	C
1	B5	810	U
1	B5	812	A
1	B5	814	A
1	B5	815	G
1	B5	824	C
1	B5	825	G
1	B5	831	A
1	B5	832	G
1	B5	835	G
1	B5	843	A
1	B5	844	A
1	B5	845	U
1	B5	856	A
1	B5	859	G
1	B5	860	A
1	B5	861	G
1	B5	866	A
1	B5	867	C
1	B5	868	C
1	B5	870	G

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Mol	Chain	Res	Type
1	B5	884	U
1	B5	983	G
1	B5	985	G
1	B5	987	C
1	B5	1072	C
1	B5	1073	C
1	B5	1074	C
1	B5	1084	C
1	B5	1091	G
1	B5	1102	G
1	B5	1105	C
1	B5	1106	U
1	B5	1124	A
1	B5	1133	C
1	B5	1202	C
1	B5	1214	A
1	B5	1215	G
1	B5	1217	G
1	B5	1219	G
1	B5	1221	G
1	B5	1228	G
1	B5	1231	G
1	B5	1238	A
1	B5	1239	U
1	B5	1240	G
1	B5	1246	U
1	B5	1247	A
1	B5	1270	A2M
1	B5	1298	A
1	B5	1299	G
1	B5	1303	G
1	B5	1309	C
1	B5	1310	G
1	B5	1323	C
1	B5	1331	A
1	B5	1341	A
1	B5	1351	G
1	B5	1367	G
1	B5	1375	A
1	B5	1391	C
1	B5	1393	C
1	B5	1401	C

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Mol	Chain	Res	Type
1	B5	1452	A
1	B5	1453	G
1	B5	1457	G
1	B5	1469	U
1	B5	1489	A2M
1	B5	1502	A
1	B5	1521	C
1	B5	1533	U
1	B5	1546	U
1	B5	1551	U
1	B5	1579	G
1	B5	1580	OMG
1	B5	1586	A
1	B5	1588	G
1	B5	1589	A
1	B5	1593	A
1	B5	1609	G
1	B5	1616	C
1	B5	1631	C
1	B5	1632	PSU
1	B5	1653	C
1	B5	1657	C
1	B5	1658	C
1	B5	1694	C
1	B5	1704	A
1	B5	1705	A
1	B5	1726	A
1	B5	1743	A
1	B5	1767	C
1	B5	1774	G
1	B5	1775	G
1	B5	1776	A
1	B5	1781	G
1	B5	1794	G
1	B5	1808	G
1	B5	1836	A
1	B5	1857	U
1	B5	1859	C
1	B5	1860	C
1	B5	1861	G
1	B5	1870	C
1	B5	1871	A

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Mol	Chain	Res	Type
1	B5	1879	G
1	B5	1887	G
1	B5	1898	U
1	B5	1900	G
1	B5	1913	U
1	B5	1922	A
1	B5	1923	A
1	B5	1926	C
1	B5	1936	U
1	B5	1942	G
1	B5	1943	U
1	B5	1963	G
1	B5	1965	A
1	B5	1985	G
1	B5	1987	U
1	B5	1994	G
1	B5	1995	G
1	B5	2008	A
1	B5	2023	U
1	B5	2032	G
1	B5	2037	G
1	B5	2041	G
1	B5	2044	A
1	B5	2045	G
1	B5	2046	A
1	B5	2132	C
1	B5	2143	A
1	B5	2144	G
1	B5	2156	A
1	B5	2157	G
1	B5	2174	G
1	B5	2191	G
1	B5	2194	OMC
1	B5	2203	A
1	B5	2207	OMG
1	B5	2238	A
1	B5	2253	C
1	B5	2264	G
1	B5	2268	U
1	B5	2327	A
1	B5	2328	U
1	B5	2330	G

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Mol	Chain	Res	Type
1	B5	2331	C
1	B5	2332	C
1	B5	2349	G
1	B5	2356	A
1	B5	2372	A
1	B5	2380	A
1	B5	2387	G
1	B5	2388	U
1	B5	2390	G
1	B5	2409	G
1	B5	2430	A
1	B5	2444	A
1	B5	2496	C
1	B5	2503	A
1	B5	2512	C
1	B5	2530	U
1	B5	2537	G
1	B5	2538	A
1	B5	2539	A
1	B5	2550	U
1	B5	2551	U
1	B5	2552	C
1	B5	2553	C
1	B5	2554	G
1	B5	2578	G
1	B5	2586	A
1	B5	2606	U
1	B5	2612	U
1	B5	2630	A2M
1	B5	2631	U
1	B5	2633	U
1	B5	2641	A
1	B5	2657	C
1	B5	2669	U
1	B5	2670	G
1	B5	2672	U
1	B5	2698	G
1	B5	2745	G
1	B5	3329	G
1	B5	3350	C
1	B5	3358	G
1	B5	3367	A

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Mol	Chain	Res	Type
1	B5	3376	U
1	B5	3385	A
1	B5	3394	A
1	B5	3443	A
1	B5	3444	A
1	B5	3485	G
1	B5	3492	A2M
1	B5	3493	C
1	B5	3498	A
1	B5	3508	G
1	B5	3509	G
1	B5	3516	A
1	B5	3543	G
1	B5	3544	C
1	B5	3546	U
1	B5	3549	A
1	B5	3551	G
1	B5	3570	U
1	B5	3572	U
1	B5	3609	A
1	B5	3610	C
1	B5	3611	G
1	B5	3629	G
1	B5	3630	G
1	B5	3633	A
1	B5	3638	A
1	B5	3639	G
1	B5	3640	A
1	B5	3647	U
1	B5	3670	G
1	B5	3687	G
1	B5	3688	G
1	B5	3689	U
1	B5	3704	A
1	B5	3785	C
1	B5	3804	G
1	B5	3823	G
1	B5	3824	C
1	B5	3825	G
1	B5	3832	G
1	B5	3833	A
1	B5	3834	G

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Mol	Chain	Res	Type
1	B5	3847	C
1	B5	3850	G
1	B5	3855	A
1	B5	3869	G
1	B5	3875	C
1	B5	3891	C
1	B5	3892	G
1	B5	3904	C
1	B5	3909	U
1	B5	3916	A
1	B5	3929	G
1	B5	3930	G
1	B5	3937	G
1	B5	3949	A
1	B5	3975	U
1	B5	3979	A
1	B5	3997	A
1	B5	4000	G
1	B5	4012	G
1	B5	4014	A
1	B5	4017	A
1	B5	4019	A
1	B5	4027	A
1	B5	4037	G
1	B5	4051	G
1	B5	4052	OMU
1	B5	4060	C
1	B5	4076	G
1	B5	4078	C
1	B5	4096	C
1	B5	4100	U
1	B5	4119	G
1	B5	4123	G
1	B5	4124	A
1	B5	4133	C
1	B5	4137	G
1	B5	4140	A
1	B5	4168	A
1	B5	4194	G
1	B5	4210	A
1	B5	4212	C
1	B5	4221	G

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Mol	Chain	Res	Type
1	B5	4258	U
1	B5	4259	A
1	B5	4270	G
1	B5	4294	A
1	B5	4306	C
1	B5	4313	G
1	B5	4321	G
1	B5	4336	A2M
1	B5	4381	A
1	B5	4382	PSU
1	B5	4383	OMG
1	B5	4402	A
1	B5	4416	C
1	B5	4418	A
1	B5	4437	A
1	B5	4440	G
1	B5	4446	A
1	B5	4454	A
1	B5	4455	U
1	B5	4465	G
1	B5	4475	A
1	B5	4476	C
1	B5	4477	G
1	B5	4478	G
1	B5	4486	G
1	B5	4487	A
1	B5	4488	A
1	B5	4489	G
1	B5	4490	G
1	B5	4492	G
1	B5	4498	G
1	B5	4501	G
1	B5	4504	C
1	B5	4506	C
1	B5	4508	G
1	B5	4512	G
1	B5	4518	C
1	B5	4609	G
1	B5	4610	C
1	B5	4614	G
1	B5	4621	U
1	B5	4622	C

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Mol	Chain	Res	Type
1	B5	4638	G
1	B5	4639	C
1	B5	4640	G
1	B5	4644	C
1	B5	4645	C
1	B5	4646	G
1	B5	4647	G
1	B5	4649	A
1	B5	4651	G
1	B5	4658	G
1	B5	4705	A
1	B5	4715	U
1	B5	4728	U
1	B5	4729	C
1	B5	4753	A
1	B5	4756	G
1	B5	4761	U
1	B5	4762	C
1	B5	4763	C
1	B5	4765	U
1	B5	4766	C
1	B5	4780	G
1	B5	4789	C
1	B5	4793	C
1	B5	4801	G
1	B5	4808	U
2	B7	7	G
2	B7	53	U
2	B7	54	A
2	B7	64	G
2	B7	110	G
2	B7	120	U
3	B8	23	C
3	B8	34	U
3	B8	35	C
3	B8	59	A
3	B8	62	A
3	B8	63	U
3	B8	83	C
3	B8	84	A
3	B8	85	U
3	B8	87	G

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Mol	Chain	Res	Type
3	B8	88	A
3	B8	94	G
3	B8	103	A
3	B8	105	C
3	B8	110	U
3	B8	114	G
3	B8	123	U
3	B8	124	U
3	B8	126	C
3	B8	156	U
52	A2	2	A
52	A2	3	C
52	A2	4	C
52	A2	33	G
52	A2	41	G
52	A2	44	U
52	A2	46	A
52	A2	56	G
52	A2	67	C
52	A2	68	A
52	A2	73	C
52	A2	74	G
52	A2	76	U
52	A2	77	A
52	A2	79	A
52	A2	103	A
52	A2	113	G
52	A2	115	U
52	A2	126	G
52	A2	130	G
52	A2	143	U
52	A2	147	A
52	A2	155	G
52	A2	163	U
52	A2	168	C
52	A2	178	C
52	A2	184	G
52	A2	188	C
52	A2	192	C
52	A2	226	A
52	A2	282	C
52	A2	306	U

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Mol	Chain	Res	Type
52	A2	310	G
52	A2	313	G
52	A2	320	C
52	A2	324	C
52	A2	325	U
52	A2	327	C
52	A2	328	G
52	A2	336	G
52	A2	348	G
52	A2	365	A
52	A2	370	C
52	A2	386	G
52	A2	387	C
52	A2	401	C
52	A2	410	C
52	A2	439	G
52	A2	449	A
52	A2	451	C
52	A2	465	A
52	A2	466	A
52	A2	472	G
52	A2	473	C
52	A2	474	A
52	A2	475	G
52	A2	488	U
52	A2	493	C
52	A2	502	C
52	A2	509	A
52	A2	526	A
52	A2	549	C
52	A2	565	A
52	A2	569	C
52	A2	584	A
52	A2	590	G
52	A2	592	U
52	A2	605	A
52	A2	607	G
52	A2	609	C
52	A2	615	C
52	A2	632	U
52	A2	644	A
52	A2	645	OMG

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Mol	Chain	Res	Type
52	A2	661	C
52	A2	669	A2M
52	A2	670	A
52	A2	672	A
52	A2	673	A
52	A2	734	C
52	A2	747	C
52	A2	748	U
52	A2	755	G
52	A2	756	C
52	A2	799	G
52	A2	802	PSU
52	A2	812	A
52	A2	822	G
52	A2	823	PSU
52	A2	831	A
52	A2	837	G
52	A2	838	A
52	A2	839	G
52	A2	840	C
52	A2	841	C
52	A2	842	G
52	A2	848	A
52	A2	871	A
52	A2	873	A
52	A2	879	G
52	A2	886	U
52	A2	892	G
52	A2	910	G
52	A2	914	A
52	A2	915	U
52	A2	921	A
52	A2	923	A
52	A2	931	C
52	A2	934	G
52	A2	944	U
52	A2	956	A
52	A2	972	G
52	A2	991	A
52	A2	993	A
52	A2	1000	G
52	A2	1003	U

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Mol	Chain	Res	Type
52	A2	1024	A
52	A2	1062	U
52	A2	1063	A
52	A2	1084	A
52	A2	1086	C
52	A2	1116	U
52	A2	1117	C
52	A2	1118	C
52	A2	1119	C
52	A2	1122	G
52	A2	1145	A
52	A2	1154	C
52	A2	1155	U
52	A2	1196	A
52	A2	1208	G
52	A2	1216	C
52	A2	1225	G
52	A2	1243	U
52	A2	1249	B8N
52	A2	1252	A
52	A2	1254	A
52	A2	1257	G
52	A2	1258	G
52	A2	1260	A
52	A2	1272	C
52	A2	1275	G
52	A2	1276	G
52	A2	1283	A
52	A2	1303	G
52	A2	1304	C
52	A2	1343	U
52	A2	1359	U
52	A2	1372	U
52	A2	1379	A
52	A2	1398	U
52	A2	1403	A
52	A2	1406	A
52	A2	1407	G
52	A2	1419	C
52	A2	1420	C
52	A2	1422	A
52	A2	1424	C

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Mol	Chain	Res	Type
52	A2	1436	C
52	A2	1455	A
52	A2	1463	U
52	A2	1464	U
52	A2	1481	A
52	A2	1490	A
52	A2	1491	OMG
52	A2	1495	U
52	A2	1498	G
52	A2	1522	C
52	A2	1523	A
52	A2	1534	A
52	A2	1553	G
52	A2	1580	A
52	A2	1581	A
52	A2	1589	A
52	A2	1602	A
52	A2	1622	U
52	A2	1624	A
52	A2	1655	G
52	A2	1666	G
52	A2	1681	G
52	A2	1699	C
52	A2	1722	U
52	A2	1723	G
52	A2	1749	G
52	A2	1783	G
52	A2	1784	C
52	A2	1785	G
52	A2	1830	G
52	A2	1832	A
52	A2	1836	A
52	A2	1837	G
52	A2	1839	U
52	A2	1850	G
52	A2	1852	MA6
52	A2	1853	C
52	A2	1862	G
52	A2	1863	G
52	A2	1864	A
52	A2	1866	C
61	AT	9	C

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Mol	Chain	Res	Type
61	AT	17	G
61	AT	18	G
61	AT	19	U
61	AT	20	U
61	AT	21	A
61	AT	60	C
61	AT	75	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	1588	G
1	B5	4445	U

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

226 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	PSU	B5	1720	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4099	95,1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	G7M	A2	1640	52,61	23,26,27	3.14	9 (39%)	35,39,42	3.31	13 (37%)
52	PSU	A2	1693	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
61	5MC	AT	48	61	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
1	OMG	B5	3524	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	B5	3573	1	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	PSU	B5	4177	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	OMG	A2	1491	52,95	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	6MZ	A2	1833	52,95	22,25,26	1.44	4 (18%)	30,36,39	2.16	9 (30%)
1	PSU	B5	4149	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
52	PSU	A2	1626	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	B5	2208	95,1	19,22,23	0.81	0	26,31,34	0.81	0
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	A2M	A2	591	52	22,25,26	1.48	4 (18%)	31,36,39	2.21	7 (22%)
3	PSU	B8	55	3	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1368	52	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3490	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4042	1	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
52	OMU	A2	116	52	19,22,23	1.20	2 (10%)	26,31,34	1.68	4 (15%)
52	PSU	A2	407	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
42	M3L	Bm	98	42	10,11,12	0.82	0	9,14,16	0.48	0
1	PSU	B5	3371	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	B5	4166	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
61	PSU	AT	54	61	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4419	95,1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	B5	3619	1	19,22,23	0.81	0	26,31,34	0.85	0
1	PSU	B5	3466	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	6MZ	B5	3966	1	22,25,26	1.44	4 (18%)	30,36,39	2.20	9 (30%)
1	PSU	B5	4188	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.66	4 (15%)
1	PSU	B5	1801	95,1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3447	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
43	MLZ	Bo	53	43	8,9,10	0.49	0	4,9,11	0.11	0
52	OMU	A2	1327	52,95	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
1	A2M	B5	3562	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
52	OMC	A2	1704	52	19,22,23	0.82	0	26,31,34	0.81	0
52	OMU	A2	429	52	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
52	PSU	A2	1233	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	172	52	19,22,23	1.19	3 (15%)	26,31,34	1.70	5 (19%)
1	PSU	B5	3652	95,1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	687	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	823	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1245	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	610	52	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	B5	2704	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
52	PSU	A2	652	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	B5	1799	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	4AC	A2	1338	52	21,24,25	1.03	1 (4%)	29,34,37	1.26	3 (10%)
52	PSU	A2	1348	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
52	A2M	A2	1679	52	22,25,26	1.47	4 (18%)	31,36,39	2.23	10 (32%)
1	PSU	B5	3585	95,1	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	34	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	A2M	A2	469	52	22,25,26	1.48	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	B5	4217	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
83	AME	Au	1	83	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
1	5MC	B5	3514	95,1	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
52	MA6	A2	1852	52	23,26,27	2.25	5 (21%)	34,38,41	3.69	14 (41%)
1	OMG	B5	1260	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	4740	95,1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	B5	3599	1	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
52	PSU	A2	1175	52,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1721	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	119	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	OMU	A2	355	52,95	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	OMU	B5	4244	95,1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
1	A2M	B5	3492	52,95,1	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
1	A2M	B5	2206	95,1	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	B5	3494	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1638	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	628	52	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	OMG	B5	2719	1	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
52	PSU	A2	1082	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	MA6	A2	1851	52	23,26,27	2.28	5 (21%)	34,38,41	3.71	13 (38%)
1	PSU	B5	1537	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	OMU	A2	1443	52,95	19,22,23	1.23	3 (15%)	26,31,34	1.69	5 (19%)
80	SAC	Ar	2	80	7,8,9	0.53	0	8,9,11	0.92	1 (12%)
1	OMC	B5	3433	95,1	19,22,23	0.79	0	26,31,34	0.75	0
52	PSU	A2	1057	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3496	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	B5	4138	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	A2M	A2	99	52,95	22,25,26	1.48	4 (18%)	31,36,39	2.13	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	B5	3616	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
62	SAC	AZ	2	62	7,8,9	0.54	0	8,9,11	0.86	1 (12%)
1	A2M	B5	2658	95,1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	OMC	B5	4202	1	19,22,23	0.82	0	26,31,34	0.82	0
52	PSU	A2	816	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	815	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1731	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4107	95,1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1047	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
3	OMG	B8	75	3	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
31	MLZ	Bb	5	31,95	8,9,10	0.49	0	4,9,11	0.16	0
52	OMC	A2	174	52,95	19,22,23	0.81	0	26,31,34	0.78	0
52	A2M	A2	485	52	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	PSU	B5	3369	95,1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	2351	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	OMC	A2	518	52	19,22,23	0.82	0	26,31,34	0.83	0
52	PSU	A2	650	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	A2M	A2	159	52	22,25,26	1.47	4 (18%)	31,36,39	2.16	10 (32%)
1	OMG	B5	1477	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4749	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	B8N	A2	1249	52	24,29,30	1.29	3 (12%)	29,42,45	1.27	3 (10%)
1	PSU	B5	4278	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
52	OMU	A2	1805	52,95	19,22,23	1.22	3 (15%)	26,31,34	1.68	5 (19%)
52	PSU	A2	1239	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	3601	1	19,22,23	0.81	0	26,31,34	0.83	0
52	A2M	A2	669	52,95	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	B5	3554	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	4317	1	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
1	A2M	B5	2630	95,1	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
52	OMU	A2	1289	52	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
1	PSU	B5	3427	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	3476	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	B5	3974	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
76	5F0	An	138	76	8,8,9	1.49	2 (25%)	7,9,11	1.70	1 (14%)
1	PSU	B5	1491	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	166	52	22,25,26	1.48	4 (18%)	31,36,39	2.13	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	B5	4364	95,1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	3583	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4711	95,1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2667	1	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
1	PSU	B5	4045	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	93	52	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4058	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	3450	1	22,25,26	1.47	4 (18%)	31,36,39	2.08	9 (29%)
5	HIC	BB	245	5	10,11,12	0.62	0	8,14,16	0.38	0
52	PSU	A2	802	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	B5	1810	95,1	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
1	PSU	B5	4246	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	B8	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	4269	95,1	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
52	OMG	A2	1329	52,95	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
81	NMM	As	67	81	9,11,12	0.60	0	6,12,14	0.39	0
52	PSU	A2	1644	52,95	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	36	52	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	B5	3359	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	B5	3502	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	1MA	B5	1266	95,1	21,25,26	1.38	4 (19%)	31,37,40	1.69	5 (16%)
1	OMG	B5	4245	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
52	OMG	A2	602	52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	OMG	A2	868	52	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
61	5MU	AT	53	61	19,22,23	1.42	5 (26%)	28,32,35	2.00	5 (17%)
1	A2M	B5	4336	1	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
52	OMC	A2	1392	52	19,22,23	0.83	0	26,31,34	0.85	1 (3%)
52	PSU	A2	967	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	B5	2244	95,1	22,25,26	1.48	4 (18%)	31,36,39	2.12	10 (32%)
52	OMG	A2	437	52	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	OMC	B5	1820	95,1	19,22,23	0.79	0	26,31,34	0.79	0
1	OMG	B5	2207	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	B5	3500	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	B5	3657	1	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
52	PSU	A2	573	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMU	B5	2258	1	19,22,23	1.23	4 (21%)	26,31,34	1.68	4 (15%)
52	OMG	A2	510	52,95	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
52	OMG	A2	1448	52	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	B5	1580	95,1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	3576	1	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	B5	2475	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1446	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	4383	95,1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	PSU	A2	867	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4298	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	1270	1	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
52	A2M	A2	1384	52	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
4	V5N	BA	216	4	9,11,12	2.10	2 (22%)	9,14,16	1.71	2 (22%)
1	PSU	B5	4435	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4369	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4374	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4116	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	A2M	B5	3456	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	PSU	B5	4039	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	B5	2680	95,1	19,22,23	1.22	2 (10%)	26,31,34	1.72	4 (15%)
1	PSU	B5	4325	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
45	SAC	Br	2	45	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
52	4AC	A2	1843	52,95	21,24,25	1.09	2 (9%)	29,34,37	1.24	3 (10%)
1	PSU	B5	4382	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	645	52	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMU	B5	4052	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
1	PSU	B5	1632	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	B5	1683	95,1	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4169	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
6	AYA	BC	2	6	6,7,8	0.72	0	5,8,10	0.33	0
1	OMU	B5	4366	1	19,22,23	1.22	3 (15%)	26,31,34	1.73	4 (15%)
52	A2M	A2	513	52	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
1	OMC	B5	2265	95,1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
30	V5N	Ba	39	30	9,11,12	2.07	2 (22%)	9,14,16	1.68	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	B5	1479	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	OMG	B5	2267	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	A2M	A2	577	52	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
1	A2M	B5	3517	1	22,25,26	1.44	4 (18%)	31,36,39	2.18	11 (35%)
85	HY3	Aw	62	85	6,8,9	2.00	1 (16%)	5,10,12	1.11	1 (20%)
52	PSU	A2	1178	52,95	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	398	1	22,25,26	1.47	4 (18%)	31,36,39	2.15	9 (29%)
52	PSU	A2	218	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	UR3	B5	4276	1	19,22,23	0.99	1 (5%)	26,32,35	1.42	1 (3%)
1	OMU	B5	3973	1	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
1	OMC	B5	3540	1	19,22,23	0.82	0	26,31,34	0.81	0
1	5MC	B5	4193	95,1	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
1	PSU	B5	3462	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	4322	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4267	95,1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
52	OMC	A2	463	52	19,22,23	0.82	0	26,31,34	0.79	0
52	PSU	A2	864	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	3942	61,1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	B5	1284	1	19,22,23	0.81	0	26,31,34	0.78	0
52	PSU	A2	105	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	684	52	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	OMC	B5	2194	95,1	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
1	A2M	B5	400	1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	OMG	B5	3676	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
52	A2M	A2	27	52,95	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	A2M	B5	1489	95,1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	OMG	B5	4240	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4203	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	210	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1005	52	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
52	A2M	A2	1032	52	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	OMG	B5	3631	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	UY1	B5	3550	95,1	19,22,23	1.40	3 (15%)	22,31,34	1.87	5 (22%)
1	OMC	B5	4282	95,1	19,22,23	0.82	0	26,31,34	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	B5	3557	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
52	PSU	A2	682	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

