



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 02:31 pm BST

PDB ID : 7O81 / pdb_00007o81
EMDB ID : EMD-12759
Title : Rabbit 80S ribosome colliding in another ribosome stalled by the SARS-CoV-2 pseudoknot
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on : 2021-04-14
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

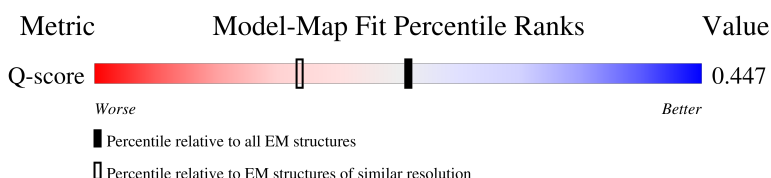
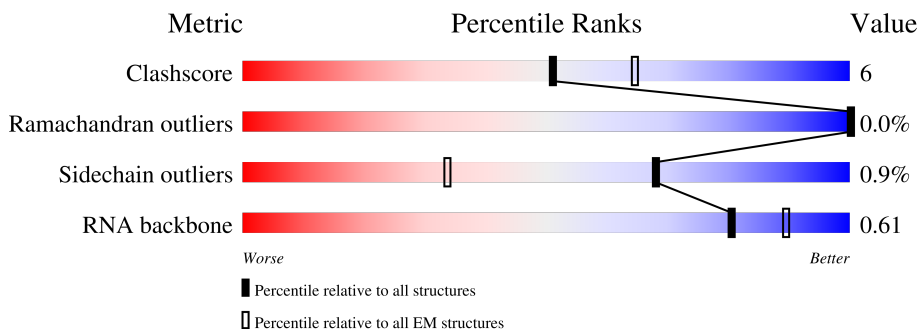
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A2	1870	
2	AA	84	
3	AB	69	

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Mol	Chain	Length	Quality of chain
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	
9	AH	217	
10	AJ	76	
11	AT	75	
12	AU	148	
13	AZ	295	
14	Aa	264	
15	Ab	293	
16	Ac	281	
17	Ad	263	
18	Ae	204	
19	Af	249	
20	Ag	432	
21	Ah	208	
22	Ai	194	
23	Aj	165	
24	Ak	158	
25	Al	132	
26	Am	151	
27	An	151	
28	Ao	145	

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Mol	Chain	Length	Quality of chain
29	Ap	172	
30	Aq	135	
31	Ar	152	
32	As	145	
33	At	119	
34	Au	83	
35	Av	130	
36	Aw	143	
37	Ax	130	
38	Ay	124	
39	Az	25	
40	B5	4808	
41	B7	120	
42	B8	158	
43	BA	257	
44	BB	403	
45	BC	413	
46	BD	297	
47	BE	291	
48	BF	247	
49	BG	266	
50	BH	192	
51	BI	214	
52	BJ	178	
53	BK	1071	

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Mol	Chain	Length	Quality of chain
54	BL	211	
55	BM	218	
56	BN	204	
57	BO	203	
58	BP	184	
59	BQ	188	
60	BR	196	
61	BS	176	
62	BT	160	
63	BU	128	
64	BV	140	
65	BW	157	
66	BX	156	
67	BY	145	
68	BZ	136	
69	Ba	148	
70	Bb	245	
71	Bc	115	
72	Bd	125	
73	Be	135	
74	Bf	110	
75	Bg	117	
76	Bh	123	
77	Bi	105	
78	Bj	97	

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Mol	Chain	Length	Quality of chain
79	Bk	70	
80	Bl	51	
81	Bm	128	
82	Bo	106	
83	Bp	92	
84	Br	137	
85	Bs	318	
86	Bt	165	
87	Bv	217	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 228361 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	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 2 is a protein called 40S ribosomal protein S27.

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

- Molecule 3 is a protein called Ribosomal protein S28.

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

- Molecule 4 is a protein called Ribosomal protein S27a.

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

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	45	Total	C	N	O	S	0	0
			369	228	84	56	1		

- Molecule 6 is a protein called Ribosomal protein eS26.

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

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	10	Total	C	N	O	P	0	0
			212	95	39	68	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called A-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	76	Total	C	N	O	P	0	0
			1622	724	290	532	76		

- Molecule 11 is a RNA chain called P-site tRNA(Pro).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	75	Total	C	N	O	P	0	0
			1604	714	284	531	75		

- Molecule 12 is a protein called EDF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AU	110	Total	C	N	O		
			864	529	169	166	0	0

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

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

- Molecule 14 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Aa	214	Total	C	N	O	S		
			1738	1104	311	309	14	0	0

- Molecule 15 is a protein called Ribosomal protein uS5.

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

- Molecule 16 is a protein called 40S ribosomal protein S3.

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

- Molecule 17 is a protein called Ribosomal protein eS4.

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

- Molecule 18 is a protein called Ribosomal protein S5.

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

- Molecule 19 is a protein called 40S ribosomal protein S6.

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

- Molecule 20 is a protein called 40S ribosomal protein S7.

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

- Molecule 21 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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 22 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 23 is a protein called Ribosomal protein eS10.

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

- Molecule 24 is a protein called 40S ribosomal protein S11.

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

- Molecule 25 is a protein called 40S ribosomal protein S12.

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

- Molecule 26 is a protein called uS15.

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

- Molecule 27 is a protein called 40S ribosomal protein uS11.

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

- Molecule 28 is a protein called 40S ribosomal protein uS19.

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

- Molecule 29 is a protein called uS9.

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

- Molecule 30 is a protein called 40S ribosomal protein eS17.

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

- Molecule 31 is a protein called 40S ribosomal protein S18.

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

- Molecule 32 is a protein called Ribosomal protein eS19.

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

- Molecule 33 is a protein called 40S ribosomal protein uS10.

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

- Molecule 34 is a protein called Ribosomal protein eS21.

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

- Molecule 35 is a protein called Ribosomal protein S15a.

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

- Molecule 36 is a protein called 40S ribosomal protein S23.

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

- Molecule 37 is a protein called 40S ribosomal protein S24.

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

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ay	73	Total	C	N	O	S	0	0
			579	372	106	100	1		

- Molecule 39 is a protein called 60s ribosomal protein l41.

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

- Molecule 40 is a RNA chain called 28S rRNA.

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

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 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

- Molecule 42 is a RNA chain called 5.8S rRNA.

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

- Molecule 43 is a protein called Ribosomal protein uL2.

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

- Molecule 44 is a protein called Ribosomal protein L3.

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

- Molecule 45 is a protein called 60S ribosomal protein L4.

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

- Molecule 46 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BD	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 47 is a protein called 60S ribosomal protein L6.

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

- Molecule 48 is a protein called Ribosomal Protein uL30.

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

- Molecule 49 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BG	232	Total	C	N	O	S	0	0
			1868	1191	359	314	4		

- Molecule 50 is a protein called 60S ribosomal protein L9.

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

- Molecule 51 is a protein called 60S ribosomal protein L10.

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

- Molecule 52 is a protein called Ribosomal protein L11.

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

- Molecule 53 is a protein called Replicase polypeptide 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	39	Total	C	N	O	S	0	0
			290	180	48	55	7		

- Molecule 54 is a protein called Ribosomal protein eL13.

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

- Molecule 55 is a protein called Ribosomal protein L14.

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

- Molecule 56 is a protein called Ribosomal protein L15.

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

- Molecule 57 is a protein called Ribosomal protein L13a.

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

- Molecule 58 is a protein called uL22.

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

- Molecule 59 is a protein called Ribosomal protein L18.

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

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

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

- Molecule 61 is a protein called Ribosomal protein L18a.

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

- Molecule 62 is a protein called eL21.

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

- Molecule 63 is a protein called Ribosomal protein eL22.

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

- Molecule 64 is a protein called Ribosomal protein L23.

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

- Molecule 65 is a protein called eL24.

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

- Molecule 66 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BX	122	Total	C	N	O	S	0	0
			1004	642	190	171	1		

- Molecule 67 is a protein called Ribosomal protein L26.

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

- Molecule 68 is a protein called 60S ribosomal protein L27.

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

- Molecule 69 is a protein called 60S ribosomal protein L27a.

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

- Molecule 70 is a protein called 60S ribosomal protein L29.

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

- Molecule 71 is a protein called eL30.

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

- Molecule 72 is a protein called eL31.

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

- Molecule 73 is a protein called eL32.

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

- Molecule 74 is a protein called eL33.

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

- Molecule 75 is a protein called 60S ribosomal protein L34.

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

- Molecule 76 is a protein called uL29.

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

- Molecule 77 is a protein called 60S ribosomal protein L36.

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

- Molecule 78 is a protein called Ribosomal protein L37.

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

- Molecule 79 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	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 80 is a protein called eL39.

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

- Molecule 81 is a protein called 60S ribosomal protein L40.

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

- Molecule 82 is a protein called eL42.

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

- Molecule 83 is a protein called eL43.

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

- Molecule 84 is a protein called Ribosomal protein eL28.

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

- Molecule 85 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 86 is a protein called Ribosomal protein L12.

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

- Molecule 87 is a protein called Ribosomal protein uL1.

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

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

Mol	Chain	Residues	Atoms		AltConf
88	A2	84	Total	Mg	0
			84	84	
88	B5	250	Total	Mg	0
			250	250	
88	B7	7	Total	Mg	0
			7	7	
88	B8	5	Total	Mg	0
			5	5	
88	BP	1	Total	Mg	0
			1	1	
88	BV	1	Total	Mg	0
			1	1	
88	Ba	1	Total	Mg	0
			1	1	

- Molecule 89 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
89	A2	62	Total	X	0
			62	62	
89	AT	1	Total	X	0
			1	1	
89	An	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
89	B5	175	Total 175	X 175	0
89	B7	6	Total 6	X 6	0
89	B8	4	Total 4	X 4	0
89	BA	4	Total 4	X 4	0
89	BB	1	Total 1	X 1	0
89	BH	1	Total 1	X 1	0
89	BI	1	Total 1	X 1	0
89	BL	1	Total 1	X 1	0
89	BN	3	Total 3	X 3	0
89	BO	1	Total 1	X 1	0
89	BT	2	Total 2	X 2	0
89	Be	1	Total 1	X 1	0
89	Bf	1	Total 1	X 1	0
89	Bg	1	Total 1	X 1	0

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

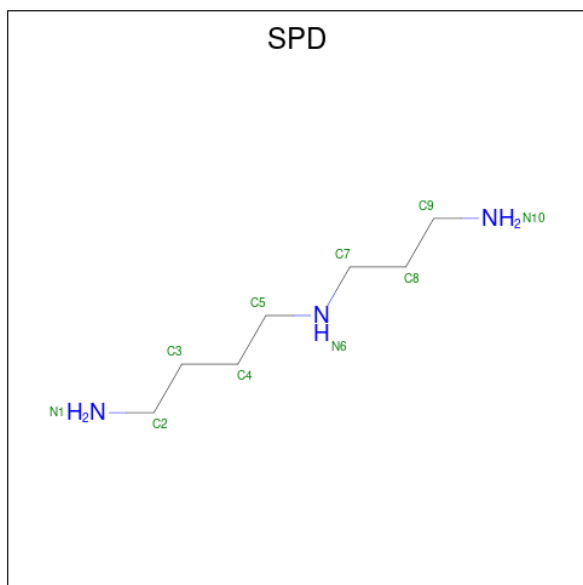
Mol	Chain	Residues	Atoms		AltConf
90	AC	1	Total 1	Zn 1	0
90	AE	1	Total 1	Zn 1	0
90	AG	1	Total 1	Zn 1	0
90	Bg	1	Total 1	Zn 1	0
90	Bj	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
90	Bm	1	Total	Zn	0
			1	1	
90	Bo	1	Total	Zn	0
			1	1	
90	Bp	1	Total	Zn	0
			1	1	

- Molecule 91 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	391	Total	O	0
			391	391	
92	AE	1	Total	O	0
			1	1	
92	Ab	1	Total	O	0
			1	1	
92	Af	1	Total	O	0
			1	1	
92	Ak	2	Total	O	0
			2	2	

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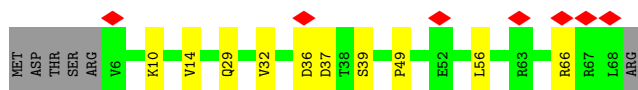
Mol	Chain	Residues	Atoms		AltConf
92	An	1	Total 1	O 1	0
92	Ap	2	Total 2	O 2	0
92	Ar	1	Total 1	O 1	0
92	As	2	Total 2	O 2	0
92	Aw	5	Total 5	O 5	0
92	B5	1197	Total 1197	O 1197	0
92	B7	35	Total 35	O 35	0
92	B8	35	Total 35	O 35	0
92	BA	4	Total 4	O 4	0
92	BB	3	Total 3	O 3	0
92	BC	3	Total 3	O 3	0
92	BD	1	Total 1	O 1	0
92	BF	2	Total 2	O 2	0
92	BH	1	Total 1	O 1	0
92	BI	1	Total 1	O 1	0
92	BL	1	Total 1	O 1	0
92	BN	2	Total 2	O 2	0
92	BO	1	Total 1	O 1	0
92	BP	3	Total 3	O 3	0
92	BR	5	Total 5	O 5	0
92	BV	3	Total 3	O 3	0

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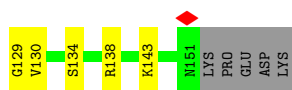
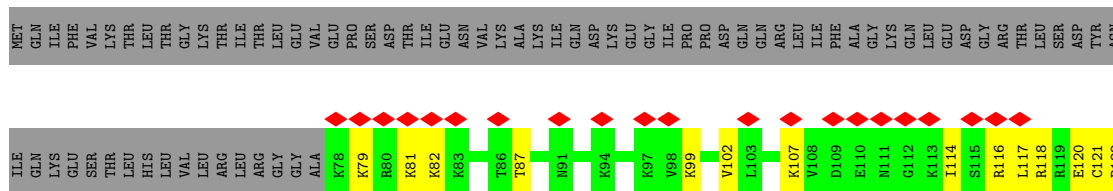
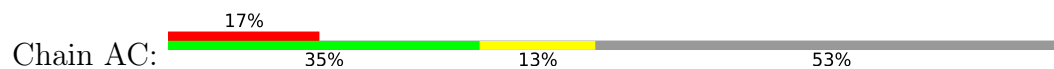
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Mol	Chain	Residues	Atoms		AltConf
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92	BY	1	Total 1	O 1	0
92	Ba	7	Total 7	O 7	0
92	Bb	1	Total 1	O 1	0
92	Be	4	Total 4	O 4	0
92	Bg	2	Total 2	O 2	0
92	Bj	3	Total 3	O 3	0
92	Bm	1	Total 1	O 1	0

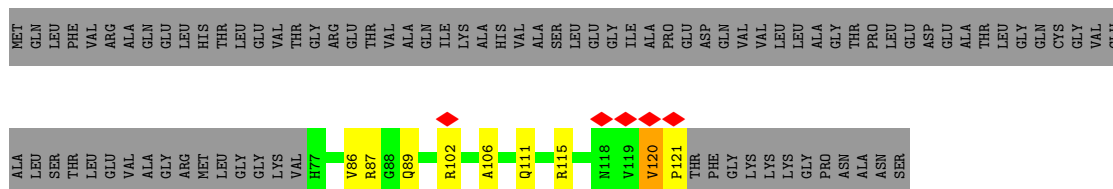




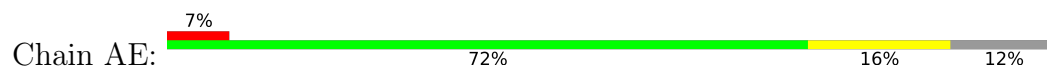
• Molecule 4: Ribosomal protein S27a



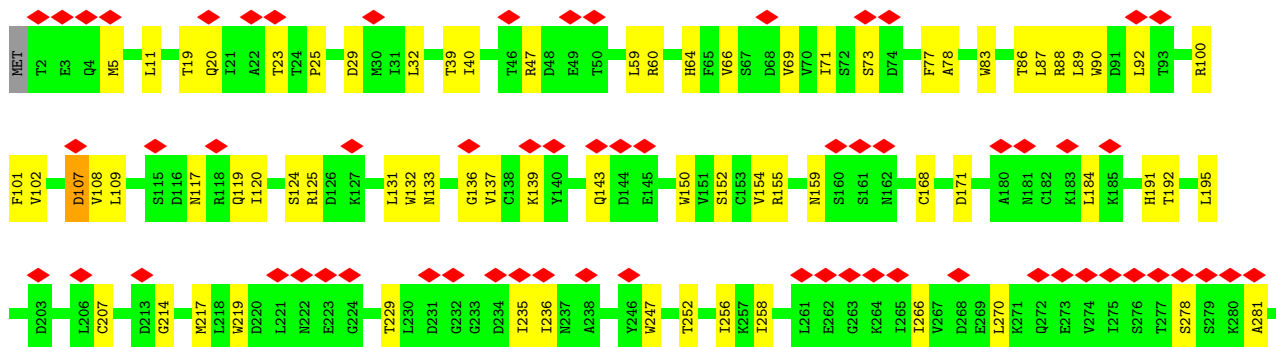
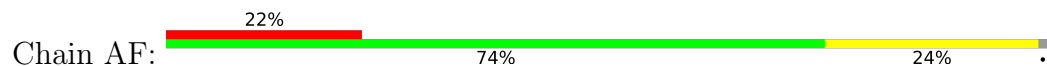
• Molecule 5: 40S ribosomal protein S30

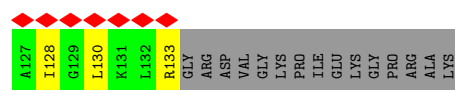


• Molecule 6: Ribosomal protein eS26

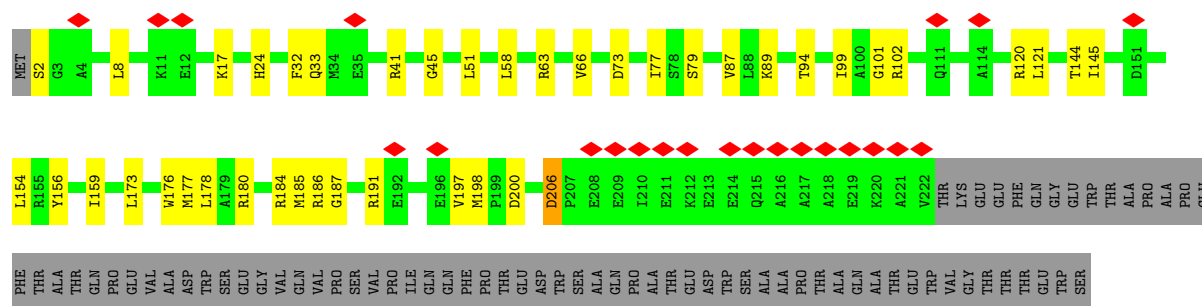


• Molecule 7: RACK1

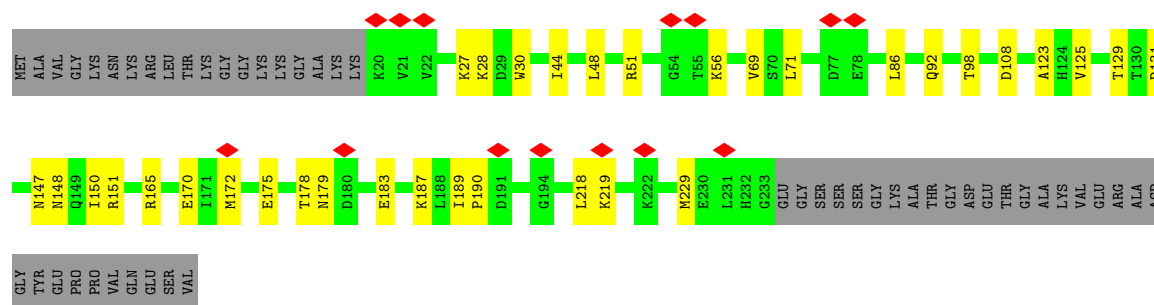




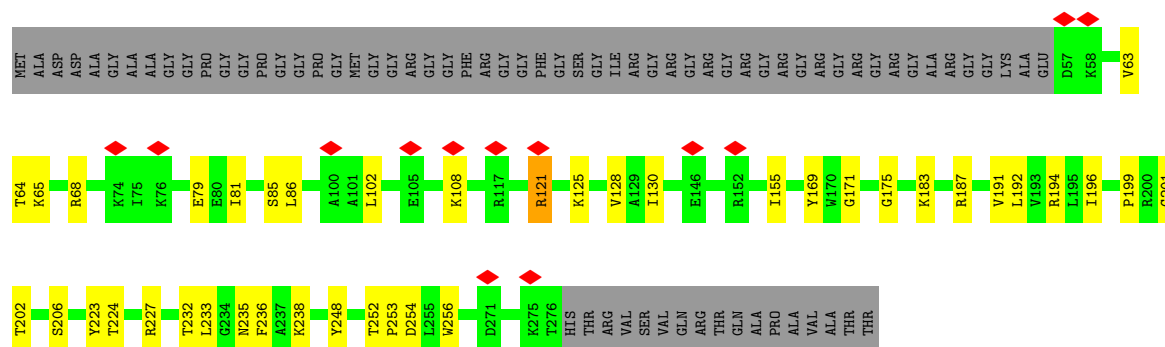
• Molecule 13: 40S ribosomal protein SA



• Molecule 14: 40S ribosomal protein S3a

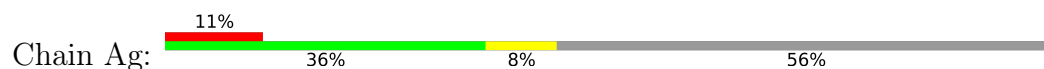


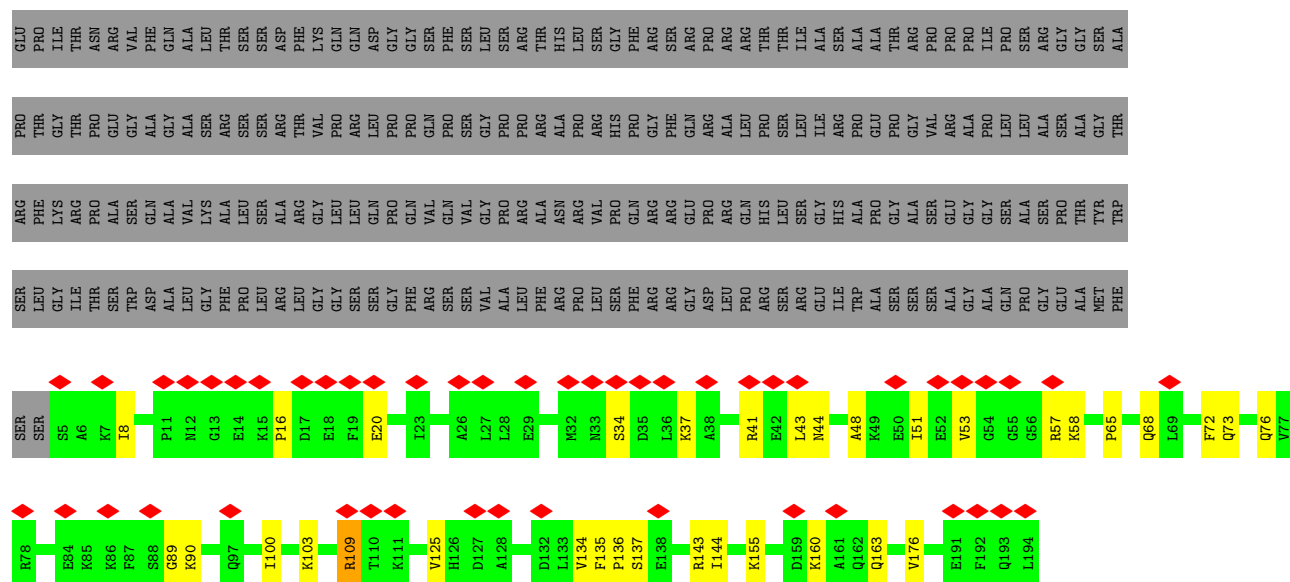
• Molecule 15: Ribosomal protein uS5



• Molecule 16: 40S ribosomal protein S3

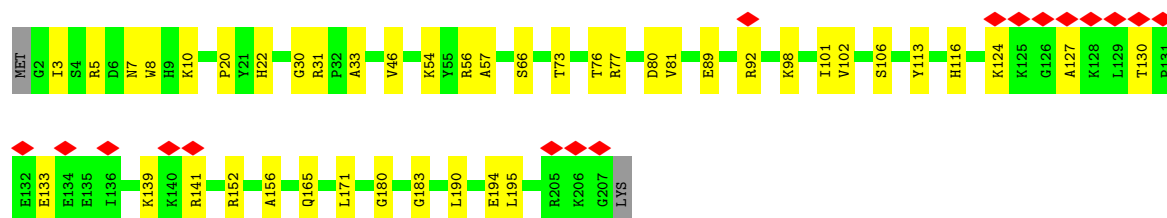






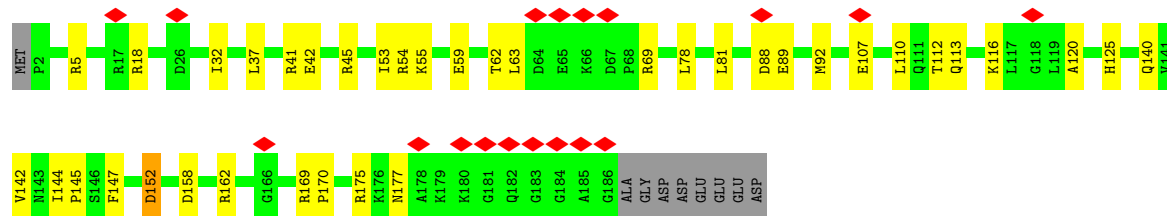
• Molecule 21: 40S ribosomal protein S8

Chain Ah: 8% 78% 21%



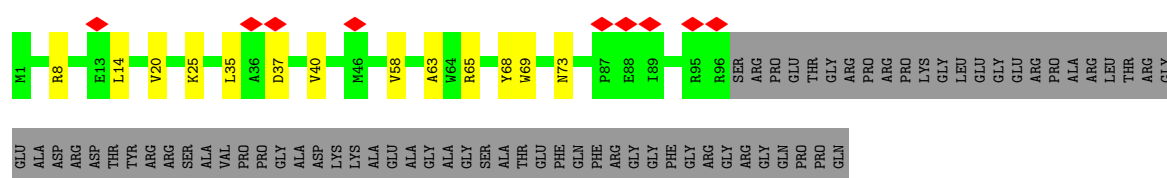
• Molecule 22: Ribosomal protein S9 (Predicted)