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	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4099	95,1	-	0/7/25/26	0/2/2/2
52	G7M	A2	1640	52,61	-	2/7/25/26	0/3/3/3
52	PSU	A2	1693	52	-	0/7/25/26	0/2/2/2
61	5MC	AT	48	61	-	0/7/25/26	0/2/2/2
1	OMG	B5	3524	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3573	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2
52	OMG	A2	1491	52,95	-	0/9/27/28	0/3/3/3
52	6MZ	A2	1833	52,95	-	0/9/27/28	0/3/3/3
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1626	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	2208	95,1	-	0/9/27/28	0/2/2/2
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	591	52	-	3/9/27/28	0/3/3/3
3	PSU	B8	55	3	-	0/7/25/26	0/2/2/2
52	PSU	A2	1368	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	116	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	407	52	-	0/7/25/26	0/2/2/2
42	M3L	Bm	98	42	-	0/9/10/12	-
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4166	1	-	0/7/25/26	0/2/2/2
61	PSU	AT	54	61	-	0/7/25/26	0/2/2/2
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4419	95,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3619	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
1	6MZ	B5	3966	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	1801	95,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
43	MLZ	Bo	53	43	-	0/7/8/10	-
52	OMU	A2	1327	52,95	-	0/9/27/28	0/2/2/2
1	A2M	B5	3562	1	-	0/9/27/28	0/3/3/3
52	OMC	A2	1704	52	-	1/9/27/28	0/2/2/2
52	OMU	A2	429	52	-	4/9/27/28	0/2/2/2
52	PSU	A2	1233	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	3652	95,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	687	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	823	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1245	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	610	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	2704	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	652	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
52	4AC	A2	1338	52	-	4/11/29/30	0/2/2/2
52	PSU	A2	1348	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	1679	52	-	1/9/27/28	0/3/3/3
1	PSU	B5	3585	95,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	469	52	-	2/9/27/28	0/3/3/3
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2
83	AME	Au	1	83	-	2/9/10/12	-
1	5MC	B5	3514	95,1	-	0/7/25/26	0/2/2/2
52	MA6	A2	1852	52	-	4/11/29/30	0/3/3/3
1	OMG	B5	1260	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4740	95,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3599	1	-	1/9/27/28	0/3/3/3
52	PSU	A2	1175	52,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	355	52,95	-	0/9/27/28	0/2/2/2
1	OMU	B5	4244	95,1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3492	52,95,1	-	1/9/27/28	0/3/3/3
1	A2M	B5	2206	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3494	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	628	52	-	4/9/27/28	0/2/2/2
1	OMG	B5	2719	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	1082	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	MA6	A2	1851	52	-	0/11/29/30	0/3/3/3
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	1443	52,95	-	1/9/27/28	0/2/2/2
80	SAC	Ar	2	80	-	0/7/8/10	-
1	OMC	B5	3433	95,1	-	4/9/27/28	0/2/2/2
52	PSU	A2	1057	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4138	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	99	52,95	-	2/9/27/28	0/3/3/3
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2
62	SAC	AZ	2	62	-	2/7/8/10	-
1	A2M	B5	2658	95,1	-	0/9/27/28	0/3/3/3
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	816	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4107	95,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1047	52	-	0/7/25/26	0/2/2/2
3	OMG	B8	75	3	-	0/9/27/28	0/3/3/3
31	MLZ	Bb	5	31,95	-	2/7/8/10	-
52	OMC	A2	174	52,95	-	0/9/27/28	0/2/2/2
52	A2M	A2	485	52	-	0/9/27/28	0/3/3/3
1	PSU	B5	3369	95,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	518	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	650	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	159	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	1477	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
52	B8N	A2	1249	52	-	4/16/34/35	0/2/2/2
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	1805	52,95	-	0/9/27/28	0/2/2/2
52	PSU	A2	1239	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
52	A2M	A2	669	52,95	-	2/9/27/28	0/3/3/3
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4317	1	-	1/9/27/28	0/3/3/3
1	A2M	B5	2630	95,1	-	2/9/27/28	0/3/3/3
52	OMU	A2	1289	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3476	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	B5	3974	1	-	0/9/27/28	0/3/3/3
76	5F0	An	138	76	-	4/9/9/10	-
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	166	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	4364	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4711	95,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2667	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3450	1	-	0/9/27/28	0/3/3/3
5	HIC	BB	245	5	-	2/5/6/8	0/1/1/1
52	PSU	A2	802	52	-	2/7/25/26	0/2/2/2
1	A2M	B5	1810	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4246	1	-	1/7/25/26	0/2/2/2
3	PSU	B8	69	3	-	0/7/25/26	0/2/2/2
1	A2M	B5	4269	95,1	-	0/9/27/28	0/3/3/3
52	OMG	A2	1329	52,95	-	0/9/27/28	0/3/3/3
81	NMM	As	67	81	-	0/9/11/13	-
52	PSU	A2	1644	52,95	-	0/7/25/26	0/2/2/2
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3359	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
1	1MA	B5	1266	95,1	-	0/7/25/26	0/3/3/3
1	OMG	B5	4245	1	-	0/9/27/28	0/3/3/3
52	OMG	A2	602	52	-	0/9/27/28	0/3/3/3
52	OMG	A2	868	52	-	1/9/27/28	0/3/3/3
61	5MU	AT	53	61	-	0/7/25/26	0/2/2/2
1	A2M	B5	4336	1	-	1/9/27/28	0/3/3/3
52	OMC	A2	1392	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	967	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	2244	95,1	-	0/9/27/28	0/3/3/3
52	OMG	A2	437	52	-	0/9/27/28	0/3/3/3
1	OMC	B5	1820	95,1	-	1/9/27/28	0/2/2/2
1	OMG	B5	2207	1	-	2/9/27/28	0/3/3/3
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3657	1	-	1/9/27/28	0/2/2/2
52	PSU	A2	573	52	-	0/7/25/26	0/2/2/2
1	OMU	B5	2258	1	-	0/9/27/28	0/2/2/2
52	OMG	A2	510	52,95	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	OMG	A2	1448	52	-	2/9/27/28	0/3/3/3
1	OMG	B5	1580	95,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1446	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	4383	95,1	-	0/9/27/28	0/3/3/3
52	PSU	A2	867	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1270	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	1384	52	-	0/9/27/28	0/3/3/3
4	V5N	BA	216	4	-	2/9/10/12	0/1/1/1
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4369	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4116	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	3456	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	2680	95,1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
45	SAC	Br	2	45	-	0/7/8/10	-
52	4AC	A2	1843	52,95	-	4/11/29/30	0/2/2/2
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
52	OMG	A2	645	52	-	3/9/27/28	0/3/3/3
1	OMU	B5	4052	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1683	95,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2
6	AYA	BC	2	6	-	3/4/6/8	-
1	OMU	B5	4366	1	-	1/9/27/28	0/2/2/2
52	A2M	A2	513	52	-	2/9/27/28	0/3/3/3
1	OMC	B5	2265	95,1	-	0/9/27/28	0/2/2/2
1	OMC	B5	2647	1	-	0/9/27/28	0/2/2/2
30	V5N	Ba	39	30	-	0/9/10/12	0/1/1/1
1	A2M	B5	1479	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	2267	1	-	1/9/27/28	0/3/3/3
52	A2M	A2	577	52	-	2/9/27/28	0/3/3/3
1	A2M	B5	3517	1	-	2/9/27/28	0/3/3/3
85	HY3	Aw	62	85	-	1/1/12/14	0/1/1/1
52	PSU	A2	1178	52,95	-	0/7/25/26	0/2/2/2
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	398	1	-	4/9/27/28	0/3/3/3
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
1	5MC	B5	4193	95,1	-	4/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4267	95,1	-	0/7/25/26	0/2/2/2
52	OMC	A2	463	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	864	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3942	61,1	-	0/9/27/28	0/3/3/3
1	OMC	B5	1284	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	684	52	-	1/9/27/28	0/3/3/3
1	OMC	B5	2194	95,1	-	2/9/27/28	0/2/2/2
1	A2M	B5	400	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	3676	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	27	52,95	-	2/9/27/28	0/3/3/3
1	A2M	B5	1489	95,1	-	2/9/27/28	0/3/3/3
1	OMG	B5	4240	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1005	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	1032	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	3631	1	-	1/9/27/28	0/3/3/3
1	UY1	B5	3550	95,1	-	1/9/27/28	0/2/2/2
1	OMC	B5	4282	95,1	-	1/9/27/28	0/2/2/2
1	A2M	B5	3557	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	682	52	-	0/7/25/26	0/2/2/2

All (521) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1640	G7M	C4-N9	7.81	1.58	1.38
52	A2	1640	G7M	O6-C6	7.69	1.38	1.23
52	A2	1851	MA6	C5-N7	6.90	1.52	1.39
52	A2	1852	MA6	C5-N7	6.80	1.51	1.39
52	A2	1640	G7M	C5-C4	6.25	1.54	1.38
52	A2	1851	MA6	C8-N9	-5.47	1.27	1.37
52	A2	1852	MA6	C8-N9	-5.33	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BA	216	V5N	CG-ND1	-4.92	1.33	1.37
30	Ba	39	V5N	CG-ND1	-4.89	1.33	1.37
52	A2	591	A2M	C5-C4	4.69	1.47	1.39
52	A2	166	A2M	C5-C4	4.61	1.47	1.39
52	A2	577	A2M	C5-C4	4.59	1.47	1.39
52	A2	513	A2M	C5-C4	4.58	1.47	1.39
1	B5	2244	A2M	C5-C4	4.57	1.47	1.39
52	A2	469	A2M	C5-C4	4.56	1.47	1.39
52	A2	485	A2M	C5-C4	4.56	1.47	1.39
52	A2	1032	A2M	C5-C4	4.55	1.47	1.39
1	B5	1479	A2M	C5-C4	4.55	1.47	1.39
52	A2	99	A2M	C5-C4	4.55	1.47	1.39
1	B5	2658	A2M	C5-C4	4.55	1.47	1.39
52	A2	27	A2M	C5-C4	4.55	1.47	1.39
52	A2	669	A2M	C5-C4	4.55	1.47	1.39
52	A2	1384	A2M	C5-C4	4.55	1.47	1.39
1	B5	3492	A2M	C5-C4	4.55	1.47	1.39
52	A2	159	A2M	C5-C4	4.54	1.47	1.39
52	A2	1833	6MZ	C5-C4	4.54	1.47	1.39
1	B5	2630	A2M	C5-C4	4.54	1.47	1.39
1	B5	398	A2M	C5-C4	4.53	1.47	1.39
1	B5	3966	6MZ	C5-C4	4.53	1.47	1.39
85	Aw	62	HY3	C3-CA	-4.52	1.50	1.55
1	B5	400	A2M	C5-C4	4.52	1.47	1.39
1	B5	4336	A2M	C5-C4	4.52	1.47	1.39
1	B5	3557	A2M	C5-C4	4.52	1.47	1.39
52	A2	1679	A2M	C5-C4	4.51	1.47	1.39
1	B5	3450	A2M	C5-C4	4.50	1.47	1.39
1	B5	3562	A2M	C5-C4	4.50	1.47	1.39
1	B5	4317	A2M	C5-C4	4.50	1.47	1.39
1	B5	2206	A2M	C5-C4	4.49	1.47	1.39
1	B5	3599	A2M	C5-C4	4.49	1.47	1.39
1	B5	1810	A2M	C5-C4	4.48	1.47	1.39
52	A2	1640	G7M	C2-N2	4.48	1.44	1.34
1	B5	1270	A2M	C5-C4	4.48	1.47	1.39
1	B5	1489	A2M	C5-C4	4.47	1.47	1.39
1	B5	3456	A2M	C5-C4	4.47	1.47	1.39
1	B5	4269	A2M	C5-C4	4.46	1.47	1.39
1	B5	3517	A2M	C5-C4	4.37	1.47	1.39
52	A2	1640	G7M	C2-N1	3.88	1.47	1.37
1	B5	3550	UY1	C6-C5	3.74	1.39	1.35
52	A2	1852	MA6	C4-N9	-3.57	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1851	MA6	C4-N9	-3.55	1.29	1.37
52	A2	1851	MA6	C5-C4	3.34	1.45	1.39
52	A2	1852	MA6	C5-C4	3.33	1.45	1.39
52	A2	1640	G7M	C2-N3	3.31	1.41	1.33
52	A2	1245	PSU	C6-C5	3.27	1.39	1.35
1	B5	3500	PSU	C6-C5	3.27	1.39	1.35
52	A2	93	PSU	C6-C5	3.27	1.39	1.35
52	A2	967	PSU	C6-C5	3.26	1.39	1.35
61	AT	54	PSU	C6-C5	3.26	1.39	1.35
1	B5	3502	PSU	C6-C5	3.25	1.39	1.35
52	A2	1047	PSU	C6-C5	3.24	1.39	1.35
52	A2	210	PSU	C6-C5	3.23	1.39	1.35
52	A2	610	PSU	C6-C5	3.23	1.39	1.35
1	B5	3496	PSU	C6-C5	3.23	1.39	1.35
1	B5	4166	PSU	C6-C5	3.23	1.39	1.35
52	A2	34	PSU	C6-C5	3.23	1.39	1.35
52	A2	816	PSU	C6-C5	3.23	1.39	1.35
52	A2	119	PSU	C6-C5	3.22	1.39	1.35
1	B5	1266	1MA	C6-N6	3.22	1.35	1.28
52	A2	823	PSU	C6-C5	3.22	1.39	1.35
1	B5	4278	PSU	C6-C5	3.22	1.39	1.35
52	A2	1644	PSU	C6-C5	3.22	1.39	1.35
52	A2	1233	PSU	C6-C5	3.21	1.39	1.35
1	B5	4382	PSU	C6-C5	3.21	1.39	1.35
52	A2	109	PSU	C6-C5	3.21	1.39	1.35
52	A2	867	PSU	C6-C5	3.21	1.39	1.35
52	A2	105	PSU	C6-C5	3.21	1.39	1.35
1	B5	1721	PSU	C6-C5	3.20	1.39	1.35
1	B5	4169	PSU	C6-C5	3.20	1.39	1.35
52	A2	573	PSU	C6-C5	3.20	1.39	1.35
52	A2	1446	PSU	C6-C5	3.20	1.39	1.35
1	B5	1537	PSU	C6-C5	3.20	1.39	1.35
1	B5	4374	PSU	C6-C5	3.20	1.39	1.35
1	B5	3494	PSU	C6-C5	3.19	1.39	1.35
1	B5	1632	PSU	C6-C5	3.19	1.39	1.35
1	B5	3554	PSU	C6-C5	3.19	1.39	1.35
1	B5	3490	PSU	C6-C5	3.19	1.39	1.35
52	A2	1046	PSU	C6-C5	3.19	1.39	1.35
52	A2	1348	PSU	C6-C5	3.19	1.39	1.35
1	B5	4188	PSU	C6-C5	3.19	1.39	1.35
52	A2	1626	PSU	C6-C5	3.19	1.39	1.35
1	B5	3583	PSU	C6-C5	3.19	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	218	PSU	C6-C5	3.19	1.39	1.35
1	B5	3447	PSU	C6-C5	3.18	1.39	1.35
52	A2	802	PSU	C6-C5	3.18	1.39	1.35
1	B5	4107	PSU	C6-C5	3.18	1.39	1.35
1	B5	2351	PSU	C6-C5	3.18	1.39	1.35
1	B5	4325	PSU	C6-C5	3.18	1.39	1.35
52	A2	815	PSU	C6-C5	3.17	1.39	1.35
1	B5	4435	PSU	C6-C5	3.17	1.39	1.35
1	B5	3652	PSU	C6-C5	3.17	1.39	1.35
52	A2	652	PSU	C6-C5	3.17	1.39	1.35
52	A2	36	PSU	C6-C5	3.17	1.39	1.35
1	B5	4203	PSU	C6-C5	3.17	1.39	1.35
52	A2	407	PSU	C6-C5	3.17	1.39	1.35
52	A2	687	PSU	C6-C5	3.17	1.39	1.35
1	B5	1799	PSU	C6-C5	3.17	1.39	1.35
1	B5	4749	PSU	C6-C5	3.17	1.39	1.35
52	A2	1239	PSU	C6-C5	3.17	1.39	1.35
1	B5	4217	PSU	C6-C5	3.16	1.39	1.35
3	B8	69	PSU	C6-C5	3.16	1.39	1.35
52	A2	1368	PSU	C6-C5	3.16	1.39	1.35
1	B5	1720	PSU	C6-C5	3.16	1.39	1.35
52	A2	1693	PSU	C6-C5	3.16	1.39	1.35
52	A2	682	PSU	C6-C5	3.16	1.39	1.35
1	B5	4039	PSU	C6-C5	3.15	1.39	1.35
52	A2	1175	PSU	C6-C5	3.15	1.39	1.35
52	A2	864	PSU	C6-C5	3.15	1.39	1.35
1	B5	4322	PSU	C6-C5	3.15	1.39	1.35
3	B8	55	PSU	C6-C5	3.15	1.39	1.35
52	A2	1005	PSU	C6-C5	3.15	1.39	1.35
1	B5	3585	PSU	C6-C5	3.14	1.39	1.35
52	A2	1178	PSU	C6-C5	3.14	1.39	1.35
52	A2	437	OMG	C5-C4	3.14	1.47	1.38
1	B5	3466	PSU	C6-C5	3.14	1.39	1.35
1	B5	2475	PSU	C6-C5	3.14	1.39	1.35
1	B5	3369	PSU	C6-C5	3.14	1.39	1.35
1	B5	4099	PSU	C6-C5	3.14	1.39	1.35
1	B5	4298	PSU	C6-C5	3.14	1.39	1.35
1	B5	4116	OMG	C5-C4	3.14	1.47	1.38
52	A2	1491	OMG	C5-C4	3.14	1.47	1.38
52	A2	650	PSU	C6-C5	3.14	1.39	1.35
1	B5	3462	PSU	C6-C5	3.14	1.39	1.35
52	A2	1329	OMG	C5-C4	3.13	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1448	OMG	C5-C4	3.13	1.47	1.38
52	A2	602	OMG	C5-C4	3.13	1.47	1.38
1	B5	4711	PSU	C6-C5	3.13	1.39	1.35
1	B5	4740	PSU	C6-C5	3.13	1.39	1.35
1	B5	2719	OMG	C5-C4	3.13	1.47	1.38
1	B5	4045	PSU	C6-C5	3.13	1.39	1.35
1	B5	1718	PSU	C6-C5	3.12	1.39	1.35
1	B5	4419	PSU	C6-C5	3.12	1.39	1.35
52	A2	510	OMG	C5-C4	3.12	1.47	1.38
1	B5	3427	PSU	C6-C5	3.12	1.39	1.35
1	B5	3371	PSU	C6-C5	3.12	1.39	1.35
1	B5	3576	PSU	C6-C5	3.12	1.39	1.35
1	B5	1266	1MA	C5-C4	3.11	1.47	1.38
1	B5	1580	OMG	C5-C4	3.11	1.47	1.38
1	B5	3676	OMG	C5-C4	3.11	1.47	1.38
1	B5	1477	OMG	C5-C4	3.11	1.47	1.38
52	A2	645	OMG	C5-C4	3.11	1.47	1.38
52	A2	1057	PSU	C6-C5	3.11	1.38	1.35
52	A2	684	OMG	C5-C4	3.11	1.47	1.38
52	A2	1082	PSU	C6-C5	3.10	1.38	1.35
52	A2	868	OMG	C5-C4	3.10	1.47	1.38
1	B5	1801	PSU	C6-C5	3.10	1.38	1.35
1	B5	1638	PSU	C6-C5	3.10	1.38	1.35
1	B5	4245	OMG	C5-C4	3.10	1.47	1.38
52	A2	1851	MA6	C6-N6	3.10	1.46	1.36
1	B5	3524	OMG	C5-C4	3.10	1.47	1.38
1	B5	4240	OMG	C5-C4	3.10	1.47	1.38
1	B5	1491	PSU	C6-C5	3.10	1.38	1.35
1	B5	3942	OMG	C5-C4	3.09	1.47	1.38
1	B5	3359	OMG	C5-C4	3.09	1.47	1.38
1	B5	4383	OMG	C5-C4	3.09	1.47	1.38
1	B5	1731	PSU	C6-C5	3.08	1.38	1.35
1	B5	4267	PSU	C6-C5	3.08	1.38	1.35
1	B5	4369	OMG	C5-C4	3.08	1.47	1.38
1	B5	4138	OMG	C5-C4	3.08	1.47	1.38
1	B5	4058	PSU	C6-C5	3.08	1.38	1.35
1	B5	4364	OMG	C5-C4	3.07	1.47	1.38
1	B5	4149	PSU	C6-C5	3.07	1.38	1.35
52	A2	1249	B8N	C6-C5	3.07	1.39	1.34
1	B5	4246	PSU	C6-C5	3.07	1.38	1.35
1	B5	4177	PSU	C6-C5	3.07	1.38	1.35
1	B5	3476	OMG	C5-C4	3.07	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	2207	OMG	C5-C4	3.07	1.47	1.38
1	B5	2267	OMG	C5-C4	3.07	1.47	1.38
3	B8	75	OMG	C5-C4	3.06	1.47	1.38
1	B5	3974	OMG	C5-C4	3.06	1.47	1.38
1	B5	3616	PSU	C6-C5	3.06	1.38	1.35
1	B5	3631	OMG	C5-C4	3.04	1.47	1.38
1	B5	1683	PSU	C6-C5	3.04	1.38	1.35
1	B5	4042	PSU	C6-C5	3.04	1.38	1.35
52	A2	1852	MA6	C6-N6	3.03	1.45	1.36
1	B5	1260	OMG	C5-C4	3.01	1.47	1.38
76	An	138	5F0	OD1-C1	2.98	1.40	1.33
52	A2	1843	4AC	C4-N4	-2.95	1.35	1.39
52	A2	1249	B8N	C4-N3	-2.95	1.34	1.40
1	B5	4193	5MC	C6-C5	2.85	1.39	1.34
4	BA	216	V5N	CD2-NE2	-2.82	1.33	1.37
30	Ba	39	V5N	CD2-NE2	-2.78	1.33	1.37
61	AT	53	5MU	C6-C5	2.76	1.39	1.34
52	A2	166	A2M	C5-C6	2.74	1.48	1.41
52	A2	159	A2M	C5-C6	2.74	1.48	1.41
52	A2	469	A2M	C5-C6	2.74	1.48	1.41
52	A2	1679	A2M	C5-C6	2.74	1.48	1.41
1	B5	3550	UY1	C2-N1	2.74	1.40	1.36
1	B5	3514	5MC	C6-C5	2.73	1.39	1.34
1	B5	1489	A2M	C5-C6	2.73	1.48	1.41
52	A2	591	A2M	C5-C6	2.73	1.48	1.41
52	A2	485	A2M	C5-C6	2.72	1.48	1.41
1	B5	398	A2M	C5-C6	2.72	1.48	1.41
61	AT	48	5MC	C6-C5	2.72	1.39	1.34
1	B5	3557	A2M	C5-C6	2.71	1.48	1.41
52	A2	27	A2M	C5-C6	2.71	1.48	1.41
1	B5	2658	A2M	C5-C6	2.71	1.48	1.41
1	B5	1638	PSU	C4-N3	-2.71	1.33	1.38
52	A2	99	A2M	C5-C6	2.71	1.48	1.41
1	B5	2244	A2M	C5-C6	2.71	1.48	1.41
1	B5	3599	A2M	C5-C6	2.70	1.48	1.41
1	B5	3450	A2M	C5-C6	2.70	1.48	1.41
52	A2	513	A2M	C5-C6	2.70	1.48	1.41
52	A2	577	A2M	C5-C6	2.70	1.48	1.41
1	B5	3562	A2M	C5-C6	2.70	1.48	1.41
1	B5	4336	A2M	C5-C6	2.70	1.48	1.41
52	A2	669	A2M	C5-C6	2.69	1.48	1.41
1	B5	3456	A2M	C5-C6	2.69	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	3371	PSU	C4-N3	-2.69	1.33	1.38
3	B8	69	PSU	C4-N3	-2.68	1.33	1.38
1	B5	400	A2M	C5-C6	2.68	1.48	1.41
52	A2	1384	A2M	C5-C6	2.68	1.48	1.41
1	B5	4246	PSU	C4-N3	-2.68	1.33	1.38
1	B5	2206	A2M	C5-C6	2.68	1.48	1.41
1	B5	3585	PSU	C4-N3	-2.68	1.33	1.38
1	B5	3492	A2M	C5-C6	2.68	1.48	1.41
1	B5	4203	PSU	C4-N3	-2.67	1.33	1.38
1	B5	1810	A2M	C5-C6	2.67	1.48	1.41
1	B5	3369	PSU	C4-N3	-2.67	1.33	1.38
52	A2	1032	A2M	C5-C6	2.67	1.48	1.41
1	B5	4269	A2M	C5-C6	2.67	1.48	1.41
1	B5	4317	A2M	C5-C6	2.67	1.48	1.41
1	B5	4325	PSU	C4-N3	-2.67	1.33	1.38
1	B5	4149	PSU	C4-N3	-2.67	1.33	1.38
1	B5	4435	PSU	C4-N3	-2.66	1.33	1.38
1	B5	4188	PSU	C4-N3	-2.66	1.33	1.38
1	B5	3616	PSU	C4-N3	-2.66	1.33	1.38
1	B5	1270	A2M	C5-C6	2.66	1.48	1.41
1	B5	1799	PSU	C4-N3	-2.66	1.33	1.38
1	B5	1479	A2M	C5-C6	2.66	1.48	1.41
52	A2	1082	PSU	C4-N3	-2.65	1.33	1.38
1	B5	2351	PSU	C4-N3	-2.65	1.33	1.38
1	B5	4382	PSU	C4-N3	-2.65	1.33	1.38
1	B5	4740	PSU	C4-N3	-2.65	1.33	1.38
1	B5	4419	PSU	C4-N3	-2.65	1.33	1.38
1	B5	4039	PSU	C4-N3	-2.65	1.33	1.38
1	B5	4749	PSU	C4-N3	-2.64	1.33	1.38
1	B5	4711	PSU	C4-N3	-2.64	1.33	1.38
1	B5	2630	A2M	C5-C6	2.64	1.48	1.41
1	B5	4298	PSU	C4-N3	-2.64	1.33	1.38
1	B5	1721	PSU	C4-N3	-2.64	1.33	1.38
52	A2	682	PSU	C4-N3	-2.64	1.33	1.38
52	A2	1175	PSU	C4-N3	-2.64	1.33	1.38
52	A2	1178	PSU	C4-N3	-2.64	1.33	1.38
52	A2	1338	4AC	C4-N4	-2.64	1.35	1.39
1	B5	1731	PSU	C4-N3	-2.64	1.33	1.38
1	B5	3490	PSU	C4-N3	-2.64	1.33	1.38
1	B5	4177	PSU	C4-N3	-2.64	1.33	1.38
1	B5	4217	PSU	C4-N3	-2.64	1.33	1.38
52	A2	407	PSU	C4-N3	-2.64	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	3447	PSU	C4-N3	-2.64	1.33	1.38
1	B5	1683	PSU	C4-N3	-2.63	1.33	1.38
1	B5	3554	PSU	C4-N3	-2.63	1.33	1.38
1	B5	3652	PSU	C4-N3	-2.63	1.33	1.38
61	AT	54	PSU	C4-N3	-2.63	1.33	1.38
1	B5	4045	PSU	C4-N3	-2.63	1.34	1.38
52	A2	610	PSU	C4-N3	-2.63	1.34	1.38
1	B5	3462	PSU	C4-N3	-2.63	1.34	1.38
3	B8	55	PSU	C4-N3	-2.63	1.34	1.38
1	B5	1801	PSU	C4-N3	-2.63	1.34	1.38
1	B5	4267	PSU	C4-N3	-2.63	1.34	1.38
1	B5	4042	PSU	C4-N3	-2.63	1.34	1.38
52	A2	93	PSU	C4-N3	-2.63	1.34	1.38
1	B5	4107	PSU	C4-N3	-2.63	1.34	1.38
52	A2	802	PSU	C4-N3	-2.62	1.34	1.38
52	A2	218	PSU	C4-N3	-2.62	1.34	1.38
52	A2	210	PSU	C4-N3	-2.62	1.34	1.38
52	A2	1005	PSU	C4-N3	-2.62	1.34	1.38
1	B5	2475	PSU	C4-N3	-2.62	1.34	1.38
1	B5	4099	PSU	C4-N3	-2.62	1.34	1.38
1	B5	1491	PSU	C4-N3	-2.62	1.34	1.38
1	B5	1718	PSU	C4-N3	-2.62	1.34	1.38
52	A2	1057	PSU	C4-N3	-2.62	1.34	1.38
1	B5	4058	PSU	C4-N3	-2.62	1.34	1.38
52	A2	650	PSU	C4-N3	-2.62	1.34	1.38
1	B5	1632	PSU	C4-N3	-2.62	1.34	1.38
1	B5	3496	PSU	C4-N3	-2.62	1.34	1.38
1	B5	4322	PSU	C4-N3	-2.62	1.34	1.38
52	A2	1239	PSU	C4-N3	-2.62	1.34	1.38
1	B5	3583	PSU	C4-N3	-2.62	1.34	1.38
52	A2	815	PSU	C4-N3	-2.62	1.34	1.38
1	B5	3576	PSU	C4-N3	-2.61	1.34	1.38
1	B5	1720	PSU	C4-N3	-2.61	1.34	1.38
1	B5	4169	PSU	C4-N3	-2.61	1.34	1.38
52	A2	652	PSU	C4-N3	-2.61	1.34	1.38
1	B5	4278	PSU	C4-N3	-2.61	1.34	1.38
52	A2	1368	PSU	C4-N3	-2.61	1.34	1.38
1	B5	3502	PSU	C4-N3	-2.61	1.34	1.38
1	B5	4374	PSU	C4-N3	-2.61	1.34	1.38
52	A2	1446	PSU	C4-N3	-2.61	1.34	1.38
52	A2	1693	PSU	C4-N3	-2.61	1.34	1.38
1	B5	3517	A2M	C5-C6	2.61	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1046	PSU	C4-N3	-2.60	1.34	1.38
1	B5	4166	PSU	C4-N3	-2.60	1.34	1.38
1	B5	3500	PSU	C4-N3	-2.60	1.34	1.38
52	A2	1626	PSU	C4-N3	-2.60	1.34	1.38
52	A2	1348	PSU	C4-N3	-2.60	1.34	1.38
52	A2	687	PSU	C4-N3	-2.60	1.34	1.38
1	B5	3466	PSU	C4-N3	-2.59	1.34	1.38
52	A2	823	PSU	C4-N3	-2.59	1.34	1.38
52	A2	967	PSU	C4-N3	-2.59	1.34	1.38
52	A2	105	PSU	C4-N3	-2.59	1.34	1.38
52	A2	119	PSU	C4-N3	-2.59	1.34	1.38
1	B5	3427	PSU	C4-N3	-2.59	1.34	1.38
52	A2	1233	PSU	C4-N3	-2.59	1.34	1.38
52	A2	816	PSU	C4-N3	-2.59	1.34	1.38
61	AT	53	5MU	C4-N3	-2.59	1.34	1.38
1	B5	1537	PSU	C4-N3	-2.58	1.34	1.38
52	A2	34	PSU	C4-N3	-2.57	1.34	1.38
52	A2	1047	PSU	C4-N3	-2.57	1.34	1.38
52	A2	1644	PSU	C4-N3	-2.57	1.34	1.38
52	A2	867	PSU	C4-N3	-2.57	1.34	1.38
52	A2	573	PSU	C4-N3	-2.57	1.34	1.38
52	A2	1245	PSU	C4-N3	-2.57	1.34	1.38
52	A2	109	PSU	C4-N3	-2.57	1.34	1.38
52	A2	36	PSU	C4-N3	-2.56	1.34	1.38
1	B5	3494	PSU	C4-N3	-2.56	1.34	1.38
52	A2	864	PSU	C4-N3	-2.55	1.34	1.38
1	B5	2258	OMU	C4-N3	-2.54	1.34	1.38
1	B5	4052	OMU	C4-N3	-2.53	1.34	1.38
1	B5	4138	OMG	C6-N1	-2.53	1.34	1.38
1	B5	3942	OMG	C6-N1	-2.52	1.34	1.38
1	B5	1477	OMG	C6-N1	-2.52	1.34	1.38
1	B5	4366	OMU	C4-N3	-2.51	1.34	1.38
1	B5	3657	OMU	C4-N3	-2.50	1.34	1.38
52	A2	1833	6MZ	C5-C6	2.50	1.48	1.41
52	A2	429	OMU	C4-N3	-2.49	1.34	1.38
1	B5	3524	OMG	C6-N1	-2.49	1.34	1.38
1	B5	3973	OMU	C4-N3	-2.49	1.34	1.38
3	B8	75	OMG	C6-N1	-2.49	1.34	1.38
52	A2	1805	OMU	C4-N3	-2.48	1.34	1.38
1	B5	3966	6MZ	C5-C6	2.48	1.48	1.41
1	B5	2207	OMG	C6-N1	-2.48	1.34	1.38
52	A2	1289	OMU	C4-N3	-2.47	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1491	OMG	C6-N1	-2.47	1.34	1.38
1	B5	3359	OMG	C6-N1	-2.47	1.34	1.38
1	B5	4369	OMG	C6-N1	-2.47	1.34	1.38
1	B5	3476	OMG	C6-N1	-2.47	1.34	1.38
1	B5	2719	OMG	C6-N1	-2.46	1.34	1.38
1	B5	4383	OMG	C6-N1	-2.46	1.34	1.38
52	A2	1443	OMU	C4-N3	-2.46	1.34	1.38
1	B5	4244	OMU	C4-N3	-2.46	1.34	1.38
52	A2	355	OMU	C4-N3	-2.46	1.34	1.38
1	B5	4116	OMG	C6-N1	-2.46	1.34	1.38
1	B5	1260	OMG	C6-N1	-2.46	1.34	1.38
52	A2	628	OMU	C4-N3	-2.45	1.34	1.38
1	B5	1489	A2M	C8-N7	2.45	1.36	1.31
1	B5	2680	OMU	C4-N3	-2.45	1.34	1.38
1	B5	1580	OMG	C6-N1	-2.45	1.34	1.38
1	B5	2244	A2M	C8-N7	2.45	1.36	1.31
52	A2	99	A2M	C8-N7	2.45	1.36	1.31
52	A2	602	OMG	C6-N1	-2.45	1.34	1.38
52	A2	1329	OMG	C6-N1	-2.45	1.34	1.38
1	B5	4240	OMG	C6-N1	-2.44	1.34	1.38
52	A2	1679	A2M	C8-N7	2.44	1.36	1.31
1	B5	2267	OMG	C6-N1	-2.44	1.34	1.38
1	B5	3974	OMG	C6-N1	-2.44	1.34	1.38
52	A2	437	OMG	C6-N1	-2.44	1.34	1.38
1	B5	4364	OMG	C6-N1	-2.44	1.34	1.38
52	A2	1448	OMG	C6-N1	-2.44	1.34	1.38
52	A2	485	A2M	C8-N7	2.44	1.36	1.31
1	B5	3456	A2M	C8-N7	2.44	1.36	1.31
1	B5	3631	OMG	C6-N1	-2.43	1.34	1.38
52	A2	469	A2M	C8-N7	2.43	1.36	1.31
52	A2	159	A2M	C8-N7	2.42	1.36	1.31
1	B5	3450	A2M	C8-N7	2.42	1.36	1.31
52	A2	27	A2M	C8-N7	2.42	1.36	1.31
52	A2	1640	G7M	C5-N7	2.42	1.42	1.39
1	B5	3676	OMG	C6-N1	-2.42	1.34	1.38
52	A2	121	OMU	C4-N3	-2.42	1.34	1.38
52	A2	868	OMG	C6-N1	-2.42	1.34	1.38
1	B5	4245	OMG	C6-N1	-2.41	1.34	1.38
52	A2	645	OMG	C6-N1	-2.41	1.34	1.38
52	A2	172	OMU	C4-N3	-2.41	1.34	1.38
1	B5	1810	A2M	C8-N7	2.41	1.36	1.31
1	B5	3517	A2M	C8-N7	2.41	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	1479	A2M	C8-N7	2.41	1.36	1.31
1	B5	398	A2M	C8-N7	2.41	1.36	1.31
1	B5	4336	A2M	C8-N7	2.41	1.36	1.31
1	B5	1270	A2M	C8-N7	2.40	1.36	1.31
1	B5	2206	A2M	C8-N7	2.40	1.36	1.31
61	AT	53	5MU	C4-C5	2.40	1.48	1.44
52	A2	513	A2M	C8-N7	2.40	1.36	1.31
52	A2	1032	A2M	C8-N7	2.40	1.36	1.31
52	A2	684	OMG	C6-N1	-2.39	1.34	1.38
52	A2	669	A2M	C8-N7	2.39	1.36	1.31
52	A2	116	OMU	C4-N3	-2.39	1.34	1.38
1	B5	400	A2M	C8-N7	2.38	1.36	1.31
52	A2	510	OMG	C6-N1	-2.38	1.34	1.38
1	B5	3562	A2M	C8-N7	2.38	1.36	1.31
52	A2	1327	OMU	C4-N3	-2.38	1.34	1.38
1	B5	3966	6MZ	C8-N7	2.38	1.36	1.31
1	B5	4269	A2M	C8-N7	2.38	1.36	1.31
1	B5	2658	A2M	C8-N7	2.38	1.36	1.31
1	B5	4317	A2M	C8-N7	2.38	1.36	1.31
52	A2	577	A2M	C8-N7	2.38	1.36	1.31
52	A2	1249	B8N	C2-N3	-2.38	1.34	1.38
52	A2	1443	OMU	C2-N1	2.38	1.42	1.38
52	A2	1384	A2M	C8-N7	2.37	1.36	1.31
1	B5	3557	A2M	C8-N7	2.37	1.36	1.31
1	B5	3599	A2M	C8-N7	2.37	1.36	1.31
52	A2	166	A2M	C8-N7	2.37	1.36	1.31
1	B5	3492	A2M	C8-N7	2.36	1.36	1.31
1	B5	2630	A2M	C8-N7	2.34	1.36	1.31
52	A2	591	A2M	C8-N7	2.33	1.36	1.31
61	AT	53	5MU	C2-N1	2.31	1.42	1.38
1	B5	1266	1MA	C2-N3	2.30	1.34	1.30
52	A2	1833	6MZ	C8-N7	2.26	1.35	1.31
1	B5	3514	5MC	C6-N1	-2.24	1.34	1.38
1	B5	3550	UY1	C6-N1	-2.23	1.32	1.36
52	A2	1289	OMU	C2-N1	2.22	1.42	1.38
52	A2	1833	6MZ	C5-N7	-2.20	1.34	1.39
3	B8	75	OMG	C5-N7	-2.20	1.34	1.39
61	AT	53	5MU	C6-N1	-2.19	1.34	1.38
52	A2	1640	G7M	C4-N3	2.19	1.39	1.34
1	B5	1270	A2M	C5-N7	-2.19	1.34	1.39
61	AT	48	5MC	C6-N1	-2.19	1.34	1.38
1	B5	3966	6MZ	C5-N7	-2.19	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	591	A2M	C5-N7	-2.19	1.34	1.39
1	B5	3450	A2M	C5-N7	-2.19	1.34	1.39
1	B5	2719	OMG	C5-N7	-2.19	1.34	1.39
1	B5	2630	A2M	C5-N7	-2.19	1.34	1.39
1	B5	1580	OMG	C5-N7	-2.18	1.34	1.39
1	B5	4269	A2M	C5-N7	-2.18	1.34	1.39
1	B5	1479	A2M	C5-N7	-2.18	1.34	1.39
52	A2	99	A2M	C5-N7	-2.18	1.34	1.39
1	B5	4240	OMG	C5-N7	-2.18	1.34	1.39
1	B5	3562	A2M	C5-N7	-2.18	1.34	1.39
52	A2	669	A2M	C5-N7	-2.18	1.34	1.39
52	A2	513	A2M	C5-N7	-2.17	1.34	1.39
52	A2	1805	OMU	C2-N1	2.17	1.41	1.38
1	B5	3942	OMG	C5-N7	-2.17	1.34	1.39
1	B5	4317	A2M	C5-N7	-2.17	1.34	1.39
52	A2	1329	OMG	C5-N7	-2.17	1.34	1.39
1	B5	1489	A2M	C5-N7	-2.17	1.34	1.39
1	B5	398	A2M	C5-N7	-2.17	1.34	1.39
52	A2	1384	A2M	C5-N7	-2.17	1.34	1.39
1	B5	2258	OMU	C2-N3	-2.17	1.34	1.38
1	B5	4193	5MC	C6-N1	-2.17	1.34	1.38
1	B5	4366	OMU	C2-N3	-2.17	1.34	1.38
1	B5	4116	OMG	C5-N7	-2.16	1.34	1.39
1	B5	400	A2M	C5-N7	-2.16	1.34	1.39
1	B5	2680	OMU	C2-N3	-2.16	1.34	1.38
1	B5	2658	A2M	C5-N7	-2.16	1.34	1.39
52	A2	1640	G7M	C6-N1	2.16	1.42	1.38
52	A2	1032	A2M	C5-N7	-2.16	1.34	1.39
1	B5	3974	OMG	C5-N7	-2.16	1.34	1.39
1	B5	2244	A2M	C5-N7	-2.16	1.34	1.39
52	A2	1491	OMG	C5-N7	-2.16	1.34	1.39
1	B5	3599	A2M	C5-N7	-2.16	1.34	1.39
1	B5	1477	OMG	C5-N7	-2.15	1.34	1.39
52	A2	469	A2M	C5-N7	-2.15	1.35	1.39
1	B5	4383	OMG	C5-N7	-2.15	1.34	1.39
52	A2	166	A2M	C5-N7	-2.15	1.35	1.39
52	A2	577	A2M	C5-N7	-2.14	1.35	1.39
52	A2	159	A2M	C5-N7	-2.14	1.35	1.39
52	A2	27	A2M	C5-N7	-2.14	1.35	1.39
1	B5	4245	OMG	C5-N7	-2.14	1.34	1.39
1	B5	3657	OMU	C2-N3	-2.14	1.34	1.38
52	A2	1327	OMU	C2-N3	-2.14	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	437	OMG	C5-N7	-2.14	1.34	1.39
1	B5	3456	A2M	C5-N7	-2.14	1.35	1.39
1	B5	4364	OMG	C5-N7	-2.14	1.34	1.39
52	A2	485	A2M	C5-N7	-2.13	1.35	1.39
1	B5	2206	A2M	C5-N7	-2.13	1.35	1.39
52	A2	868	OMG	C5-N7	-2.13	1.35	1.39
1	B5	3973	OMU	C2-N3	-2.13	1.34	1.38
1	B5	4369	OMG	C5-N7	-2.13	1.35	1.39
1	B5	3492	A2M	C5-N7	-2.13	1.35	1.39
1	B5	4138	OMG	C5-N7	-2.13	1.35	1.39
1	B5	2267	OMG	C5-N7	-2.13	1.35	1.39
1	B5	1810	A2M	C5-N7	-2.13	1.35	1.39
1	B5	3359	OMG	C5-N7	-2.13	1.35	1.39
1	B5	4336	A2M	C5-N7	-2.12	1.35	1.39
1	B5	4052	OMU	C2-N1	2.12	1.41	1.38
1	B5	3517	A2M	C5-N7	-2.12	1.35	1.39
1	B5	1260	OMG	C5-N7	-2.12	1.35	1.39
1	B5	3524	OMG	C5-N7	-2.12	1.35	1.39
1	B5	3557	A2M	C5-N7	-2.12	1.35	1.39
52	A2	645	OMG	C5-N7	-2.12	1.35	1.39
1	B5	4244	OMU	C2-N3	-2.11	1.34	1.38
1	B5	1266	1MA	C5-N7	-2.11	1.35	1.39
1	B5	3631	OMG	C5-N7	-2.11	1.35	1.39
1	B5	3476	OMG	C5-N7	-2.11	1.35	1.39
52	A2	602	OMG	C5-N7	-2.11	1.35	1.39
76	An	138	5F0	OD1-CXT	-2.11	1.40	1.45
1	B5	2207	OMG	C5-N7	-2.11	1.35	1.39
52	A2	116	OMU	C2-N3	-2.10	1.34	1.38
52	A2	1679	A2M	C5-N7	-2.10	1.35	1.39
52	A2	510	OMG	C5-N7	-2.10	1.35	1.39
52	A2	1448	OMG	C5-N7	-2.10	1.35	1.39
52	A2	429	OMU	C2-N3	-2.09	1.34	1.38
1	B5	4052	OMU	C2-N3	-2.09	1.34	1.38
52	A2	121	OMU	C2-N1	2.09	1.41	1.38
52	A2	628	OMU	C2-N3	-2.09	1.34	1.38
52	A2	355	OMU	C2-N1	2.08	1.41	1.38
52	A2	1289	OMU	C2-N3	-2.08	1.34	1.38
52	A2	355	OMU	C2-N3	-2.08	1.34	1.38
52	A2	172	OMU	C2-N1	2.08	1.41	1.38
52	A2	121	OMU	C2-N3	-2.06	1.34	1.38
52	A2	684	OMG	C5-N7	-2.06	1.35	1.39
52	A2	429	OMU	C2-N1	2.05	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	3676	OMG	C5-N7	-2.05	1.35	1.39
1	B5	3973	OMU	C2-N1	2.04	1.41	1.38
1	B5	4366	OMU	C2-N1	2.04	1.41	1.38
52	A2	172	OMU	C2-N3	-2.04	1.34	1.38
52	A2	1443	OMU	C2-N3	-2.03	1.34	1.38
52	A2	1843	4AC	C7-N4	-2.02	1.33	1.37
52	A2	1805	OMU	C2-N3	-2.02	1.34	1.38
1	B5	2258	OMU	C2-N1	2.02	1.41	1.38
1	B5	4276	UR3	C2-N1	2.01	1.41	1.38
1	B5	2258	OMU	C5-C4	-2.00	1.39	1.43

All (966) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1851	MA6	C4-N9-C8	14.65	121.61	105.73
52	A2	1852	MA6	C4-N9-C8	14.47	121.41	105.73
52	A2	1640	G7M	C8-N7-C5	11.37	122.00	107.78
52	A2	591	A2M	C5-C4-N3	-7.05	117.55	126.75
52	A2	1852	MA6	N3-C4-N9	6.98	138.59	127.08
52	A2	1851	MA6	N3-C4-N9	6.74	138.18	127.08
52	A2	1640	G7M	N9-C4-N3	6.55	139.10	125.94
52	A2	1640	G7M	C6-C5-N7	6.50	140.11	132.25
1	B5	2719	OMG	C5-C4-N3	-6.39	118.09	128.46
1	B5	2658	A2M	C5-C4-N3	-6.39	118.41	126.75
52	A2	1833	6MZ	C5-C4-N3	-6.36	118.45	126.75
1	B5	1479	A2M	C5-C4-N3	-6.29	118.54	126.75
1	B5	3599	A2M	C5-C4-N3	-6.28	118.55	126.75
52	A2	166	A2M	C5-C4-N3	-6.28	118.56	126.75
1	B5	2206	A2M	C5-C4-N3	-6.27	118.57	126.75
1	B5	398	A2M	C5-C4-N3	-6.26	118.58	126.75
52	A2	469	A2M	C5-C4-N3	-6.25	118.59	126.75
52	A2	99	A2M	C5-C4-N3	-6.24	118.61	126.75
1	B5	1489	A2M	C5-C4-N3	-6.24	118.61	126.75
1	B5	2244	A2M	C5-C4-N3	-6.24	118.61	126.75
1	B5	3966	6MZ	C5-C4-N3	-6.22	118.63	126.75
1	B5	400	A2M	C5-C4-N3	-6.22	118.64	126.75
52	A2	513	A2M	C5-C4-N3	-6.21	118.64	126.75
52	A2	577	A2M	C5-C4-N3	-6.21	118.65	126.75
1	B5	3492	A2M	C5-C4-N3	-6.21	118.65	126.75
1	B5	1270	A2M	C5-C4-N3	-6.20	118.66	126.75
1	B5	4336	A2M	C5-C4-N3	-6.20	118.67	126.75
52	A2	485	A2M	C5-C4-N3	-6.19	118.67	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	27	A2M	C5-C4-N3	-6.19	118.68	126.75
1	B5	3562	A2M	C5-C4-N3	-6.18	118.68	126.75
52	A2	1384	A2M	C5-C4-N3	-6.18	118.69	126.75
1	B5	4317	A2M	C5-C4-N3	-6.17	118.70	126.75
52	A2	1448	OMG	C5-C4-N3	-6.17	118.45	128.46
1	B5	3942	OMG	C5-C4-N3	-6.17	118.45	128.46
1	B5	4269	A2M	C5-C4-N3	-6.16	118.71	126.75
1	B5	3456	A2M	C5-C4-N3	-6.16	118.71	126.75
52	A2	159	A2M	C5-C4-N3	-6.16	118.71	126.75
52	A2	437	OMG	C5-C4-N3	-6.16	118.47	128.46
52	A2	1491	OMG	C5-C4-N3	-6.16	118.47	128.46
1	B5	1810	A2M	C5-C4-N3	-6.15	118.72	126.75
1	B5	2630	A2M	C5-C4-N3	-6.15	118.72	126.75
1	B5	3557	A2M	C5-C4-N3	-6.15	118.73	126.75
52	A2	1679	A2M	C5-C4-N3	-6.14	118.74	126.75
1	B5	3450	A2M	C5-C4-N3	-6.14	118.74	126.75
1	B5	4116	OMG	C5-C4-N3	-6.13	118.52	128.46
1	B5	4138	OMG	C5-C4-N3	-6.13	118.52	128.46
1	B5	1580	OMG	C5-C4-N3	-6.12	118.53	128.46
1	B5	3676	OMG	C5-C4-N3	-6.12	118.54	128.46
52	A2	1329	OMG	C5-C4-N3	-6.12	118.54	128.46
52	A2	669	A2M	C5-C4-N3	-6.11	118.78	126.75
1	B5	4240	OMG	C5-C4-N3	-6.11	118.55	128.46
52	A2	645	OMG	C5-C4-N3	-6.11	118.56	128.46
1	B5	3476	OMG	C5-C4-N3	-6.11	118.56	128.46
1	B5	4245	OMG	C5-C4-N3	-6.10	118.57	128.46
1	B5	3524	OMG	C5-C4-N3	-6.09	118.58	128.46
1	B5	4383	OMG	C5-C4-N3	-6.08	118.59	128.46
1	B5	3359	OMG	C5-C4-N3	-6.08	118.59	128.46
1	B5	1477	OMG	C5-C4-N3	-6.08	118.59	128.46
1	B5	4364	OMG	C5-C4-N3	-6.08	118.60	128.46
52	A2	868	OMG	C5-C4-N3	-6.08	118.60	128.46
52	A2	510	OMG	C5-C4-N3	-6.07	118.61	128.46
52	A2	1032	A2M	C5-C4-N3	-6.07	118.83	126.75
52	A2	602	OMG	C5-C4-N3	-6.07	118.62	128.46
1	B5	4369	OMG	C5-C4-N3	-6.06	118.64	128.46
3	B8	75	OMG	C5-C4-N3	-6.05	118.64	128.46
1	B5	2207	OMG	C5-C4-N3	-6.05	118.65	128.46
1	B5	4325	PSU	N1-C2-N3	6.04	121.97	115.13
1	B5	4322	PSU	N1-C2-N3	6.03	121.96	115.13
1	B5	3369	PSU	N1-C2-N3	6.03	121.96	115.13
1	B5	3616	PSU	N1-C2-N3	6.02	121.95	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	4435	PSU	N1-C2-N3	6.02	121.95	115.13
52	A2	650	PSU	N1-C2-N3	6.02	121.95	115.13
52	A2	1446	PSU	N1-C2-N3	6.02	121.95	115.13
1	B5	4177	PSU	N1-C2-N3	6.02	121.95	115.13
52	A2	682	PSU	N1-C2-N3	6.01	121.94	115.13
1	B5	4042	PSU	N1-C2-N3	6.01	121.94	115.13
1	B5	4246	PSU	N1-C2-N3	6.01	121.94	115.13
52	A2	816	PSU	N1-C2-N3	6.01	121.93	115.13
1	B5	2267	OMG	C5-C4-N3	-6.00	118.72	128.46
1	B5	3554	PSU	N1-C2-N3	5.99	121.92	115.13
1	B5	4099	PSU	N1-C2-N3	5.99	121.92	115.13
1	B5	4374	PSU	N1-C2-N3	5.99	121.92	115.13
1	B5	3494	PSU	N1-C2-N3	5.99	121.92	115.13
1	B5	3427	PSU	N1-C2-N3	5.99	121.92	115.13
1	B5	3466	PSU	N1-C2-N3	5.99	121.92	115.13
52	A2	1640	G7M	CN7-N7-C5	-5.99	119.33	126.77
1	B5	4149	PSU	N1-C2-N3	5.98	121.91	115.13
1	B5	4039	PSU	N1-C2-N3	5.98	121.91	115.13
52	A2	823	PSU	N1-C2-N3	5.98	121.91	115.13
1	B5	1799	PSU	N1-C2-N3	5.98	121.91	115.13
52	A2	407	PSU	N1-C2-N3	5.98	121.90	115.13
1	B5	4267	PSU	N1-C2-N3	5.98	121.90	115.13
52	A2	1239	PSU	N1-C2-N3	5.98	121.90	115.13
1	B5	3652	PSU	N1-C2-N3	5.97	121.90	115.13
52	A2	1175	PSU	N1-C2-N3	5.97	121.90	115.13
3	B8	69	PSU	N1-C2-N3	5.97	121.90	115.13
52	A2	1178	PSU	N1-C2-N3	5.97	121.89	115.13
1	B5	4217	PSU	N1-C2-N3	5.97	121.89	115.13
1	B5	1801	PSU	N1-C2-N3	5.96	121.89	115.13
1	B5	3517	A2M	C5-C4-N3	-5.96	118.97	126.75
1	B5	1491	PSU	N1-C2-N3	5.96	121.89	115.13
1	B5	3500	PSU	N1-C2-N3	5.96	121.89	115.13
1	B5	4711	PSU	N1-C2-N3	5.96	121.89	115.13
1	B5	3583	PSU	N1-C2-N3	5.96	121.88	115.13
52	A2	1852	MA6	C5-C4-N3	-5.96	118.97	126.75
52	A2	1851	MA6	C4-C5-N7	-5.96	103.36	110.62
1	B5	3502	PSU	N1-C2-N3	5.96	121.88	115.13
1	B5	1721	PSU	N1-C2-N3	5.96	121.88	115.13
1	B5	1731	PSU	N1-C2-N3	5.96	121.88	115.13
52	A2	573	PSU	N1-C2-N3	5.95	121.88	115.13
52	A2	652	PSU	N1-C2-N3	5.95	121.88	115.13
1	B5	3490	PSU	N1-C2-N3	5.95	121.88	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	3585	PSU	N1-C2-N3	5.95	121.88	115.13
1	B5	4058	PSU	N1-C2-N3	5.95	121.88	115.13
1	B5	4749	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	1233	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	1082	PSU	N1-C2-N3	5.95	121.87	115.13
1	B5	1683	PSU	N1-C2-N3	5.95	121.87	115.13
1	B5	4298	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	1046	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	864	PSU	N1-C2-N3	5.95	121.87	115.13
52	A2	867	PSU	N1-C2-N3	5.95	121.87	115.13
1	B5	3631	OMG	C5-C4-N3	-5.95	118.81	128.46
52	A2	687	PSU	N1-C2-N3	5.94	121.86	115.13
52	A2	1057	PSU	N1-C2-N3	5.94	121.86	115.13
1	B5	2475	PSU	N1-C2-N3	5.94	121.86	115.13
1	B5	4382	PSU	N1-C2-N3	5.94	121.86	115.13
52	A2	93	PSU	N1-C2-N3	5.94	121.86	115.13
52	A2	967	PSU	N1-C2-N3	5.94	121.86	115.13
1	B5	1260	OMG	C5-C4-N3	-5.94	118.83	128.46
52	A2	684	OMG	C5-C4-N3	-5.94	118.83	128.46
1	B5	1638	PSU	N1-C2-N3	5.94	121.86	115.13
1	B5	1720	PSU	N1-C2-N3	5.94	121.86	115.13
1	B5	4166	PSU	N1-C2-N3	5.94	121.86	115.13
1	B5	3974	OMG	C5-C4-N3	-5.94	118.83	128.46
1	B5	4188	PSU	N1-C2-N3	5.93	121.85	115.13
3	B8	55	PSU	N1-C2-N3	5.93	121.85	115.13
52	A2	1851	MA6	N9-C8-N7	-5.93	105.80	113.91
1	B5	4107	PSU	N1-C2-N3	5.93	121.85	115.13
1	B5	2351	PSU	N1-C2-N3	5.93	121.85	115.13
52	A2	210	PSU	N1-C2-N3	5.93	121.85	115.13
52	A2	1245	PSU	N1-C2-N3	5.93	121.85	115.13
1	B5	4419	PSU	N1-C2-N3	5.93	121.85	115.13
1	B5	4169	PSU	N1-C2-N3	5.93	121.84	115.13
61	AT	54	PSU	N1-C2-N3	5.92	121.84	115.13
1	B5	3496	PSU	N1-C2-N3	5.92	121.84	115.13
52	A2	105	PSU	N1-C2-N3	5.91	121.83	115.13
52	A2	1368	PSU	N1-C2-N3	5.91	121.83	115.13
52	A2	610	PSU	N1-C2-N3	5.91	121.83	115.13
52	A2	218	PSU	N1-C2-N3	5.91	121.82	115.13
52	A2	802	PSU	N1-C2-N3	5.91	121.82	115.13
52	A2	815	PSU	N1-C2-N3	5.91	121.82	115.13
1	B5	1537	PSU	N1-C2-N3	5.90	121.82	115.13
52	A2	1047	PSU	N1-C2-N3	5.90	121.82	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	1718	PSU	N1-C2-N3	5.90	121.82	115.13
1	B5	1632	PSU	N1-C2-N3	5.90	121.81	115.13
1	B5	4203	PSU	N1-C2-N3	5.90	121.81	115.13
1	B5	4045	PSU	N1-C2-N3	5.90	121.81	115.13
1	B5	3462	PSU	N1-C2-N3	5.90	121.81	115.13
1	B5	4278	PSU	N1-C2-N3	5.89	121.81	115.13
52	A2	119	PSU	N1-C2-N3	5.89	121.81	115.13
52	A2	34	PSU	N1-C2-N3	5.89	121.80	115.13
52	A2	1626	PSU	N1-C2-N3	5.89	121.80	115.13
1	B5	4740	PSU	N1-C2-N3	5.89	121.80	115.13
52	A2	109	PSU	N1-C2-N3	5.88	121.80	115.13
52	A2	1644	PSU	N1-C2-N3	5.88	121.79	115.13
52	A2	1005	PSU	N1-C2-N3	5.88	121.79	115.13
1	B5	3447	PSU	N1-C2-N3	5.88	121.79	115.13
52	A2	1693	PSU	N1-C2-N3	5.88	121.79	115.13
1	B5	3371	PSU	N1-C2-N3	5.87	121.78	115.13
52	A2	1348	PSU	N1-C2-N3	5.87	121.78	115.13
52	A2	36	PSU	N1-C2-N3	5.86	121.78	115.13
1	B5	3576	PSU	N1-C2-N3	5.86	121.77	115.13
1	B5	4276	UR3	C4-N3-C2	-5.81	119.09	124.56
52	A2	1852	MA6	N9-C8-N7	-5.75	106.05	113.91
52	A2	1851	MA6	C5-C4-N3	-5.73	119.27	126.75
52	A2	1852	MA6	C4-C5-N7	-5.71	103.67	110.62
52	A2	591	A2M	N3-C4-N9	5.56	136.24	127.08
1	B5	1266	1MA	C5-C4-N3	-5.40	119.20	127.26
1	B5	3550	UY1	C4-N3-C2	-5.20	118.85	126.34
52	A2	1833	6MZ	N3-C4-N9	5.07	135.44	127.08
1	B5	2719	OMG	C2-N3-C4	5.05	121.31	112.30
61	AT	53	5MU	C4-N3-C2	-4.93	120.97	127.35
1	B5	2658	A2M	N3-C4-N9	4.92	135.19	127.08
1	B5	4138	OMG	C2-N3-C4	4.92	121.06	112.30
52	A2	437	OMG	C2-N3-C4	4.91	121.04	112.30
52	A2	1448	OMG	C2-N3-C4	4.91	121.04	112.30
1	B5	4240	OMG	C2-N3-C4	4.91	121.04	112.30
1	B5	3476	OMG	C2-N3-C4	4.89	121.02	112.30
52	A2	1491	OMG	C2-N3-C4	4.89	121.02	112.30
1	B5	3524	OMG	C2-N3-C4	4.89	121.01	112.30
1	B5	1477	OMG	C2-N3-C4	4.88	121.00	112.30
1	B5	3359	OMG	C2-N3-C4	4.88	121.00	112.30
1	B5	4245	OMG	C2-N3-C4	4.88	120.99	112.30
1	B5	3676	OMG	C2-N3-C4	4.88	120.99	112.30
52	A2	166	A2M	N3-C4-N9	4.88	135.12	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	645	OMG	C2-N3-C4	4.88	120.99	112.30
1	B5	3599	A2M	N3-C4-N9	4.87	135.11	127.08
1	B5	4383	OMG	C2-N3-C4	4.87	120.98	112.30
52	A2	868	OMG	C2-N3-C4	4.87	120.98	112.30
1	B5	4116	OMG	C2-N3-C4	4.87	120.98	112.30
1	B5	3966	6MZ	N3-C4-N9	4.87	135.10	127.08
1	B5	1479	A2M	N3-C4-N9	4.87	135.10	127.08
1	B5	4369	OMG	C2-N3-C4	4.87	120.97	112.30
1	B5	1580	OMG	C2-N3-C4	4.86	120.97	112.30
1	B5	2244	A2M	N3-C4-N9	4.86	135.09	127.08
1	B5	4364	OMG	C2-N3-C4	4.86	120.95	112.30
52	A2	602	OMG	C2-N3-C4	4.85	120.95	112.30
52	A2	99	A2M	N3-C4-N9	4.85	135.08	127.08
52	A2	1329	OMG	C2-N3-C4	4.85	120.94	112.30
1	B5	3492	A2M	N3-C4-N9	4.85	135.07	127.08
1	B5	3631	OMG	C2-N3-C4	4.85	120.94	112.30
52	A2	513	A2M	N3-C4-N9	4.85	135.06	127.08
52	A2	469	A2M	N3-C4-N9	4.84	135.06	127.08
1	B5	3974	OMG	C2-N3-C4	4.84	120.93	112.30
3	B8	75	OMG	C2-N3-C4	4.84	120.93	112.30
1	B5	3942	OMG	C2-N3-C4	4.84	120.93	112.30
1	B5	400	A2M	N3-C4-N9	4.84	135.06	127.08
1	B5	2267	OMG	C2-N3-C4	4.84	120.92	112.30
1	B5	398	A2M	N3-C4-N9	4.84	135.05	127.08
52	A2	485	A2M	N3-C4-N9	4.84	135.05	127.08
1	B5	2630	A2M	N3-C4-N9	4.83	135.04	127.08
1	B5	3562	A2M	N3-C4-N9	4.83	135.04	127.08
52	A2	510	OMG	C2-N3-C4	4.83	120.91	112.30
52	A2	684	OMG	C2-N3-C4	4.83	120.90	112.30
1	B5	2207	OMG	C2-N3-C4	4.82	120.89	112.30
52	A2	27	A2M	N3-C4-N9	4.81	135.01	127.08
52	A2	577	A2M	N3-C4-N9	4.81	135.01	127.08
1	B5	2206	A2M	N3-C4-N9	4.81	135.00	127.08
1	B5	1260	OMG	C2-N3-C4	4.81	120.86	112.30
1	B5	4336	A2M	N3-C4-N9	4.80	135.00	127.08
52	A2	1384	A2M	N3-C4-N9	4.80	135.00	127.08
1	B5	1270	A2M	N3-C4-N9	4.80	135.00	127.08
1	B5	4269	A2M	N3-C4-N9	4.80	135.00	127.08
1	B5	1810	A2M	N3-C4-N9	4.80	134.99	127.08
52	A2	159	A2M	N3-C4-N9	4.80	134.98	127.08
52	A2	1679	A2M	N3-C4-N9	4.79	134.98	127.08
1	B5	2719	OMG	N9-C4-N3	4.78	135.55	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	3456	A2M	N3-C4-N9	4.78	134.95	127.08
61	AT	53	5MU	N3-C2-N1	4.77	121.22	114.89
52	A2	669	A2M	N3-C4-N9	4.76	134.93	127.08
1	B5	4317	A2M	N3-C4-N9	4.75	134.92	127.08
1	B5	1489	A2M	N3-C4-N9	4.75	134.91	127.08
1	B5	3557	A2M	N3-C4-N9	4.75	134.91	127.08
52	A2	1640	G7M	C2-N3-C4	4.74	120.74	112.30
52	A2	1032	A2M	N3-C4-N9	4.73	134.87	127.08
1	B5	1266	1MA	C2-N3-C4	4.70	121.65	112.41
52	A2	1338	4AC	N4-C4-N3	4.67	121.70	113.85
1	B5	3517	A2M	N3-C4-N9	4.66	134.76	127.08
52	A2	1491	OMG	N9-C4-N3	4.66	135.29	125.94
1	B5	3450	A2M	N3-C4-N9	4.65	134.74	127.08
1	B5	3942	OMG	N9-C4-N3	4.63	135.23	125.94
52	A2	437	OMG	N9-C4-N3	4.62	135.22	125.94
1	B5	4116	OMG	N9-C4-N3	4.62	135.21	125.94
1	B5	1580	OMG	N9-C4-N3	4.61	135.20	125.94
1	B5	4138	OMG	N9-C4-N3	4.60	135.18	125.94
52	A2	1448	OMG	N9-C4-N3	4.60	135.17	125.94
52	A2	1329	OMG	N9-C4-N3	4.60	135.17	125.94
1	B5	3676	OMG	N9-C4-N3	4.58	135.15	125.94
52	A2	628	OMU	C4-N3-C2	-4.56	120.56	126.58
52	A2	645	OMG	N9-C4-N3	4.56	135.09	125.94
3	B8	75	OMG	N9-C4-N3	4.55	135.08	125.94
1	B5	3476	OMG	N9-C4-N3	4.55	135.07	125.94
1	B5	3524	OMG	N9-C4-N3	4.55	135.07	125.94
1	B5	4383	OMG	N9-C4-N3	4.54	135.05	125.94
52	A2	510	OMG	N9-C4-N3	4.54	135.05	125.94
1	B5	4240	OMG	N9-C4-N3	4.53	135.04	125.94
1	B5	4245	OMG	N9-C4-N3	4.53	135.04	125.94
1	B5	1477	OMG	N9-C4-N3	4.53	135.04	125.94
52	A2	868	OMG	N9-C4-N3	4.53	135.04	125.94
52	A2	602	OMG	N9-C4-N3	4.53	135.03	125.94
1	B5	3359	OMG	N9-C4-N3	4.52	135.02	125.94
1	B5	4369	OMG	N9-C4-N3	4.52	135.02	125.94
1	B5	4364	OMG	N9-C4-N3	4.51	135.00	125.94
1	B5	2267	OMG	N9-C4-N3	4.51	134.99	125.94
1	B5	2680	OMU	C4-N3-C2	-4.50	120.64	126.58
52	A2	1327	OMU	C4-N3-C2	-4.50	120.64	126.58
1	B5	2207	OMG	N9-C4-N3	4.49	134.96	125.94
52	A2	1843	4AC	N4-C4-N3	4.49	121.38	113.85
1	B5	4366	OMU	C4-N3-C2	-4.48	120.68	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	3657	OMU	C4-N3-C2	-4.47	120.69	126.58
1	B5	4244	OMU	C4-N3-C2	-4.47	120.69	126.58
52	A2	684	OMG	N9-C4-N3	4.43	134.83	125.94
1	B5	3631	OMG	N9-C4-N3	4.43	134.82	125.94
1	B5	1260	OMG	N9-C4-N3	4.42	134.82	125.94
1	B5	3973	OMU	C4-N3-C2	-4.40	120.78	126.58
52	A2	355	OMU	C4-N3-C2	-4.39	120.79	126.58
52	A2	429	OMU	C4-N3-C2	-4.38	120.80	126.58
1	B5	3974	OMG	N9-C4-N3	4.38	134.74	125.94
1	B5	2258	OMU	C4-N3-C2	-4.38	120.81	126.58
52	A2	172	OMU	C4-N3-C2	-4.37	120.82	126.58
52	A2	116	OMU	C4-N3-C2	-4.35	120.85	126.58
52	A2	1640	G7M	C5-C4-N3	-4.32	119.86	128.15
1	B5	4052	OMU	C4-N3-C2	-4.31	120.89	126.58
61	AT	53	5MU	C5-C4-N3	4.30	118.98	115.31
52	A2	1851	MA6	N1-C2-N3	-4.28	121.92	128.60
52	A2	1805	OMU	C4-N3-C2	-4.26	120.96	126.58
52	A2	1289	OMU	C4-N3-C2	-4.24	120.98	126.58
52	A2	121	OMU	C4-N3-C2	-4.24	120.99	126.58
52	A2	591	A2M	C2-N3-C4	4.21	121.70	111.75
1	B5	3550	UY1	N1-C2-N3	4.18	119.87	115.13
52	A2	1851	MA6	C2-N1-C6	4.16	121.58	111.75
52	A2	1679	A2M	C2'-C1'-N9	-4.15	106.54	113.53
52	A2	1443	OMU	C4-N3-C2	-4.15	121.11	126.58
52	A2	628	OMU	N3-C2-N1	4.15	120.39	114.89
1	B5	4366	OMU	N3-C2-N1	4.14	120.38	114.89
1	B5	2680	OMU	N3-C2-N1	4.13	120.37	114.89
1	B5	3657	OMU	N3-C2-N1	4.13	120.37	114.89
1	B5	4244	OMU	N3-C2-N1	4.12	120.36	114.89
52	A2	1327	OMU	N3-C2-N1	4.10	120.33	114.89
52	A2	1852	MA6	N1-C2-N3	-4.09	122.21	128.60
52	A2	429	OMU	N3-C2-N1	4.08	120.31	114.89
1	B5	2258	OMU	N3-C2-N1	4.07	120.29	114.89
1	B5	3973	OMU	N3-C2-N1	4.06	120.27	114.89
52	A2	355	OMU	N3-C2-N1	4.05	120.26	114.89
52	A2	116	OMU	N3-C2-N1	4.03	120.24	114.89
52	A2	1805	OMU	N3-C2-N1	4.02	120.22	114.89
1	B5	4052	OMU	N3-C2-N1	4.01	120.21	114.89
52	A2	172	OMU	N3-C2-N1	4.00	120.20	114.89
52	A2	1852	MA6	C2-N1-C6	4.00	121.19	111.75
52	A2	1640	G7M	CN7-N7-C8	-4.00	118.67	124.84
1	B5	4149	PSU	C4-N3-C2	-3.99	120.59	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	4325	PSU	C4-N3-C2	-3.99	120.59	126.34
1	B5	1489	A2M	C2-N3-C4	3.98	121.15	111.75
1	B5	1491	PSU	C4-N3-C2	-3.97	120.61	126.34
52	A2	1289	OMU	N3-C2-N1	3.96	120.14	114.89
52	A2	121	OMU	N3-C2-N1	3.95	120.14	114.89
1	B5	3466	PSU	C4-N3-C2	-3.95	120.65	126.34
1	B5	4042	PSU	C4-N3-C2	-3.95	120.65	126.34
1	B5	3616	PSU	C4-N3-C2	-3.94	120.66	126.34
1	B5	1638	PSU	C4-N3-C2	-3.94	120.66	126.34
1	B5	4267	PSU	C4-N3-C2	-3.94	120.67	126.34
1	B5	3369	PSU	C4-N3-C2	-3.92	120.68	126.34
1	B5	1721	PSU	C4-N3-C2	-3.92	120.69	126.34
1	B5	4246	PSU	C4-N3-C2	-3.92	120.69	126.34
52	A2	166	A2M	C2-N3-C4	3.91	121.00	111.75
1	B5	4099	PSU	C4-N3-C2	-3.91	120.70	126.34
1	B5	1801	PSU	C4-N3-C2	-3.91	120.70	126.34
1	B5	4039	PSU	C4-N3-C2	-3.91	120.71	126.34
52	A2	1175	PSU	C4-N3-C2	-3.91	120.71	126.34
1	B5	1799	PSU	C4-N3-C2	-3.91	120.71	126.34
1	B5	4107	PSU	C4-N3-C2	-3.90	120.71	126.34
1	B5	3652	PSU	C4-N3-C2	-3.90	120.72	126.34
1	B5	4298	PSU	C4-N3-C2	-3.90	120.72	126.34
52	A2	1443	OMU	N3-C2-N1	3.90	120.07	114.89
1	B5	4177	PSU	C4-N3-C2	-3.90	120.72	126.34
52	A2	407	PSU	C4-N3-C2	-3.90	120.72	126.34
52	A2	1233	PSU	C4-N3-C2	-3.90	120.72	126.34
1	B5	3427	PSU	C4-N3-C2	-3.90	120.73	126.34
1	B5	1731	PSU	C4-N3-C2	-3.89	120.73	126.34
1	B5	4322	PSU	C4-N3-C2	-3.89	120.73	126.34
1	B5	4336	A2M	C2-N3-C4	3.89	120.95	111.75
1	B5	398	A2M	C2-N3-C4	3.89	120.94	111.75
52	A2	218	PSU	C4-N3-C2	-3.89	120.73	126.34
1	B5	4711	PSU	C4-N3-C2	-3.89	120.73	126.34
1	B5	1683	PSU	C4-N3-C2	-3.89	120.74	126.34
52	A2	652	PSU	C4-N3-C2	-3.89	120.74	126.34
52	A2	1446	PSU	C4-N3-C2	-3.89	120.74	126.34
52	A2	99	A2M	C2-N3-C4	3.89	120.93	111.75
1	B5	2206	A2M	C2-N3-C4	3.89	120.93	111.75
1	B5	2658	A2M	C2-N3-C4	3.89	120.93	111.75
1	B5	4188	PSU	C4-N3-C2	-3.88	120.74	126.34
52	A2	1178	PSU	C4-N3-C2	-3.88	120.74	126.34
52	A2	1679	A2M	C2-N3-C4	3.88	120.92	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1239	PSU	C4-N3-C2	-3.88	120.75	126.34
3	B8	69	PSU	C4-N3-C2	-3.88	120.75	126.34
1	B5	3554	PSU	C4-N3-C2	-3.88	120.75	126.34
1	B5	4749	PSU	C4-N3-C2	-3.87	120.76	126.34
52	A2	469	A2M	C2-N3-C4	3.87	120.90	111.75
52	A2	27	A2M	C2-N3-C4	3.87	120.90	111.75
3	B8	55	PSU	C4-N3-C2	-3.87	120.76	126.34
1	B5	2244	A2M	C2-N3-C4	3.87	120.89	111.75
1	B5	4374	PSU	C4-N3-C2	-3.87	120.77	126.34
1	B5	400	A2M	C2-N3-C4	3.87	120.89	111.75
52	A2	650	PSU	C4-N3-C2	-3.87	120.77	126.34
1	B5	3966	6MZ	C2-N3-C4	3.87	120.88	111.75
1	B5	3562	A2M	C2-N3-C4	3.86	120.88	111.75
1	B5	1718	PSU	C4-N3-C2	-3.86	120.77	126.34
52	A2	513	A2M	C2-N3-C4	3.86	120.88	111.75
1	B5	3599	A2M	C2-N3-C4	3.86	120.87	111.75
52	A2	816	PSU	C4-N3-C2	-3.86	120.78	126.34
1	B5	4269	A2M	C2-N3-C4	3.86	120.87	111.75
52	A2	1046	PSU	C4-N3-C2	-3.86	120.78	126.34
1	B5	4740	PSU	C4-N3-C2	-3.86	120.78	126.34
52	A2	573	PSU	C4-N3-C2	-3.86	120.78	126.34
52	A2	1047	PSU	C4-N3-C2	-3.86	120.78	126.34
52	A2	867	PSU	C4-N3-C2	-3.86	120.78	126.34
1	B5	3502	PSU	C4-N3-C2	-3.86	120.78	126.34
1	B5	3583	PSU	C4-N3-C2	-3.86	120.78	126.34
1	B5	3490	PSU	C4-N3-C2	-3.85	120.79	126.34
52	A2	687	PSU	C4-N3-C2	-3.85	120.79	126.34
52	A2	1384	A2M	C2-N3-C4	3.85	120.85	111.75
52	A2	815	PSU	C4-N3-C2	-3.85	120.79	126.34
52	A2	1833	6MZ	C2-N3-C4	3.85	120.85	111.75
1	B5	4317	A2M	C2-N3-C4	3.85	120.84	111.75
1	B5	1810	A2M	C2-N3-C4	3.85	120.84	111.75
1	B5	1479	A2M	C2-N3-C4	3.85	120.84	111.75
52	A2	577	A2M	C2-N3-C4	3.85	120.84	111.75
1	B5	4058	PSU	C4-N3-C2	-3.85	120.80	126.34
1	B5	2351	PSU	C4-N3-C2	-3.84	120.80	126.34
52	A2	682	PSU	C4-N3-C2	-3.84	120.80	126.34
1	B5	1720	PSU	C4-N3-C2	-3.84	120.80	126.34
1	B5	1270	A2M	C2-N3-C4	3.84	120.83	111.75
52	A2	1032	A2M	C2-N3-C4	3.84	120.83	111.75
1	B5	3557	A2M	C2-N3-C4	3.84	120.82	111.75
52	A2	485	A2M	C2-N3-C4	3.84	120.82	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	159	A2M	C2-N3-C4	3.84	120.82	111.75
52	A2	1082	PSU	C4-N3-C2	-3.84	120.81	126.34
1	B5	3492	A2M	C2-N3-C4	3.84	120.82	111.75
1	B5	3517	A2M	C2-N3-C4	3.84	120.82	111.75
1	B5	3456	A2M	C2-N3-C4	3.84	120.81	111.75
1	B5	1537	PSU	C4-N3-C2	-3.84	120.81	126.34
1	B5	4217	PSU	C4-N3-C2	-3.83	120.81	126.34
61	AT	54	PSU	C4-N3-C2	-3.83	120.81	126.34
1	B5	4203	PSU	C4-N3-C2	-3.83	120.83	126.34
52	A2	93	PSU	C4-N3-C2	-3.83	120.83	126.34
1	B5	4045	PSU	C4-N3-C2	-3.82	120.83	126.34
52	A2	105	PSU	C4-N3-C2	-3.82	120.83	126.34
1	B5	3496	PSU	C4-N3-C2	-3.82	120.83	126.34
52	A2	864	PSU	C4-N3-C2	-3.82	120.83	126.34
1	B5	2475	PSU	C4-N3-C2	-3.82	120.83	126.34
1	B5	4419	PSU	C4-N3-C2	-3.82	120.83	126.34
1	B5	3450	A2M	C2-N3-C4	3.82	120.77	111.75
52	A2	669	A2M	C2-N3-C4	3.82	120.77	111.75
52	A2	802	PSU	C4-N3-C2	-3.81	120.84	126.34
1	B5	3585	PSU	C4-N3-C2	-3.81	120.84	126.34
1	B5	4435	PSU	C4-N3-C2	-3.81	120.84	126.34
52	A2	1368	PSU	C4-N3-C2	-3.81	120.85	126.34
1	B5	4169	PSU	C4-N3-C2	-3.81	120.86	126.34
52	A2	1057	PSU	C4-N3-C2	-3.81	120.86	126.34
1	B5	3500	PSU	C4-N3-C2	-3.80	120.86	126.34
1	B5	2630	A2M	C2-N3-C4	3.80	120.72	111.75
1	B5	3462	PSU	C4-N3-C2	-3.80	120.87	126.34
52	A2	210	PSU	C4-N3-C2	-3.79	120.88	126.34
52	A2	967	PSU	C4-N3-C2	-3.79	120.88	126.34
1	B5	3494	PSU	C4-N3-C2	-3.78	120.89	126.34
52	A2	1245	PSU	C4-N3-C2	-3.78	120.89	126.34
52	A2	1693	PSU	C4-N3-C2	-3.78	120.89	126.34
1	B5	4193	5MC	C5-C6-N1	-3.78	119.45	123.34
52	A2	1005	PSU	C4-N3-C2	-3.78	120.89	126.34
1	B5	4166	PSU	C4-N3-C2	-3.78	120.89	126.34
52	A2	34	PSU	C4-N3-C2	-3.78	120.89	126.34
1	B5	4382	PSU	C4-N3-C2	-3.77	120.90	126.34
52	A2	119	PSU	C4-N3-C2	-3.77	120.90	126.34
52	A2	1640	G7M	C5-C6-N1	3.77	119.66	111.79
52	A2	1626	PSU	C4-N3-C2	-3.77	120.91	126.34
1	B5	3576	PSU	C4-N3-C2	-3.77	120.91	126.34
52	A2	1644	PSU	C4-N3-C2	-3.77	120.91	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1640	G7M	N9-C8-N7	-3.76	102.92	112.21
61	AT	53	5MU	O4-C4-C5	-3.75	120.55	124.90
1	B5	3447	PSU	C4-N3-C2	-3.75	120.93	126.34
52	A2	109	PSU	C4-N3-C2	-3.75	120.93	126.34
52	A2	823	PSU	C4-N3-C2	-3.75	120.94	126.34
52	A2	36	PSU	C4-N3-C2	-3.75	120.94	126.34
52	A2	610	PSU	C4-N3-C2	-3.71	120.99	126.34
1	B5	1632	PSU	C4-N3-C2	-3.71	120.99	126.34
1	B5	4278	PSU	C4-N3-C2	-3.70	121.01	126.34
1	B5	3371	PSU	C4-N3-C2	-3.67	121.05	126.34
52	A2	1348	PSU	C4-N3-C2	-3.65	121.09	126.34
1	B5	4366	OMU	C5-C4-N3	3.60	120.23	114.84
52	A2	1327	OMU	C5-C4-N3	3.58	120.19	114.84
52	A2	1640	G7M	C4-C5-N7	-3.57	101.82	107.67
1	B5	2258	OMU	C5-C4-N3	3.57	120.19	114.84
1	B5	2680	OMU	C5-C4-N3	3.57	120.18	114.84
52	A2	355	OMU	C5-C4-N3	3.57	120.18	114.84
52	A2	628	OMU	C5-C4-N3	3.57	120.18	114.84
1	B5	4052	OMU	C5-C4-N3	3.56	120.17	114.84
1	B5	4244	OMU	C5-C4-N3	3.56	120.17	114.84
1	B5	3973	OMU	C5-C4-N3	3.56	120.16	114.84
52	A2	429	OMU	C5-C4-N3	3.55	120.16	114.84
52	A2	1851	MA6	C6-C5-N7	3.55	139.24	133.28
52	A2	823	PSU	O2-C2-N1	-3.54	118.89	122.79
52	A2	172	OMU	C5-C4-N3	3.54	120.14	114.84
52	A2	1289	OMU	C5-C4-N3	3.54	120.14	114.84
52	A2	116	OMU	C5-C4-N3	3.54	120.13	114.84
1	B5	3657	OMU	C5-C4-N3	3.51	120.10	114.84
52	A2	1805	OMU	C5-C4-N3	3.51	120.08	114.84
52	A2	1852	MA6	C1'-N9-C8	-3.51	119.22	127.14
52	A2	121	OMU	C5-C4-N3	3.50	120.07	114.84
52	A2	1851	MA6	C2-N3-C4	3.48	119.98	111.75
52	A2	1851	MA6	C1'-N9-C8	-3.48	119.27	127.14
52	A2	682	PSU	O2-C2-N1	-3.47	118.97	122.79
52	A2	1443	OMU	C5-C4-N3	3.47	120.03	114.84
52	A2	1852	MA6	C2-N3-C4	3.46	119.94	111.75
1	B5	3494	PSU	O2-C2-N1	-3.46	118.98	122.79
1	B5	4435	PSU	O2-C2-N1	-3.45	118.99	122.79
61	AT	53	5MU	C5-C6-N1	-3.45	119.79	123.34
52	A2	1446	PSU	O2-C2-N1	-3.45	118.99	122.79
1	B5	1491	PSU	O2-C2-N1	-3.45	119.00	122.79
52	A2	1239	PSU	O2-C2-N1	-3.45	119.00	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	4267	PSU	O2-C2-N1	-3.45	119.00	122.79
3	B8	55	PSU	O2-C2-N1	-3.44	119.00	122.79
1	B5	4177	PSU	O2-C2-N1	-3.44	119.00	122.79
1	B5	4322	PSU	O2-C2-N1	-3.44	119.00	122.79
1	B5	4058	PSU	O2-C2-N1	-3.44	119.01	122.79
1	B5	4042	PSU	O2-C2-N1	-3.43	119.01	122.79
1	B5	3966	6MZ	C9-N6-C6	-3.43	119.92	122.87
1	B5	1489	A2M	C4-C5-N7	-3.43	106.44	110.62
1	B5	3502	PSU	O2-C2-N1	-3.43	119.02	122.79
1	B5	3652	PSU	O2-C2-N1	-3.43	119.02	122.79
1	B5	1632	PSU	O2-C2-N1	-3.43	119.02	122.79
1	B5	3427	PSU	O2-C2-N1	-3.43	119.02	122.79
52	A2	816	PSU	O2-C2-N1	-3.42	119.02	122.79
1	B5	4374	PSU	O2-C2-N1	-3.42	119.02	122.79
1	B5	3585	PSU	O2-C2-N1	-3.42	119.03	122.79
1	B5	4711	PSU	O2-C2-N1	-3.41	119.03	122.79
52	A2	864	PSU	O2-C2-N1	-3.41	119.03	122.79
1	B5	3496	PSU	O2-C2-N1	-3.41	119.03	122.79
1	B5	4298	PSU	O2-C2-N1	-3.41	119.03	122.79
52	A2	650	PSU	O2-C2-N1	-3.41	119.03	122.79
52	A2	1178	PSU	O2-C2-N1	-3.41	119.04	122.79
1	B5	1720	PSU	O2-C2-N1	-3.41	119.04	122.79
1	B5	2351	PSU	O2-C2-N1	-3.41	119.04	122.79
52	A2	610	PSU	O2-C2-N1	-3.41	119.04	122.79
52	A2	1348	PSU	O2-C2-N1	-3.40	119.05	122.79
1	B5	1799	PSU	O2-C2-N1	-3.40	119.05	122.79
52	A2	1626	PSU	O2-C2-N1	-3.40	119.05	122.79
52	A2	1082	PSU	O2-C2-N1	-3.40	119.05	122.79
1	B5	1683	PSU	O2-C2-N1	-3.40	119.05	122.79
1	B5	3490	PSU	O2-C2-N1	-3.39	119.05	122.79
52	A2	210	PSU	O2-C2-N1	-3.39	119.06	122.79
4	BA	216	V5N	CD2-CG-ND1	3.39	110.16	105.71
1	B5	4382	PSU	O2-C2-N1	-3.39	119.06	122.79
1	B5	4749	PSU	O2-C2-N1	-3.39	119.06	122.79
1	B5	3554	PSU	O2-C2-N1	-3.39	119.06	122.79
3	B8	69	PSU	O2-C2-N1	-3.39	119.06	122.79
52	A2	687	PSU	O2-C2-N1	-3.39	119.06	122.79
52	A2	867	PSU	O2-C2-N1	-3.38	119.07	122.79
30	Ba	39	V5N	CD2-CG-ND1	3.38	110.15	105.71
1	B5	3466	PSU	O2-C2-N1	-3.38	119.07	122.79
52	A2	1368	PSU	O2-C2-N1	-3.38	119.07	122.79
52	A2	36	PSU	O2-C2-N1	-3.38	119.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1175	PSU	O2-C2-N1	-3.38	119.07	122.79
1	B5	3500	PSU	O2-C2-N1	-3.38	119.07	122.79
1	B5	4419	PSU	O2-C2-N1	-3.38	119.07	122.79
52	A2	1693	PSU	O2-C2-N1	-3.38	119.07	122.79
1	B5	4246	PSU	O2-C2-N1	-3.37	119.08	122.79
52	A2	573	PSU	O2-C2-N1	-3.37	119.08	122.79
52	A2	407	PSU	O2-C2-N1	-3.37	119.08	122.79
1	B5	4278	PSU	O2-C2-N1	-3.37	119.08	122.79
52	A2	1057	PSU	O2-C2-N1	-3.37	119.08	122.79
1	B5	4325	PSU	O2-C2-N1	-3.37	119.08	122.79
1	B5	1721	PSU	O2-C2-N1	-3.37	119.08	122.79
1	B5	2475	PSU	O2-C2-N1	-3.37	119.08	122.79
1	B5	4099	PSU	O2-C2-N1	-3.37	119.08	122.79
52	A2	1245	PSU	O2-C2-N1	-3.37	119.08	122.79
1	B5	4217	PSU	O2-C2-N1	-3.36	119.09	122.79
1	B5	4336	A2M	C4-C5-N7	-3.36	106.53	110.62
1	B5	3369	PSU	O2-C2-N1	-3.36	119.09	122.79
52	A2	93	PSU	O2-C2-N1	-3.36	119.09	122.79
1	B5	1537	PSU	O2-C2-N1	-3.36	119.09	122.79
1	B5	1810	A2M	C2'-C1'-N9	-3.36	107.88	113.53
1	B5	4039	PSU	O2-C2-N1	-3.36	119.10	122.79
1	B5	4166	PSU	O2-C2-N1	-3.35	119.10	122.79
1	B5	4169	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	109	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	652	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	218	PSU	O2-C2-N1	-3.35	119.10	122.79
52	A2	1233	PSU	O2-C2-N1	-3.35	119.10	122.79
1	B5	2206	A2M	C4-C5-N7	-3.35	106.54	110.62
1	B5	3557	A2M	C4-C5-N7	-3.35	106.54	110.62
1	B5	1638	PSU	O2-C2-N1	-3.35	119.11	122.79
1	B5	4149	PSU	O2-C2-N1	-3.35	119.11	122.79
52	A2	105	PSU	O2-C2-N1	-3.35	119.11	122.79
52	A2	1679	A2M	C4-C5-N7	-3.35	106.54	110.62
1	B5	3447	PSU	O2-C2-N1	-3.34	119.11	122.79
52	A2	802	PSU	O2-C2-N1	-3.34	119.11	122.79
52	A2	967	PSU	O2-C2-N1	-3.34	119.11	122.79
1	B5	4188	PSU	O2-C2-N1	-3.34	119.11	122.79
52	A2	1046	PSU	O2-C2-N1	-3.34	119.11	122.79
52	A2	1644	PSU	O2-C2-N1	-3.34	119.12	122.79
1	B5	2658	A2M	C4-C5-N7	-3.33	106.56	110.62
61	AT	54	PSU	O2-C2-N1	-3.33	119.12	122.79
1	B5	398	A2M	C2'-C1'-N9	-3.33	107.92	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1005	PSU	O2-C2-N1	-3.33	119.12	122.79
1	B5	3462	PSU	O2-C2-N1	-3.33	119.12	122.79
52	A2	577	A2M	C4-C5-N7	-3.33	106.56	110.62
1	B5	398	A2M	C4-C5-N7	-3.33	106.57	110.62
52	A2	1640	G7M	O6-C6-C5	-3.33	120.56	128.06
1	B5	4045	PSU	O2-C2-N1	-3.33	119.13	122.79
1	B5	3492	A2M	C4-C5-N7	-3.32	106.57	110.62
52	A2	1384	A2M	C2'-C1'-N9	-3.32	107.94	113.53
76	An	138	5F0	OD1-C1-CA	3.32	120.02	111.52
1	B5	3371	PSU	O2-C2-N1	-3.32	119.13	122.79
52	A2	1384	A2M	C4-C5-N7	-3.32	106.58	110.62
1	B5	3450	A2M	C4-C5-N7	-3.32	106.58	110.62
52	A2	119	PSU	O2-C2-N1	-3.32	119.14	122.79
52	A2	166	A2M	C4-C5-N7	-3.32	106.58	110.62
1	B5	1810	A2M	C4-C5-N7	-3.31	106.58	110.62
1	B5	4317	A2M	C4-C5-N7	-3.31	106.58	110.62
52	A2	1249	B8N	C4-N3-C2	-3.31	121.28	125.46
1	B5	3583	PSU	O2-C2-N1	-3.31	119.15	122.79
52	A2	159	A2M	C4-C5-N7	-3.31	106.59	110.62
1	B5	3966	6MZ	C6-C5-N7	3.31	135.97	132.39
1	B5	1731	PSU	O2-C2-N1	-3.31	119.15	122.79
52	A2	34	PSU	O2-C2-N1	-3.31	119.15	122.79
1	B5	1801	PSU	O2-C2-N1	-3.30	119.15	122.79
1	B5	400	A2M	C4-C5-N7	-3.30	106.60	110.62
1	B5	2244	A2M	C4-C5-N7	-3.30	106.60	110.62
52	A2	684	OMG	C6-C5-N7	3.30	136.38	130.25
52	A2	469	A2M	C4-C5-N7	-3.30	106.60	110.62
1	B5	3576	PSU	O2-C2-N1	-3.30	119.16	122.79
52	A2	669	A2M	C4-C5-N7	-3.30	106.60	110.62
52	A2	1047	PSU	O2-C2-N1	-3.29	119.17	122.79
1	B5	3599	A2M	C4-C5-N7	-3.29	106.61	110.62
1	B5	4269	A2M	C4-C5-N7	-3.29	106.61	110.62
52	A2	1032	A2M	C4-C5-N7	-3.29	106.61	110.62
52	A2	99	A2M	C4-C5-N7	-3.28	106.62	110.62
1	B5	1266	1MA	N9-C4-N3	3.28	134.59	126.94
1	B5	3616	PSU	O2-C2-N1	-3.28	119.18	122.79
52	A2	27	A2M	C4-C5-N7	-3.28	106.63	110.62
52	A2	513	A2M	C4-C5-N7	-3.28	106.63	110.62
1	B5	4740	PSU	O2-C2-N1	-3.27	119.19	122.79
1	B5	3974	OMG	C6-C5-N7	3.27	136.33	130.25
1	B5	1270	A2M	C4-C5-N7	-3.27	106.64	110.62
1	B5	1479	A2M	C4-C5-N7	-3.27	106.64	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	4107	PSU	O2-C2-N1	-3.26	119.20	122.79
1	B5	3517	A2M	C4-C5-N7	-3.26	106.65	110.62
1	B5	3562	A2M	C4-C5-N7	-3.26	106.65	110.62
52	A2	815	PSU	O2-C2-N1	-3.26	119.21	122.79
1	B5	1718	PSU	O2-C2-N1	-3.25	119.21	122.79
1	B5	3456	A2M	C4-C5-N7	-3.25	106.66	110.62
1	B5	4203	PSU	O2-C2-N1	-3.25	119.21	122.79
1	B5	2630	A2M	C2'-C1'-N9	-3.25	108.06	113.53
1	B5	3514	5MC	C5-C6-N1	-3.25	120.00	123.34
61	AT	48	5MC	C5-C6-N1	-3.24	120.00	123.34
1	B5	1489	A2M	N3-C2-N1	-3.24	123.53	128.60
1	B5	3631	OMG	C6-C5-N7	3.24	136.28	130.25
52	A2	485	A2M	C4-C5-N7	-3.24	106.67	110.62
1	B5	3557	A2M	C2'-C1'-N9	-3.24	108.08	113.53
1	B5	3966	6MZ	C4-C5-N7	-3.22	106.69	110.62
52	A2	1032	A2M	N3-C2-N1	-3.22	123.57	128.60
1	B5	1477	OMG	C6-C5-N7	3.22	136.24	130.25
1	B5	1260	OMG	C6-C5-N7	3.22	136.23	130.25
1	B5	3359	OMG	C6-C5-N7	3.22	136.23	130.25
1	B5	3517	A2M	N3-C2-N1	-3.21	123.58	128.60
1	B5	2207	OMG	C6-C5-N7	3.21	136.22	130.25
1	B5	4245	OMG	C6-C5-N7	3.20	136.20	130.25
52	A2	591	A2M	N3-C2-N1	-3.20	123.60	128.60
1	B5	3524	OMG	C6-C5-N7	3.20	136.20	130.25
52	A2	868	OMG	C6-C5-N7	3.20	136.19	130.25
1	B5	4369	OMG	C6-C5-N7	3.19	136.19	130.25
1	B5	4383	OMG	C6-C5-N7	3.18	136.17	130.25
52	A2	1679	A2M	N3-C2-N1	-3.18	123.63	128.60
1	B5	2630	A2M	C4-C5-N7	-3.18	106.75	110.62
52	A2	1852	MA6	C6-C5-N7	3.17	138.61	133.28
1	B5	4240	OMG	C6-C5-N7	3.17	136.15	130.25
52	A2	602	OMG	C6-C5-N7	3.17	136.14	130.25
52	A2	645	OMG	C6-C5-N7	3.17	136.14	130.25
1	B5	4138	OMG	C6-C5-N7	3.16	136.13	130.25
1	B5	2206	A2M	C2'-C1'-N9	-3.16	108.21	113.53
1	B5	4269	A2M	C2'-C1'-N9	-3.16	108.21	113.53
52	A2	510	OMG	C6-C5-N7	3.16	136.12	130.25
1	B5	3476	OMG	C6-C5-N7	3.16	136.12	130.25
52	A2	1032	A2M	C2'-C1'-N9	-3.16	108.22	113.53
1	B5	4336	A2M	N3-C2-N1	-3.15	123.67	128.60
3	B8	75	OMG	C6-C5-N7	3.15	136.11	130.25
52	A2	591	A2M	C4-C5-N7	-3.15	106.78	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	27	A2M	N3-C2-N1	-3.15	123.68	128.60
1	B5	3562	A2M	N3-C2-N1	-3.15	123.68	128.60
1	B5	2267	OMG	C6-C5-N7	3.14	136.09	130.25
52	A2	1329	OMG	C6-C5-N7	3.14	136.09	130.25
52	A2	166	A2M	N3-C2-N1	-3.14	123.70	128.60
52	A2	1851	MA6	C4-N9-C1'	-3.13	119.12	126.59
1	B5	400	A2M	N3-C2-N1	-3.13	123.70	128.60
52	A2	1448	OMG	C6-C5-N7	3.13	136.07	130.25
1	B5	2206	A2M	N3-C2-N1	-3.13	123.71	128.60
1	B5	4317	A2M	N3-C2-N1	-3.13	123.71	128.60
52	A2	99	A2M	N3-C2-N1	-3.12	123.72	128.60
1	B5	1810	A2M	N3-C2-N1	-3.12	123.72	128.60
1	B5	4364	OMG	C6-C5-N7	3.12	136.05	130.25
52	A2	159	A2M	C2'-C1'-N9	-3.12	108.28	113.53
52	A2	437	OMG	C6-C5-N7	3.12	136.05	130.25
52	A2	1384	A2M	N3-C2-N1	-3.12	123.72	128.60
1	B5	3676	OMG	C6-C5-N7	3.12	136.05	130.25
1	B5	4269	A2M	N3-C2-N1	-3.12	123.73	128.60
52	A2	159	A2M	N3-C2-N1	-3.11	123.74	128.60
1	B5	3456	A2M	N3-C2-N1	-3.11	123.74	128.60
1	B5	3966	6MZ	N1-C2-N3	-3.11	123.74	128.60
52	A2	513	A2M	N3-C2-N1	-3.11	123.74	128.60
1	B5	4116	OMG	C6-C5-N7	3.10	136.02	130.25
1	B5	2244	A2M	N3-C2-N1	-3.10	123.76	128.60
52	A2	469	A2M	N3-C2-N1	-3.10	123.76	128.60
1	B5	3492	A2M	N3-C2-N1	-3.09	123.76	128.60
1	B5	3557	A2M	N3-C2-N1	-3.09	123.76	128.60
1	B5	398	A2M	N3-C2-N1	-3.09	123.77	128.60
52	A2	577	A2M	N3-C2-N1	-3.09	123.77	128.60
1	B5	1580	OMG	C6-C5-N7	3.09	136.00	130.25
52	A2	485	A2M	N3-C2-N1	-3.09	123.77	128.60
52	A2	1491	OMG	C6-C5-N7	3.08	135.98	130.25
1	B5	1270	A2M	N3-C2-N1	-3.08	123.79	128.60
1	B5	2630	A2M	N3-C2-N1	-3.08	123.79	128.60
52	A2	669	A2M	N3-C2-N1	-3.07	123.79	128.60
52	A2	1833	6MZ	C4-C5-N7	-3.07	106.88	110.62
1	B5	3599	A2M	N3-C2-N1	-3.07	123.81	128.60
1	B5	3942	OMG	C6-C5-N7	3.06	135.94	130.25
1	B5	3450	A2M	N3-C2-N1	-3.06	123.82	128.60
1	B5	2658	A2M	N3-C2-N1	-3.05	123.84	128.60
52	A2	1833	6MZ	N1-C2-N3	-3.03	123.86	128.60
52	A2	1852	MA6	C4-N9-C1'	-3.03	119.38	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	99	A2M	C2'-C1'-N9	-3.03	108.43	113.53
52	A2	116	OMU	O4-C4-C5	-3.02	119.85	125.16
52	A2	1327	OMU	O4-C4-C5	-3.02	119.85	125.16
1	B5	2719	OMG	C6-C5-N7	3.01	135.85	130.25
1	B5	3456	A2M	C2'-C1'-N9	-3.00	108.48	113.53
1	B5	3562	A2M	C2'-C1'-N9	-3.00	108.48	113.53
1	B5	1479	A2M	N3-C2-N1	-3.00	123.91	128.60
52	A2	1249	B8N	N3-C2-N1	3.00	121.00	116.76
1	B5	4244	OMU	O4-C4-C5	-3.00	119.89	125.16
1	B5	4317	A2M	C2'-C1'-N9	-2.99	108.49	113.53
52	A2	355	OMU	O4-C4-C5	-2.99	119.90	125.16
52	A2	1443	OMU	O4-C4-C5	-2.99	119.90	125.16
1	B5	3973	OMU	O4-C4-C5	-2.99	119.90	125.16
52	A2	1289	OMU	O4-C4-C5	-2.99	119.91	125.16
1	B5	3657	OMU	O4-C4-C5	-2.98	119.92	125.16
1	B5	4366	OMU	O4-C4-C5	-2.97	119.94	125.16
1	B5	2258	OMU	O4-C4-C5	-2.97	119.94	125.16
1	B5	2680	OMU	O4-C4-C5	-2.96	119.95	125.16
52	A2	1833	6MZ	C9-N6-C6	-2.96	120.33	122.87
52	A2	121	OMU	O4-C4-C5	-2.95	119.96	125.16
52	A2	429	OMU	O4-C4-C5	-2.95	119.97	125.16
1	B5	4052	OMU	O4-C4-C5	-2.95	119.97	125.16
52	A2	628	OMU	O4-C4-C5	-2.95	119.97	125.16
52	A2	172	OMU	O4-C4-C5	-2.95	119.98	125.16
52	A2	1805	OMU	O4-C4-C5	-2.94	119.99	125.16
1	B5	2244	A2M	C2'-C1'-N9	-2.94	108.58	113.53
52	A2	1833	6MZ	C6-C5-N7	2.93	135.57	132.39
52	A2	1640	G7M	C2-N1-C6	-2.93	119.76	125.10
1	B5	3450	A2M	C2'-C1'-N9	-2.93	108.60	113.53
1	B5	4336	A2M	C2'-C1'-N9	-2.92	108.61	113.53
1	B5	3517	A2M	O4'-C1'-N9	2.90	113.77	108.06
52	A2	1852	MA6	C5-C4-N9	-2.87	102.44	105.78
1	B5	1489	A2M	C5-N7-C8	2.84	107.55	103.51
1	B5	3492	A2M	C5-N7-C8	2.84	107.55	103.51
52	A2	1679	A2M	C5-N7-C8	2.84	107.54	103.51
1	B5	4336	A2M	C5-N7-C8	2.82	107.51	103.51
52	A2	1384	A2M	C5-N7-C8	2.82	107.51	103.51
52	A2	159	A2M	C5-N7-C8	2.81	107.50	103.51
1	B5	4269	A2M	C5-N7-C8	2.80	107.49	103.51
52	A2	166	A2M	C2'-C1'-N9	-2.80	108.81	113.53
1	B5	3557	A2M	C5-N7-C8	2.80	107.48	103.51
52	A2	166	A2M	C5-N7-C8	2.79	107.48	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	3517	A2M	C4-N9-C8	2.79	108.75	105.73
52	A2	669	A2M	C5-N7-C8	2.78	107.46	103.51
1	B5	2206	A2M	C5-N7-C8	2.78	107.46	103.51
52	A2	469	A2M	C5-N7-C8	2.78	107.45	103.51
52	A2	1851	MA6	C5-C4-N9	-2.78	102.55	105.78
1	B5	398	A2M	C5-N7-C8	2.78	107.45	103.51
1	B5	1810	A2M	C5-N7-C8	2.78	107.45	103.51
52	A2	577	A2M	C5-N7-C8	2.77	107.45	103.51
1	B5	2658	A2M	C5-N7-C8	2.77	107.44	103.51
1	B5	2244	A2M	C5-N7-C8	2.77	107.44	103.51
52	A2	27	A2M	C5-N7-C8	2.77	107.44	103.51
52	A2	99	A2M	C5-N7-C8	2.77	107.44	103.51
1	B5	400	A2M	C5-N7-C8	2.76	107.44	103.51
52	A2	1032	A2M	C5-N7-C8	2.76	107.44	103.51
52	A2	513	A2M	C2'-C1'-N9	-2.76	108.88	113.53
1	B5	3517	A2M	C5-N7-C8	2.76	107.43	103.51
52	A2	27	A2M	C2'-C1'-N9	-2.76	108.89	113.53
52	A2	513	A2M	C5-N7-C8	2.76	107.43	103.51
52	A2	1443	OMU	C1'-N1-C2	2.75	122.55	117.57
1	B5	3599	A2M	C5-N7-C8	2.74	107.41	103.51
1	B5	3562	A2M	C5-N7-C8	2.74	107.40	103.51
1	B5	4317	A2M	C5-N7-C8	2.73	107.39	103.51
1	B5	1270	A2M	C5-N7-C8	2.73	107.39	103.51
52	A2	485	A2M	C5-N7-C8	2.72	107.37	103.51
1	B5	3966	6MZ	C5-N7-C8	2.71	107.36	103.51
1	B5	1479	A2M	C5-N7-C8	2.71	107.36	103.51
52	A2	1679	A2M	C4-N9-C8	2.71	108.66	105.73
1	B5	3456	A2M	C5-N7-C8	2.70	107.34	103.51
52	A2	591	A2M	C5-N7-C8	2.69	107.34	103.51
1	B5	3450	A2M	C5-N7-C8	2.69	107.33	103.51
1	B5	2630	A2M	C5-N7-C8	2.69	107.32	103.51
1	B5	1810	A2M	C4-N9-C8	2.65	108.60	105.73
1	B5	4245	OMG	C4-C5-N7	-2.64	106.54	110.72
1	B5	3359	OMG	C4-C5-N7	-2.64	106.54	110.72
1	B5	3492	A2M	C4-N9-C8	2.64	108.58	105.73
52	A2	684	OMG	C4-C5-N7	-2.63	106.56	110.72
1	B5	1477	OMG	C4-C5-N7	-2.63	106.56	110.72
1	B5	4383	OMG	C4-C5-N7	-2.62	106.57	110.72
52	A2	868	OMG	C4-C5-N7	-2.62	106.57	110.72
1	B5	2207	OMG	C4-C5-N7	-2.62	106.57	110.72
52	A2	510	OMG	C4-C5-N7	-2.62	106.57	110.72
1	B5	4269	A2M	C4-N9-C8	2.62	108.56	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	645	OMG	C4-C5-N7	-2.62	106.58	110.72
52	A2	1448	OMG	C4-C5-N7	-2.62	106.58	110.72
1	B5	3524	OMG	C4-C5-N7	-2.61	106.59	110.72
1	B5	4240	OMG	C4-C5-N7	-2.61	106.60	110.72
1	B5	3476	OMG	C4-C5-N7	-2.60	106.60	110.72
52	A2	602	OMG	C4-C5-N7	-2.60	106.60	110.72
52	A2	1833	6MZ	C5-N7-C8	2.60	107.21	103.51
1	B5	3974	OMG	C4-C5-N7	-2.60	106.60	110.72
1	B5	400	A2M	C2'-C1'-N9	-2.60	109.15	113.53
1	B5	4369	OMG	C4-C5-N7	-2.60	106.61	110.72
52	A2	1329	OMG	C4-C5-N7	-2.59	106.62	110.72
1	B5	4364	OMG	C4-C5-N7	-2.59	106.62	110.72
1	B5	4336	A2M	C4-N9-C8	2.59	108.53	105.73
1	B5	4138	OMG	C4-C5-N7	-2.58	106.63	110.72
52	A2	437	OMG	C4-C5-N7	-2.58	106.63	110.72
1	B5	3631	OMG	C4-C5-N7	-2.58	106.63	110.72
1	B5	3676	OMG	C4-C5-N7	-2.58	106.63	110.72
1	B5	1260	OMG	C4-C5-N7	-2.58	106.63	110.72
1	B5	2719	OMG	C4-C5-N7	-2.58	106.64	110.72
1	B5	4116	OMG	C4-C5-N7	-2.57	106.65	110.72
1	B5	1266	1MA	C4-C5-N7	-2.57	106.65	110.72
3	B8	75	OMG	C4-C5-N7	-2.57	106.66	110.72
1	B5	3514	5MC	C5-C4-N3	-2.57	118.91	121.67
52	A2	669	A2M	C4-N9-C8	2.56	108.51	105.73
1	B5	3942	OMG	C4-C5-N7	-2.56	106.67	110.72
1	B5	2244	A2M	C4-N9-C8	2.56	108.50	105.73
1	B5	3557	A2M	C4-N9-C8	2.56	108.50	105.73
1	B5	1580	OMG	C4-C5-N7	-2.55	106.69	110.72
52	A2	485	A2M	C2'-C1'-N9	-2.55	109.24	113.53
1	B5	400	A2M	C4-N9-C8	2.54	108.48	105.73
52	A2	1032	A2M	C4-N9-C8	2.54	108.48	105.73
52	A2	99	A2M	C4-N9-C8	2.53	108.47	105.73
52	A2	159	A2M	C4-N9-C8	2.53	108.47	105.73
52	A2	485	A2M	C4-N9-C8	2.53	108.47	105.73
1	B5	3562	A2M	C4-N9-C8	2.52	108.46	105.73
1	B5	2267	OMG	C4-C5-N7	-2.52	106.73	110.72
52	A2	27	A2M	C4-N9-C8	2.51	108.45	105.73
1	B5	3966	6MZ	C4-N9-C8	2.51	108.44	105.73
52	A2	1384	A2M	C4-N9-C8	2.51	108.44	105.73
52	A2	1491	OMG	C4-C5-N7	-2.50	106.76	110.72
52	A2	577	A2M	C2'-C1'-N9	-2.50	109.32	113.53
1	B5	3456	A2M	C4-N9-C8	2.50	108.44	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	3599	A2M	C4-N9-C8	2.50	108.44	105.73
52	A2	513	A2M	C4-N9-C8	2.50	108.43	105.73
61	AT	48	5MC	C5-C4-N3	-2.49	118.98	121.67
1	B5	4193	5MC	C5-C4-N3	-2.49	118.99	121.67
1	B5	398	A2M	C4-N9-C8	2.49	108.42	105.73
80	Ar	2	SAC	O-C-CA	-2.48	118.28	124.78
1	B5	3550	UY1	C6-C5-C4	2.48	119.93	118.20
1	B5	1489	A2M	C4-N9-C8	2.48	108.41	105.73
1	B5	2630	A2M	C4-N9-C8	2.48	108.41	105.73
52	A2	577	A2M	C4-N9-C8	2.48	108.41	105.73
1	B5	4317	A2M	C4-N9-C8	2.46	108.39	105.73
52	A2	469	A2M	C4-N9-C8	2.46	108.39	105.73
1	B5	1270	A2M	C4-N9-C8	2.46	108.39	105.73
1	B5	2206	A2M	C4-N9-C8	2.46	108.39	105.73
83	Au	1	AME	O-C-CA	-2.45	118.36	124.78
1	B5	3517	A2M	C2'-C1'-N9	-2.43	109.43	113.53
52	A2	1338	4AC	C6-C5-C4	2.43	119.94	116.96
4	BA	216	V5N	O-C-CA	-2.42	118.43	124.78
52	A2	166	A2M	C4-N9-C8	2.42	108.35	105.73
52	A2	1338	4AC	C5-C4-N4	-2.42	118.72	122.92
52	A2	1843	4AC	C5-C4-N4	-2.41	118.72	122.92
52	A2	1833	6MZ	C4-N9-C8	2.40	108.33	105.73
1	B5	1479	A2M	C4-N9-C8	2.39	108.32	105.73
1	B5	2658	A2M	C4-N9-C8	2.39	108.32	105.73
1	B5	1489	A2M	C6-C5-N7	2.37	136.44	132.02
1	B5	3517	A2M	C6-C5-N7	2.36	136.42	132.02
1	B5	3492	A2M	C2'-C1'-N9	-2.36	109.56	113.53
1	B5	3550	UY1	O2-C2-N1	-2.36	120.20	122.79
1	B5	3450	A2M	C4-N9-C8	2.35	108.27	105.73
1	B5	3514	5MC	O2-C2-N3	-2.35	118.52	122.33
62	AZ	2	SAC	O-C-CA	-2.34	118.64	124.78
1	B5	2658	A2M	C2'-C1'-N9	-2.33	109.61	113.53
30	Ba	39	V5N	O-C-CA	-2.30	118.74	124.78
45	Br	2	SAC	O-C-CA	-2.30	118.76	124.78
52	A2	1843	4AC	C6-C5-C4	2.29	119.77	116.96
52	A2	1679	A2M	C6-C5-N7	2.28	136.28	132.02
52	A2	1289	OMU	C1'-N1-C2	2.28	121.70	117.57
1	B5	4336	A2M	C6-C5-N7	2.26	136.23	132.02
52	A2	628	OMU	O2-C2-N1	-2.25	119.80	122.79
52	A2	1032	A2M	C6-C5-N7	2.24	136.19	132.02
1	B5	3557	A2M	C6-C5-N7	2.24	136.19	132.02
52	A2	669	A2M	C2'-C1'-N9	-2.24	109.77	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1851	MA6	C5-N7-C8	2.23	106.68	103.51
52	A2	1327	OMU	O2-C2-N1	-2.22	119.83	122.79
1	B5	4269	A2M	C6-C5-N7	2.22	136.15	132.02
52	A2	669	A2M	C6-C5-N7	2.21	136.15	132.02
52	A2	1640	G7M	C5-C4-N9	-2.21	101.04	105.89
1	B5	3517	A2M	N9-C8-N7	-2.21	110.89	113.91
1	B5	2194	OMC	O2-C2-N3	-2.21	118.73	122.33
1	B5	1810	A2M	C6-C5-N7	2.21	136.14	132.02
85	Aw	62	HY3	O-C-CA	-2.21	118.68	124.83
52	A2	159	A2M	C6-C5-N7	2.21	136.13	132.02
1	B5	2206	A2M	C6-C5-N7	2.20	136.12	132.02
52	A2	166	A2M	C6-C5-N7	2.20	136.12	132.02
52	A2	27	A2M	C6-C5-N7	2.20	136.12	132.02
52	A2	577	A2M	C6-C5-N7	2.19	136.11	132.02
1	B5	1479	A2M	C2'-C1'-N9	-2.19	109.84	113.53
1	B5	398	A2M	C6-C5-N7	2.19	136.10	132.02
1	B5	2704	OMC	O2-C2-N3	-2.19	118.77	122.33
52	A2	1384	A2M	C6-C5-N7	2.19	136.10	132.02
1	B5	3450	A2M	C6-C5-N7	2.18	136.09	132.02
1	B5	3562	A2M	C6-C5-N7	2.18	136.08	132.02
1	B5	4317	A2M	C6-C5-N7	2.18	136.08	132.02
52	A2	1491	OMG	O6-C6-C5	-2.18	120.82	126.60
1	B5	2244	A2M	C6-C5-N7	2.18	136.08	132.02
1	B5	3492	A2M	C6-C5-N7	2.18	136.07	132.02
52	A2	99	A2M	C6-C5-N7	2.17	136.07	132.02
52	A2	1852	MA6	C5-C6-N6	-2.17	121.52	125.30
1	B5	400	A2M	C6-C5-N7	2.17	136.06	132.02
52	A2	513	A2M	C6-C5-N7	2.16	136.04	132.02
1	B5	3456	A2M	C6-C5-N7	2.16	136.04	132.02
52	A2	1679	A2M	N9-C8-N7	-2.16	110.97	113.91
1	B5	1479	A2M	C6-C5-N7	2.15	136.03	132.02
1	B5	2267	OMG	O6-C6-C5	-2.15	120.89	126.60
52	A2	1249	B8N	C5-C4-N3	2.15	120.15	116.17
3	B8	75	OMG	O6-C6-C5	-2.14	120.92	126.60
52	A2	469	A2M	C6-C5-N7	2.14	136.01	132.02
1	B5	1580	OMG	O6-C6-C5	-2.14	120.92	126.60
1	B5	4369	OMG	O6-C6-C5	-2.14	120.93	126.60
52	A2	1329	OMG	O6-C6-C5	-2.14	120.93	126.60
1	B5	3550	UY1	CM2-O2'-C2'	-2.13	108.92	114.52
1	B5	3676	OMG	O6-C6-C5	-2.13	120.94	126.60
1	B5	1260	OMG	O6-C6-C5	-2.13	120.94	126.60
1	B5	1270	A2M	C6-C5-N7	2.13	135.99	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	437	OMG	O6-C6-C5	-2.13	120.96	126.60
1	B5	2719	OMG	O6-C6-C5	-2.13	120.96	126.60
52	A2	485	A2M	C6-C5-N7	2.13	135.98	132.02
1	B5	3631	OMG	O6-C6-C5	-2.13	120.96	126.60
1	B5	3524	OMG	O6-C6-C5	-2.12	120.96	126.60
1	B5	4116	OMG	O6-C6-C5	-2.12	120.96	126.60
1	B5	3359	OMG	O6-C6-C5	-2.12	120.97	126.60
1	B5	3599	A2M	C6-C5-N7	2.12	135.97	132.02
1	B5	1477	OMG	O6-C6-C5	-2.12	120.97	126.60
1	B5	4138	OMG	O6-C6-C5	-2.12	120.98	126.60
52	A2	645	OMG	O6-C6-C5	-2.11	120.99	126.60
1	B5	3942	OMG	O6-C6-C5	-2.11	121.00	126.60
52	A2	1448	OMG	O6-C6-C5	-2.11	121.00	126.60
52	A2	684	OMG	O6-C6-C5	-2.11	121.00	126.60
1	B5	4052	OMU	C1'-N1-C2	2.11	121.39	117.57
1	B5	3492	A2M	N9-C8-N7	-2.11	111.03	113.91
52	A2	868	OMG	O6-C6-C5	-2.11	121.01	126.60
1	B5	2207	OMG	O6-C6-C5	-2.11	121.01	126.60
1	B5	1266	1MA	C6-C5-N7	2.11	136.03	132.20
1	B5	4245	OMG	O6-C6-C5	-2.11	121.01	126.60
1	B5	3974	OMG	O6-C6-C5	-2.10	121.02	126.60
1	B5	2658	A2M	C6-C5-N7	2.10	135.94	132.02
1	B5	4269	A2M	N9-C8-N7	-2.10	111.04	113.91
1	B5	4240	OMG	O6-C6-C5	-2.10	121.03	126.60
1	B5	2630	A2M	C6-C5-N7	2.10	135.93	132.02
52	A2	602	OMG	O6-C6-C5	-2.10	121.04	126.60
52	A2	1805	OMU	C1'-N1-C2	2.10	121.36	117.57
1	B5	4383	OMG	O6-C6-C5	-2.09	121.04	126.60
1	B5	4364	OMG	O6-C6-C5	-2.09	121.05	126.60
1	B5	3599	A2M	C2'-C1'-N9	-2.09	110.01	113.53
1	B5	2265	OMC	O2-C2-N3	-2.09	118.94	122.33
1	B5	4244	OMU	O2-C2-N1	-2.08	120.02	122.79
1	B5	3476	OMG	O6-C6-C5	-2.08	121.08	126.60
1	B5	1810	A2M	N9-C8-N7	-2.07	111.08	113.91
52	A2	510	OMG	O6-C6-C5	-2.07	121.10	126.60
52	A2	1852	MA6	C5-N7-C8	2.07	106.44	103.51
52	A2	469	A2M	C2'-C1'-N9	-2.06	110.06	113.53
52	A2	591	A2M	C4-N9-C8	2.06	107.96	105.73
1	B5	1632	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	B5	4336	A2M	N9-C8-N7	-2.06	111.10	113.91
52	A2	172	OMU	C1'-N1-C2	2.06	121.29	117.57
1	B5	2647	OMC	O2-C2-N3	-2.05	119.00	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	3557	A2M	N9-C8-N7	-2.05	111.12	113.91
1	B5	1489	A2M	N9-C8-N7	-2.04	111.12	113.91
1	B5	1270	A2M	C2'-C1'-N9	-2.04	110.10	113.53
1	B5	2667	OMC	O2-C2-N3	-2.03	119.03	122.33
52	A2	669	A2M	N9-C8-N7	-2.03	111.14	113.91
52	A2	159	A2M	N9-C8-N7	-2.03	111.14	113.91
52	A2	99	A2M	N9-C8-N7	-2.02	111.15	113.91
52	A2	1384	A2M	N9-C8-N7	-2.01	111.16	113.91
1	B5	2244	A2M	N9-C8-N7	-2.01	111.16	113.91
1	B5	4149	PSU	C5-C6-N1	-2.01	119.09	122.11
52	A2	1032	A2M	N9-C8-N7	-2.00	111.17	113.91
1	B5	3573	OMC	O2-C2-N3	-2.00	119.07	122.33
52	A2	27	A2M	N9-C8-N7	-2.00	111.17	113.91
52	A2	1392	OMC	O2-C2-N3	-2.00	119.08	122.33