Chain Ai: 9% 76% 19% 5%

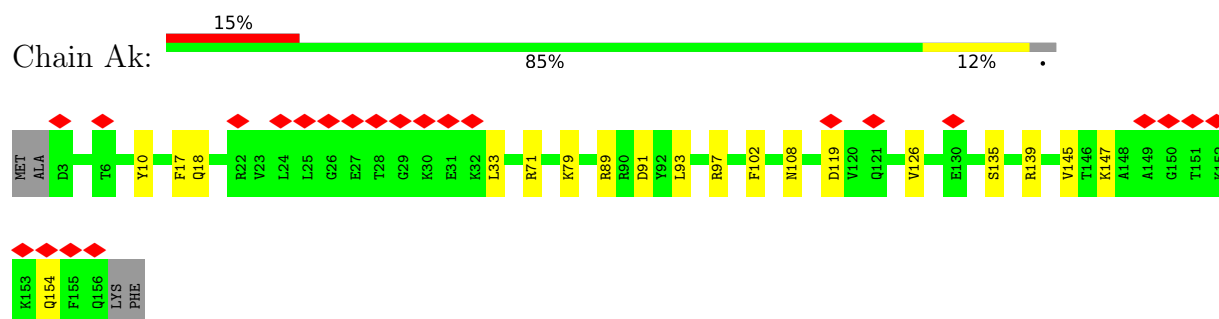


• Molecule 23: Ribosomal protein eS10

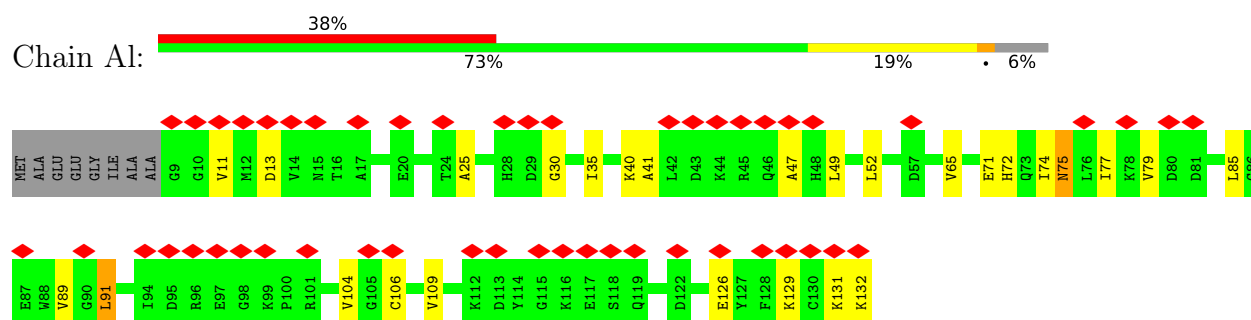
Chain Aj: 5% 50% 8% 42%



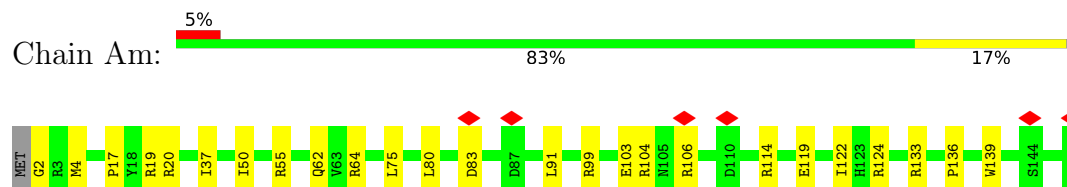
- Molecule 24: 40S ribosomal protein S11



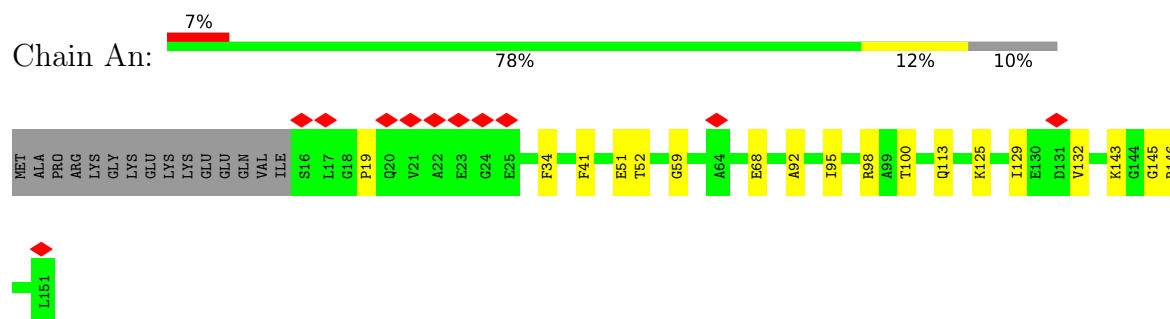
- Molecule 25: 40S ribosomal protein S12



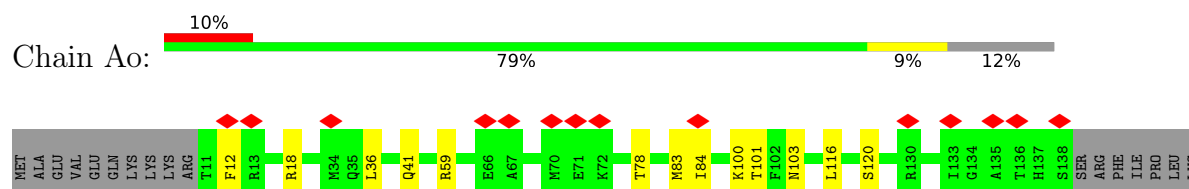
- Molecule 26: uS15



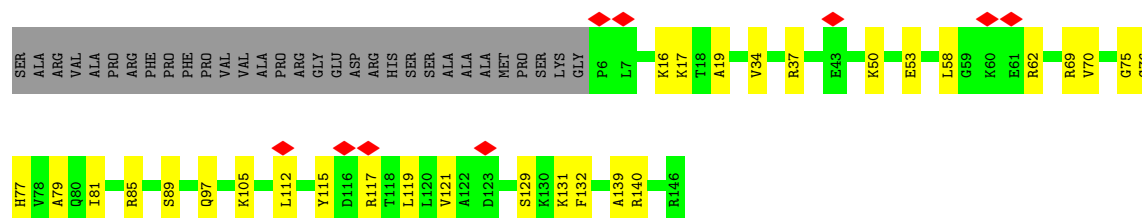
- Molecule 27: 40S ribosomal protein uS11



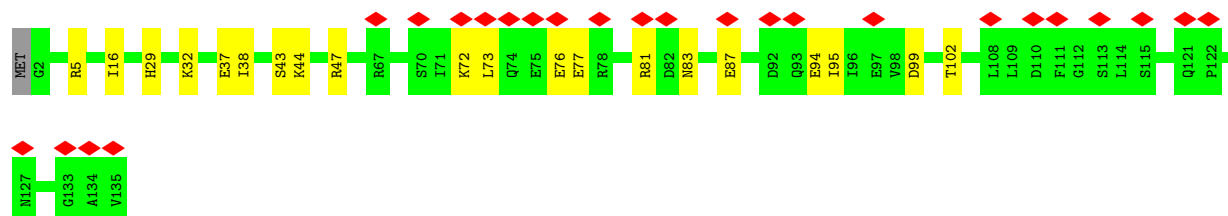
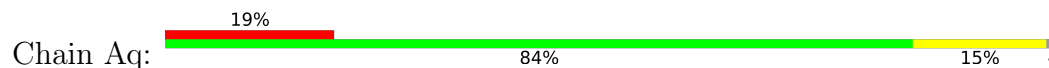
- Molecule 28: 40S ribosomal protein uS19



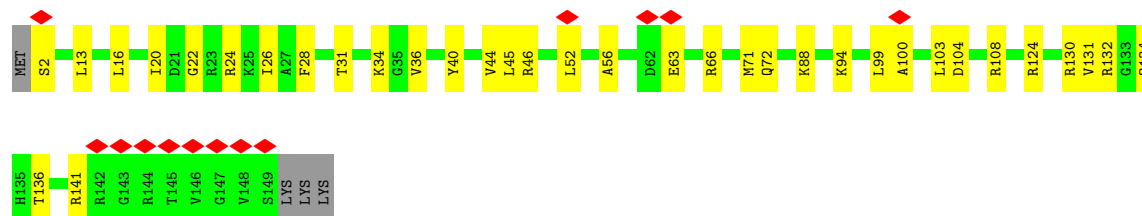
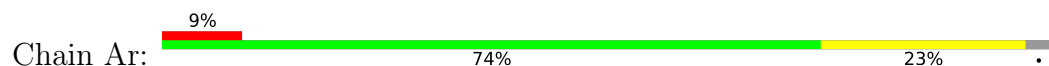
- Molecule 29: uS9



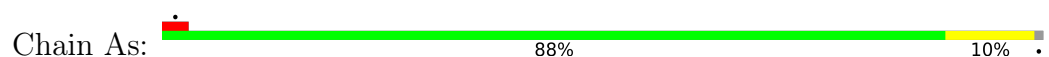
- Molecule 30: 40S ribosomal protein eS17



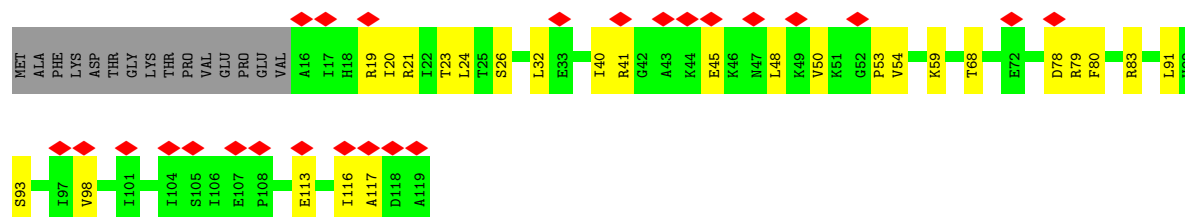
- Molecule 31: 40S ribosomal protein S18



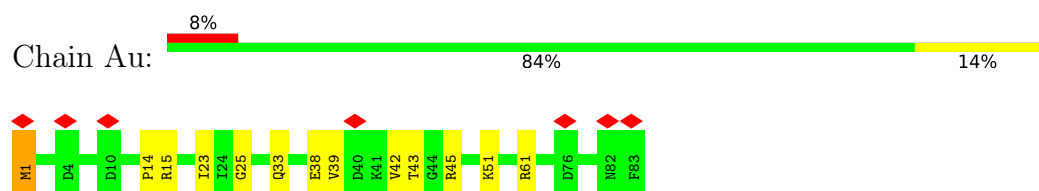
- Molecule 32: Ribosomal protein eS19



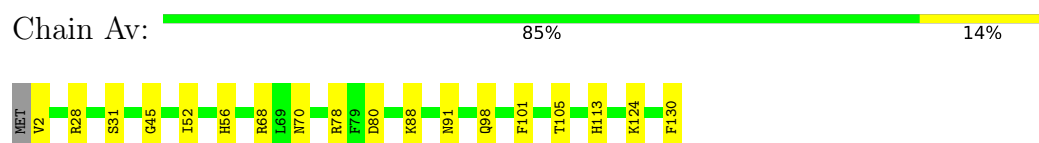
- Molecule 33: 40S ribosomal protein uS10



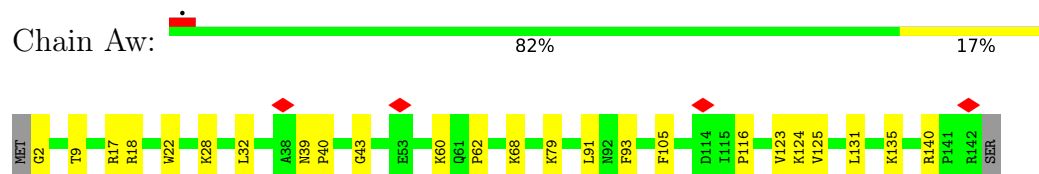
- Molecule 34: Ribosomal protein eS21



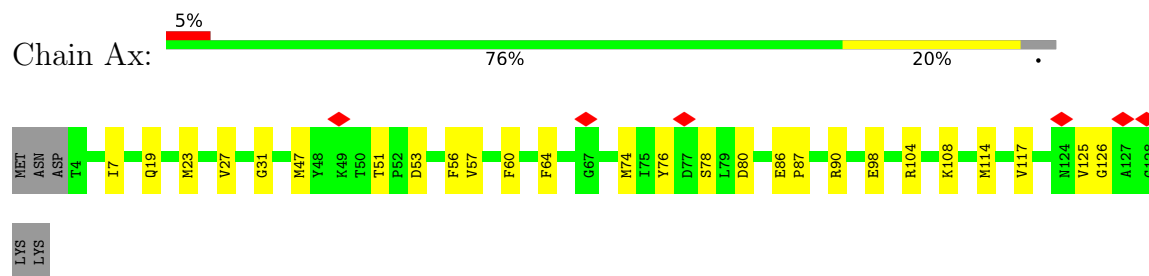
- Molecule 35: Ribosomal protein S15a



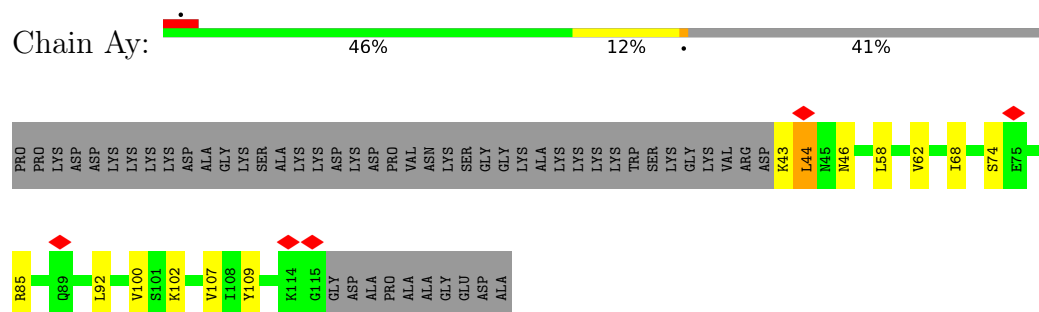
- Molecule 36: 40S ribosomal protein S23



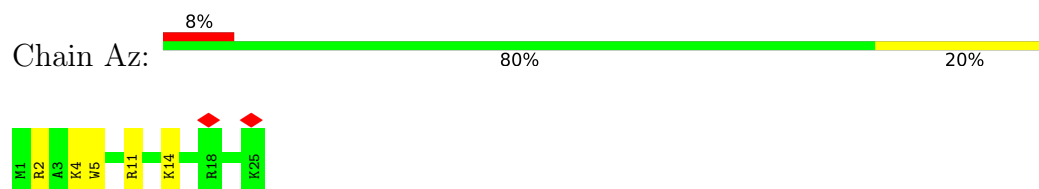
- Molecule 37: 40S ribosomal protein S24



- Molecule 38: 40S ribosomal protein S25



- Molecule 39: 60s ribosomal protein l41

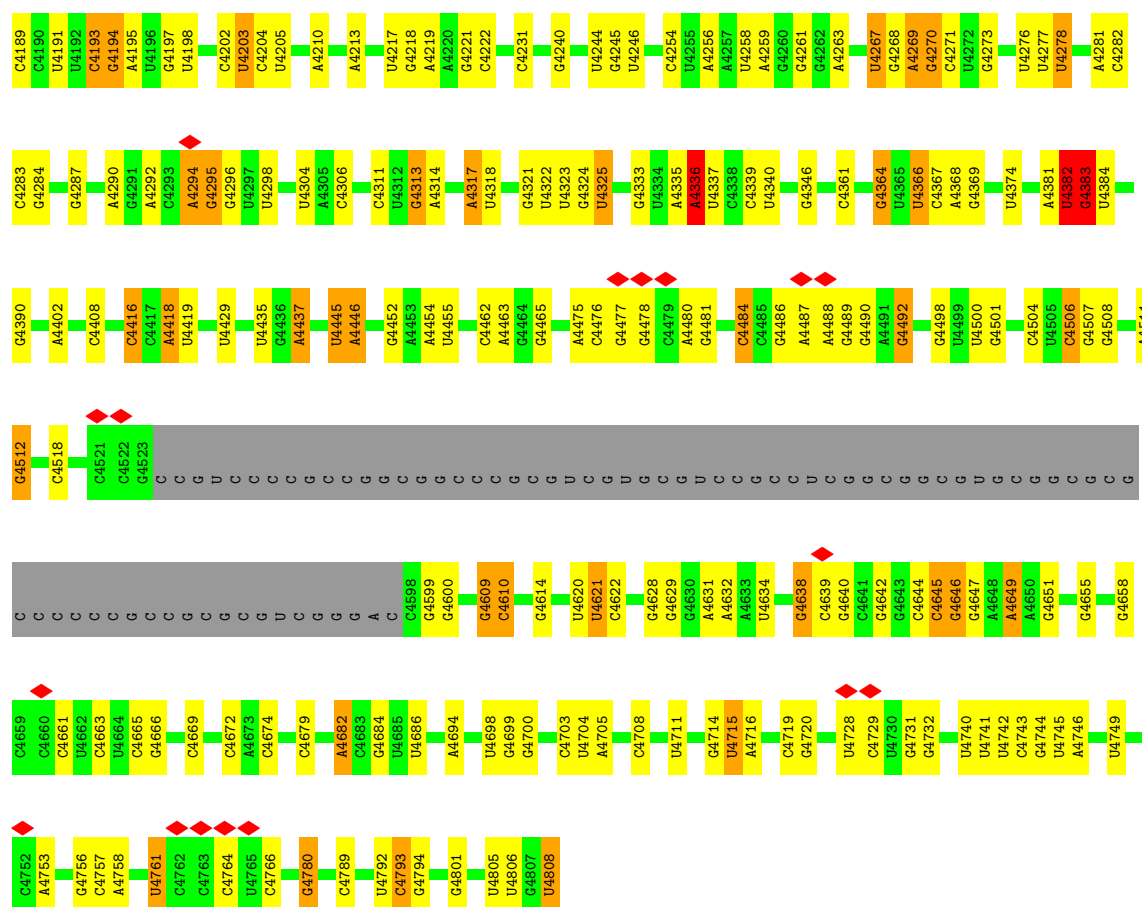


Chain B5:

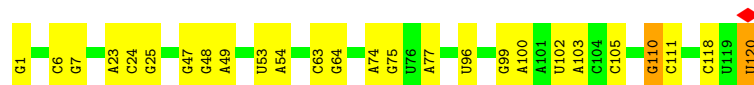
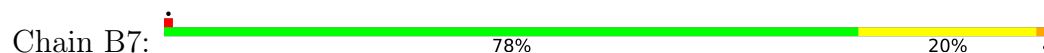


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G	A2641	U2504	C2363	A2260	C2133	G	C1955	G1879	C1766	U1687	C1545	U1400	A1286
G	C2647	G2511	G2364	A2261	G2142	C	A1956	G1887	G1772	G1689	U1546	C1401	C1287
C	C2648	G2512	G2365	G2264	A2143	G	C1958	G1890	U1773	G1694	G1550	G1406	A1288
C	A2649	C2515	G2366	A2266	G2144	C	U1959	G1891	G1774	C1695	U1551	C1413	A1289
G	A2650	G2515	U2373	G2267	G2145	C	G1960	G1899	G1775	U1699	C1565	G1412	G1297
A	G2651	C2515	U2373	U2268	G2146	G	G1963	G1899	A1776	G1699	C1568	C1415	G1298
A	G2652	U2530	A2380	U2269	A2156	G	A1964	U1898	G1781	G1700	A1568	G1414	G1299
C	C2657	G2537	U2381	A2270	C2157	G	A1965	G1900	U1784	C1701	G1572	G1420	C1309
C	A2658	G2538	C2382	A2271	G2161	G	A1968	G1907	G1785	C1702	G1579	G1421	G1310
G	G2659	A2539	C2383	A2272	G2164	C	C1970	G1908	C1786	G1703	G1580	C1422	C1311
G	G2665	G2544	G2385	G2277	G2169	U	A1980	A1909	U1791	A1704	G1584	C1423	A1312
G	G2666	C2545	U2386	C2289	G2172	C	A1984	C1910	G1792	A1705	G1586	C1438	A1316
U	C2667	G2546	U2388	G2293	U2172	C	G1985	G1911	G1793	A1706	A1585	G1439	A1317
G	A2668	C2547	G2389	G2294	C2178	C	A1986	G1912	G1794	C1707	A1586	U1449	G1318
G	U2669	G2548	G2390	A2296	G2179	C	U1987	U1913	U1799	G1708	A1587	G1450	C1319
G	G2670	G2549	U2397	G2300	G2191	G	G1988	G1914	U1800	A1709	G1588	G1451	C1320
C	U2671	U2550	G2400	C2301	G2195	G	G1991	G1915	U1801	U1710	C1590	A1452	G1323
C	U2672	C2552	C2401	G2302	C2194	G	G1994	C1917	G1804	U1712	G1591	G1453	G1326
C	U2680	G2553	G2402	C2305	U2195	G	A1995	A1918	U1805	C1713	G1609	G1457	G1326
G	A2688	G2554	C2406	G2317	G2203	G	A1996	U1919	A1806	A1714	A1458	G1459	A1331
C	G2689	G2564	G2407	G2318	G2204	U	A1999	G1920	G1807	G1715	U1468	U1473	G1334
C	G2690	U2584	A2408	G2319	G2205	C	C2001	G1921	G1808	C1716	A1478	A1479	G1337
C	G2698	G2585	U2409	C2321	A2206	C	C2007	A1922	A1810	G1717	A1479	A1480	G1341
G	C2699	A2586	G2410	G2322	G2207	C	A2008	A1923	G1811	U1718	C1630	G1485	G1351
C	A2700	A2587	G2411	G2323	C2208	G	C2012	A1924	U1815	U1720	C1631	U1491	G1354
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G	G2705	G2593	A2416	C2325	G2221	C	G2014	G1926	G1822	A1726	U1638	U	U
G	G2706	G2594	G2422	G2326	A2224	C	G2015	G1927	U1827	A1727	U1642	C	C
A	U2712	G2599	U2423	U2327	A2225	C	U2023	G1928	G1829	U1731	U1643	C	C
C	G2719	G2601	A2424	C2332	A2232	C	G2024	A1929	A1830	A1732	G1646	A1502	G1361
C	A2724	U2604	A2425	U2333	A2239	C	G2028	U1931	A1831	A1733	U1648	A1509	C1362
G	C2742	G2605	G2429	U2336	A2240	C	G2032	C1932	C1832	G1736	G1652	G1529	G1367
G	U2745	U2607	A2444	U2337	G2241	C	C2033	G1934	A1836	G1737	C1653	U1524	A1375
C	G	A2608	U2469	U2338	G2242	C	A2034	U1935	G1842	A1741	C1654	G1532	A1381
C	U	G	C2470	G2346	G2243	C	G2035	U1936	G1846	G1742	A1655	U1533	C1391
C	C	G	U2473	C2347	A2244	C	A2036	A1937	U1857	A1743	C1656	C1534	C1392
C	C	G	U2474	G2348	G2245	C	G2037	G1938	G1858	A1744	C1657	U1536	U1394
C	C	G	U2475	A2350	G2249	C	G2039	G1939	C1859	G1745	C1658	G1532	C1391
C	C	G	U2475	U2351	G2250	C	A2040	G1940	C1860	G1754	C1658	C1534	C1392
C	G	A2630	G2483	U2356	U2251	C	A2042	G1941	G1861	G1757	C1672	C1536	U1395
C	G	A2632	C2496	A2356	U2252	C	A2043	U1943	U1869	G1760	G1680	U1536	U1395
C	G	U2633	U2499	G2369	C2253	C	A2044	U1944	C1870	G1762	G1680	U1536	U1395
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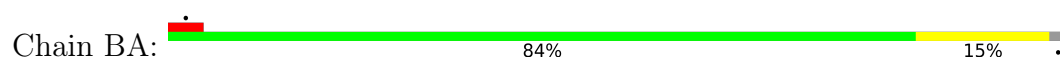
• Molecule 41: 5S rRNA

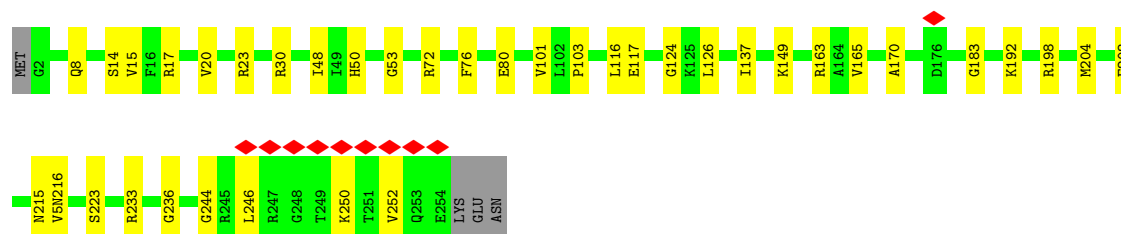


• Molecule 42: 5.8S rRNA



• Molecule 43: Ribosomal protein uL2





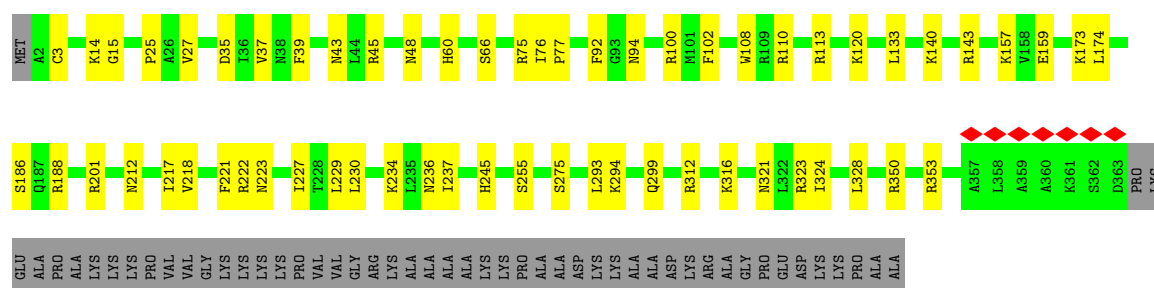
• Molecule 44: Ribosomal protein L3

Chain BB: 82% 16% .