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	2207	OMG	O4'-C4'-C5'-O5'
1	B5	3433	OMC	C2'-C1'-N1-C2
1	B5	3433	OMC	C2'-C1'-N1-C6
1	B5	4193	5MC	C2'-C1'-N1-C6
1	B5	4382	PSU	O4'-C1'-C5-C4
1	B5	4382	PSU	O4'-C1'-C5-C6
1	B5	4382	PSU	C3'-C4'-C5'-O5'
4	BA	216	V5N	O-C-CA-CB
52	A2	429	OMU	C2'-C1'-N1-C2
52	A2	429	OMU	C2'-C1'-N1-C6
52	A2	628	OMU	C2'-C1'-N1-C2
52	A2	628	OMU	C2'-C1'-N1-C6
52	A2	645	OMG	O4'-C4'-C5'-O5'
52	A2	1852	MA6	C5-C6-N6-C9
52	A2	1852	MA6	C5-C6-N6-C10
52	A2	1249	B8N	N34-C33-C34-O35
52	A2	1338	4AC	N3-C4-N4-C7
52	A2	1338	4AC	C5-C4-N4-C7
52	A2	1338	4AC	O7-C7-N4-C4
52	A2	1338	4AC	CM7-C7-N4-C4
52	A2	1843	4AC	N3-C4-N4-C7
52	A2	1843	4AC	C5-C4-N4-C7
76	An	138	5F0	CA-C1-OD1-CXT

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Mol	Chain	Res	Type	Atoms
76	An	138	5F0	O1-C1-OD1-CXT
1	B5	4193	5MC	C2'-C1'-N1-C2
1	B5	4336	A2M	C4'-C5'-O5'-P
1	B5	1489	A2M	O4'-C4'-C5'-O5'
1	B5	3517	A2M	O4'-C4'-C5'-O5'
1	B5	3517	A2M	C3'-C4'-C5'-O5'
52	A2	645	OMG	C3'-C4'-C5'-O5'
52	A2	669	A2M	O4'-C4'-C5'-O5'
52	A2	669	A2M	C3'-C4'-C5'-O5'
6	BC	2	AYA	CM-CT-N-CA
83	Au	1	AME	CT2-CT1-N-CA
83	Au	1	AME	OT-CT1-N-CA
6	BC	2	AYA	OT-CT-N-CA
52	A2	1249	B8N	N34-C33-C34-O36
1	B5	398	A2M	O4'-C4'-C5'-O5'
1	B5	2207	OMG	C3'-C4'-C5'-O5'
1	B5	4382	PSU	O4'-C4'-C5'-O5'
52	A2	513	A2M	O4'-C4'-C5'-O5'
52	A2	1448	OMG	C3'-C4'-C5'-O5'
52	A2	1852	MA6	N1-C6-N6-C9
52	A2	99	A2M	O4'-C4'-C5'-O5'
52	A2	802	PSU	C3'-C4'-C5'-O5'
1	B5	1489	A2M	C3'-C4'-C5'-O5'
52	A2	513	A2M	C3'-C4'-C5'-O5'
1	B5	398	A2M	C3'-C4'-C5'-O5'
52	A2	469	A2M	O4'-C4'-C5'-O5'
52	A2	1448	OMG	O4'-C4'-C5'-O5'
52	A2	1640	G7M	O4'-C4'-C5'-O5'
52	A2	1640	G7M	C3'-C4'-C5'-O5'
52	A2	429	OMU	O4'-C1'-N1-C6
5	BB	245	HIC	CA-CB-CG-ND1
52	A2	802	PSU	O4'-C4'-C5'-O5'
52	A2	429	OMU	O4'-C1'-N1-C2
52	A2	1249	B8N	C32-C33-C34-O36
52	A2	1843	4AC	O7-C7-N4-C4
52	A2	1843	4AC	CM7-C7-N4-C4
6	BC	2	AYA	C-CA-N-CT
1	B5	3433	OMC	O4'-C1'-N1-C6
1	B5	3576	PSU	C4'-C5'-O5'-P
52	A2	645	OMG	C4'-C5'-O5'-P
1	B5	3550	UY1	C4'-C5'-O5'-P
52	A2	591	A2M	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
1	B5	2630	A2M	C2'-C1'-N9-C8
52	A2	591	A2M	C2'-C1'-N9-C8
62	AZ	2	SAC	C-CA-N-C1A
62	AZ	2	SAC	CB-CA-N-C1A
1	B5	3476	OMG	C3'-C2'-O2'-CM2
1	B5	3657	OMU	C3'-C2'-O2'-CM2
1	B5	4366	OMU	C3'-C2'-O2'-CM2
52	A2	1679	A2M	C3'-C2'-O2'-CM'
52	A2	1704	OMC	C3'-C2'-O2'-CM2
1	B5	4246	PSU	C4'-C5'-O5'-P
31	Bb	5	MLZ	N-CA-CB-CG
52	A2	577	A2M	C3'-C4'-C5'-O5'
52	A2	1249	B8N	C32-C33-C34-O35
31	Bb	5	MLZ	C-CA-CB-CG
1	B5	3619	OMC	C4'-C5'-O5'-P
52	A2	1852	MA6	C4'-C5'-O5'-P
52	A2	27	A2M	O4'-C4'-C5'-O5'
1	B5	4193	5MC	O4'-C1'-N1-C6
1	B5	4193	5MC	O4'-C1'-N1-C2
52	A2	628	OMU	O4'-C1'-N1-C6
4	BA	216	V5N	O2-CB-CG-CD2
1	B5	3599	A2M	C3'-C4'-C5'-O5'
1	B5	398	A2M	C3'-C2'-O2'-CM'
1	B5	2667	OMC	C3'-C2'-O2'-CM2
1	B5	2680	OMU	C3'-C2'-O2'-CM2
76	An	138	5F0	O-C-CB-CA
1	B5	3433	OMC	O4'-C1'-N1-C2
5	BB	245	HIC	CA-CB-CG-CD2
1	B5	1820	OMC	C3'-C2'-O2'-CM2
1	B5	4282	OMC	C3'-C2'-O2'-CM2
52	A2	510	OMG	C3'-C2'-O2'-CM2
52	A2	684	OMG	C3'-C2'-O2'-CM2
52	A2	868	OMG	C3'-C2'-O2'-CM2
52	A2	99	A2M	C3'-C4'-C5'-O5'
52	A2	577	A2M	O4'-C4'-C5'-O5'
1	B5	3492	A2M	O4'-C4'-C5'-O5'
52	A2	469	A2M	C3'-C4'-C5'-O5'
1	B5	398	A2M	C1'-C2'-O2'-CM'
76	An	138	5F0	OD1-C1-CA-N
1	B5	3631	OMG	C3'-C2'-O2'-CM2
52	A2	1443	OMU	C2'-C1'-N1-C2
1	B5	2630	A2M	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
52	A2	628	OMU	O4'-C1'-N1-C2
1	B5	3494	PSU	C3'-C4'-C5'-O5'
1	B5	4317	A2M	O4'-C4'-C5'-O5'
85	Aw	62	HY3	O-C-CA-C3
52	A2	591	A2M	O4'-C1'-N9-C8
1	B5	2194	OMC	O4'-C4'-C5'-O5'
1	B5	2194	OMC	C2'-C1'-N1-C2
1	B5	2267	OMG	C3'-C2'-O2'-CM2
1	B5	4052	OMU	C3'-C2'-O2'-CM2
52	A2	27	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