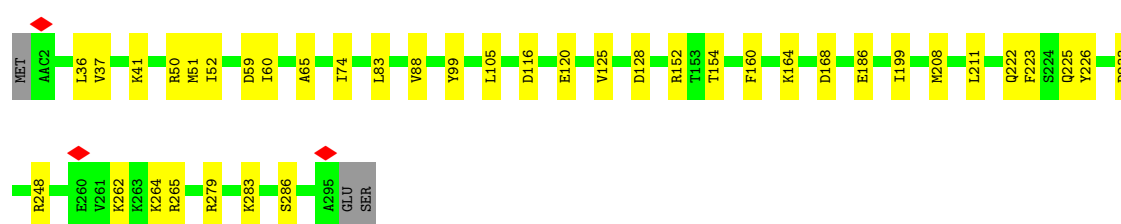
• Molecule 45: 60S ribosomal protein L4

Chain BC: 73% 15% 12%



• Molecule 46: Ribosomal_L18_c domain-containing protein

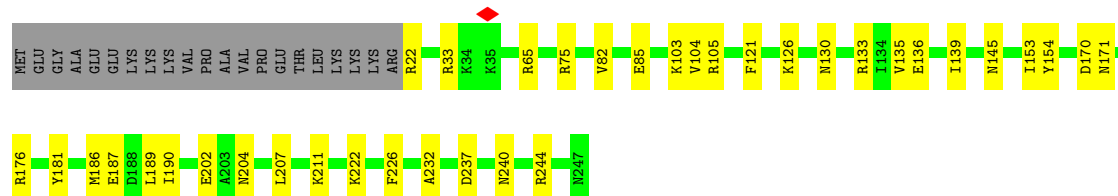
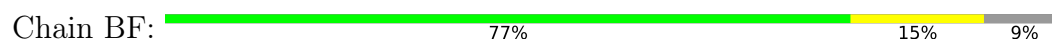
Chain BD: 86% 13% .



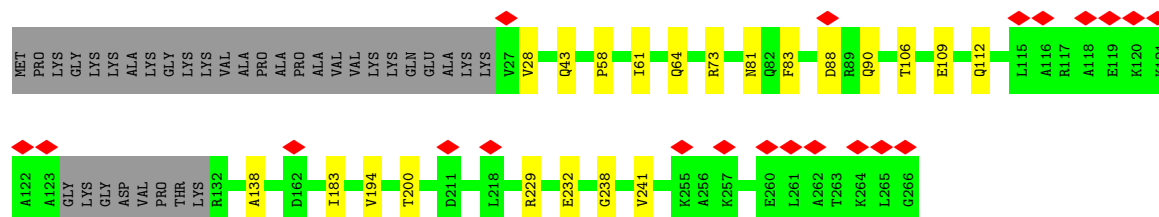
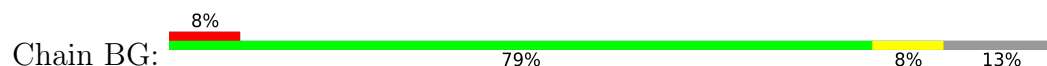
• Molecule 47: 60S ribosomal protein L6

Chain BE: 9% 69% 14% 16%

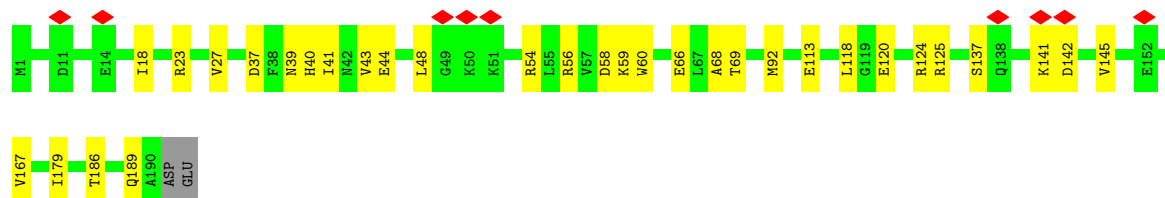
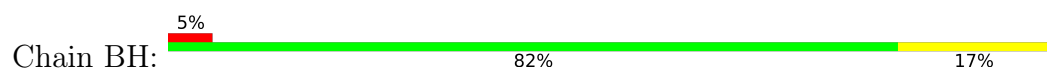
- Molecule 48: Ribosomal Protein uL30



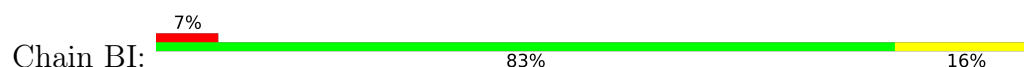
- Molecule 49: Ribosomal protein eL8

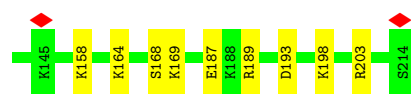


- Molecule 50: 60S ribosomal protein L9



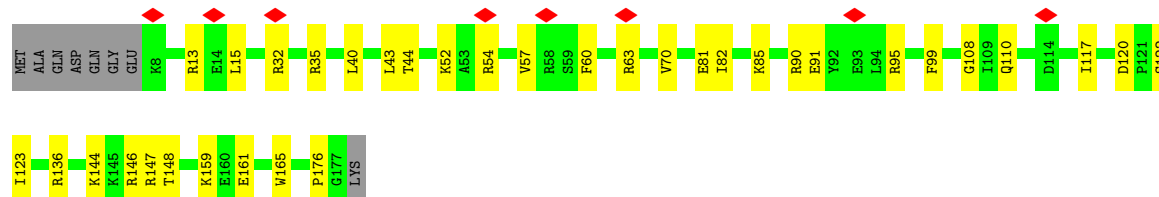
- Molecule 51: 60S ribosomal protein L10





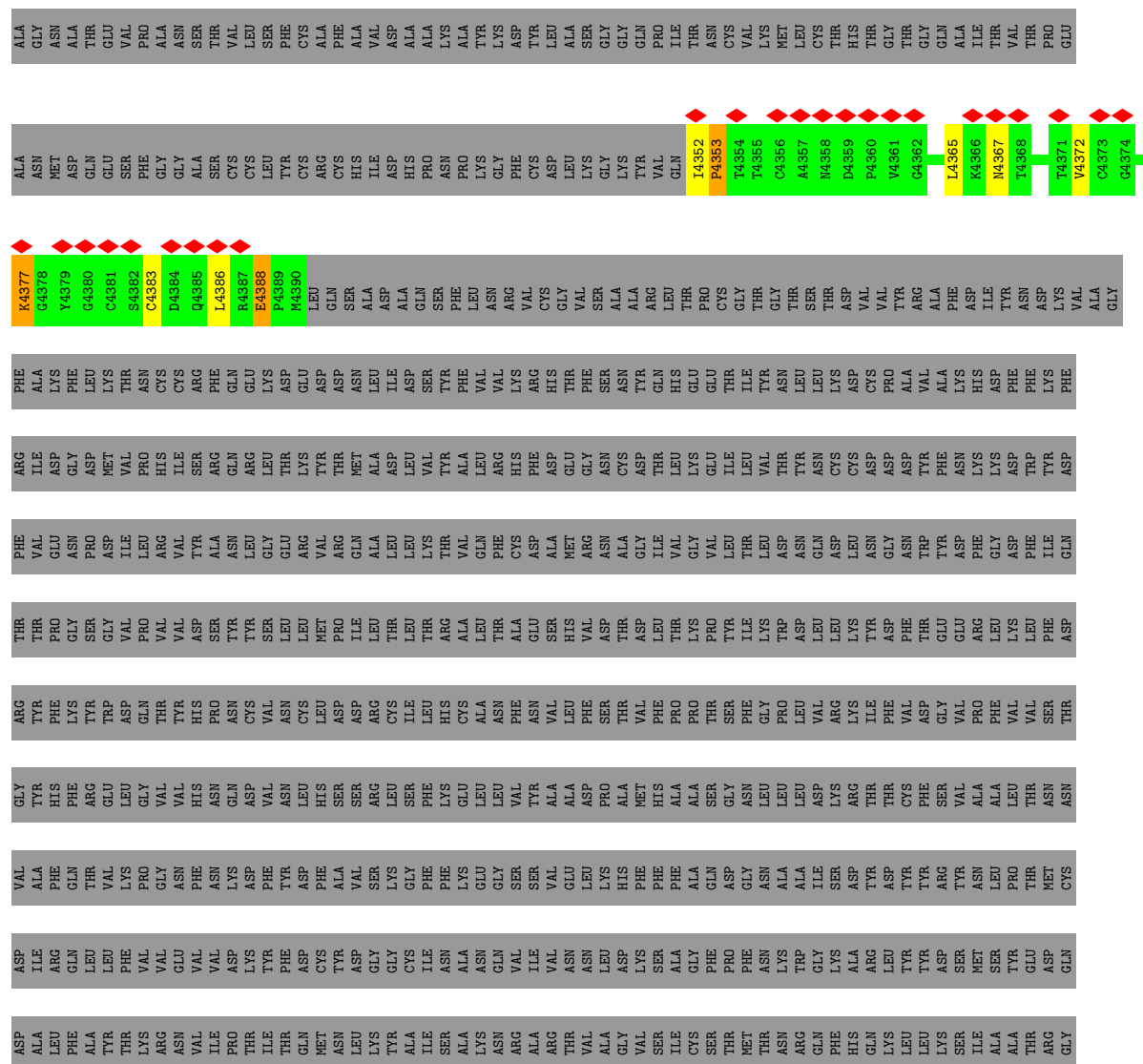
• Molecule 52: Ribosomal protein L11

Chain BJ: 76% 20% .



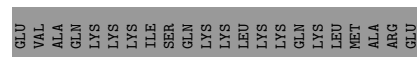
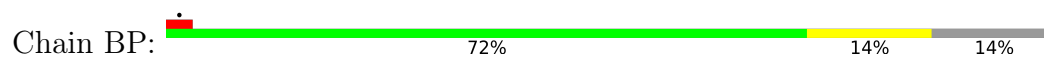
• Molecule 53: Replicase polyprotein 1ab

Chain BK: 96%

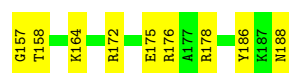
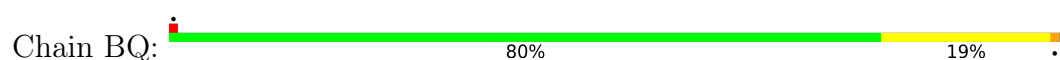




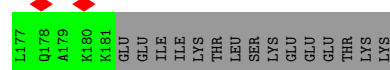
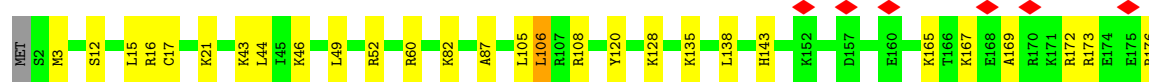
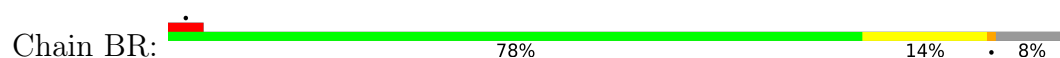
- Molecule 58: uL22



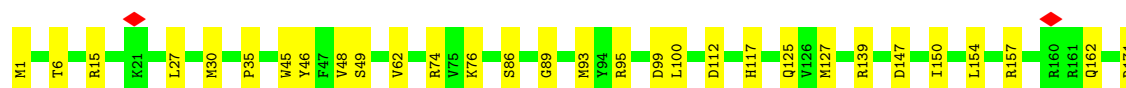
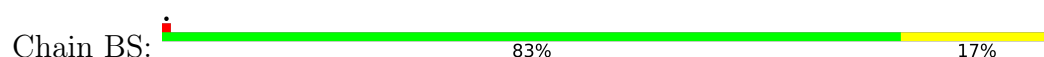
- Molecule 59: Ribosomal protein L18



- Molecule 60: 60S ribosomal protein L19

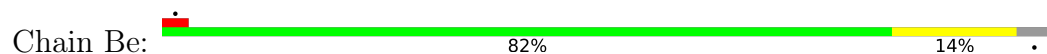


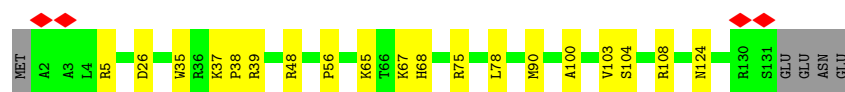
- Molecule 61: Ribosomal protein L18a



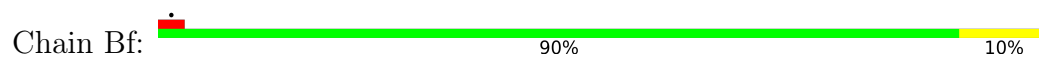
- Molecule 62: eL21



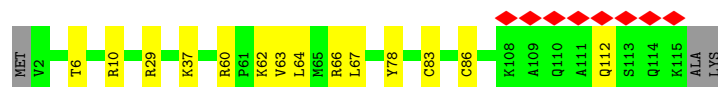
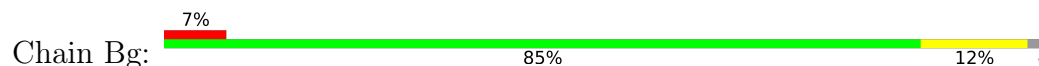




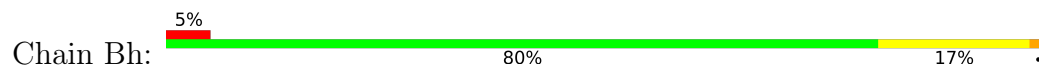
- Molecule 74: eL33



- Molecule 75: 60S ribosomal protein L34



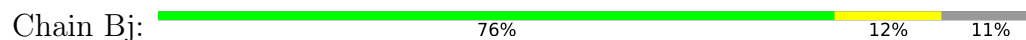
- Molecule 76: uL29



- Molecule 77: 60S ribosomal protein L36



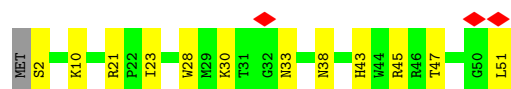
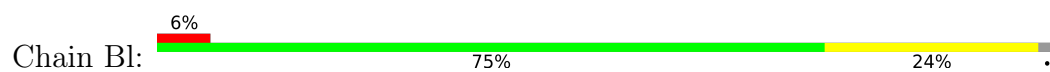
- Molecule 78: Ribosomal protein L37



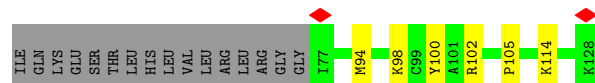
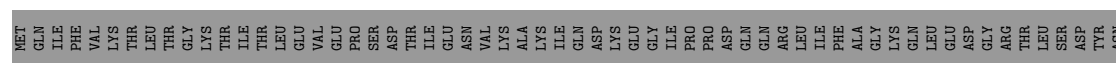
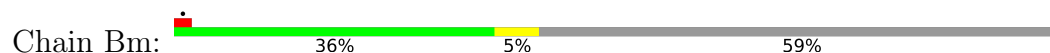
- Molecule 79: eL38



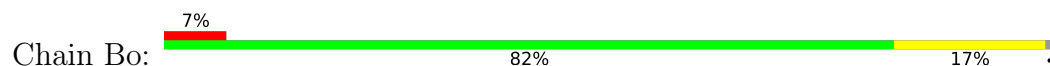
- Molecule 80: eL39



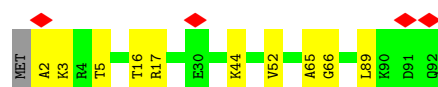
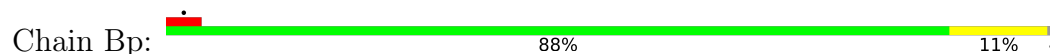
- Molecule 81: 60S ribosomal protein L40



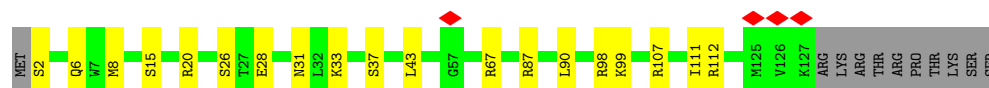
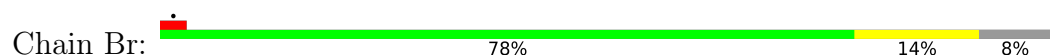
- Molecule 82: eL42



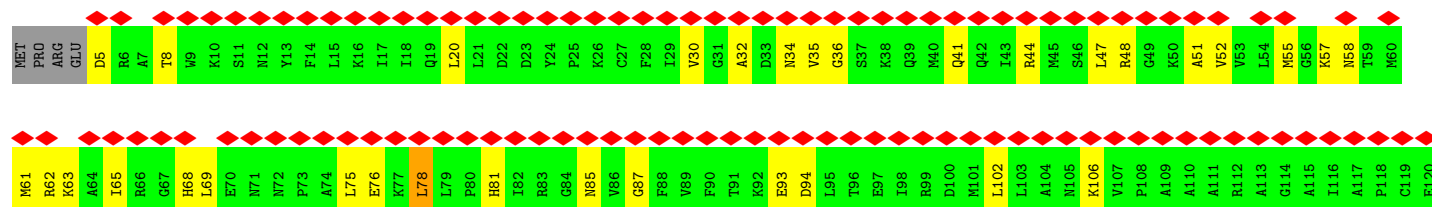
- Molecule 83: eL43

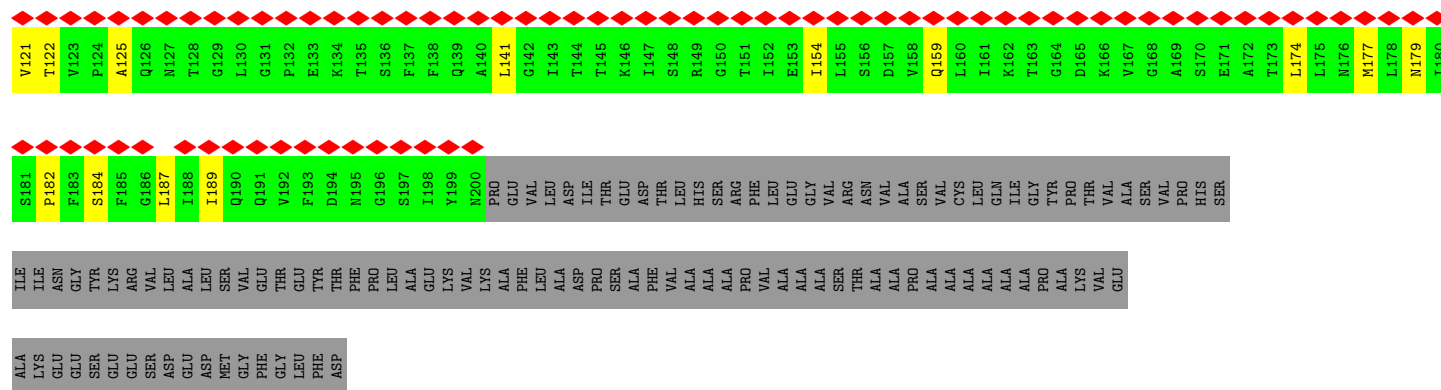


- Molecule 84: Ribosomal protein eL28

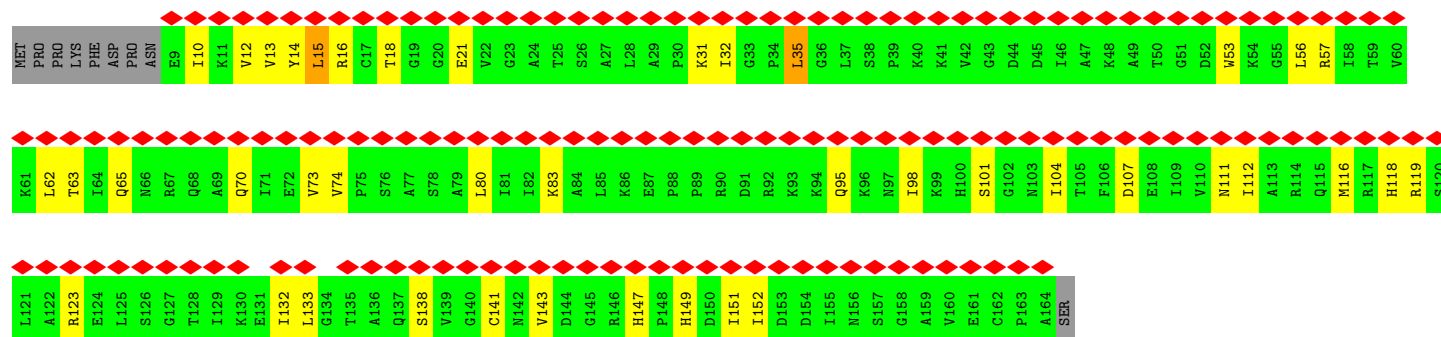
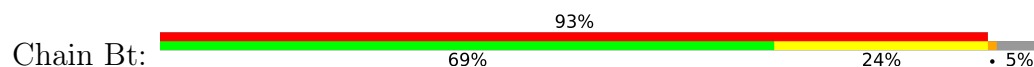