113 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	1693	PSU	1	0
61	AT	48	5MC	2	0
1	B5	3524	OMG	1	0
1	B5	4177	PSU	1	0
52	A2	1491	OMG	1	0
52	A2	1833	6MZ	1	0
1	B5	4149	PSU	1	0
1	B5	2208	OMC	2	0
1	B5	4042	PSU	1	0
52	A2	116	OMU	1	0
42	Bm	98	M3L	1	0
1	B5	3371	PSU	1	0
1	B5	4166	PSU	1	0
1	B5	3619	OMC	1	0
52	A2	121	OMU	2	0
1	B5	3562	A2M	2	0
52	A2	1704	OMC	2	0
52	A2	1233	PSU	1	0
52	A2	172	OMU	1	0
52	A2	1245	PSU	1	0
52	A2	610	PSU	1	0
1	B5	2704	OMC	1	0
52	A2	1338	4AC	2	0
52	A2	1348	PSU	1	0
52	A2	1679	A2M	2	0
1	B5	3585	PSU	1	0
52	A2	469	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	Au	1	AME	1	0
52	A2	1852	MA6	1	0
1	B5	1260	OMG	1	0
52	A2	119	PSU	1	0
52	A2	355	OMU	1	0
1	B5	3492	A2M	1	0
1	B5	2206	A2M	1	0
1	B5	1638	PSU	2	0
52	A2	1082	PSU	1	0
52	A2	1443	OMU	1	0
1	B5	3433	OMC	1	0
1	B5	4138	OMG	2	0
52	A2	99	A2M	2	0
1	B5	2658	A2M	2	0
1	B5	4202	OMC	1	0
3	B8	75	OMG	1	0
52	A2	485	A2M	2	0
1	B5	3369	PSU	1	0
52	A2	518	OMC	1	0
52	A2	650	PSU	1	0
52	A2	1249	B8N	1	0
1	B5	4278	PSU	1	0
52	A2	1805	OMU	2	0
1	B5	4317	A2M	1	0
1	B5	2630	A2M	1	0
52	A2	1289	OMU	2	0
1	B5	3476	OMG	1	0
1	B5	3974	OMG	1	0
52	A2	166	A2M	2	0
1	B5	4364	OMG	2	0
1	B5	2667	OMC	1	0
1	B5	4058	PSU	1	0
1	B5	3450	A2M	2	0
5	BB	245	HIC	1	0
1	B5	1810	A2M	2	0
1	B5	4269	A2M	1	0
52	A2	1329	OMG	1	0
52	A2	36	PSU	2	0
52	A2	602	OMG	1	0
1	B5	4336	A2M	1	0
52	A2	1392	OMC	1	0
1	B5	2244	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	437	OMG	1	0
1	B5	2207	OMG	1	0
1	B5	2258	OMU	1	0
52	A2	510	OMG	1	0
52	A2	1448	OMG	2	0
52	A2	1446	PSU	1	0
1	B5	4383	OMG	1	0
1	B5	4298	PSU	1	0
1	B5	1270	A2M	2	0
52	A2	1384	A2M	1	0
1	B5	3456	A2M	2	0
1	B5	4039	PSU	1	0
52	A2	1843	4AC	2	0
1	B5	4382	PSU	1	0
52	A2	645	OMG	1	0
1	B5	4052	OMU	2	0
1	B5	4366	OMU	3	0
52	A2	513	A2M	2	0
1	B5	2265	OMC	1	0
1	B5	2647	OMC	2	0
30	Ba	39	V5N	1	0
1	B5	2267	OMG	1	0
52	A2	577	A2M	2	0
1	B5	3517	A2M	1	0
1	B5	1718	PSU	2	0
1	B5	398	A2M	1	0
1	B5	3973	OMU	1	0
1	B5	3540	OMC	1	0
1	B5	4193	5MC	1	0
52	A2	864	PSU	1	0
1	B5	3942	OMG	2	0
1	B5	1284	OMC	2	0
1	B5	2194	OMC	1	0
1	B5	400	A2M	1	0
1	B5	3676	OMG	2	0
52	A2	27	A2M	2	0
1	B5	1489	A2M	1	0
1	B5	4203	PSU	1	0
52	A2	1032	A2M	2	0
1	B5	3631	OMG	1	0
1	B5	3550	UY1	1	0
1	B5	4282	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	3557	A2M	1	0
52	A2	682	PSU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 793 ligands modelled in this entry, 758 are monoatomic - leaving 35 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	$\#\|Z\| > 2$
93	SPD	B5	4922	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPM	B5	4911	-	13,13,13	0.15	0	12,12,12	0.18	0
93	SPD	BN	301	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1906	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4915	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.16	0
93	SPD	B5	4920	-	9,9,9	0.16	0	8,8,8	0.19	0
97	AAC	BD	301	7	6,6,7	0.89	0	6,6,8	1.11	1 (16%)
93	SPD	B5	4919	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.21	0
93	SPD	A2	1908	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.16	0
93	SPD	B5	4912	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1904	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	4923	-	9,9,9	0.16	0	8,8,8	0.15	0
93	SPD	A2	1901	-	9,9,9	0.15	0	8,8,8	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
93	SPD	A2	1903	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4902	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1902	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4909	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	A2	1905	-	9,9,9	0.15	0	8,8,8	0.17	0
93	SPD	B5	4904	-	9,9,9	0.16	0	8,8,8	0.18	0
96	GTP	B7	201	2	30,34,34	0.49	0	46,54,54	0.57	0
93	SPD	B5	4916	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPM	B5	4914	-	13,13,13	0.15	0	12,12,12	0.15	0
93	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.14	0
93	SPD	B5	4913	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	4905	-	9,9,9	0.16	0	8,8,8	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	B5	4922	-	-	0/7/7/7	-
93	SPD	B5	4917	-	-	0/7/7/7	-
93	SPD	A2	1907	-	-	1/7/7/7	-
93	SPD	B5	4903	-	-	1/7/7/7	-
94	SPM	B5	4911	-	-	1/11/11/11	-
93	SPD	BN	301	-	-	1/7/7/7	-
93	SPD	A2	1906	-	-	0/7/7/7	-
93	SPD	B5	4915	-	-	0/7/7/7	-
93	SPD	B5	4910	-	-	0/7/7/7	-
93	SPD	B5	4920	-	-	0/7/7/7	-
97	AAC	BD	301	7	-	0/3/4/5	-
93	SPD	B5	4919	-	-	1/7/7/7	-
93	SPD	B5	4907	-	-	0/7/7/7	-
93	SPD	B5	4918	-	-	0/7/7/7	-
93	SPD	A2	1908	-	-	0/7/7/7	-
93	SPD	B5	4906	-	-	0/7/7/7	-
94	SPM	A2	1909	-	-	1/11/11/11	-
93	SPD	B5	4912	-	-	0/7/7/7	-
93	SPD	A2	1904	-	-	0/7/7/7	-
93	SPD	B5	4923	-	-	1/7/7/7	-
93	SPD	A2	1901	-	-	1/7/7/7	-
93	SPD	A2	1903	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	B5	4902	-	-	2/7/7/7	-
93	SPD	A2	1902	-	-	0/7/7/7	-
93	SPD	B5	4909	-	-	1/7/7/7	-
93	SPD	A2	1905	-	-	0/7/7/7	-
93	SPD	B5	4904	-	-	0/7/7/7	-
96	GTP	B7	201	2	-	0/22/38/38	0/3/3/3
93	SPD	B5	4916	-	-	0/7/7/7	-
93	SPD	B5	4921	-	-	1/7/7/7	-
94	SPM	B5	4914	-	-	0/11/11/11	-
93	SPD	B5	4908	-	-	0/7/7/7	-
93	SPD	B5	4901	-	-	2/7/7/7	-
93	SPD	B5	4913	-	-	0/7/7/7	-
93	SPD	B5	4905	-	-	1/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
97	BD	301	AAC	O2-C1-C2	-2.27	118.86	125.42

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	A2	1909	SPM	C8-C9-N10-C11
93	B5	4902	SPD	C2-C3-C4-C5
93	B5	4921	SPD	C2-C3-C4-C5
94	B5	4911	SPM	C6-C7-C8-C9
93	A2	1901	SPD	C2-C3-C4-C5
93	B5	4923	SPD	C2-C3-C4-C5
93	BN	301	SPD	C2-C3-C4-C5
93	A2	1907	SPD	C2-C3-C4-C5
93	B5	4905	SPD	C2-C3-C4-C5
93	B5	4901	SPD	C4-C5-N6-C7
93	B5	4902	SPD	C4-C5-N6-C7
93	B5	4903	SPD	C2-C3-C4-C5
93	B5	4901	SPD	C2-C3-C4-C5
93	B5	4909	SPD	C2-C3-C4-C5
93	B5	4919	SPD	C2-C3-C4-C5

There are no ring outliers.

18 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	A2	1907	SPD	2	0
93	B5	4903	SPD	2	0
94	B5	4911	SPM	2	0
93	A2	1906	SPD	1	0
93	B5	4915	SPD	2	0
93	B5	4919	SPD	1	0
93	B5	4907	SPD	1	0
93	B5	4918	SPD	1	0
93	B5	4906	SPD	1	0
94	A2	1909	SPM	1	0
93	A2	1904	SPD	2	0
93	B5	4923	SPD	3	0
93	A2	1901	SPD	1	0
93	A2	1903	SPD	1	0
93	A2	1902	SPD	1	0
93	A2	1905	SPD	1	0
93	B5	4916	SPD	2	0
94	B5	4914	SPM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

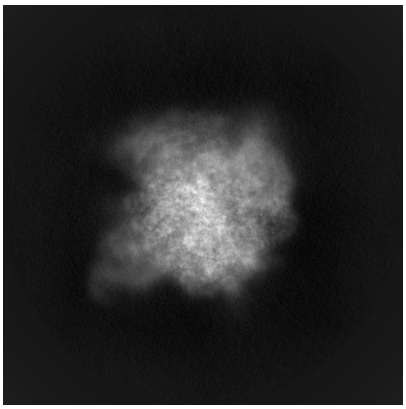
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16232. These allow visual inspection of the internal detail of the map and identification of artifacts.

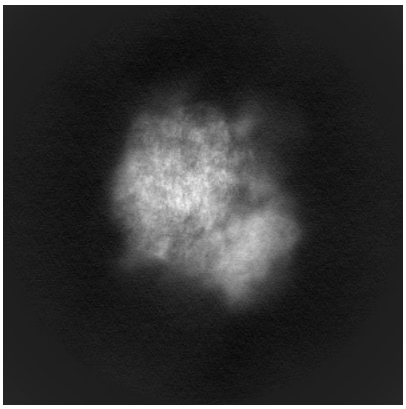
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

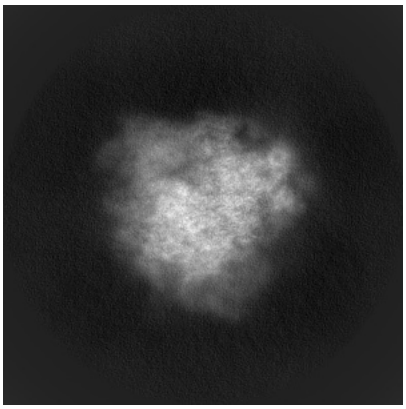
6.1.1 Primary map



X

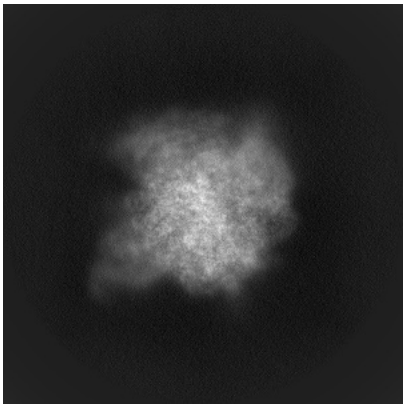


Y

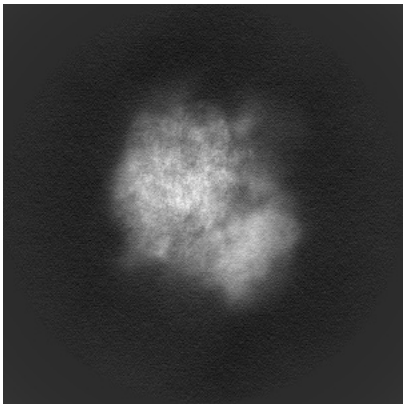


Z

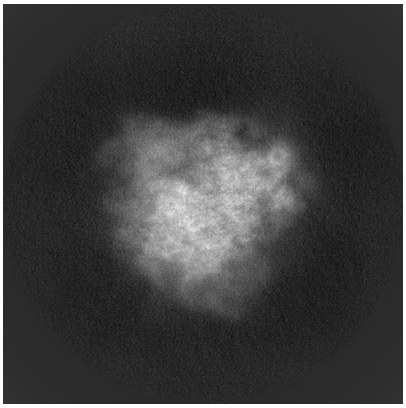
6.1.2 Raw map



X



Y

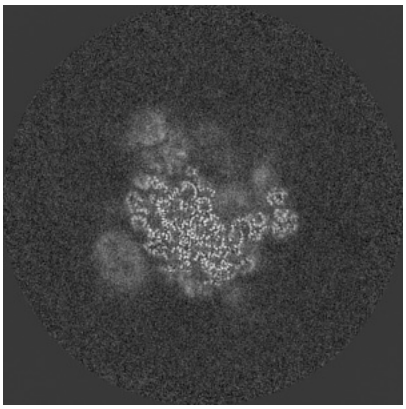


Z

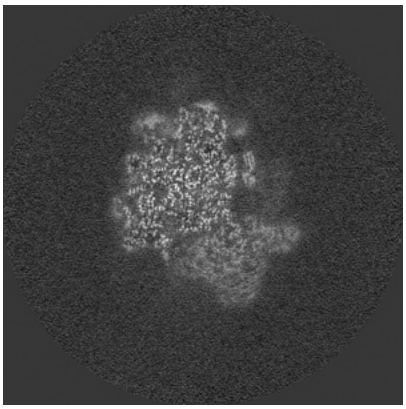
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

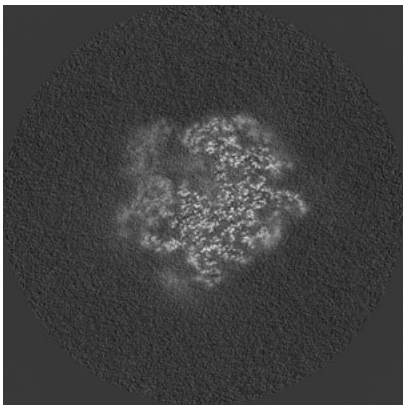
6.2.1 Primary map



X Index: 256

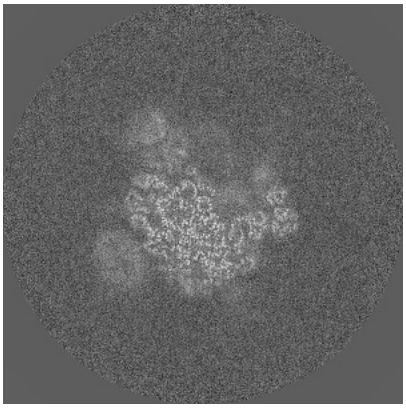


Y Index: 256

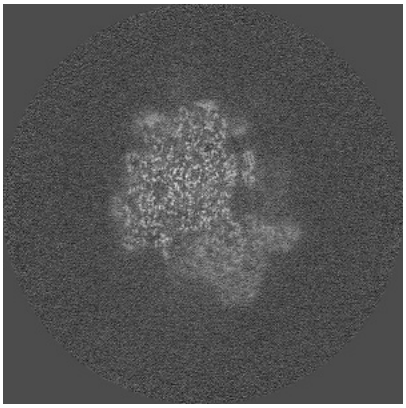


Z Index: 256

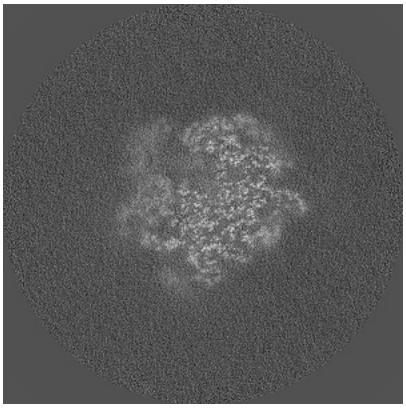
6.2.2 Raw map



X Index: 256



Y Index: 256

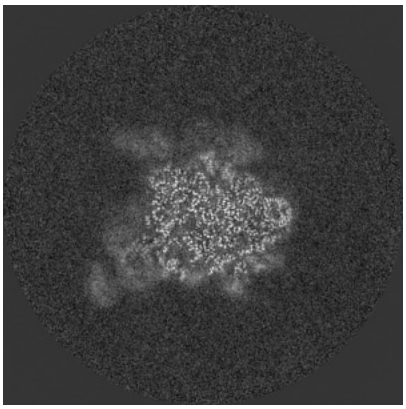


Z Index: 256

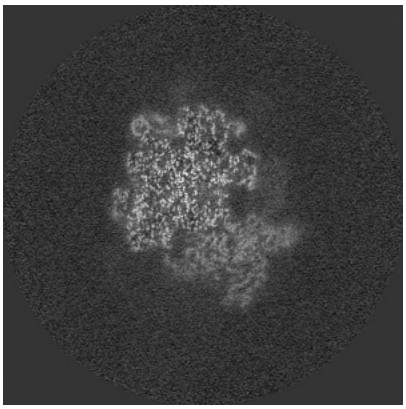
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

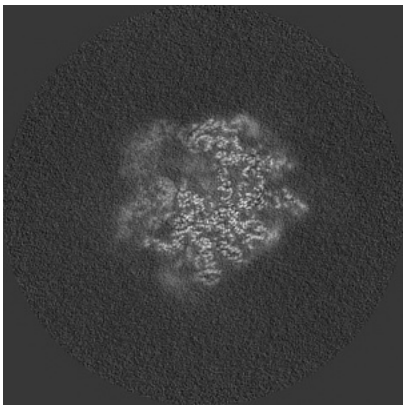
6.3.1 Primary map



X Index: 283

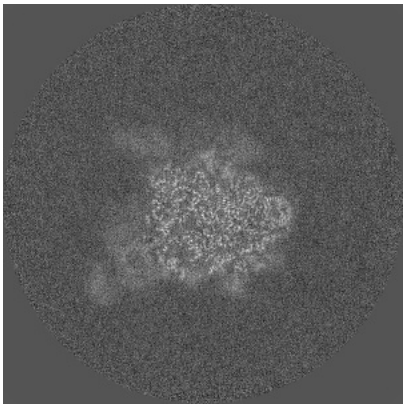


Y Index: 261

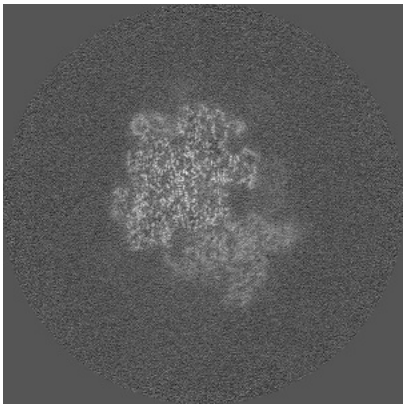


Z Index: 259

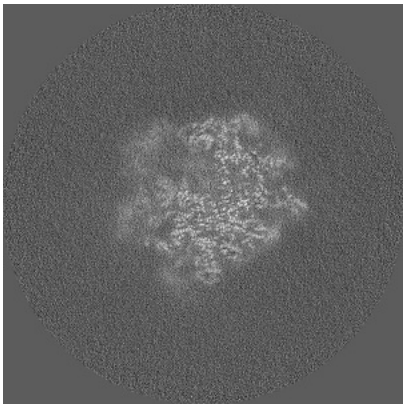
6.3.2 Raw map



X Index: 283



Y Index: 261

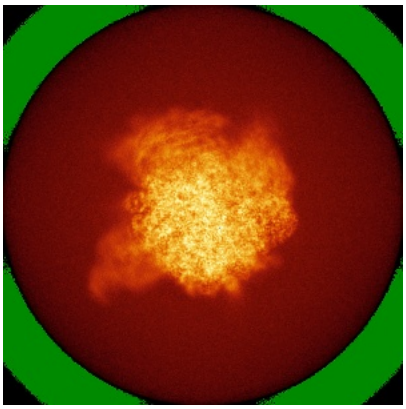


Z Index: 260

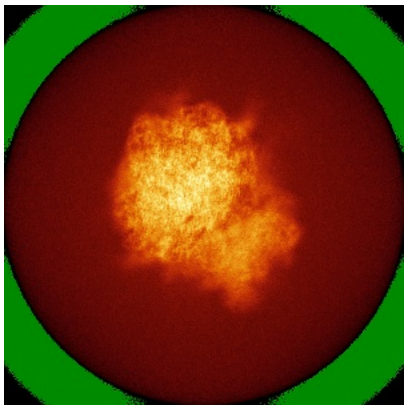
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

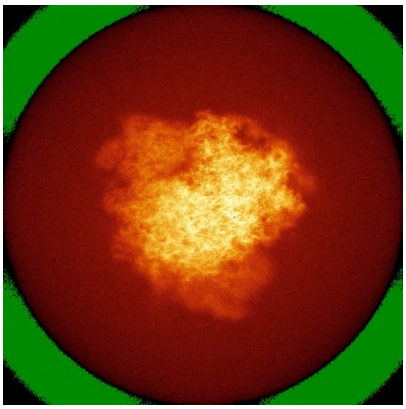
6.4.1 Primary map



X

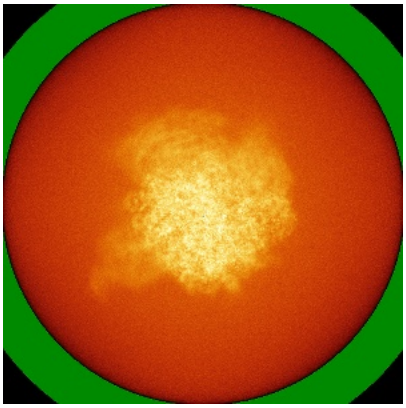


Y

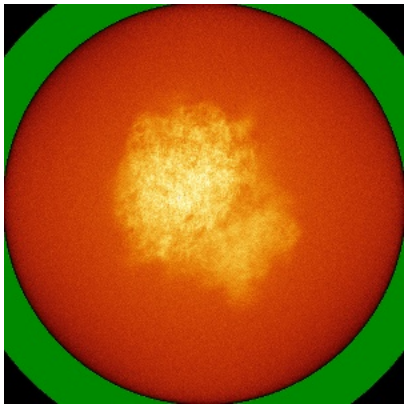


Z

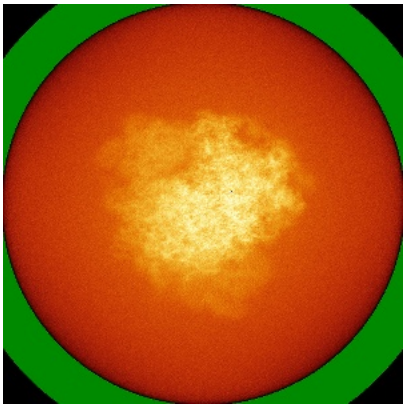
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

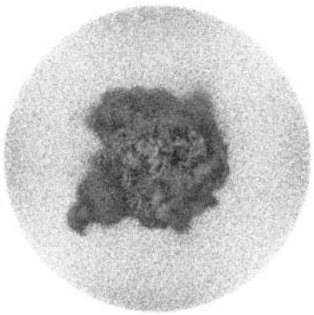
X

Y

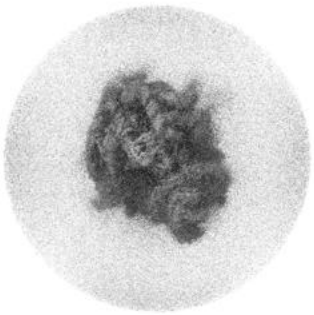
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