- Molecule 85: 60S acidic ribosomal protein P0

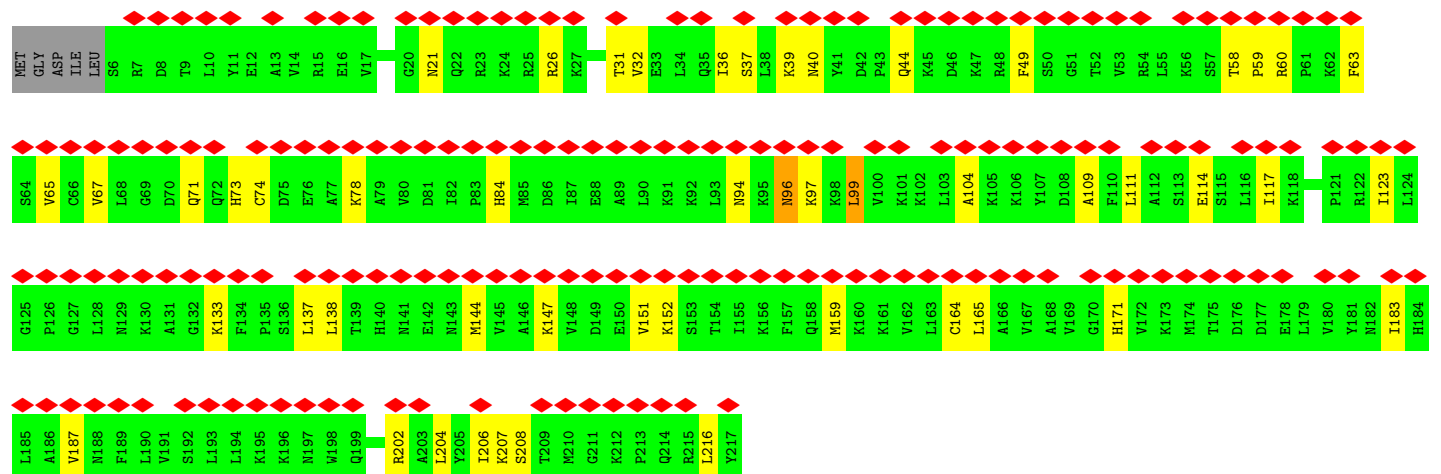
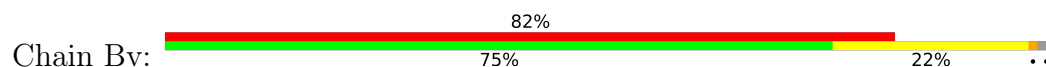




• Molecule 86: Ribosomal protein L12



• Molecule 87: Ribosomal protein uL1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19009	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.676	Depositor
Minimum map value	-1.120	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A2	0.14	3/40342 (0.0%)	0.13	0/62877
2	AA	0.08	0/665	0.26	0/891
3	AB	0.08	0/497	0.22	0/666
4	AC	0.08	0/622	0.24	0/822
5	AD	0.07	0/372	0.18	0/489
6	AE	0.09	0/828	0.23	0/1109
7	AF	0.08	0/2493	0.23	0/3394
8	AG	0.09	0/470	0.24	0/623
9	AH	0.06	0/236	0.13	0/365
10	AJ	0.05	0/1767	0.11	0/2751
11	AT	0.06	0/1746	0.11	0/2720
12	AU	0.09	0/871	0.22	0/1166
13	AZ	0.08	0/1771	0.22	0/2406
14	Aa	0.08	0/1765	0.22	0/2361
15	Ab	0.09	0/1742	0.24	0/2354
16	Ac	0.09	0/1779	0.26	0/2395
17	Ad	0.09	0/2118	0.23	0/2849
18	Ae	0.08	0/1531	0.23	0/2059
19	Af	0.08	0/1946	0.22	0/2590
20	Ag	0.09	0/1552	0.24	0/2079
21	Ah	0.08	0/1715	0.22	0/2287
22	Ai	0.09	0/1550	0.28	0/2069
23	Aj	0.09	0/834	0.25	0/1125
24	Ak	0.08	0/1284	0.22	0/1717
25	Al	0.08	0/968	0.23	0/1296
26	Am	0.08	0/1232	0.23	0/1656
27	An	0.09	0/1029	0.23	0/1380
28	Ao	0.10	0/1069	0.27	0/1429
29	Ap	0.10	0/1142	0.28	0/1528
30	Aq	0.08	0/1094	0.22	0/1469
31	Ar	0.08	0/1226	0.21	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	As	0.07	0/1119	0.18	0/1498
33	At	0.09	0/831	0.23	0/1115
34	Au	0.08	0/636	0.21	0/852
35	Av	0.09	0/1051	0.22	0/1406
36	Aw	0.09	0/1107	0.22	0/1475
37	Ax	0.08	0/1032	0.20	0/1371
38	Ay	0.08	0/585	0.19	0/785
39	Az	0.07	0/240	0.18	0/305
40	B5	0.11	5/87403 (0.0%)	0.13	0/136359
41	B7	0.07	0/2835	0.10	0/4418
42	B8	0.07	0/3635	0.12	0/5661
43	BA	0.12	0/1965	0.32	1/2633 (0.0%)
44	BB	0.09	0/3261	0.23	0/4364
45	BC	0.09	0/2932	0.23	0/3939
46	BD	0.08	0/2437	0.23	0/3264
47	BE	0.09	0/1998	0.23	0/2673
48	BF	0.09	0/1922	0.22	0/2563
49	BG	0.09	0/1899	0.21	0/2555
50	BH	0.08	0/1535	0.21	0/2063
51	BI	0.09	0/1756	0.22	0/2346
52	BJ	0.10	0/1385	0.25	0/1852
53	BK	0.57	1/296 (0.3%)	0.62	0/402
54	BL	0.10	0/1733	0.24	0/2316
55	BM	0.08	0/1158	0.19	0/1547
56	BN	0.09	0/1746	0.22	0/2338
57	BO	0.09	0/1662	0.22	0/2222
58	BP	0.09	0/1317	0.25	0/1768
59	BQ	0.09	0/1539	0.23	0/2054
60	BR	0.07	0/1524	0.19	0/2013
61	BS	0.10	0/1497	0.22	0/2008
62	BT	0.09	0/1326	0.21	0/1770
63	BU	0.08	0/820	0.22	0/1100
64	BV	0.11	0/1048	0.25	0/1402
65	BW	0.08	0/1006	0.22	0/1334
66	BX	0.08	0/1022	0.22	0/1371
67	BY	0.08	0/1132	0.22	0/1504
68	BZ	0.08	0/1130	0.20	0/1507
69	Ba	0.09	0/1179	0.25	0/1572
70	Bb	0.07	0/884	0.21	0/1169
71	Bc	0.08	0/847	0.23	0/1134
72	Bd	0.08	0/903	0.22	0/1216
73	Be	0.09	0/1088	0.25	0/1451
74	Bf	0.09	0/903	0.22	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Bg	0.08	0/916	0.22	0/1220
76	Bh	0.08	0/1021	0.21	0/1348
77	Bi	0.08	0/841	0.22	0/1112
78	Bj	0.09	0/720	0.24	0/952
79	Bk	0.08	0/575	0.20	0/761
80	Bl	0.08	0/459	0.20	0/608
81	Bm	0.08	0/426	0.23	0/564
82	Bo	0.09	0/866	0.21	0/1141
83	Bp	0.09	0/718	0.24	0/953
84	Br	0.08	0/1020	0.23	0/1366
85	Bs	0.08	0/1530	0.20	0/2064
86	Bt	0.08	0/1193	0.25	0/1609
87	Bv	0.09	0/1735	0.26	0/2328
All	All	0.11	9/237600 (0.0%)	0.18	1/348494 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
82	Bo	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BK	4353	PRO	N-CD	7.01	1.57	1.47
40	B5	4761	U	C4-O4	5.15	1.33	1.23
40	B5	4276	UR3	O3'-P	5.08	1.61	1.56
1	A2	1032	A2M	O3'-P	5.05	1.61	1.56
1	A2	1443	OMU	O3'-P	5.04	1.61	1.56
40	B5	2258	OMU	O3'-P	5.03	1.61	1.56
40	B5	4269	A2M	O3'-P	5.03	1.61	1.56
1	A2	485	A2M	O3'-P	5.02	1.61	1.56
40	B5	2658	A2M	O3'-P	5.00	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	BA	15	VAL	N-CA-C	-5.74	108.25	113.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	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	A2	37833	0	19168	366	0
2	AA	651	0	672	4	0
3	AB	495	0	523	6	0
4	AC	610	0	634	15	0
5	AD	369	0	412	8	0
6	AE	814	0	863	12	0
7	AF	2436	0	2393	44	0
8	AG	459	0	448	19	0
9	AH	212	0	110	2	0
10	AJ	1622	0	822	15	0
11	AT	1604	0	811	9	0
12	AU	864	0	897	15	0
13	AZ	1743	0	1748	24	0
14	Aa	1738	0	1816	23	0
15	Ab	1706	0	1796	28	0
16	Ac	1751	0	1846	21	0
17	Ad	2076	0	2177	22	0
18	Ae	1509	0	1563	17	0
19	Af	1923	0	2089	40	0
20	Ag	1529	0	1627	19	0
21	Ah	1686	0	1772	29	0
22	Ai	1525	0	1640	25	0
23	Aj	810	0	836	9	0
24	Ak	1262	0	1335	14	0
25	Al	958	0	993	19	0
26	Am	1208	0	1294	20	0
27	An	1016	0	1039	13	0
28	Ao	1048	0	1093	10	0
29	Ap	1124	0	1193	20	0
30	Aq	1080	0	1135	12	0
31	Ar	1217	0	1279	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	As	1113	0	1145	13	0
33	At	821	0	883	18	0
34	Au	640	0	633	9	0
35	Av	1034	0	1080	15	0
36	Aw	1099	0	1162	15	0
37	Ax	1015	0	1086	16	0
38	Ay	579	0	639	12	0
39	Az	239	0	289	5	0
40	B5	80772	0	40880	687	0
41	B7	2570	0	1293	16	0
42	B8	3319	0	1684	31	0
43	BA	1940	0	2029	27	0
44	BB	3206	0	3353	48	0
45	BC	2886	0	3057	42	0
46	BD	2398	0	2430	28	0
47	BE	1960	0	2153	25	0
48	BF	1886	0	2008	32	0
49	BG	1868	0	2010	13	0
50	BH	1516	0	1597	20	0
51	BI	1717	0	1764	22	0
52	BJ	1362	0	1399	24	0
53	BK	290	0	281	6	0
54	BL	1702	0	1820	13	0
55	BM	1137	0	1211	20	0
56	BN	1701	0	1749	30	0
57	BO	1630	0	1778	16	0
58	BP	1289	0	1329	17	0
59	BQ	1515	0	1634	27	0
60	BR	1508	0	1664	22	0
61	BS	1457	0	1492	19	0
62	BT	1298	0	1366	17	0
63	BU	806	0	827	12	0
64	BV	1034	0	1097	18	0
65	BW	991	0	1048	12	0
66	BX	1004	0	1086	6	0
67	BY	1115	0	1205	9	0
68	BZ	1107	0	1182	18	0
69	Ba	1163	0	1202	18	0
70	Bb	881	0	957	12	0
71	Bc	836	0	888	8	0
72	Bd	888	0	930	14	0
73	Be	1070	0	1165	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	Bf	884	0	923	8	0
75	Bg	906	0	998	11	0
76	Bh	1013	0	1147	19	0
77	Bi	830	0	916	5	0
78	Bj	705	0	737	14	0
79	Bk	569	0	637	5	0
80	Bl	447	0	479	9	0
81	Bm	432	0	470	5	0
82	Bo	863	0	929	13	0
83	Bp	708	0	756	8	0
84	Br	1014	0	1083	16	0
85	Bs	1507	0	1564	32	0
86	Bt	1178	0	1235	24	0
87	Bv	1707	0	1815	33	0
88	A2	84	0	0	0	0
88	B5	250	0	0	0	0
88	B7	7	0	0	0	0
88	B8	5	0	0	0	0
88	BP	1	0	0	0	0
88	BV	1	0	0	0	0
88	Ba	1	0	0	0	0
89	A2	62	0	0	0	0
89	AT	1	0	0	0	0
89	An	1	0	0	0	0
89	B5	175	0	0	0	0
89	B7	6	0	0	0	0
89	B8	4	0	0	0	0
89	BA	4	0	0	0	0
89	BB	1	0	0	0	0
89	BH	1	0	0	0	0
89	BI	1	0	0	0	0
89	BL	1	0	0	0	0
89	BN	3	0	0	0	0
89	BO	1	0	0	0	0
89	BT	2	0	0	0	0
89	Be	1	0	0	0	0
89	Bf	1	0	0	0	0
89	Bg	1	0	0	0	0
90	AC	1	0	0	0	0
90	AE	1	0	0	0	0
90	AG	1	0	0	0	0
90	Bg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Bj	1	0	0	0	0
90	Bm	1	0	0	0	0
90	Bo	1	0	0	0	0
90	Bp	1	0	0	0	0
91	B5	10	0	19	1	0
92	A2	391	0	0	11	0
92	AE	1	0	0	0	0
92	Ab	1	0	0	0	0
92	Af	1	0	0	0	0
92	Ak	2	0	0	0	0
92	An	1	0	0	0	0
92	Ap	2	0	0	0	0
92	Ar	1	0	0	0	0
92	As	2	0	0	0	0
92	Aw	5	0	0	0	0
92	B5	1197	0	0	32	0
92	B7	35	0	0	0	0
92	B8	35	0	0	0	0
92	BA	4	0	0	0	0
92	BB	3	0	0	0	0
92	BC	3	0	0	1	0
92	BD	1	0	0	0	0
92	BF	2	0	0	0	0
92	BH	1	0	0	0	0
92	BI	1	0	0	0	0
92	BL	1	0	0	0	0
92	BN	2	0	0	0	0
92	BO	1	0	0	0	0
92	BP	3	0	0	0	0
92	BR	5	0	0	1	0
92	BV	3	0	0	0	0
92	BX	2	0	0	0	0
92	BY	1	0	0	1	0
92	Ba	7	0	0	0	0
92	Bb	1	0	0	0	0
92	Be	4	0	0	0	0
92	Bg	2	0	0	0	0
92	Bj	3	0	0	1	0
92	Bm	1	0	0	0	0
All	All	228361	0	168217	2013	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 (2013) 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)
1:A2:1034:G:H1	1:A2:1081:A:HO2'	1.11	0.94
60:BR:87:ALA:O	92:BR:201:HOH:O	1.88	0.89
1:A2:1092:C:HO2'	35:Av:2:VAL:N	1.81	0.79
1:A2:1491:OMG:HM22	1:A2:1492:G:H5'	1.66	0.78
1:A2:1758:G:H1	1:A2:1776:U:H3	1.33	0.77
40:B5:41:C:P	92:B5:5406:HOH:O	2.44	0.75
48:BF:85:GLU:HB2	62:BT:135:PRO:HB3	1.69	0.75
40:B5:3373:U:OP2	40:B5:3378:A:N6	2.19	0.74
40:B5:3547:G:OP1	92:B5:5415:HOH:O	2.04	0.74
40:B5:1565:C:P	92:B5:5405:HOH:O	2.43	0.73
64:BV:69:LYS:HG2	64:BV:71:GLU:HG2	1.71	0.73
40:B5:2143:A:N7	45:BC:143:ARG:NH1	2.35	0.73
40:B5:3824:C:H3'	75:Bg:112:GLN:HE21	1.52	0.73
85:Bs:65:ILE:HG23	85:Bs:75:LEU:HB3	1.71	0.72
40:B5:3640:A:N6	53:BK:4383:CYS:SG	2.63	0.72
40:B5:1810:A2M:HM'2	40:B5:1811:G:H5'	1.71	0.72
1:A2:664:C:P	92:A2:2143:HOH:O	2.48	0.71
1:A2:745:G:H21	20:Ag:109:ARG:HA	1.55	0.71
1:A2:1518:G:C6	92:A2:2102:HOH:O	2.43	0.71
87:Bv:117:ILE:HD13	87:Bv:137:LEU:HD21	1.71	0.70
1:A2:926:G:H1	1:A2:1018:U:H3	1.39	0.70
27:An:34:PHE:HB3	27:An:41:PHE:HB2	1.72	0.70
40:B5:1630:C:P	92:B5:5414:HOH:O	2.49	0.70
40:B5:4610:C:N4	61:BS:171:ARG:O	2.24	0.70
40:B5:4366:OMU:HM22	40:B5:4367:C:H5'	1.74	0.70
40:B5:2106:A:OP1	84:Br:107:ARG:NH2	2.25	0.70
7:AF:247:TRP:HB3	7:AF:258:ILE:HD11	1.74	0.70
1:A2:1397:A:O2'	1:A2:1399:G:N7	2.24	0.69
44:BB:224:LYS:HG2	44:BB:340:THR:HG22	1.74	0.69
1:A2:1392:OMC:HM22	1:A2:1393:U:H5'	1.74	0.69
17:Ad:125:LYS:H	17:Ad:142:HIS:HD2	1.39	0.69
40:B5:1133:C:O2	40:B5:1207:G:N2	2.25	0.69
42:B8:81:C:HO2'	76:Bh:2:ALA:N	1.91	0.69
40:B5:4271:C:OP1	44:BB:246:ARG:NH1	2.26	0.69
40:B5:2704:OMC:HM22	40:B5:2705:G:H5'	1.75	0.68
40:B5:4366:OMU:OP2	40:B5:4416:C:N4	2.26	0.68
86:Bt:63:THR:HB	86:Bt:70:GLN:HB2	1.74	0.68
1:A2:166:A2M:HM'2	1:A2:167:G:H5'	1.74	0.68
18:Ae:58:ALA:HB3	18:Ae:62:ARG:HH21	1.58	0.68
55:BM:40:GLY:HA3	55:BM:45:VAL:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Bs:47:LEU:HB3	85:Bs:51:ALA:HB3	1.74	0.68
40:B5:61:A:P	92:B5:5408:HOH:O	2.50	0.68
1:A2:577:A2M:HM'2	1:A2:578:U:H5'	1.76	0.68
40:B5:4645:C:O2	40:B5:4655:G:N2	2.26	0.68
40:B5:1237:G:OP2	40:B5:1237:G:N2	2.23	0.68
7:AF:120:ILE:HB	7:AF:132:TRP:HB2	1.77	0.67
33:At:23:THR:HB	33:At:113:GLU:HB2	1.76	0.67
4:AC:126:CYS:HB3	4:AC:143:LYS:HD3	1.76	0.67
40:B5:3557:A2M:HM'2	40:B5:3558:C:H5'	1.77	0.67
82:Bo:36:GLN:OE1	82:Bo:39:ARG:NH2	2.28	0.67
59:BQ:16:LYS:O	59:BQ:33:ARG:NH2	2.23	0.67
40:B5:3909:U:H5'	40:B5:3910:C:H5''	1.76	0.67
12:AU:43:LYS:HB2	12:AU:46:ALA:HB2	1.77	0.67
40:B5:3985:A:P	92:B5:5452:HOH:O	2.52	0.67
1:A2:1143:G:OP1	15:Ab:187:ARG:NH1	2.28	0.67
49:BG:58:PRO:HD2	49:BG:61:ILE:HD12	1.75	0.67
7:AF:87:LEU:HB2	7:AF:101:PHE:HB2	1.77	0.67
12:AU:55:THR:HG23	12:AU:56:LYS:HD2	1.75	0.66
40:B5:4663:C:O2	40:B5:4665:C:N4	2.27	0.66
40:B5:3449:A:OP2	40:B5:3467:G:N2	2.27	0.66
40:B5:4202:OMC:HM22	40:B5:4203:PSU:H5''	1.76	0.66
40:B5:2444:A:N6	40:B5:2587:A:OP2	2.28	0.66
7:AF:40:ILE:HB	7:AF:59:LEU:HB2	1.75	0.66
40:B5:3669:C:H1'	56:BN:125:SER:HB3	1.76	0.66
40:B5:4416:C:O2'	64:BV:15:ARG:NH2	2.28	0.66
40:B5:1260:OMG:HM22	40:B5:1261:U:H5'	1.77	0.66
17:Ad:11:ARG:HA	17:Ad:28:ALA:HB2	1.77	0.66
1:A2:1031:A:H2'	1:A2:1032:A2M:H8	1.78	0.65
1:A2:1337:C:N4	1:A2:1338:4AC:O7	2.28	0.65
6:AE:51:ARG:NH1	6:AE:55:GLU:OE2	2.29	0.65
18:Ae:71:ARG:NH2	18:Ae:148:ASN:OD1	2.29	0.65
26:Am:136:PRO:HG2	26:Am:139:TRP:HB2	1.77	0.65
19:Af:22:ARG:HG2	19:Af:25:ARG:HH22	1.59	0.65
40:B5:1924:G:N2	40:B5:1924:G:OP1	2.28	0.65
40:B5:4267:PSU:P	92:B5:5437:HOH:O	2.53	0.65
1:A2:1131:G:N2	1:A2:1131:G:OP2	2.29	0.65
40:B5:1793:G:OP2	92:B5:5419:HOH:O	2.14	0.65
19:Af:129:VAL:O	65:BW:80:ARG:NH2	2.27	0.65
1:A2:126:G:OP2	19:Af:195:LYS:NZ	2.29	0.65
40:B5:39:A:OP1	91:B5:4901:SPD:N1	2.30	0.65
40:B5:1809:C:H2'	40:B5:1810:A2M:H8	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Bd:64:ILE:HG23	72:Bd:68:LEU:HD23	1.77	0.65
40:B5:2689:G:N7	92:B5:5473:HOH:O	2.29	0.65
34:Au:43:THR:OG1	34:Au:45:ARG:NH1	2.30	0.65
40:B5:3612:G:C8	92:B5:5497:HOH:O	2.49	0.65
40:B5:4361:C:H5''	44:BB:357:ARG:HE	1.62	0.65
87:Bv:67:VAL:HG12	87:Bv:84:HIS:HD2	1.62	0.65
40:B5:1588:G:O6	40:B5:3650:G:O2'	2.15	0.64
1:A2:165:G:OP2	1:A2:165:G:N2	2.31	0.64
40:B5:4194:G:H5''	40:B5:4195:A:H5''	1.78	0.64
17:Ad:44:LEU:HD21	17:Ad:72:ILE:HD11	1.78	0.64
1:A2:1600:U:OP2	38:Ay:46:ASN:ND2	2.30	0.64
7:AF:11:LEU:HB2	7:AF:307:VAL:HB	1.79	0.64
20:Ag:144:ILE:HB	35:Av:52:ILE:HB	1.79	0.64
40:B5:1846:A:H4'	48:BF:222:LYS:HE3	1.80	0.64
40:B5:2266:A:N7	92:B5:5483:HOH:O	2.30	0.64
1:A2:929:G:H1	1:A2:1014:U:H3	1.46	0.64
1:A2:1843:4AC:O7	39:Az:4:LYS:NZ	2.30	0.64
40:B5:4018:G:OP2	40:B5:4018:G:N2	2.29	0.64
64:BV:13:LYS:HB3	64:BV:128:LEU:HD11	1.80	0.64
16:Ac:75:LYS:NZ	23:Aj:20:VAL:O	2.31	0.64
31:Ar:36:VAL:HG21	31:Ar:71:MET:HE3	1.79	0.64
8:AG:17:GLY:O	8:AG:27:ARG:NH1	2.31	0.64
50:BH:113:GLU:HG2	50:BH:125:ARG:HG2	1.79	0.64
63:BU:105:ASN:ND2	63:BU:111:GLU:OE1	2.31	0.64
1:A2:1249:B8N:O3'	1:A2:1250:C:OP2	2.15	0.63
18:Ae:49:LEU:HD12	29:Ap:50:LYS:HG2	1.79	0.63
29:Ap:58:LEU:HB3	29:Ap:62:ARG:HD2	1.81	0.63
40:B5:1922:A:H1'	40:B5:1949:A:H4'	1.80	0.63
6:AE:44:ILE:O	27:An:113:GLN:NE2	2.31	0.63
25:Al:75:ASN:N	25:Al:75:ASN:OD1	2.31	0.63
40:B5:3555:G:N2	40:B5:3555:G:OP2	2.31	0.63
15:Ab:201:GLY:O	22:Ai:54:ARG:NH2	2.22	0.63
40:B5:1311:C:N4	45:BC:229:LEU:O	2.31	0.63
40:B5:1915:G:N3	86:Bt:138:SER:OG	2.31	0.63
40:B5:3637:A:H5'	53:BK:4377:LYS:HE2	1.80	0.63
40:B5:2400:G:H1	40:B5:2413:U:H3	1.46	0.63
40:B5:1701:C:H42	40:B5:1709:A:H61	1.47	0.63
40:B5:308:G:OP2	40:B5:308:G:N2	2.25	0.63
16:Ac:70:THR:HG22	16:Ac:86:LEU:HD13	1.81	0.62
31:Ar:124:ARG:NE	31:Ar:130:ARG:O	2.30	0.62
40:B5:1394:U:HO2'	48:BF:33:ARG:HE	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ab:196:ILE:HB	15:Ab:223:TYR:HB2	1.80	0.62
28:Ao:18:ARG:NH1	31:Ar:88:LYS:O	2.32	0.62
1:A2:1594:C:H1'	32:As:12:GLN:HE22	1.64	0.62
40:B5:1652:G:N2	40:B5:2024:G:OP1	2.30	0.62
40:B5:1960:G:OP1	85:Bs:58:ASN:ND2	2.32	0.62
40:B5:1399:G:OP2	40:B5:1399:G:N2	2.31	0.62
40:B5:1908:G:H4'	85:Bs:36:GLY:HA2	1.81	0.62
1:A2:1663:U:O4	1:A2:1664:A:N6	2.33	0.62
8:AG:44:ARG:NH1	33:At:78:ASP:OD2	2.32	0.62
40:B5:3329:G:O4'	60:BR:143:HIS:NE2	2.33	0.62
40:B5:3812:G:O6	43:BA:72:ARG:NH2	2.33	0.62
50:BH:23:ARG:HE	50:BH:39:ASN:HA	1.64	0.62
32:As:60:THR:HG23	32:As:75:MET:HE2	1.82	0.62
46:BD:125:VAL:HG11	46:BD:199:ILE:HG21	1.81	0.62
59:BQ:119:LYS:HE3	59:BQ:121:LEU:HD21	1.81	0.62
74:Bf:43:LEU:O	74:Bf:109:ARG:NH1	2.29	0.62
87:Bv:183:ILE:HD13	87:Bv:206:ILE:HD13	1.81	0.62
50:BH:186:THR:O	50:BH:189:GLN:NE2	2.32	0.62
1:A2:513:A2M:HM'2	1:A2:514:G:H5'	1.82	0.62
1:A2:953:G:H21	27:An:52:THR:HG21	1.64	0.62
12:AU:73:VAL:HG23	12:AU:112:GLY:HA2	1.81	0.62
31:Ar:72:GLN:HG2	31:Ar:99:LEU:HD11	1.80	0.62
1:A2:437:OMG:HM22	1:A2:438:G:H5'	1.80	0.61
42:B8:81:C:O2'	76:Bh:2:ALA:N	2.33	0.61
44:BB:19:ARG:HB2	44:BB:234:ARG:HH21	1.65	0.61
44:BB:213:GLN:NE2	44:BB:285:TYR:O	2.32	0.61
51:BI:87:ILE:HG12	51:BI:138:ILE:HG12	1.82	0.61
72:Bd:38:PHE:HB3	72:Bd:78:ARG:HG2	1.82	0.61
79:Bk:13:LEU:HD23	79:Bk:16:ARG:HH21	1.65	0.61
85:Bs:32:ALA:O	85:Bs:85:ASN:ND2	2.32	0.61
40:B5:1937:A:N3	40:B5:1958:C:O2'	2.31	0.61
40:B5:2250:G:N2	80:Bl:51:LEU:OXT	2.33	0.61
40:B5:4282:OMC:HM22	40:B5:4283:C:H5'	1.81	0.61
40:B5:4287:G:N2	40:B5:4290:A:OP2	2.30	0.61
42:B8:85:U:O4	67:BY:50:ARG:NH2	2.34	0.61
15:Ab:171:GLY:O	35:Av:98:GLN:NE2	2.33	0.61
40:B5:198:A:OP2	67:BY:126:ARG:NH2	2.34	0.61
59:BQ:79:THR:HB	59:BQ:136:THR:HG22	1.83	0.61
73:Be:78:LEU:O	84:Br:20:ARG:NH1	2.33	0.61
24:Ak:119:ASP:O	24:Ak:147:LYS:NZ	2.28	0.61
29:Ap:53:GLU:OE1	29:Ap:85:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:2261:A:P	92:B5:5402:HOH:O	2.49	0.61
40:B5:4364:OMG:H5''	64:BV:15:ARG:HB2	1.82	0.61
47:BE:104:ASN:OD1	47:BE:108:ARG:NH2	2.34	0.61
87:Bv:65:VAL:HG22	87:Bv:109:ALA:HB3	1.82	0.61
2:AA:11:SER:OG	2:AA:14:GLU:OE1	2.19	0.61
40:B5:842:G:OP1	48:BF:145:ASN:ND2	2.33	0.61
40:B5:1391:C:O2'	70:Bb:106:ARG:NH2	2.34	0.61
40:B5:4336:A2M:HM'2	40:B5:4337:U:H5'	1.83	0.61
1:A2:1844:G:N7	39:Az:4:LYS:NZ	2.48	0.61
48:BF:104:VAL:HG13	48:BF:135:VAL:HG12	1.83	0.61
1:A2:1569:C:OP1	32:As:96:SER:OG	2.18	0.61
40:B5:1757:G:N2	40:B5:1757:G:OP2	2.34	0.61
1:A2:856:G:O2'	24:Ak:71:ARG:NH1	2.34	0.60
8:AG:22:ARG:HH11	16:Ac:16:ILE:HG21	1.64	0.60
21:Ah:101:ILE:HD12	21:Ah:190:LEU:HD11	1.82	0.60
30:Aq:94:GLU:HG2	30:Aq:95:ILE:HG13	1.81	0.60
40:B5:856:A:H1'	40:B5:2015:G:H5''	1.83	0.60
40:B5:4304:U:OP2	44:BB:246:ARG:NH2	2.33	0.60
57:BO:81:TRP:HB2	57:BO:104:VAL:HG21	1.83	0.60
22:Ai:170:PRO:O	22:Ai:175:ARG:NH1	2.34	0.60
40:B5:1934:G:H21	85:Bs:41:GLN:HE22	1.49	0.60
65:BW:2:LYS:NZ	65:BW:4:GLU:OE2	2.34	0.60
21:Ah:56:ARG:NH1	21:Ah:180:GLY:O	2.34	0.60
34:Au:15:ARG:NH1	34:Au:33:GLN:OE1	2.34	0.60
40:B5:1394:U:O2'	48:BF:33:ARG:NE	2.30	0.60
51:BI:51:HIS:CD2	51:BI:168:SER:HB2	2.36	0.60
87:Bv:63:PHE:O	87:Bv:152:LYS:NZ	2.34	0.60
1:A2:1522:C:OP2	31:Ar:136:THR:OG1	2.19	0.60
1:A2:1730:U:H3	1:A2:1806:G:H1	1.48	0.60
40:B5:228:C:O2'	67:BY:14:ASN:ND2	2.35	0.60
40:B5:1334:G:N2	40:B5:1337:G:OP2	2.27	0.60
40:B5:4068:G:N2	40:B5:4071:A:OP2	2.33	0.60
1:A2:282:C:H2'	1:A2:892:G:H1'	1.83	0.60
1:A2:1842:C:H2'	1:A2:1843:4AC:H6	1.82	0.60
40:B5:2250:G:N2	40:B5:2250:G:OP2	2.30	0.60
40:B5:2473:U:O4	63:BU:89:LYS:NZ	2.34	0.60
40:B5:3374:A:HO2'	78:Bj:2:THR:N	2.00	0.60
41:B7:6:C:H4'	46:BD:52:ILE:HD13	1.82	0.60
58:BP:8:PRO:HG3	58:BP:149:ILE:HD13	1.84	0.60
1:A2:1399:G:O2'	7:AF:88:ARG:NH2	2.35	0.60
1:A2:1548:C:N4	1:A2:1587:U:O4	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1551:G:H3'	1:A2:1580:A:H61	1.66	0.60
40:B5:178:C:H42	40:B5:258:G:H1	1.49	0.60
1:A2:561:A:OP2	22:Ai:177:ASN:ND2	2.35	0.60
40:B5:992:C:OP1	40:B5:1106:U:O2'	2.20	0.60
40:B5:1631:C:OP2	92:B5:5420:HOH:O	2.17	0.60
1:A2:430:C:O2'	1:A2:812:A:N1	2.34	0.60
1:A2:635:A:OP1	5:AD:87:ARG:NH2	2.35	0.60
10:AJ:28:C:H42	10:AJ:42:G:H1	1.49	0.60
40:B5:2293:G:OP1	43:BA:17:ARG:NH1	2.35	0.60
1:A2:421:G:OP1	35:Av:88:LYS:NZ	2.34	0.59
8:AG:54:LYS:NZ	33:At:78:ASP:OD1	2.33	0.59
31:Ar:13:LEU:HB2	31:Ar:20:ILE:HB	1.84	0.59
34:Au:38:GLU:OE2	34:Au:51:LYS:NZ	2.35	0.59
40:B5:4744:G:N2	40:B5:4780:G:O2'	2.35	0.59
1:A2:194:C:H42	1:A2:205:G:H1	1.49	0.59
24:Ak:135:SER:O	24:Ak:139:ARG:NH1	2.35	0.59
37:Ax:57:VAL:HB	37:Ax:60:PHE:HE1	1.67	0.59
40:B5:3420:U:OP2	43:BA:198:ARG:NH2	2.35	0.59
40:B5:458:C:OP2	47:BE:117:ARG:NH1	2.36	0.59
40:B5:1297:G:N7	59:BQ:104:ARG:NH2	2.50	0.59
40:B5:3387:C:N4	92:B5:5458:HOH:O	2.34	0.59
40:B5:4383:OMG:HM22	40:B5:4384:U:H5'	1.84	0.59
40:B5:4621:U:OP1	55:BM:117:LYS:NZ	2.34	0.59
54:BL:56:ARG:NH1	54:BL:74:ARG:O	2.35	0.59
40:B5:1529:G:N7	92:B5:5501:HOH:O	2.32	0.59
40:B5:4231:C:O2'	81:Bm:114:LYS:NZ	2.34	0.59
40:B5:4666:G:N2	40:B5:4666:G:OP2	2.36	0.59
43:BA:101:VAL:HG22	43:BA:165:VAL:HG22	1.82	0.59
1:A2:1148:C:OP1	6:AE:6:ARG:NH1	2.35	0.59
7:AF:217:MET:HG2	7:AF:229:THR:HG22	1.85	0.59
40:B5:2221:G:N2	40:B5:2224:A:OP2	2.35	0.59
44:BB:261:ARG:HB2	57:BO:64:THR:HG21	1.83	0.59
10:AJ:58:A:O2'	10:AJ:60:C:OP2	2.20	0.59
13:AZ:94:THR:HG23	13:AZ:186:ARG:HH12	1.68	0.59
40:B5:707:C:O2	47:BE:133:LYS:NZ	2.36	0.59
40:B5:2205:U:H2'	40:B5:2206:A2M:H8	1.83	0.59
40:B5:2688:A:H61	40:B5:3575:C:H42	1.51	0.59
42:B8:38:U:O2'	76:Bh:86:LYS:NZ	2.32	0.59
1:A2:153:G:N3	19:Af:13:GLN:NE2	2.50	0.59
1:A2:1161:U:O4	36:Aw:2:GLY:N	2.35	0.59
40:B5:492:G:H4'	45:BC:3:CYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:375:G:OP2	78:Bj:52:LYS:NZ	2.36	0.59
40:B5:4218:G:O2'	81:Bm:100:TYR:O	2.20	0.59
40:B5:496:C:H42	40:B5:653:G:H1	1.49	0.59
40:B5:2366:G:OP1	60:BR:16:ARG:NH2	2.36	0.59
40:B5:734:G:OP2	55:BM:71:LYS:NZ	2.35	0.58
40:B5:2300:G:OP1	56:BN:65:ARG:NH2	2.35	0.58
40:B5:3930:G:H5'	43:BA:233:ARG:HB2	1.85	0.58
87:Bv:49:PHE:HB2	87:Bv:159:MET:HB2	1.84	0.58
1:A2:602:OMG:HM22	1:A2:603:G:H5'	1.83	0.58
14:Aa:71:LEU:HD11	14:Aa:189:ILE:HG23	1.84	0.58
15:Ab:102:LEU:HD22	15:Ab:130:ILE:HG12	1.85	0.58
1:A2:1661:C:OP1	8:AG:19:ARG:NH2	2.36	0.58
26:Am:103:GLU:HA	26:Am:106:ARG:HE	1.68	0.58
29:Ap:129:SER:O	29:Ap:131:LYS:NZ	2.36	0.58
40:B5:74:G:H1'	54:BL:62:PRO:HG3	1.84	0.58
40:B5:369:G:N2	40:B5:372:A:OP2	2.33	0.58
40:B5:2658:A2M:HM'2	40:B5:2659:G:H5'	1.85	0.58
52:BJ:90:ARG:NH2	52:BJ:110:GLN:OE1	2.37	0.58
2:AA:84:HIS:OXT	26:Am:19:ARG:NH1	2.36	0.58
40:B5:2637:C:P	92:B5:5435:HOH:O	2.60	0.58
64:BV:85:ARG:NH1	64:BV:99:GLU:O	2.32	0.58
1:A2:382:C:OP2	21:Ah:31:ARG:NH2	2.36	0.58
40:B5:4780:G:N1	44:BB:389:MET:O	2.34	0.58
1:A2:1446:PSU:O2	1:A2:1447:A:N6	2.37	0.58
19:Af:2:LYS:HG2	19:Af:17:GLU:HG2	1.84	0.58
40:B5:4292:A:N7	43:BA:215:ASN:ND2	2.51	0.58
72:Bd:54:MET:HE3	72:Bd:60:PRO:HA	1.86	0.58
1:A2:1601:G:H4'	38:Ay:43:LYS:HE3	1.84	0.58
40:B5:1631:C:H41	40:B5:4124:A:H5''	1.68	0.58
40:B5:1737:G:O2'	62:BT:60:LYS:NZ	2.37	0.58
40:B5:4761:U:H3	40:B5:4766:C:H42	1.51	0.58
46:BD:83:LEU:HB3	46:BD:88:VAL:HB	1.86	0.58
45:BC:221:PHE:HB3	45:BC:227:ILE:HG21	1.85	0.58
61:BS:46:TYR:OH	61:BS:125:GLN:NE2	2.37	0.58
1:A2:588:A:H5'	1:A2:593:C:H41	1.69	0.58
1:A2:1651:A:H5''	29:Ap:139:ALA:HB2	1.85	0.58
8:AG:52:PHE:HB3	33:At:80:PHE:HB3	1.85	0.58
40:B5:308:G:H2'	77:Bi:41:ARG:HH12	1.69	0.58
1:A2:43:U:OP2	1:A2:486:A:N6	2.35	0.58
41:B7:1:GTP:O1G	46:BD:265:ARG:NH1	2.36	0.58
72:Bd:19:GLU:OE1	72:Bd:92:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1014:U:OP1	1:A2:1130:G:O2'	2.22	0.57
1:A2:1289:OMU:HN3	1:A2:1312:C:H42	1.51	0.57
40:B5:1942:G:N2	40:B5:1943:U:O4	2.36	0.57
40:B5:3843:G:H4'	40:B5:3844:C:H5'	1.84	0.57
56:BN:5:LYS:HG3	77:Bi:40:VAL:HG11	1.85	0.57
40:B5:1736:G:C8	92:B5:5606:HOH:O	2.53	0.57
40:B5:2652:G:O2'	40:B5:4390:G:OP1	2.20	0.57
4:AC:116:ARG:NH1	4:AC:120:GLU:OE2	2.37	0.57
1:A2:1157:U:O4	15:Ab:194:ARG:NH1	2.38	0.57
38:Ay:74:SER:OG	38:Ay:79:ILE:O	2.21	0.57
40:B5:1804:G:N2	40:B5:1807:A:OP2	2.33	0.57
47:BE:181:PRO:HD2	47:BE:184:LEU:HD12	1.86	0.57
1:A2:1566:C:OP2	32:As:101:ARG:NH1	2.37	0.57
40:B5:3852:G:N2	49:BG:43:GLN:O	2.37	0.57
87:Bv:21:ASN:HB2	87:Bv:26:ARG:HD3	1.86	0.57
40:B5:1535:C:P	92:B5:5403:HOH:O	2.53	0.57
1:A2:371:G:O2'	21:Ah:10:LYS:NZ	2.37	0.57
28:Ao:12:PHE:H	52:BJ:91:GLU:HG2	1.68	0.57
31:Ar:46:ARG:HG2	32:As:35:ASP:HB2	1.85	0.57
40:B5:1101:C:N3	48:BF:65:ARG:NH2	2.53	0.57
40:B5:1341:A:HO2'	40:B5:1422:C:HO2'	1.53	0.57
40:B5:1415:C:H5''	59:BQ:144:LYS:HG2	1.86	0.57
40:B5:2546:G:H5''	63:BU:113:ARG:HH22	1.70	0.57
43:BA:30:ARG:O	43:BA:163:ARG:NH2	2.38	0.57
45:BC:316:LYS:HB2	45:BC:324:ILE:HG13	1.86	0.57
87:Bv:73:HIS:ND1	87:Bv:144:MET:SD	2.77	0.57
1:A2:360:U:OP2	36:Aw:18:ARG:NH1	2.36	0.57
1:A2:381:G:N1	1:A2:384:G:OP2	2.31	0.57
1:A2:1448:OMG:HM22	1:A2:1449:A:H5'	1.86	0.57
1:A2:1525:G:OP2	31:Ar:141:ARG:NH1	2.38	0.57
40:B5:1280:G:N7	92:B5:5506:HOH:O	2.33	0.57
40:B5:4631:A:H5''	57:BO:188:LYS:HD2	1.87	0.57
87:Bv:32:VAL:HA	87:Bv:208:SER:HA	1.87	0.57
1:A2:532:A:N6	1:A2:553:G:O6	2.38	0.57
1:A2:1220:C:O3'	18:Ae:127:ARG:NH2	2.38	0.57
13:AZ:198:MET:HG2	13:AZ:200:ASP:H	1.70	0.57
31:Ar:22:GLY:HA2	31:Ar:56:ALA:HB3	1.86	0.57
48:BF:126:LYS:HB2	62:BT:133:ALA:HB3	1.87	0.57
76:Bh:80:PRO:HD2	76:Bh:83:LEU:HD12	1.87	0.57
1:A2:469:A2M:HM'2	1:A2:470:A:H5'	1.87	0.56
30:Aq:29:HIS:HA	30:Aq:32:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1143:G:N2	1:A2:1146:A:OP2	2.34	0.56
1:A2:1256:G:O3'	8:AG:40:ARG:NH2	2.38	0.56
7:AF:214:GLY:HA2	7:AF:236:ILE:HG13	1.87	0.56
20:Ag:44:ASN:O	20:Ag:68:GLN:NE2	2.38	0.56
40:B5:2647:OMC:HM22	40:B5:2648:C:H5'	1.87	0.56
59:BQ:157:GLY:O	59:BQ:188:ASN:ND2	2.38	0.56
1:A2:1861:A:N7	6:AE:34:LYS:NZ	2.53	0.56
13:AZ:17:LYS:HB3	13:AZ:173:LEU:HD11	1.86	0.56
25:Al:79:VAL:HG11	25:Al:85:LEU:HB2	1.86	0.56
40:B5:375:G:N7	78:Bj:56:ARG:NH2	2.49	0.56
40:B5:709:G:OP1	45:BC:321:ASN:ND2	2.34	0.56
40:B5:1326:G:P	92:B5:5410:HOH:O	2.59	0.56
40:B5:1811:G:O2'	40:B5:3965:A:N3	2.37	0.56
40:B5:3456:A2M:HM'2	40:B5:3457:G:H5'	1.88	0.56
40:B5:3892:G:H2'	40:B5:3893:G:H8	1.70	0.56
40:B5:4794:G:N2	72:Bd:118:GLN:OE1	2.38	0.56
48:BF:189:LEU:HD21	48:BF:207:LEU:HD21	1.87	0.56
58:BP:118:GLN:NE2	58:BP:147:GLU:OE2	2.37	0.56
61:BS:15:ARG:HB3	61:BS:27:LEU:HD23	1.87	0.56
1:A2:689:U:H5'	20:Ag:103:LYS:HB2	1.88	0.56
40:B5:1879:G:N2	40:B5:4180:C:OP1	2.38	0.56
40:B5:3682:U:H2'	40:B5:3683:G:H8	1.71	0.56
40:B5:3699:G:N2	87:Bv:164:CYS:SG	2.79	0.56
47:BE:115:MET:O	84:Br:87:ARG:NH1	2.39	0.56
63:BU:28:PRO:HB2	63:BU:34:MET:HG2	1.87	0.56
70:Bb:56:LYS:O	70:Bb:60:ASN:ND2	2.34	0.56
1:A2:1273:C:HO2'	8:AG:2:GLY:N	2.04	0.56
16:Ac:177:LEU:HD13	16:Ac:182:LEU:HD13	1.88	0.56
21:Ah:113:TYR:OH	21:Ah:156:ALA:O	2.22	0.56
40:B5:184:U:H3	40:B5:253:G:H1	1.53	0.56
44:BB:95:THR:OG1	44:BB:98:GLY:O	2.22	0.56
70:Bb:48:LYS:O	70:Bb:51:LYS:NZ	2.39	0.56
1:A2:386:G:H5''	1:A2:388:C:H41	1.69	0.56
40:B5:2363:C:O2	40:B5:2483:G:N2	2.39	0.56
40:B5:3660:A:OP1	56:BN:90:ASN:ND2	2.37	0.56
40:B5:4416:C:O2'	40:B5:4418:A:OP2	2.23	0.56
1:A2:753:G:O2'	1:A2:754:C:O2	2.24	0.56
1:A2:1264:U:O2	8:AG:16:GLN:NE2	2.38	0.56
40:B5:3518:U:OP1	40:B5:4296:G:O2'	2.23	0.56
40:B5:4672:C:OP2	47:BE:265:LYS:NZ	2.39	0.56
71:Bc:9:LYS:HA	71:Bc:13:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Bs:48:ARG:HD3	86:Bt:123:ARG:HG2	1.88	0.56
13:AZ:63:ARG:HH21	34:Au:38:GLU:HA	1.69	0.56
20:Ag:57:ARG:NH2	20:Ag:89:GLY:O	2.39	0.56
42:B8:57:C:OP2	78:Bj:68:LYS:NZ	2.38	0.56
68:BZ:95:VAL:HG13	68:BZ:96:VAL:HG23	1.87	0.56
33:At:40:ILE:HD11	33:At:53:PRO:HD3	1.87	0.56
40:B5:4268:G:O2'	40:B5:4271:C:OP2	2.23	0.56
41:B7:120:U:H3'	46:BD:262:LYS:HE2	1.88	0.56
87:Bv:36:ILE:HD11	87:Bv:165:LEU:HD12	1.88	0.56
20:Ag:34:SER:HA	20:Ag:37:LYS:HB2	1.88	0.56
40:B5:481:G:O2'	40:B5:483:G:OP1	2.23	0.56
44:BB:215:GLU:OE2	44:BB:349:LYS:NZ	2.35	0.56
1:A2:1125:C:H5''	14:Aa:150:ILE:HG12	1.87	0.55
12:AU:82:GLN:OE1	12:AU:85:ARG:NH2	2.38	0.55
40:B5:1284:OMC:HM22	40:B5:1285:U:H5'	1.87	0.55
86:Bt:107:ASP:O	86:Bt:111:ASN:ND2	2.40	0.55
1:A2:189:U:H3	1:A2:210:PSU:HN3	1.54	0.55
1:A2:538:C:O2	1:A2:548:G:N2	2.39	0.55
1:A2:1680:A:H2'	18:Ae:60:ARG:HD2	1.88	0.55
2:AA:33:MET:HE2	2:AA:48:SER:HA	1.88	0.55
19:Af:98:ARG:NH2	19:Af:103:ASP:OD1	2.38	0.55
40:B5:4073:C:OP1	62:BT:70:HIS:NE2	2.38	0.55
52:BJ:90:ARG:NH2	52:BJ:108:GLY:O	2.38	0.55
84:Br:26:SER:OG	84:Br:28:GLU:OE1	2.19	0.55
1:A2:746:C:H42	1:A2:797:G:H1	1.53	0.55
1:A2:910:G:OP1	60:BR:176:ARG:NH2	2.36	0.55
13:AZ:176:TRP:HE1	13:AZ:197:VAL:HG23	1.71	0.55
40:B5:2469:U:O4	63:BU:97:ARG:NH1	2.35	0.55
40:B5:3386:G:O2'	40:B5:3425:U:OP1	2.23	0.55
81:Bm:94:MET:HG2	81:Bm:105:PRO:HA	1.87	0.55
86:Bt:18:THR:OG1	86:Bt:21:GLU:O	2.24	0.55
1:A2:1544:U:H5''	29:Ap:37:ARG:HH12	1.70	0.55
7:AF:133:ASN:HD21	7:AF:137:VAL:HB	1.70	0.55
40:B5:1545:C:H4'	40:B5:2700:A:H5'	1.88	0.55
40:B5:1624:A:N3	40:B5:1791:U:O2'	2.34	0.55
1:A2:142:C:N4	1:A2:330:G:OP1	2.39	0.55
13:AZ:77:ILE:HD11	13:AZ:99:ILE:HD12	1.89	0.55
40:B5:1458:A:H4'	40:B5:1459:G:H5'	1.88	0.55
40:B5:4294:A:H4'	40:B5:4295:G:O5'	2.05	0.55
50:BH:59:LYS:HE2	50:BH:66:GLU:HB3	1.88	0.55
87:Bv:96:ASN:HB3	87:Bv:99:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:510:OMG:HM22	1:A2:511:G:H5'	1.88	0.55
12:AU:66:GLU:OE1	16:Ac:94:ARG:NE	2.39	0.55
40:B5:3688:G:N2	40:B5:3785:C:O2	2.40	0.55
40:B5:3908:C:H5	49:BG:73:ARG:HH12	1.54	0.55
41:B7:77:A:H62	41:B7:99:G:H21	1.54	0.55
42:B8:102:G:OP1	78:Bj:20:ARG:NH1	2.36	0.55
51:BI:54:SER:HB2	51:BI:135:ILE:HD11	1.89	0.55
51:BI:55:ASP:OD2	51:BI:164:LYS:NZ	2.38	0.55
1:A2:839:G:O2'	1:A2:841:C:OP1	2.25	0.55
1:A2:879:G:H22	1:A2:909:A:H2	1.55	0.55
10:AJ:48:C:HO2'	10:AJ:59:G:HO2'	1.54	0.55
40:B5:1395:U:OP2	48:BF:33:ARG:NH2	2.39	0.55
40:B5:2105:G:OP2	84:Br:98:ARG:NH2	2.39	0.55
40:B5:4203:PSU:OP1	64:BV:50:ASN:ND2	2.35	0.55
40:B5:4708:C:O2'	58:BP:75:GLN:NE2	2.40	0.55
58:BP:14:SER:O	58:BP:105:LYS:NZ	2.38	0.55
1:A2:908:G:OP1	60:BR:165:LYS:NZ	2.40	0.55
14:Aa:189:ILE:HB	14:Aa:190:PRO:HD3	1.88	0.55
18:Ae:102:LEU:HD21	38:Ay:100:VAL:HG21	1.88	0.55
19:Af:58:LYS:HA	19:Af:107:SER:HB2	1.89	0.55
40:B5:1919:U:O4	86:Bt:57:ARG:NH2	2.40	0.55
40:B5:2422:G:N2	40:B5:2425:A:OP2	2.29	0.55
40:B5:3679:A:N6	40:B5:3793:G:O6	2.39	0.55
55:BM:11:ARG:NH1	55:BM:58:THR:O	2.38	0.55
85:Bs:125:ALA:HA	85:Bs:154:ILE:HB	1.88	0.55
19:Af:57:ASP:OD1	19:Af:61:PHE:N	2.40	0.55
19:Af:156:TYR:OH	65:BW:101:ARG:NH1	2.40	0.55
40:B5:4004:C:OP2	52:BJ:54:ARG:NH1	2.39	0.55
55:BM:29:ASP:OD1	55:BM:30:VAL:N	2.39	0.55
86:Bt:10:ILE:HG12	86:Bt:65:GLN:HG2	1.89	0.55
40:B5:4197:G:P	92:B5:5404:HOH:O	2.56	0.55
51:BI:48:LEU:HB2	51:BI:142:LEU:HD23	1.88	0.55
64:BV:13:LYS:HD2	64:BV:128:LEU:HD21	1.87	0.55
1:A2:116:OMU:HM22	1:A2:117:C:H5'	1.88	0.54
21:Ah:89:GLU:OE1	21:Ah:92:ARG:NH2	2.39	0.54
30:Aq:37:GLU:HG3	30:Aq:38:ILE:HG23	1.89	0.54
40:B5:373:G:OP2	78:Bj:36:LYS:NZ	2.32	0.54
40:B5:1741:A:H5''	40:B5:1742:G:H5'	1.87	0.54
40:B5:4679:C:OP1	47:BE:159:ARG:NH1	2.40	0.54
48:BF:126:LYS:HE2	48:BF:130:ASN:HD21	1.73	0.54
87:Bv:204:LEU:HD22	87:Bv:216:LEU:HD23	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:635:A:N7	92:A2:2129:HOH:O	2.32	0.54
1:A2:868:OMG:HM22	1:A2:869:G:H5'	1.89	0.54
3:AB:29:GLN:NE2	3:AB:66:ARG:O	2.40	0.54
6:AE:44:ILE:HD12	6:AE:65:PRO:HG2	1.88	0.54
40:B5:1924:G:H1'	40:B5:1942:G:H2'	1.89	0.54
40:B5:2499:U:H5''	68:BZ:38:TYR:HB3	1.89	0.54
42:B8:52:A:OP1	80:BI:21:ARG:NH1	2.38	0.54
65:BW:81:ALA:HB2	65:BW:87:LEU:HB2	1.90	0.54
1:A2:800:U:O4'	1:A2:868:OMG:N2	2.40	0.54
13:AZ:145:ILE:HG12	13:AZ:159:ILE:HB	1.89	0.54
40:B5:4175:C:N3	51:BI:158:LYS:NZ	2.55	0.54
50:BH:118:LEU:HD11	50:BH:167:VAL:HG22	1.90	0.54
70:Bb:36:ASP:HB3	70:Bb:39:PHE:HB3	1.90	0.54
87:Bv:138:LEU:HD21	87:Bv:147:LYS:HG2	1.89	0.54
19:Af:161:PRO:HD3	65:BW:84:GLY:HA2	1.88	0.54
40:B5:1805:U:OP1	51:BI:4:ARG:NH1	2.40	0.54
46:BD:208:MET:HE3	46:BD:233:PRO:HG3	1.90	0.54
1:A2:355:OMU:HM22	1:A2:356:G:H5'	1.89	0.54
7:AF:87:LEU:HD21	7:AF:108:VAL:HG11	1.88	0.54
40:B5:1341:A:O2'	40:B5:1422:C:O2'	2.21	0.54
47:BE:193:HIS:HB3	47:BE:196:PHE:HD2	1.71	0.54
1:A2:49:C:H2'	1:A2:473:C:H41	1.73	0.54
1:A2:1481:A:O2'	8:AG:56:ASP:OXT	2.26	0.54
14:Aa:179:ASN:ND2	14:Aa:183:GLU:OE1	2.40	0.54
28:Ao:103:ASN:ND2	28:Ao:120:SER:OG	2.41	0.54
40:B5:741:A:H2	40:B5:815:G:H22	1.54	0.54
40:B5:2194:OMC:HM22	40:B5:2195:U:H5'	1.90	0.54
40:B5:3831:C:H2'	40:B5:3832:G:H4'	1.88	0.54
54:BL:205:GLN:HG3	54:BL:209:LYS:HE3	1.89	0.54
40:B5:512:U:OP2	69:Ba:85:GLN:NE2	2.34	0.54
40:B5:2207:OMG:HM22	40:B5:2208:OMC:H5''	1.87	0.54
40:B5:4333:G:N2	44:BB:15:GLY:O	2.37	0.54
48:BF:121:PHE:O	48:BF:204:ASN:ND2	2.40	0.54
1:A2:1311:U:H5''	4:AC:130:VAL:HG13	1.89	0.54
40:B5:483:G:O2'	40:B5:486:C:OP2	2.21	0.54
40:B5:1899:A:H1'	85:Bs:63:LYS:HD2	1.89	0.54
43:BA:53:GLY:O	43:BA:192:LYS:NZ	2.33	0.54
51:BI:53:VAL:HG11	62:BT:158:PHE:HZ	1.73	0.54
14:Aa:44:ILE:HD12	14:Aa:69:VAL:HG21	1.90	0.54
20:Ag:65:PRO:HD2	20:Ag:68:GLN:HE21	1.72	0.54
27:An:92:ALA:HA	27:An:125:LYS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Av:45:GLY:O	35:Av:68:ARG:NH2	2.40	0.54
40:B5:3450:A2M:HM'2	40:B5:3451:A:H5'	1.90	0.54
45:BC:230:LEU:HD21	45:BC:236:ASN:H	1.73	0.54
50:BH:92:MET:HE2	50:BH:179:ILE:HG22	1.89	0.54
57:BO:125:LYS:HG2	57:BO:129:LEU:HD12	1.89	0.54
59:BQ:178:ARG:H	69:Ba:51:GLY:HA2	1.73	0.54
1:A2:1329:OMG:HM22	1:A2:1330:U:H5'	1.90	0.54
4:AC:118:ARG:NH1	4:AC:134:SER:OG	2.41	0.54
23:Aj:63:ALA:HB3	23:Aj:68:TYR:HE2	1.73	0.54
25:Al:11:VAL:HG13	25:Al:13:ASP:H	1.71	0.54
40:B5:2232:A:H4'	72:Bd:70:LYS:HG3	1.90	0.54
40:B5:3619:OMC:HM22	40:B5:3620:G:H5'	1.88	0.54
48:BF:226:PHE:N	48:BF:232:ALA:O	2.41	0.54
1:A2:68:A:OP2	19:Af:164:LYS:NZ	2.37	0.53
1:A2:1315:U:O2'	23:Aj:8:ARG:NH2	2.37	0.53
1:A2:1662:A:OP1	8:AG:19:ARG:NH1	2.38	0.53
1:A2:1824:A:OP1	36:Aw:60:LYS:NZ	2.41	0.53
40:B5:58:G:H4'	40:B5:59:A:H4'	1.90	0.53
40:B5:1125:C:H5	47:BE:62:SER:HB2	1.73	0.53
40:B5:2028:G:OP2	45:BC:294:LYS:NZ	2.40	0.53
40:B5:2470:C:OP1	63:BU:92:LYS:NZ	2.41	0.53
52:BJ:144:LYS:O	52:BJ:148:THR:OG1	2.19	0.53
54:BL:63:THR:HG21	69:Ba:66:ASN:HD22	1.73	0.53
86:Bt:13:VAL:HB	86:Bt:62:LEU:HB2	1.89	0.53
1:A2:75:G:O2'	1:A2:77:A:OP1	2.25	0.53
1:A2:956:A:N6	1:A2:972:G:O2'	2.40	0.53
3:AB:32:VAL:HG11	3:AB:56:LEU:HD12	1.90	0.53
46:BD:51:MET:HE3	46:BD:105:LEU:HD23	1.91	0.53
52:BJ:120:ASP:OD2	52:BJ:122:SER:OG	2.22	0.53
53:BK:4352:ILE:O	53:BK:4352:ILE:HG13	2.07	0.53
54:BL:91:ALA:HB1	54:BL:96:ILE:HB	1.89	0.53
62:BT:94:GLU:OE1	62:BT:94:GLU:N	2.39	0.53
1:A2:547:G:H21	1:A2:549:C:H42	1.54	0.53
14:Aa:219:LYS:NZ	83:Bp:89:LEU:O	2.41	0.53
40:B5:2161:G:N2	40:B5:2164:G:OP2	2.37	0.53
40:B5:3476:OMG:HM22	40:B5:3477:U:H5'	1.91	0.53
40:B5:3890:G:O2'	40:B5:3892:G:OP1	2.23	0.53
59:BQ:35:LEU:HB3	59:BQ:44:ASN:HD22	1.73	0.53
87:Bv:94:ASN:O	87:Bv:97:LYS:NZ	2.35	0.53
1:A2:109:PSU:O4	24:Ak:71:ARG:NH2	2.41	0.53
13:AZ:8:LEU:HD11	34:Au:39:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Ag:58:LYS:HB2	20:Ag:90:LYS:HG2	1.90	0.53
22:Ai:152:ASP:OD1	22:Ai:152:ASP:N	2.38	0.53
40:B5:724:G:OP2	48:BF:75:ARG:NE	2.41	0.53
40:B5:2243:G:H21	75:Bg:6:THR:HG22	1.73	0.53
40:B5:4792:U:OP1	40:B5:4793:C:N4	2.42	0.53
52:BJ:63:ARG:HH22	82:Bo:106:PHE:H	1.56	0.53
80:Bl:23:ILE:HG23	80:Bl:38:ASN:HB2	1.90	0.53
82:Bo:97:LYS:O	82:Bo:99:ARG:NH1	2.40	0.53
1:A2:397:U:OP2	24:Ak:79:LYS:NZ	2.40	0.53
1:A2:1205:A:N6	1:A2:1694:G:O6	2.41	0.53
1:A2:1805:OMU:HM22	1:A2:1806:G:H5'	1.91	0.53
14:Aa:175:GLU:OE1	14:Aa:187:LYS:NZ	2.35	0.53
17:Ad:174:LYS:O	17:Ad:179:ASN:ND2	2.42	0.53
33:At:19:ARG:HB2	33:At:117:ALA:HB3	1.90	0.53
40:B5:1584:G:N1	43:BA:208:GLU:OE1	2.36	0.53
45:BC:201:ARG:NH2	92:BC:502:HOH:O	2.41	0.53
86:Bt:14:TYR:O	86:Bt:31:LYS:NZ	2.41	0.53
40:B5:630:G:H2'	40:B5:631:G:C8	2.43	0.53
46:BD:152:ARG:HG3	46:BD:154:THR:HG23	1.90	0.53
82:Bo:59:LYS:NZ	82:Bo:61:LYS:O	2.41	0.53
1:A2:121:OMU:HM22	1:A2:122:G:H5'	1.91	0.53
19:Af:142:ARG:HA	19:Af:147:LEU:HB2	1.91	0.53
35:Av:80:ASP:OD1	35:Av:124:LYS:NZ	2.37	0.53
40:B5:115:C:OP1	56:BN:2:GLY:N	2.42	0.53
40:B5:1653:C:O2'	48:BF:176:ARG:NH2	2.42	0.53
40:B5:4052:OMU:HM22	40:B5:4053:A:H5'	1.90	0.53
68:BZ:92:ASP:HB3	68:BZ:95:VAL:HG12	1.90	0.53
13:AZ:33:GLN:HB3	13:AZ:154:LEU:HD12	1.91	0.53
40:B5:4484:C:OP1	40:B5:4808:U:O2'	2.23	0.53
76:Bh:4:ILE:HD12	76:Bh:53:SER:HB3	1.90	0.53
1:A2:531:U:H2'	1:A2:532:A:H8	1.74	0.53
1:A2:554:U:O4	1:A2:555:A:N6	2.41	0.53
30:Aq:44:LYS:HG3	30:Aq:47:ARG:HH21	1.72	0.53
40:B5:2599:G:O6	68:BZ:51:ARG:NH2	2.37	0.53
42:B8:75:OMG:HM22	42:B8:76:C:H5'	1.91	0.53
45:BC:140:LYS:HE3	45:BC:245:HIS:HB2	1.91	0.53
49:BG:229:ARG:NE	49:BG:232:GLU:OE2	2.42	0.53
1:A2:127:C:O2	17:Ad:134:LYS:NZ	2.38	0.53
1:A2:518:OMC:HM22	1:A2:519:G:H5'	1.90	0.53
1:A2:1084:A:N7	1:A2:1842:C:O2'	2.40	0.53
1:A2:1289:OMU:HM22	1:A2:1290:U:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Ad:100:ARG:HB2	17:Ad:114:ILE:HD13	1.91	0.53
26:Am:20:ARG:HH21	35:Av:56:HIS:HB3	1.73	0.53
29:Ap:97:GLN:HB2	29:Ap:105:LYS:HG3	1.91	0.53
42:B8:141:C:OP1	56:BN:38:ARG:NH1	2.41	0.53
45:BC:60:HIS:HA	45:BC:92:PHE:HE1	1.73	0.53
66:BX:82:THR:HG22	66:BX:155:ILE:HG23	1.90	0.53
74:Bf:41:PHE:HE1	74:Bf:110:ILE:HD13	1.74	0.53
87:Bv:74:CYS:SG	87:Bv:78:LYS:NZ	2.82	0.53
36:Aw:93:PHE:O	36:Aw:140:ARG:NH1	2.41	0.52
40:B5:2625:U:OP2	80:Bl:10:LYS:NZ	2.35	0.52
50:BH:44:GLU:OE2	55:BM:2:VAL:N	2.42	0.52
52:BJ:52:LYS:NZ	82:Bo:101:GLY:O	2.38	0.52
1:A2:26:U:H2'	1:A2:27:A2M:H8	1.91	0.52
1:A2:473:C:O2	1:A2:476:C:N4	2.41	0.52
1:A2:953:G:OP1	14:Aa:56:LYS:NZ	2.41	0.52
1:A2:1124:C:OP1	14:Aa:151:ARG:NH2	2.42	0.52
7:AF:133:ASN:HB3	7:AF:139:LYS:HE3	1.90	0.52
14:Aa:179:ASN:HB3	14:Aa:183:GLU:HB2	1.90	0.52
15:Ab:183:LYS:HD3	15:Ab:194:ARG:HH21	1.75	0.52
16:Ac:132:LYS:HD3	16:Ac:156:LEU:HD12	1.91	0.52
18:Ae:45:TYR:OH	18:Ae:65:GLN:NE2	2.42	0.52
29:Ap:132:PHE:O	29:Ap:140:ARG:NH2	2.37	0.52
40:B5:70:A:OP2	69:Ba:64:LYS:NZ	2.38	0.52
40:B5:404:U:O3'	67:BY:87:ARG:NH2	2.42	0.52
40:B5:3868:C:H2'	40:B5:3869:G:H8	1.74	0.52
1:A2:319:A:N1	19:Af:186:GLN:NE2	2.57	0.52
7:AF:20:GLN:HG2	7:AF:69:VAL:H	1.74	0.52
11:AT:57:A:O2'	11:AT:59:U:OP2	2.27	0.52
40:B5:137:G:H2'	40:B5:138:G:H8	1.74	0.52
60:BR:44:LEU:HD22	60:BR:49:LEU:HD12	1.90	0.52
84:Br:90:LEU:HD22	84:Br:111:ILE:HG23	1.91	0.52
85:Bs:65:ILE:HA	85:Bs:75:LEU:HD23	1.91	0.52
40:B5:67:C:N4	40:B5:325:U:O3'	2.41	0.52
40:B5:382:G:N1	40:B5:385:A:OP2	2.42	0.52
40:B5:1960:G:OP2	85:Bs:57:LYS:NZ	2.41	0.52
46:BD:65:ALA:HB2	46:BD:74:ILE:HD13	1.92	0.52
50:BH:141:LYS:NZ	50:BH:142:ASP:OD2	2.41	0.52
64:BV:69:LYS:NZ	64:BV:71:GLU:OE2	2.38	0.52
1:A2:528:C:O2	1:A2:560:G:N2	2.42	0.52
1:A2:1260:A:N6	1:A2:1520:U:OP1	2.38	0.52
1:A2:1416:C:O2'	32:As:132:ASP:OD2	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ab:191:VAL:HG11	15:Ab:236:PHE:HA	1.91	0.52
17:Ad:87:MET:HE2	17:Ad:123:LEU:HB2	1.92	0.52
40:B5:4437:A:O2'	50:BH:68:ALA:O	2.24	0.52
73:Be:37:LYS:HD2	73:Be:38:PRO:HD2	1.91	0.52
24:Ak:18:GLN:HG2	24:Ak:33:LEU:HD21	1.92	0.52
40:B5:4138:OMG:HM21	40:B5:4140:A:H2'	1.92	0.52
40:B5:4507:G:OP1	57:BO:117:ARG:NH2	2.43	0.52
45:BC:39:PHE:O	45:BC:43:ASN:ND2	2.35	0.52
17:Ad:131:VAL:HA	17:Ad:137:PRO:HA	1.91	0.52
40:B5:150:U:OP2	49:BG:200:THR:OG1	2.24	0.52
40:B5:1736:G:OP1	48:BF:103:LYS:NZ	2.42	0.52
40:B5:2100:C:O2'	40:B5:2102:G:OP2	2.22	0.52
40:B5:4071:A:H1'	46:BD:36:LEU:HD23	1.92	0.52
40:B5:4324:G:H2'	40:B5:4325:PSU:H6	1.75	0.52
47:BE:120:PRO:O	84:Br:112:ARG:NH1	2.40	0.52
48:BF:130:ASN:OD1	48:BF:133:ARG:NH1	2.43	0.52
58:BP:102:ALA:HB1	58:BP:107:LEU:HB2	1.92	0.52
61:BS:147:ASP:HB3	61:BS:150:ILE:HB	1.91	0.52
72:Bd:24:GLU:OE2	72:Bd:87:ARG:NH2	2.38	0.52
85:Bs:69:LEU:HD22	85:Bs:76:GLU:HB2	1.92	0.52
1:A2:1783:G:OP2	65:BW:71:ARG:NH2	2.43	0.52
11:AT:20:A:H61	11:AT:45:G:H2'	1.75	0.52
32:As:108:GLU:OE2	32:As:115:LYS:NZ	2.40	0.52
40:B5:2103:C:O2	84:Br:99:LYS:NZ	2.43	0.52
40:B5:4715:U:O2	44:BB:343:ARG:NH1	2.43	0.52
45:BC:186:SER:O	45:BC:188:ARG:NH1	2.43	0.52
59:BQ:30:LYS:NZ	84:Br:8:MET:SD	2.76	0.52
61:BS:99:ASP:OD1	61:BS:100:LEU:N	2.43	0.52
68:BZ:25:ILE:HA	68:BZ:43:VAL:HG12	1.92	0.52
1:A2:71:G:O6	19:Af:170:ARG:NH1	2.43	0.52
1:A2:1355:G:N2	1:A2:1358:A:OP2	2.39	0.52
1:A2:1356:C:O3'	15:Ab:238:LYS:NZ	2.43	0.52
1:A2:1520:U:OP2	92:A2:2107:HOH:O	2.19	0.52
3:AB:10:LYS:NZ	3:AB:36:ASP:OD2	2.39	0.52
5:AD:86:VAL:HA	5:AD:89:GLN:HE21	1.74	0.52
13:AZ:89:LYS:NZ	30:Aq:83:ASN:OD1	2.43	0.52
1:A2:599:G:O2'	1:A2:606:A:N1	2.39	0.51
1:A2:727:C:H2'	1:A2:728:G:H8	1.75	0.51
40:B5:1869:U:OP2	57:BO:49:ARG:NH1	2.34	0.51
47:BE:189:LEU:HD21	47:BE:256:VAL:HG21	1.92	0.51
82:Bo:26:TYR:HB3	82:Bo:67:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1618:G:N1	1:A2:1621:A:OP2	2.42	0.51
25:Al:91:LEU:HD22	25:Al:106:CYS:HB2	1.90	0.51
40:B5:2131:G:O2'	40:B5:2133:C:O5'	2.28	0.51
40:B5:3573:OMC:HM22	40:B5:3574:C:H5'	1.92	0.51
40:B5:4368:A:H4'	44:BB:13:SER:HB2	1.91	0.51
47:BE:45:HIS:ND1	47:BE:46:CYS:O	2.43	0.51
1:A2:462:U:H2'	1:A2:463:OMC:H6	1.76	0.51
1:A2:1286:G:O2'	4:AC:99:LYS:NZ	2.39	0.51
11:AT:17:G:N2	11:AT:57:A:O4'	2.42	0.51
40:B5:4311:C:O2	44:BB:268:ARG:NH2	2.43	0.51
12:AU:117:ASN:HD22	12:AU:120:VAL:HG23	1.74	0.51
40:B5:3997:A:H5''	52:BJ:108:GLY:HA3	1.92	0.51
44:BB:220:ILE:HB	44:BB:346:THR:HB	1.93	0.51
20:Ag:8:ILE:HD13	20:Ag:16:PRO:HB3	1.92	0.51
38:Ay:92:LEU:HD22	38:Ay:109:TYR:HE1	1.75	0.51
40:B5:706:C:OP1	47:BE:142:LYS:NZ	2.36	0.51
40:B5:2385:G:H4'	42:B8:128:C:H4'	1.93	0.51
40:B5:3631:OMG:HM22	40:B5:3632:G:H5'	1.93	0.51
86:Bt:95:GLN:HG3	86:Bt:98:ILE:HG12	1.91	0.51
1:A2:1675:G:N7	29:Ap:17:LYS:NZ	2.59	0.51
41:B7:6:C:O2'	46:BD:50:ARG:NH2	2.43	0.51
41:B7:48:G:OP1	46:BD:226:TYR:OH	2.28	0.51
48:BF:153:ILE:HD12	48:BF:190:ILE:HG12	1.92	0.51
1:A2:64:A:H2	1:A2:83:A:H62	1.58	0.51
10:AJ:18:G:N2	10:AJ:58:A:O4'	2.44	0.51
12:AU:122:GLY:O	12:AU:126:ARG:NE	2.36	0.51
40:B5:184:U:H3	40:B5:253:G:H22	1.57	0.51
40:B5:514:U:O2'	40:B5:516:U:O4	2.25	0.51
40:B5:1299:G:OP1	59:BQ:108:ARG:NH2	2.32	0.51
40:B5:1766:C:H1'	70:Bb:50:ASN:HD21	1.74	0.51
79:Bk:26:LYS:NZ	79:Bk:28:ASN:OD1	2.34	0.51
86:Bt:116:MET:HG3	86:Bt:132:ILE:HD11	1.92	0.51
36:Aw:68:LYS:HB3	36:Aw:91:LEU:HD22	1.91	0.51
40:B5:24:G:N7	78:Bj:46:LYS:NZ	2.58	0.51
40:B5:837:U:OP2	55:BM:48:GLN:NE2	2.44	0.51
40:B5:1713:C:H2'	40:B5:1714:A:H8	1.75	0.51
40:B5:1879:G:H22	40:B5:4180:C:H5''	1.76	0.51
40:B5:3609:A:OP1	92:B5:5422:HOH:O	2.19	0.51
40:B5:4381:A:OP1	40:B5:4382:PSU:O2'	2.28	0.51
1:A2:682:PSU:H4'	36:Aw:9:THR:HG22	1.93	0.51
40:B5:237:G:N7	92:B5:5533:HOH:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:751:G:H2'	40:B5:752:G:H8	1.76	0.51
40:B5:2253:C:H42	40:B5:2277:G:H1	1.59	0.51
40:B5:2258:OMU:HM22	40:B5:2259:G:H5'	1.93	0.51
40:B5:2365:G:OP2	75:Bg:29:ARG:NH2	2.39	0.51
40:B5:2402:G:H1	40:B5:2411:C:H42	1.58	0.51
42:B8:47:C:H1'	42:B8:61:A:H2'	1.92	0.51
45:BC:133:LEU:HD13	84:Br:6:GLN:HE21	1.76	0.51
40:B5:2539:A:H62	79:Bk:35:LYS:NZ	2.09	0.51
40:B5:4263:A:OP2	44:BB:2:SER:N	2.44	0.51
40:B5:4273:G:OP2	40:B5:4273:G:N2	2.40	0.51
45:BC:14:LYS:HA	45:BC:173:LYS:HD3	1.93	0.51
1:A2:1330:U:O2'	1:A2:1333:A:OP2	2.22	0.50
1:A2:1498:G:N7	23:Aj:25:LYS:NZ	2.54	0.50
36:Aw:131:LEU:HD11	36:Aw:135:LYS:HE3	1.93	0.50
40:B5:1741:A:O2'	40:B5:1776:A:OP1	2.27	0.50
52:BJ:35:ARG:HD2	52:BJ:123:ILE:HA	1.92	0.50
55:BM:24:LEU:HB2	55:BM:43:THR:HG21	1.93	0.50
56:BN:155:VAL:O	56:BN:162:ARG:NH2	2.33	0.50
78:Bj:30:GLN:NE2	92:Bj:202:HOH:O	2.38	0.50
1:A2:378:G:H5'	21:Ah:98:LYS:HB3	1.92	0.50
1:A2:463:OMC:HM22	1:A2:464:C:H5'	1.93	0.50
1:A2:630:A:O2'	1:A2:632:U:OP1	2.29	0.50
37:Ax:117:VAL:HG11	37:Ax:125:VAL:HG21	1.93	0.50
40:B5:261:G:H2'	40:B5:262:G:C8	2.47	0.50
40:B5:1061:G:H1	40:B5:1082:C:H42	1.59	0.50
50:BH:41:ILE:HG22	50:BH:43:VAL:HG13	1.92	0.50
60:BR:169:ALA:HA	60:BR:172:ARG:HE	1.76	0.50
64:BV:87:SER:HB3	65:BW:19:ARG:HH21	1.75	0.50
76:Bh:67:GLU:HG2	76:Bh:71:LYS:HE3	1.93	0.50
16:Ac:42:THR:OG1	16:Ac:45:ARG:O	2.25	0.50
40:B5:308:G:O6	56:BN:12:ARG:NH1	2.45	0.50
40:B5:1988:G:HO2'	40:B5:3616:PSU:HO2'	1.58	0.50
40:B5:3480:A:O2'	43:BA:223:SER:OG	2.20	0.50
45:BC:328:LEU:HB3	48:BF:186:MET:HG3	1.92	0.50
47:BE:209:VAL:HG23	47:BE:263:LYS:HZ2	1.75	0.50
50:BH:37:ASP:OD2	50:BH:39:ASN:ND2	2.45	0.50
76:Bh:13:LYS:NZ	76:Bh:16:GLU:OE2	2.44	0.50
13:AZ:41:ARG:HE	13:AZ:45:GLY:HA2	1.76	0.50
27:An:98:ARG:HB3	27:An:132:VAL:HG23	1.93	0.50
36:Aw:39:ASN:HD22	36:Aw:43:GLY:H	1.59	0.50
37:Ax:76:TYR:OH	37:Ax:86:GLU:OE1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:526:C:H2'	40:B5:527:G:H8	1.75	0.50
40:B5:1310:G:O6	45:BC:222:ARG:NH1	2.45	0.50
40:B5:4682:A:OP1	47:BE:158:GLY:N	2.36	0.50
57:BO:128:ARG:NH1	61:BS:162:GLN:OE1	2.44	0.50
58:BP:40:HIS:NE2	58:BP:110:ASP:O	2.39	0.50
86:Bt:32:ILE:HB	86:Bt:35:LEU:HD11	1.93	0.50
1:A2:380:C:H5'	21:Ah:33:ALA:HA	1.92	0.50
1:A2:1357:G:O3'	15:Ab:125:LYS:NZ	2.44	0.50
37:Ax:7:ILE:HG22	37:Ax:27:VAL:HG22	1.92	0.50
40:B5:1208:C:H2'	40:B5:1209:G:H8	1.76	0.50
40:B5:3979:A:H4'	82:Bo:98:LYS:HD2	1.91	0.50
52:BJ:35:ARG:NH1	52:BJ:123:ILE:O	2.45	0.50
52:BJ:81:GLU:OE2	52:BJ:85:LYS:NZ	2.40	0.50
62:BT:18:PRO:HG2	62:BT:21:LYS:HB2	1.92	0.50
13:AZ:79:SER:HA	13:AZ:101:GLY:HA2	1.92	0.50
35:Av:101:PHE:HA	35:Av:113:HIS:CE1	2.46	0.50
40:B5:2548:G:O6	60:BR:46:LYS:NZ	2.31	0.50
1:A2:35:C:H2'	1:A2:36:PSU:H6	1.77	0.50
1:A2:464:C:O2'	1:A2:467:G:O6	2.27	0.50
1:A2:1715:U:H2'	1:A2:1716:A:C8	2.46	0.50
12:AU:68:LEU:HD22	16:Ac:104:SER:HA	1.93	0.50
32:As:40:ALA:HB3	32:As:43:LYS:HG2	1.94	0.50
33:At:20:ILE:HG12	33:At:98:VAL:HG21	1.94	0.50
38:Ay:58:LEU:HD12	38:Ay:62:VAL:HG21	1.94	0.50
40:B5:1827:A:N6	40:B5:3605:G:O2'	2.45	0.50
40:B5:2301:C:O2'	40:B5:3403:G:N3	2.45	0.50
40:B5:4649:A:H4'	44:BB:95:THR:HG22	1.93	0.50
46:BD:59:ASP:OD1	46:BD:60:ILE:N	2.45	0.50
68:BZ:81:MET:HE1	71:Bc:59:GLU:HG3	1.93	0.50
72:Bd:37:GLY:O	72:Bd:41:ARG:HG3	2.12	0.50
1:A2:17:C:O2'	1:A2:1195:A:N1	2.44	0.50
1:A2:220:U:H2'	1:A2:221:A:C8	2.47	0.50
1:A2:280:G:H2'	1:A2:281:G:C8	2.47	0.50
21:Ah:124:LYS:HB2	21:Ah:127:ALA:HB2	1.94	0.50
40:B5:257:C:H2'	40:B5:258:G:H8	1.75	0.50
40:B5:1713:C:H2'	40:B5:1714:A:C8	2.47	0.50
40:B5:3892:G:H2'	40:B5:3893:G:C8	2.47	0.50
41:B7:23:A:N3	41:B7:118:C:O2'	2.43	0.50
48:BF:105:ARG:NH1	59:BQ:4:ASP:OD1	2.45	0.50
58:BP:42:ARG:HH12	58:BP:109:VAL:HG12	1.77	0.50
12:AU:128:ILE:HG13	12:AU:130:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Af:85:ARG:O	19:Af:87:ARG:NH1	2.44	0.50
19:Af:192:ILE:HG22	19:Af:196:LYS:HE2	1.94	0.50
40:B5:448:G:OP2	40:B5:449:C:O2'	2.29	0.50
40:B5:1550:G:P	92:B5:5439:HOH:O	2.70	0.50
40:B5:3677:A:H61	40:B5:3796:U:H3	1.59	0.50
45:BC:110:ARG:O	45:BC:113:ARG:NH1	2.34	0.50
45:BC:159:GLU:HA	45:BC:217:ILE:HB	1.93	0.50
56:BN:53:TYR:HB2	56:BN:133:ILE:HD13	1.93	0.50
63:BU:48:LYS:HG2	63:BU:53:ALA:HB2	1.94	0.50
1:A2:523:A:H5''	22:Ai:145:PRO:HD2	1.92	0.49
25:Al:49:LEU:HD11	25:Al:77:ILE:HD13	1.93	0.49
40:B5:2272:A:H5''	80:Bl:43:HIS:HE2	1.77	0.49
51:BI:169:LYS:NZ	62:BT:157:GLU:OE2	2.35	0.49
56:BN:116:LEU:HD22	56:BN:135:ILE:HD11	1.93	0.49
60:BR:15:LEU:HD13	60:BR:52:ARG:HB2	1.94	0.49
1:A2:935:G:H22	1:A2:1009:A:H2	1.60	0.49
1:A2:1598:C:OP2	38:Ay:85:ARG:NH2	2.34	0.49
1:A2:1804:U:H2'	1:A2:1805:OMU:H6	1.94	0.49
18:Ae:40:ALA:HB1	18:Ae:45:TYR:CG	2.47	0.49
40:B5:261:G:H2'	40:B5:262:G:H8	1.77	0.49
40:B5:1211:G:N7	70:Bb:111:ARG:NH1	2.57	0.49
41:B7:47:G:H21	46:BD:222:GLN:HE22	1.60	0.49
52:BJ:32:ARG:HD2	52:BJ:35:ARG:HH22	1.77	0.49
1:A2:191:A:H3'	1:A2:192:C:H5''	1.93	0.49
9:AH:3435:G:H1	10:AJ:34:C:H42	1.61	0.49
28:Ao:41:GLN:HG3	28:Ao:84:ILE:HD13	1.94	0.49
31:Ar:36:VAL:HG13	31:Ar:40:TYR:HD2	1.77	0.49
40:B5:3457:G:N2	40:B5:3460:A:OP2	2.33	0.49
40:B5:4051:G:O5'	62:BT:83:LYS:NZ	2.44	0.49
40:B5:4429:U:OP2	40:B5:4452:G:N1	2.36	0.49
47:BE:170:GLN:HE21	47:BE:174:GLY:HA2	1.77	0.49
73:Be:65:LYS:O	73:Be:75:ARG:NH2	2.45	0.49
1:A2:923:A:OP2	35:Av:28:ARG:NH2	2.45	0.49
1:A2:1443:OMU:HM22	1:A2:1444:C:H5'	1.94	0.49
1:A2:1492:G:OP1	92:A2:2105:HOH:O	2.18	0.49
1:A2:1704:OMC:HM22	1:A2:1705:C:H5'	1.94	0.49
40:B5:1223:A:O2'	40:B5:1225:G:N7	2.38	0.49
40:B5:1610:C:OP2	69:Ba:26:ARG:NH1	2.45	0.49
40:B5:4254:C:H5''	64:BV:43:LYS:HD3	1.93	0.49
45:BC:293:LEU:O	45:BC:299:GLN:NE2	2.44	0.49
52:BJ:15:LEU:HD12	52:BJ:165:TRP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BK:4365:LEU:O	53:BK:4367:ASN:ND2	2.44	0.49
1:A2:1041:G:H2'	1:A2:1042:G:H8	1.78	0.49
1:A2:1659:G:OP2	1:A2:1661:C:N4	2.45	0.49
4:AC:102:VAL:HG21	25:Al:35:ILE:HG21	1.95	0.49
7:AF:29:ASP:OD1	7:AF:47:ARG:NH1	2.38	0.49
26:Am:83:ASP:OD1	26:Am:83:ASP:N	2.45	0.49
40:B5:74:G:H5'	54:BL:59:VAL:HB	1.93	0.49
40:B5:630:G:H2'	40:B5:631:G:H8	1.76	0.49
40:B5:859:G:O2'	40:B5:2106:A:N6	2.45	0.49
40:B5:1420:G:OP1	70:Bb:44:ARG:NH1	2.45	0.49
40:B5:3352:G:OP1	40:B5:3354:C:N4	2.46	0.49
1:A2:1666:G:P	32:As:91:HIS:HE2	2.35	0.49
19:Af:103:ASP:OD2	19:Af:105:ASN:ND2	2.35	0.49
40:B5:280:G:OP2	56:BN:44:ARG:NH2	2.41	0.49
40:B5:1898:U:H1'	40:B5:1900:G:C2	2.48	0.49
46:BD:186:GLU:N	46:BD:186:GLU:OE1	2.44	0.49
56:BN:8:GLN:OE1	56:BN:50:ARG:NH2	2.46	0.49
74:Bf:36:ARG:HB2	74:Bf:80:ASN:HA	1.93	0.49
13:AZ:187:GLY:HA2	34:Au:45:ARG:HE	1.76	0.49
38:Ay:79:ILE:HB	38:Ay:83:LEU:HD23	1.94	0.49
40:B5:2745:G:OP2	40:B5:3328:A:N6	2.41	0.49
40:B5:4317:A2M:HM'2	40:B5:4318:U:H5'	1.94	0.49
47:BE:273:TYR:OH	55:BM:106:ASP:OD2	2.28	0.49
54:BL:81:LEU:HD12	54:BL:86:ILE:HB	1.94	0.49
75:Bg:83:CYS:SG	75:Bg:86:CYS:HB2	2.52	0.49
1:A2:398:G:OP2	24:Ak:108:ASN:ND2	2.46	0.49
1:A2:589:G:OP2	1:A2:589:G:N2	2.37	0.49
1:A2:1417:C:OP1	32:As:129:ARG:NH1	2.45	0.49
1:A2:1845:U:OP1	39:Az:11:ARG:NH2	2.40	0.49
7:AF:154:VAL:O	7:AF:155:ARG:NH1	2.41	0.49
15:Ab:121:ARG:NH1	15:Ab:121:ARG:O	2.46	0.49
20:Ag:143:ARG:HB2	20:Ag:155:LYS:HB2	1.95	0.49
22:Ai:107:GLU:O	22:Ai:113:GLN:NE2	2.46	0.49
29:Ap:34:VAL:HG22	29:Ap:70:VAL:HB	1.95	0.49
40:B5:375:G:O6	78:Bj:56:ARG:NE	2.41	0.49
40:B5:512:U:O5'	54:BL:163:LYS:NZ	2.45	0.49
40:B5:1724:C:OP1	51:BI:133:GLN:NE2	2.44	0.49
40:B5:2408:A:C5	40:B5:2409:G:H1'	2.47	0.49
40:B5:4632:A:OP1	57:BO:188:LYS:NZ	2.45	0.49
1:A2:875:G:H2'	1:A2:876:A:C8	2.47	0.49
1:A2:1018:U:H5'	26:Am:55:ARG:HE	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AF:78:ALA:HB3	7:AF:90:TRP:HB2	1.95	0.49
7:AF:119:GLN:HB3	7:AF:131:LEU:HD11	1.95	0.49
7:AF:150:TRP:NE1	30:Aq:37:GLU:OE1	2.46	0.49
11:AT:16:G:H21	11:AT:58:A:H2'	1.77	0.49
40:B5:423:G:OP1	58:BP:62:ARG:NH1	2.43	0.49
40:B5:1215:G:H5''	70:Bb:110:ALA:HB1	1.94	0.49
40:B5:1268:A:O2'	40:B5:1270:A2M:OP1	2.24	0.49
40:B5:1772:G:OP1	62:BT:120:LYS:NZ	2.45	0.49
40:B5:2665:G:OP2	60:BR:21:LYS:NZ	2.42	0.49
40:B5:181:C:H42	40:B5:256:G:H1	1.61	0.49
40:B5:1214:A:H61	40:B5:2054:G:H21	1.61	0.49
40:B5:1815:U:H2'	40:B5:1816:G:C8	2.48	0.49
40:B5:4512:G:O6	55:BM:4:ARG:NH2	2.42	0.49
61:BS:74:ARG:O	61:BS:76:LYS:NZ	2.46	0.49
1:A2:28:U:H2'	1:A2:29:G:H8	1.78	0.48
1:A2:65:C:H4'	19:Af:172:LYS:HD3	1.95	0.48
1:A2:1036:A:O2'	1:A2:1857:C:O2	2.30	0.48
16:Ac:172:VAL:HG22	16:Ac:185:LYS:HG2	1.95	0.48
40:B5:85:G:N2	40:B5:98:A:OP2	2.42	0.48
40:B5:526:C:H2'	40:B5:527:G:C8	2.48	0.48
40:B5:2409:G:H2'	40:B5:2410:G:H8	1.77	0.48
40:B5:4741:U:OP2	44:BB:385:LYS:NZ	2.40	0.48
42:B8:36:G:C5	76:Bh:89:ARG:HD3	2.47	0.48
44:BB:317:LEU:HB2	44:BB:372:SER:HB2	1.95	0.48
80:Bl:28:TRP:HA	80:Bl:33:ASN:HD22	1.77	0.48
40:B5:755:G:H1	40:B5:800:U:H3	1.60	0.48
40:B5:3868:C:H2'	40:B5:3869:G:C8	2.48	0.48
40:B5:4189:C:O3'	92:B5:5425:HOH:O	2.20	0.48
67:BY:30:MET:HB3	67:BY:101:PRO:HG2	1.95	0.48
85:Bs:106:LYS:HB3	85:Bs:184:SER:HB3	1.95	0.48
1:A2:434:A:H5''	21:Ah:22:HIS:HB3	1.95	0.48
1:A2:831:A:OP2	1:A2:847:G:N2	2.43	0.48
1:A2:1674:U:O2'	18:Ae:84:GLY:O	2.29	0.48
32:As:104:LEU:HD13	32:As:121:ARG:HD3	1.94	0.48
35:Av:70:ASN:ND2	35:Av:130:PHE:OXT	2.40	0.48
40:B5:23:C:OP2	78:Bj:46:LYS:NZ	2.41	0.48
40:B5:480:C:OP1	84:Br:67:ARG:NH1	2.44	0.48
40:B5:1394:U:HO2'	48:BF:33:ARG:NE	2.08	0.48
40:B5:1423:C:OP1	69:Ba:132:ARG:NH2	2.43	0.48
40:B5:1568:A:H5'	43:BA:183:GLY:HA2	1.96	0.48
40:B5:1907:G:H4'	85:Bs:34:ASN:HD22	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:B8:60:G:OP1	66:BX:68:ARG:NH2	2.40	0.48
1:A2:1093:G:OP1	26:Am:2:GLY:N	2.46	0.48
1:A2:1260:A:H1'	1:A2:1265:C:H42	1.78	0.48
36:Aw:28:LYS:HE2	36:Aw:32:LEU:HD22	1.95	0.48
40:B5:1680:G:O6	41:B7:103:A:O2'	2.26	0.48
40:B5:2546:G:H5'	63:BU:113:ARG:HH12	1.78	0.48
86:Bt:112:ILE:HG22	86:Bt:132:ILE:HD13	1.95	0.48
1:A2:1564:G:OP1	32:As:121:ARG:NH1	2.47	0.48
7:AF:77:PHE:HB3	7:AF:89:LEU:HD11	1.95	0.48
10:AJ:63:C:H2'	10:AJ:64:A:C8	2.49	0.48
13:AZ:184:ARG:HD3	13:AZ:191:ARG:HG2	1.93	0.48
14:Aa:129:THR:OG1	14:Aa:131:ASP:OD1	2.26	0.48
15:Ab:183:LYS:NZ	35:Av:91:ASN:O	2.46	0.48
40:B5:238:C:OP2	67:BY:45:ARG:NH2	2.47	0.48
40:B5:399:G:H2'	40:B5:400:A2M:H8	1.95	0.48
40:B5:1829:G:OP2	40:B5:1829:G:N2	2.33	0.48
1:A2:485:A2M:O5'	1:A2:485:A2M:H8	2.13	0.48
1:A2:1338:4AC:H2'	1:A2:1339:G:C8	2.48	0.48
1:A2:1809:U:H2'	1:A2:1810:A:C8	2.49	0.48
3:AB:49:PRO:HG2	18:Ae:144:LEU:HD23	1.94	0.48
40:B5:3432:C:O2'	40:B5:3506:A:N3	2.42	0.48
48:BF:154:TYR:OH	48:BF:187:GLU:OE2	2.32	0.48
55:BM:5:ARG:NE	55:BM:59:ASP:OD1	2.45	0.48
61:BS:1:MET:HE3	61:BS:35:PRO:HD3	1.96	0.48
1:A2:5:U:H2'	1:A2:6:G:H8	1.79	0.48
1:A2:1173:U:H5''	39:Az:14:LYS:HD2	1.95	0.48
22:Ai:107:GLU:HA	22:Ai:112:THR:HG21	1.95	0.48
45:BC:94:ASN:HD22	45:BC:102:PHE:HB2	1.77	0.48
59:BQ:151:HIS:ND1	59:BQ:164:LYS:O	2.47	0.48
87:Bv:204:LEU:N	87:Bv:216:LEU:O	2.40	0.48
17:Ad:137:PRO:HG2	17:Ad:150:PRO:HD2	1.96	0.48
40:B5:1270:A2M:OP2	40:B5:4191:U:O2'	2.31	0.48
40:B5:2712:U:O2'	40:B5:2724:A:N7	2.41	0.48
49:BG:88:ASP:OD1	49:BG:88:ASP:N	2.40	0.48
51:BI:51:HIS:HD2	51:BI:168:SER:HB2	1.76	0.48
51:BI:101:LYS:NZ	51:BI:102:MET:O	2.46	0.48
7:AF:287:THR:N	7:AF:301:GLY:O	2.42	0.48
17:Ad:151:ASP:HB3	17:Ad:154:ILE:HG13	1.96	0.48
40:B5:2194:OMC:N4	92:B5:5626:HOH:O	2.46	0.48
40:B5:4313:G:H5'	44:BB:20:LYS:HB3	1.95	0.48
44:BB:248:LEU:HD12	44:BB:249:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BG:73:ARG:NH1	49:BG:241:VAL:O	2.47	0.48
59:BQ:178:ARG:N	69:Ba:51:GLY:HA2	2.28	0.48
85:Bs:30:VAL:HG21	85:Bs:187:LEU:HD13	1.95	0.48
1:A2:584:A:OP1	22:Ai:169:ARG:NH1	2.46	0.48
1:A2:1098:G:H4'	13:AZ:32:PHE:CD1	2.49	0.48
1:A2:1602:A:O2'	1:A2:1605:G:O6	2.24	0.48
14:Aa:123:ALA:HB2	14:Aa:165:ARG:HG3	1.95	0.48
20:Ag:20:GLU:HG2	20:Ag:48:ALA:HB3	1.95	0.48
40:B5:2584:U:H2'	43:BA:50:HIS:HD2	1.79	0.48
40:B5:3335:G:H2'	40:B5:3336:A:C8	2.49	0.48
42:B8:90:C:H2'	42:B8:91:A:C8	2.48	0.48
49:BG:83:PHE:HA	49:BG:183:ILE:HD13	1.94	0.48
1:A2:126:G:O6	19:Af:196:LYS:NZ	2.29	0.47
1:A2:925:G:H1	1:A2:1019:U:H3	1.62	0.47
1:A2:1832:A:H2'	1:A2:1833:6MZ:H8	1.96	0.47
7:AF:131:LEU:O	7:AF:139:LYS:N	2.45	0.47
26:Am:4:MET:SD	26:Am:124:ARG:NH2	2.87	0.47
40:B5:779:G:H2'	40:B5:780:G:H8	1.79	0.47
40:B5:1458:A:H62	59:BQ:87:THR:HG21	1.79	0.47
40:B5:2547:C:H2'	40:B5:2548:G:H8	1.79	0.47
40:B5:3562:A2M:HM'2	40:B5:3563:U:H5'	1.95	0.47
40:B5:4314:A:O3'	44:BB:21:ARG:NH2	2.47	0.47
40:B5:4745:U:H4'	40:B5:4746:A:H5'	1.96	0.47
41:B7:105:C:OP2	51:BI:203:ARG:NH1	2.43	0.47
48:BF:170:ASP:OD1	48:BF:171:ASN:N	2.47	0.47
52:BJ:13:ARG:O	52:BJ:136:ARG:NH1	2.47	0.47
69:Ba:72:THR:HG22	69:Ba:110:LYS:HB3	1.96	0.47
71:Bc:38:ILE:HD11	71:Bc:46:VAL:HG21	1.96	0.47
72:Bd:42:ALA:HB3	72:Bd:77:ILE:HG13	1.96	0.47
85:Bs:106:LYS:HD3	85:Bs:184:SER:HB2	1.95	0.47
1:A2:1118:C:O2'	1:A2:1119:C:O4'	2.31	0.47
1:A2:1666:G:OP1	32:As:91:HIS:NE2	2.40	0.47
13:AZ:66:VAL:HG21	13:AZ:185:MET:HB2	1.95	0.47
19:Af:102:VAL:HG13	19:Af:106:LEU:HD12	1.96	0.47
20:Ag:134:VAL:O	20:Ag:137:SER:OG	2.25	0.47
27:An:95:ILE:HB	27:An:129:ILE:HG12	1.96	0.47
33:At:48:LEU:HD22	33:At:93:SER:HB3	1.95	0.47
40:B5:435:A:O2'	73:Be:26:ASP:OD2	2.26	0.47
40:B5:1822:G:O2'	73:Be:48:ARG:O	2.29	0.47
72:Bd:65:ASP:OD1	72:Bd:66:THR:N	2.47	0.47
75:Bg:64:LEU:HD23	75:Bg:67:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Bs:20:LEU:HD22	85:Bs:52:VAL:HG11	1.96	0.47
1:A2:381:G:OP1	21:Ah:31:ARG:NE	2.33	0.47
1:A2:1048:C:H5''	27:An:143:LYS:HB2	1.96	0.47
5:AD:102:ARG:HD3	5:AD:106:ALA:HB1	1.95	0.47
40:B5:4261:G:H5''	44:BB:3:HIS:CE1	2.49	0.47
40:B5:4281:A:H2'	40:B5:4282:OMC:H6	1.79	0.47
40:B5:4719:C:N3	58:BP:69:ARG:NH2	2.56	0.47
44:BB:119:TYR:OH	44:BB:129:ALA:N	2.47	0.47
50:BH:41:ILE:HD13	50:BH:69:THR:HB	1.95	0.47
60:BR:106:LEU:HB3	60:BR:120:TYR:HE1	1.80	0.47
1:A2:239:C:H2'	1:A2:240:G:C8	2.49	0.47
40:B5:108:A:N1	40:B5:333:U:O2'	2.41	0.47
40:B5:2601:G:O2'	40:B5:2608:A:N3	2.38	0.47
85:Bs:141:LEU:HD12	85:Bs:174:LEU:HD12	1.97	0.47
87:Bv:111:LEU:HD21	87:Bv:151:VAL:HG21	1.97	0.47
1:A2:1180:G:N2	1:A2:1183:A:OP2	2.43	0.47
21:Ah:81:VAL:HG22	21:Ah:102:VAL:HG12	1.96	0.47
40:B5:2547:C:H2'	40:B5:2548:G:C8	2.49	0.47
42:B8:82:A:H1'	76:Bh:49:VAL:HG21	1.97	0.47
52:BJ:40:LEU:HD12	52:BJ:70:VAL:HG22	1.96	0.47
71:Bc:47:ILE:HD12	71:Bc:94:LEU:HD11	1.97	0.47
85:Bs:177:MET:O	85:Bs:179:ASN:ND2	2.48	0.47
1:A2:901:C:H2'	1:A2:902:G:H8	1.78	0.47
1:A2:925:G:H5'	26:Am:4:MET:HE3	1.96	0.47
1:A2:1405:U:OP1	33:At:21:ARG:NH2	2.38	0.47
5:AD:120:VAL:HG22	5:AD:121:PRO:HD2	1.95	0.47
6:AE:22:ARG:NH2	27:An:145:GLY:O	2.48	0.47
17:Ad:55:ALA:HB1	17:Ad:60:GLU:HB2	1.97	0.47
18:Ae:176:GLU:OE2	18:Ae:187:SER:OG	2.31	0.47
31:Ar:34:LYS:HB3	31:Ar:100:ALA:HA	1.96	0.47
40:B5:68:U:OP1	56:BN:178:HIS:ND1	2.39	0.47
40:B5:1891:G:OP1	61:BS:139:ARG:NE	2.40	0.47
40:B5:3497:G:O2'	40:B5:3499:C:N4	2.48	0.47
40:B5:4006:U:H2'	40:B5:4007:C:C6	2.50	0.47
40:B5:4481:G:H1	40:B5:4703:C:H42	1.63	0.47
40:B5:4506:C:OP2	57:BO:171:LYS:NZ	2.40	0.47
59:BQ:12:LYS:HB2	59:BQ:14:ARG:HH11	1.79	0.47
68:BZ:136:PHE:O	75:Bg:78:TYR:OH	2.31	0.47
86:Bt:14:TYR:HE2	86:Bt:74:VAL:HG21	1.78	0.47
1:A2:907:U:H2'	1:A2:908:G:C8	2.49	0.47
1:A2:1093:G:H2'	1:A2:1094:A:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1865:U:H3'	6:AE:5:ARG:HH21	1.80	0.47
2:AA:28:PRO:HG3	26:Am:17:PRO:HG3	1.97	0.47
7:AF:86:THR:HG22	7:AF:102:VAL:HG12	1.97	0.47
31:Ar:24:ARG:HH21	31:Ar:28:PHE:HB3	1.78	0.47
40:B5:158:A:H5''	40:B5:159:C:H2'	1.96	0.47
40:B5:417:G:OP1	40:B5:2172:U:O2'	2.27	0.47
40:B5:1935:C:H42	40:B5:1939:G:H22	1.62	0.47
40:B5:2322:G:H2'	40:B5:2323:G:H8	1.80	0.47
40:B5:2706:G:O2'	60:BR:82:LYS:O	2.27	0.47
40:B5:3600:G:H22	40:B5:3632:G:H1'	1.80	0.47
40:B5:3871:C:H2'	40:B5:3872:G:C8	2.50	0.47
40:B5:3995:G:H1	40:B5:4005:C:H42	1.61	0.47
40:B5:4698:U:H2'	40:B5:4699:G:C8	2.50	0.47
46:BD:120:GLU:O	46:BD:248:ARG:NH1	2.44	0.47
58:BP:116:HIS:CE1	58:BP:118:GLN:HB2	2.49	0.47
65:BW:96:GLN:O	65:BW:101:ARG:NH2	2.48	0.47
68:BZ:76:ASN:OD1	68:BZ:77:TYR:N	2.47	0.47
1:A2:1216:C:H42	1:A2:1221:A:H61	1.63	0.47
1:A2:1653:G:H1	1:A2:1673:U:H3	1.63	0.47
17:Ad:152:PRO:HG2	19:Af:216:ARG:HG3	1.97	0.47
40:B5:2658:A2M:P	40:B5:2658:A2M:H8	2.55	0.47
40:B5:3478:A:H5''	43:BA:244:GLY:HA3	1.96	0.47
40:B5:4323:U:H2'	40:B5:4324:G:C8	2.49	0.47
43:BA:80:GLU:HB2	43:BA:170:ALA:HA	1.97	0.47
64:Bv:21:PRO:HA	64:Bv:54:ALA:HA	1.96	0.47
87:Bv:94:ASN:HB2	87:Bv:123:ILE:HB	1.97	0.47
15:Ab:65:LYS:HA	15:Ab:68:ARG:HE	1.79	0.47
20:Ag:100:ILE:HG12	20:Ag:125:VAL:HG21	1.96	0.47
22:Ai:59:GLU:O	22:Ai:62:THR:OG1	2.27	0.47
28:Ao:83:MET:HB3	28:Ao:116:LEU:HD12	1.96	0.47
40:B5:4197:G:O6	40:B5:4268:G:H2'	2.15	0.47
42:B8:94:G:H21	78:Bj:82:THR:HB	1.80	0.47
43:BA:116:LEU:HB3	43:BA:126:LEU:HB2	1.96	0.47
44:BB:92:TYR:HB2	44:BB:159:VAL:HB	1.96	0.47
47:BE:156:LEU:HD11	47:BE:198:ILE:HG13	1.97	0.47
59:BQ:172:ARG:HA	59:BQ:176:ARG:HD2	1.96	0.47
75:Bg:60:ARG:HB2	75:Bg:63:VAL:HG23	1.97	0.47
85:Bs:122:THR:HG22	85:Bs:159:GLN:HG2	1.97	0.47
87:Bv:96:ASN:HD22	87:Bv:99:LEU:H	1.63	0.47
1:A2:996:G:O3'	26:Am:114:ARG:NH2	2.46	0.47
1:A2:1008:C:O2'	26:Am:104:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1279:A:H61	1:A2:1320:U:H3	1.62	0.47
7:AF:256:ILE:HB	7:AF:270:LEU:HB2	1.96	0.47
31:Ar:46:ARG:HH22	31:Ar:52:LEU:HD11	1.80	0.47
40:B5:417:G:O2'	42:B8:17:A:N6	2.48	0.47
40:B5:788:G:H2'	40:B5:789:G:C8	2.50	0.47
40:B5:1341:A:N1	40:B5:1453:G:O2'	2.47	0.47
40:B5:1485:G:O2'	78:Bj:45:ARG:NH2	2.46	0.47
40:B5:4069:A:H1'	46:BD:160:PHE:HE1	1.80	0.47
40:B5:4792:U:H3'	40:B5:4793:C:C6	2.49	0.47
72:Bd:23:ARG:HG2	72:Bd:121:ASN:HA	1.97	0.47
86:Bt:133:LEU:HD11	86:Bt:151:ILE:HG13	1.96	0.47
7:AF:23:THR:HG21	7:AF:292:SER:HA	1.97	0.46
34:Au:1:AME:HT23	34:Au:1:AME:HA	1.51	0.46
46:BD:41:LYS:NZ	62:BT:32:ARG:O	2.31	0.46
50:BH:120:GLU:OE1	50:BH:124:ARG:NH2	2.40	0.46
63:BU:47:ILE:HD12	63:BU:63:ILE:HD11	1.96	0.46
1:A2:65:C:C6	19:Af:174:PRO:HB3	2.51	0.46
1:A2:1776:U:H2'	1:A2:1777:G:H8	1.81	0.46
7:AF:5:MET:HG2	7:AF:312:VAL:HG22	1.98	0.46
7:AF:236:ILE:HG12	7:AF:252:THR:HG22	1.97	0.46
25:Al:126:GLU:HA	25:Al:129:LYS:HZ3	1.80	0.46
33:At:26:SER:HB3	33:At:32:LEU:HD22	1.97	0.46
40:B5:637:C:H2'	40:B5:638:G:C8	2.50	0.46
40:B5:1449:U:H2'	40:B5:1450:G:H8	1.79	0.46
40:B5:3588:A:H5''	58:BP:83:TRP:O	2.15	0.46
40:B5:4124:A:P	92:B5:5436:HOH:O	2.73	0.46
45:BC:60:HIS:NE2	45:BC:100:ARG:HD3	2.30	0.46
52:BJ:95:ARG:NH2	52:BJ:176:PRO:O	2.48	0.46
55:BM:86:TRP:O	55:BM:89:THR:OG1	2.33	0.46
79:Bk:17:ARG:NH2	79:Bk:19:ASP:OD2	2.49	0.46
1:A2:99:A2M:HM'2	1:A2:100:U:H5'	1.96	0.46
1:A2:206:G:H2'	1:A2:207:G:C8	2.50	0.46
1:A2:521:A:O2'	1:A2:826:A:N3	2.34	0.46
1:A2:691:G:H2'	1:A2:692:G:C8	2.49	0.46
1:A2:1026:U:P	92:A2:2117:HOH:O	2.72	0.46
1:A2:1293:C:N3	4:AC:138:ARG:NH2	2.56	0.46
1:A2:1754:C:H2'	1:A2:1755:G:H8	1.79	0.46
8:AG:23:VAL:HG21	8:AG:38:MET:HE3	1.97	0.46
17:Ad:211:LYS:NZ	17:Ad:215:GLY:O	2.39	0.46
27:An:59:GLY:HA2	27:An:68:GLU:HG2	1.97	0.46
31:Ar:16:LEU:HD13	31:Ar:99:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:4269:A2M:H5''	40:B5:4270:G:H5'	1.96	0.46
43:BA:20:VAL:HG12	43:BA:23:ARG:HD2	1.95	0.46
68:BZ:11:VAL:HG12	68:BZ:82:PRO:HA	1.98	0.46
1:A2:1018:U:OP1	26:Am:62:GLN:NE2	2.49	0.46
1:A2:1080:C:O2'	1:A2:1183:A:N1	2.45	0.46
13:AZ:24:HIS:HB3	13:AZ:51:LEU:HD21	1.98	0.46
28:Ao:18:ARG:HB2	28:Ao:36:LEU:HD22	1.97	0.46
40:B5:753:G:H4'	50:BH:54:ARG:HH12	1.80	0.46
40:B5:1316:A:OP1	56:BN:202:ARG:NH2	2.37	0.46
40:B5:1317:A:H2	45:BC:234:LYS:HD2	1.80	0.46
40:B5:2249:G:N7	80:Bl:2:SER:N	2.64	0.46
40:B5:2539:A:H62	79:Bk:35:LYS:HZ2	1.63	0.46
40:B5:2594:G:H2'	40:B5:2595:G:H8	1.80	0.46
43:BA:80:GLU:HG3	83:Bp:66:GLY:HA2	1.97	0.46
45:BC:108:TRP:O	56:BN:204:ARG:NH2	2.48	0.46
52:BJ:136:ARG:NH2	52:BJ:161:GLU:OE1	2.48	0.46
54:BL:116:ARG:NH2	54:BL:155:MET:O	2.43	0.46
57:BO:74:ARG:NH1	57:BO:145:VAL:O	2.48	0.46
1:A2:172:OMU:H6	1:A2:315:U:H1'	1.97	0.46
7:AF:19:THR:OG1	7:AF:66:VAL:O	2.31	0.46
10:AJ:18:G:O2'	10:AJ:57:G:N2	2.46	0.46
17:Ad:80:ILE:HG13	17:Ad:81:THR:HG23	1.96	0.46
40:B5:795:A:H3'	40:B5:796:C:C6	2.50	0.46
40:B5:2102:G:O2'	40:B5:2104:G:N2	2.48	0.46
40:B5:2691:G:O2'	40:B5:3570:U:O4	2.28	0.46
40:B5:3702:G:O2'	87:Bv:31:THR:OG1	2.30	0.46
40:B5:4628:G:H2'	40:B5:4629:G:H8	1.80	0.46
42:B8:30:U:OP1	54:BL:34:ARG:NH2	2.43	0.46
59:BQ:122:THR:OG1	59:BQ:124:ASP:OD1	2.27	0.46
86:Bt:147:HIS:HD2	86:Bt:149:HIS:HB2	1.80	0.46
1:A2:1049:G:N1	1:A2:1070:U:OP2	2.37	0.46
1:A2:1806:G:H2'	1:A2:1807:A:C8	2.51	0.46
7:AF:88:ARG:HH12	7:AF:100:ARG:HH21	1.63	0.46
16:Ac:50:ILE:HD11	16:Ac:86:LEU:HD23	1.97	0.46
40:B5:252:C:H2'	40:B5:253:G:C8	2.50	0.46
40:B5:1624:A:OP1	70:Bb:18:ARG:NH1	2.49	0.46
40:B5:1743:A:H5'	40:B5:1745:G:O4'	2.16	0.46
45:BC:66:SER:HA	45:BC:77:PRO:HA	1.97	0.46
47:BE:246:THR:HG22	47:BE:248:GLN:H	1.80	0.46
61:BS:127:MET:HG2	62:BT:153:PRO:HB2	1.98	0.46
16:Ac:105:LEU:HG	16:Ac:122:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:637:C:H2'	40:B5:638:G:H8	1.81	0.46
40:B5:2216:C:H5'	72:Bd:46:LEU:HD22	1.98	0.46
40:B5:4367:C:OP1	64:BV:48:ARG:HD2	2.16	0.46
1:A2:222:U:H5''	24:Ak:17:PHE:CG	2.50	0.46
1:A2:1508:G:N2	4:AC:87:THR:O	2.40	0.46
1:A2:1600:U:H3'	38:Ay:44:LEU:HD11	1.97	0.46
15:Ab:63:VAL:HG23	15:Ab:64:THR:HG23	1.98	0.46
22:Ai:78:LEU:HD13	22:Ai:92:MET:HG2	1.96	0.46
40:B5:4:G:H2'	40:B5:5:A:C8	2.51	0.46
40:B5:1473:A:N6	54:BL:19:GLN:OE1	2.49	0.46
40:B5:2332:C:H4'	40:B5:2333:U:H5	1.81	0.46
40:B5:2362:U:O2'	40:B5:2373:U:O2	2.31	0.46
40:B5:2592:C:H2'	40:B5:2593:G:C8	2.51	0.46
40:B5:2613:C:H2'	40:B5:2614:G:H8	1.80	0.46
40:B5:2632:A:H1'	80:Bl:45:ARG:HH22	1.81	0.46
40:B5:3682:U:H2'	40:B5:3683:G:C8	2.51	0.46
50:BH:137:SER:HB2	50:BH:145:VAL:HG23	1.97	0.46
85:Bs:68:HIS:HB3	85:Bs:75:LEU:HD22	1.96	0.46
1:A2:607:G:N3	12:AU:51:GLN:NE2	2.63	0.46
1:A2:1846:A:H2'	1:A2:1847:G:C8	2.51	0.46
8:AG:20:SER:OG	23:Aj:65:ARG:NH1	2.47	0.46
40:B5:772:C:H2'	40:B5:773:G:C8	2.51	0.46
40:B5:1072:C:H4'	40:B5:1073:C:C5	2.50	0.46
40:B5:1591:U:OP2	92:B5:5424:HOH:O	2.20	0.46
40:B5:2225:A:N1	40:B5:2672:U:O2'	2.37	0.46
55:BM:41:PRO:HB3	55:BM:70:GLN:HG3	1.97	0.46
86:Bt:133:LEU:HD22	86:Bt:152:ILE:HD12	1.97	0.46
87:Bv:104:ALA:O	87:Bv:133:LYS:NZ	2.35	0.46
3:AB:36:ASP:OD1	3:AB:36:ASP:N	2.49	0.46
17:Ad:43:PRO:HD2	17:Ad:46:ILE:HD12	1.97	0.46
40:B5:1572:G:H1'	40:B5:2356:A:N6	2.31	0.46
40:B5:1943:U:H2'	40:B5:1944:G:C8	2.51	0.46
40:B5:1980:A:N7	40:B5:4180:C:O2'	2.49	0.46
44:BB:77:THR:HG21	44:BB:337:VAL:HG22	1.97	0.46
44:BB:90:VAL:HG13	44:BB:161:ARG:HB2	1.97	0.46
48:BF:237:ASP:O	48:BF:240:ASN:ND2	2.48	0.46
51:BI:187:GLU:HG3	51:BI:189:ARG:HG3	1.97	0.46
57:BO:130:LYS:HB2	57:BO:133:ARG:HG2	1.98	0.46
85:Bs:58:ASN:O	85:Bs:62:ARG:HG3	2.15	0.46
1:A2:192:C:H4'	1:A2:192:C:OP1	2.15	0.45
1:A2:838:A:N7	37:Ax:47:MET:HE3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1387:A:OP2	16:Ac:160:SER:OG	2.23	0.45
1:A2:1758:G:H2'	1:A2:1759:G:H8	1.82	0.45
13:AZ:144:THR:OG1	13:AZ:156:TYR:O	2.27	0.45
31:Ar:132:ARG:HB2	31:Ar:134:GLN:HE22	1.81	0.45
40:B5:1509:A:OP1	83:Bp:5:THR:OG1	2.30	0.45
40:B5:3529:C:OP1	64:BV:74:LYS:NZ	2.34	0.45
42:B8:149:G:H21	49:BG:64:GLN:HE22	1.64	0.45
43:BA:250:LYS:HE2	43:BA:252:VAL:HG22	1.98	0.45
1:A2:911:G:OP1	60:BR:173:ARG:NH1	2.48	0.45
4:AC:114:ILE:HD12	25:Al:71:GLU:HG2	1.97	0.45
13:AZ:102:ARG:HD2	13:AZ:102:ARG:HA	1.83	0.45
17:Ad:141:THR:OG1	17:Ad:143:ASP:OD1	2.32	0.45
31:Ar:104:ASP:O	31:Ar:108:ARG:HG2	2.16	0.45
40:B5:4:G:H2'	40:B5:5:A:H8	1.80	0.45
40:B5:1388:A:N6	40:B5:1406:G:O2'	2.49	0.45
40:B5:2258:OMU:HM21	53:BK:4353:PRO:HG3	1.97	0.45
43:BA:103:PRO:HA	43:BA:163:ARG:HA	1.99	0.45
45:BC:35:ASP:OD1	45:BC:35:ASP:N	2.49	0.45
51:BI:61:SER:HA	51:BI:126:VAL:HG12	1.98	0.45
73:Be:124:ASN:O	73:Be:124:ASN:ND2	2.49	0.45
86:Bt:104:ILE:HB	86:Bt:143:VAL:HG22	1.97	0.45
87:Bv:71:GLN:HA	87:Bv:74:CYS:HB3	1.99	0.45
1:A2:1383:A:H2'	1:A2:1384:A2M:H8	1.98	0.45
8:AG:22:ARG:HH21	8:AG:37:ASN:HD22	1.63	0.45
10:AJ:63:C:H2'	10:AJ:64:A:H8	1.82	0.45
21:Ah:139:LYS:HB3	21:Ah:141:ARG:CZ	2.47	0.45
40:B5:1842:G:OP1	74:Bf:87:LYS:NZ	2.34	0.45
40:B5:3680:C:H2'	40:B5:3681:A:C8	2.51	0.45
43:BA:117:GLU:HG2	43:BA:124:GLY:H	1.81	0.45
48:BF:181:TYR:CZ	48:BF:202:GLU:HG2	2.52	0.45
69:Ba:103:VAL:HB	69:Ba:108:TYR:HB2	1.98	0.45
1:A2:686:A:H5''	35:Av:31:SER:HB3	1.98	0.45
1:A2:1390:C:OP1	30:Aq:43:SER:OG	2.32	0.45
18:Ae:14:THR:HB	18:Ae:15:PRO:HD3	1.98	0.45
24:Ak:126:VAL:HG12	24:Ak:145:VAL:HG22	1.98	0.45
31:Ar:28:PHE:O	31:Ar:31:THR:OG1	2.31	0.45
33:At:24:LEU:HB3	33:At:32:LEU:HD11	1.99	0.45
40:B5:48:G:OP1	56:BN:192:TRP:NE1	2.36	0.45
40:B5:398:A2M:H8	40:B5:398:A2M:O5'	2.17	0.45
40:B5:2146:C:H5''	73:Be:104:SER:HB3	1.97	0.45
40:B5:2651:G:O3'	60:BR:60:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:3945:C:H42	51:BI:116:ARG:HH12	1.65	0.45
41:B7:96:U:O2'	48:BF:136:GLU:OE1	2.33	0.45
44:BB:86:VAL:HG13	44:BB:162:VAL:HG13	1.98	0.45
45:BC:25:PRO:HB2	45:BC:27:VAL:HG12	1.97	0.45
46:BD:99:TYR:OH	46:BD:168:ASP:OD2	2.33	0.45
85:Bs:85:ASN:OD1	85:Bs:85:ASN:N	2.49	0.45
1:A2:65:C:N4	19:Af:134:GLY:O	2.44	0.45
1:A2:835:C:O2'	1:A2:837:G:O6	2.32	0.45
3:AB:37:ASP:OD1	3:AB:39:SER:OG	2.29	0.45
40:B5:419:A:N3	40:B5:1276:C:O2'	2.45	0.45
40:B5:4065:C:H4'	82:Bo:9:ARG:HH12	1.82	0.45
64:BV:45:ILE:HG21	64:BV:53:PRO:HB3	1.98	0.45
10:AJ:48:C:O2'	10:AJ:59:G:O2'	2.29	0.45
40:B5:223:G:N3	45:BC:223:ASN:ND2	2.64	0.45
40:B5:260:C:H2'	40:B5:261:G:C8	2.51	0.45
40:B5:1718:PSU:H2'	40:B5:1719:A:C8	2.51	0.45
40:B5:1733:A:H5''	40:B5:3960:A:H61	1.80	0.45
40:B5:2302:G:N2	40:B5:2305:C:OP2	2.42	0.45
40:B5:2742:C:OP1	60:BR:108:ARG:NH2	2.46	0.45
40:B5:4137:G:OP1	45:BC:75:ARG:NH1	2.40	0.45
40:B5:4620:U:C4	55:BM:113:MET:HG3	2.51	0.45
40:B5:4757:C:H2'	40:B5:4758:A:C8	2.52	0.45
44:BB:378:ARG:HE	65:BW:32:LEU:HD21	1.81	0.45
55:BM:24:LEU:O	55:BM:43:THR:OG1	2.33	0.45
63:BU:84:LYS:HG3	63:BU:102:VAL:HG11	1.97	0.45
73:Be:35:TRP:CZ2	73:Be:56:PRO:HD2	2.51	0.45
19:Af:138:ALA:HA	19:Af:176:ILE:HD11	1.98	0.45
40:B5:474:C:H2'	40:B5:475:G:C8	2.52	0.45
40:B5:2014:G:OP1	45:BC:312:ARG:NH2	2.50	0.45
40:B5:3360:G:H2'	40:B5:3361:A:H8	1.82	0.45
46:BD:211:LEU:HD12	46:BD:223:PHE:HE2	1.82	0.45
56:BN:42:PRO:HG3	56:BN:61:