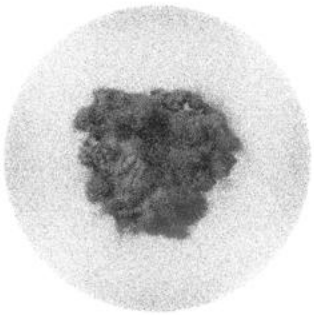
6.5.2 Raw map



X



Y



Z

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

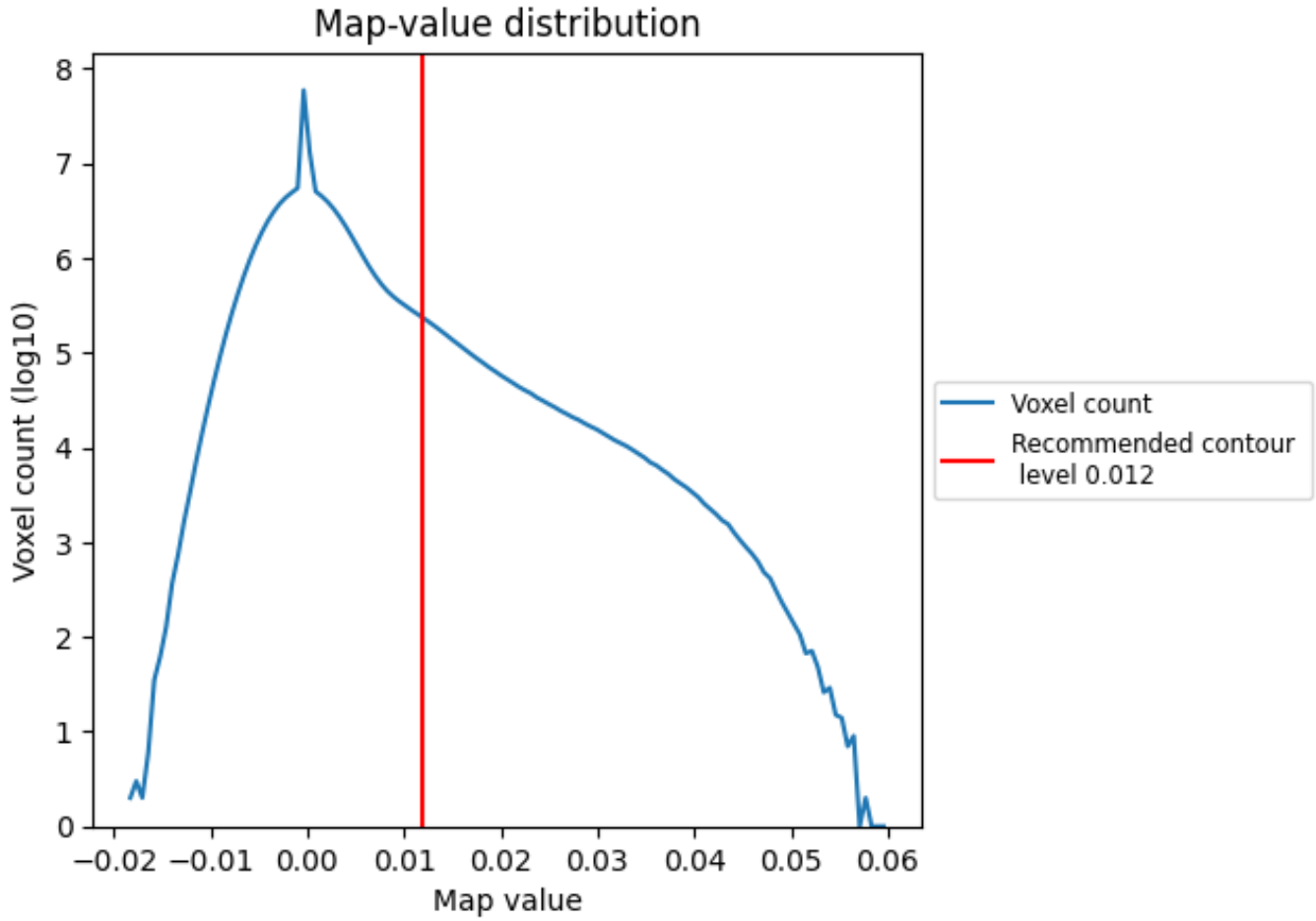
6.6 Mask visualisation (i)

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

7 Map analysis

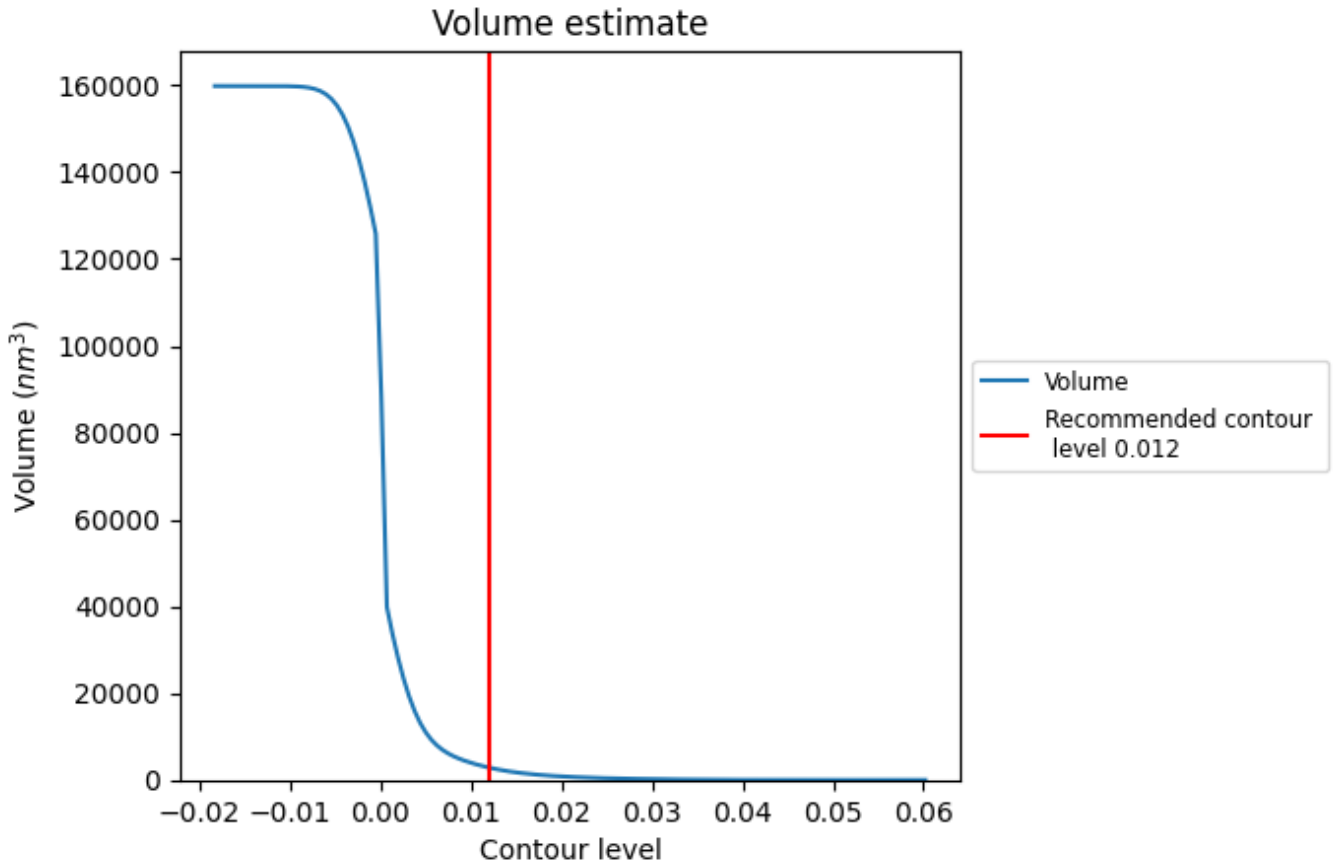
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

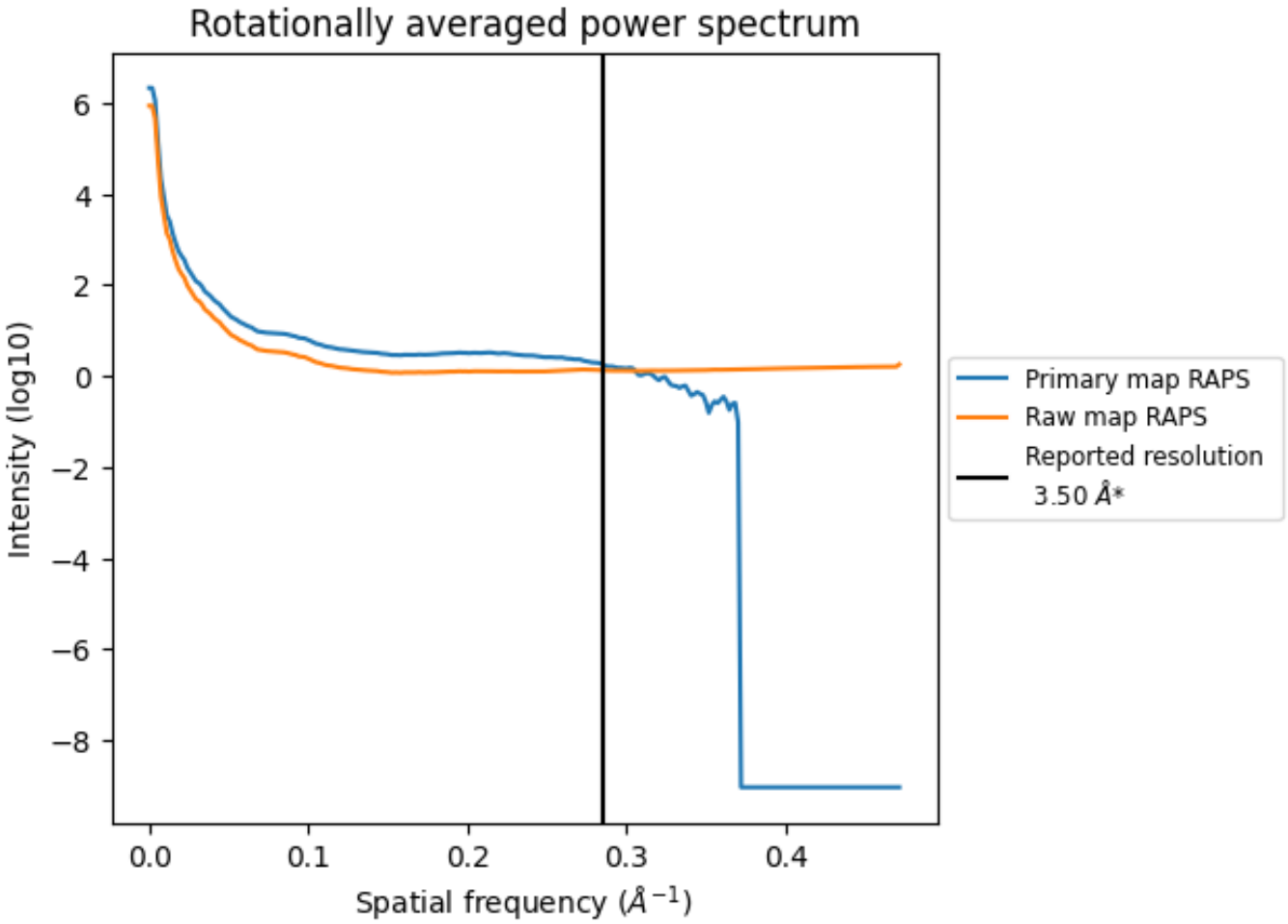
7.2 Volume estimate



The volume at the recommended contour level is 2852 nm^3; this corresponds to an approximate mass of 2576 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 (i)

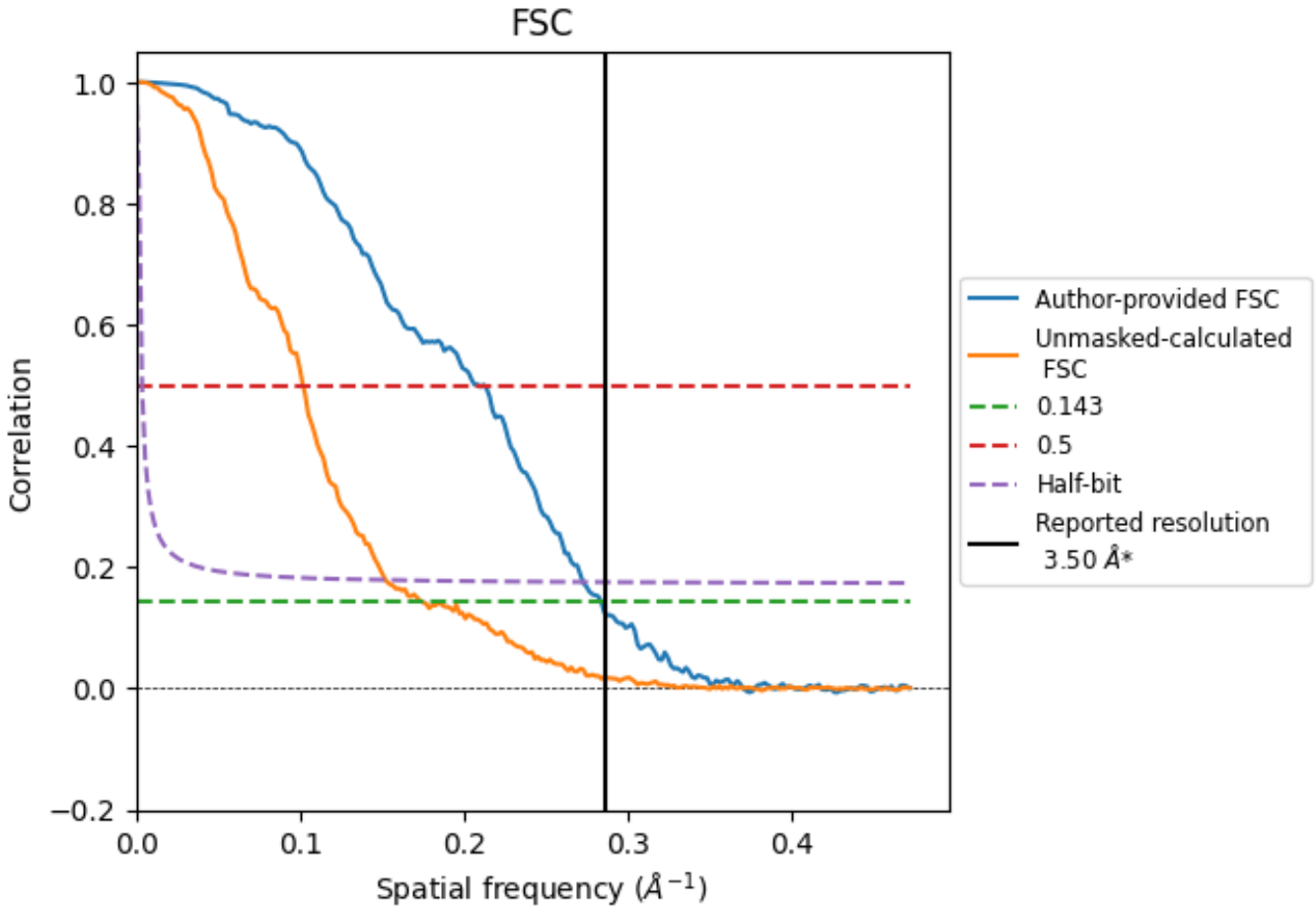


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

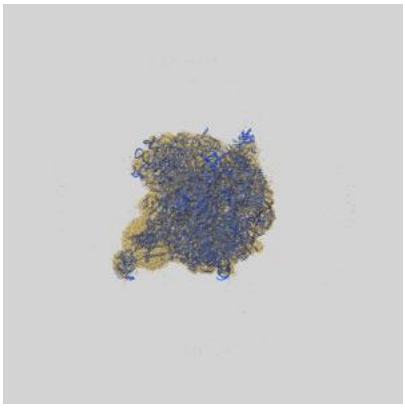
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	4.79	3.67
Unmasked-calculated*	5.74	9.82	6.57

*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 5.74 differs from the reported value 3.5 by more than 10 %

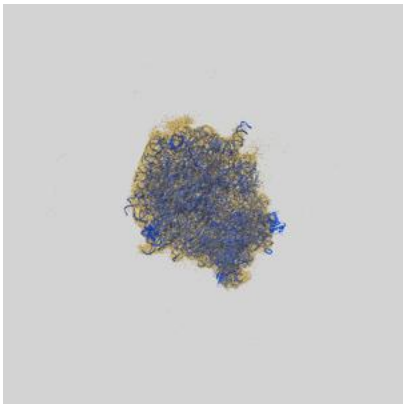
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16232 and PDB model 8BTK. Per-residue inclusion information can be found in section 3 on page 29.

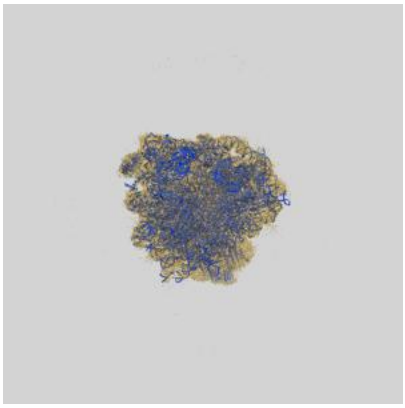
9.1 Map-model overlay



X



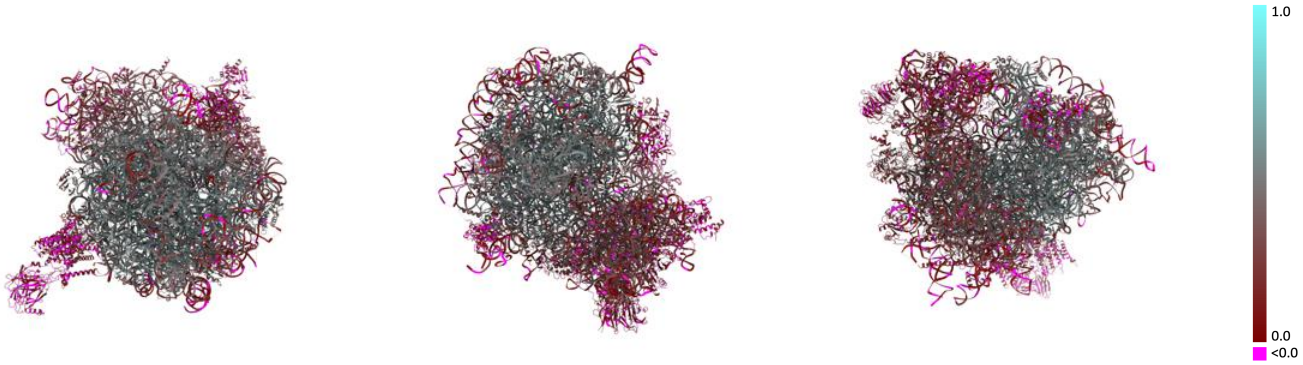
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

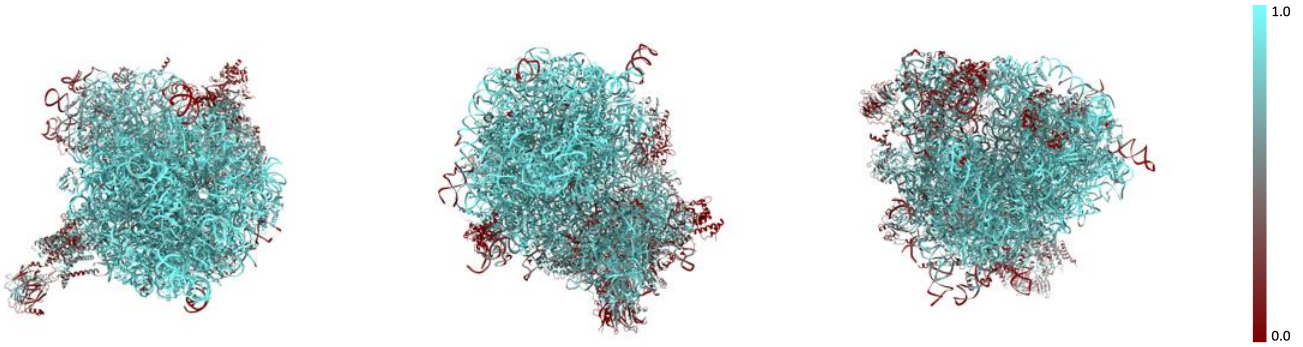
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

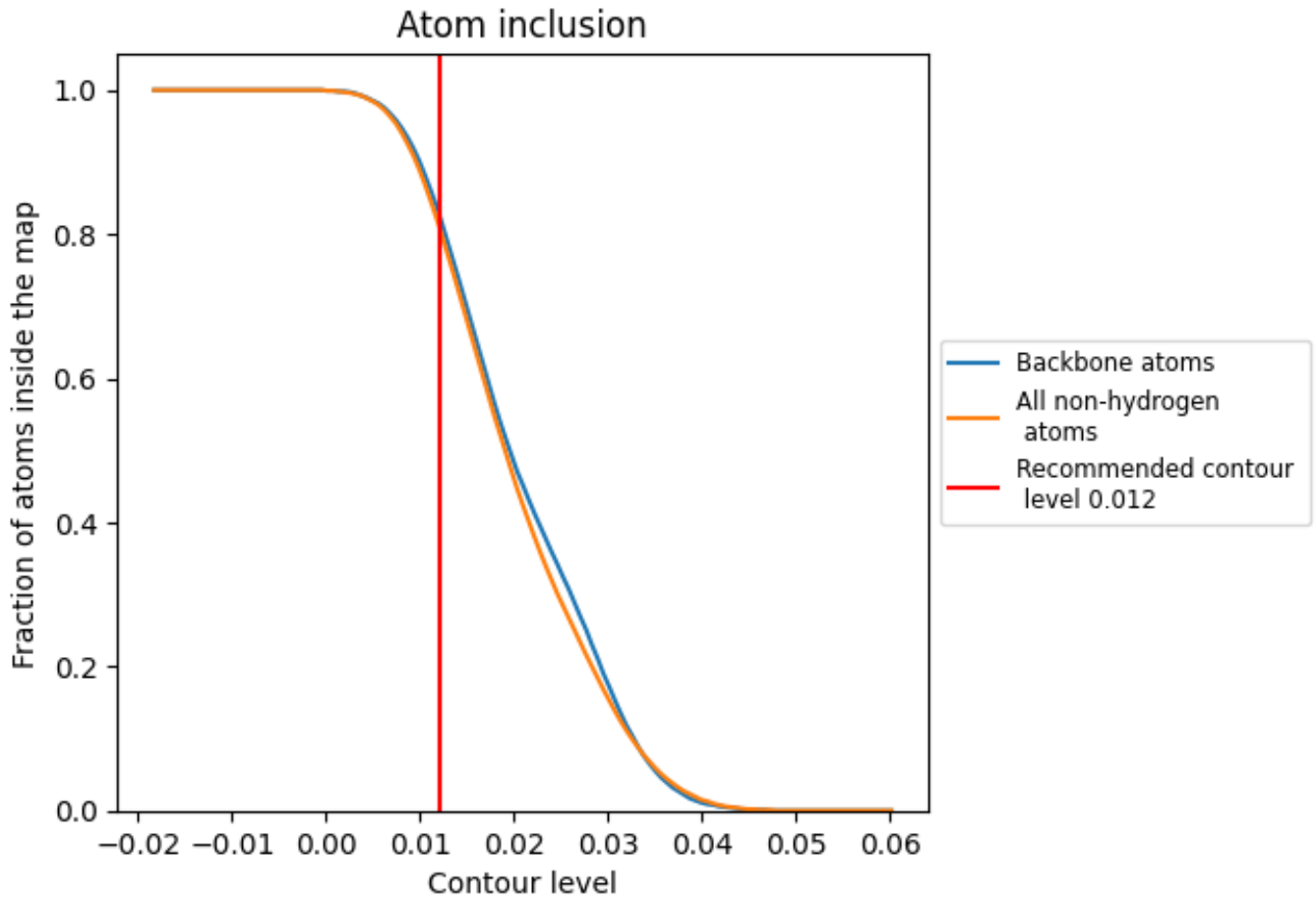
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.3620
A2	0.8260	0.2850
AA	0.6120	0.2480
AB	0.4950	0.1730
AC	0.1480	0.0390
AD	0.5960	0.2210
AE	0.7810	0.3420
AF	0.3110	0.1180
AG	0.6240	0.2030
AH	0.1940	0.0250
AT	0.4880	0.1690
AZ	0.6640	0.2980
Aa	0.6470	0.3000
Ab	0.7530	0.3250
Ac	0.4050	0.1730
Ad	0.7170	0.2710
Ae	0.5430	0.2010
Af	0.5790	0.2120
Ag	0.4930	0.2280
Ah	0.6090	0.2620
Ai	0.6870	0.2630
Aj	0.3700	0.1210
Ak	0.6280	0.2850
Al	0.0140	0.0620
Am	0.7240	0.3290
An	0.6940	0.3100
Ao	0.5050	0.1730
Ap	0.6240	0.2030
Aq	0.5170	0.2240
Ar	0.5520	0.1950
As	0.5560	0.1870
At	0.5550	0.1670
Au	0.6760	0.2890
Av	0.7850	0.3410
Aw	0.7720	0.3290

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Chain	Atom inclusion	Q-score
Ax	0.5930	0.1760
Ay	0.4210	0.1720
Az	0.8530	0.4140
B5	0.9300	0.4300
B7	0.9940	0.5030
B8	0.9850	0.4620
BA	0.9370	0.5160
BB	0.9340	0.5000
BC	0.9580	0.5070
BD	0.9010	0.4540
BE	0.8570	0.4000
BF	0.9400	0.4960
BG	0.8680	0.4280
BH	0.8950	0.4450
BI	0.8900	0.4670
BJ	0.8390	0.3870
BK	0.9170	0.3470
BL	0.8980	0.4610
BM	0.8980	0.4480
BN	0.9720	0.5310
BO	0.9470	0.5050
BP	0.9230	0.5120
BQ	0.9660	0.5220
BR	0.8590	0.4220
BS	0.9550	0.5090
BT	0.9190	0.4980
BU	0.8520	0.3690
BV	0.9090	0.4810
BW	0.5920	0.2990
BX	0.9110	0.4800
BY	0.9090	0.4810
BZ	0.9080	0.4500
Ba	0.9610	0.5210
Bb	0.8180	0.3850
Bc	0.8330	0.3990
Bd	0.9050	0.4880
Be	0.9530	0.5190
Bf	0.9500	0.5340
Bg	0.9150	0.4650
Bh	0.9000	0.4670
Bi	0.9070	0.4390
Bj	0.9620	0.5270

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Chain	Atom inclusion	Q-score
Bk	0.7900	0.4050
Bl	0.9490	0.5040
Bm	0.8160	0.4060
Bo	0.8840	0.4750
Bp	0.9200	0.4980
Br	0.9480	0.4990
Bs	0.3620	0.1160
Bt	0.1570	0.0760
Bv	0.0600	0.0630
SX	0.5620	0.1520
SY	0.6650	0.2130
SZ	0.2760	0.0800
TA	0.3920	0.0740
TB	0.3550	0.0590
TC	0.3960	0.0780
TD	0.2000	0.0470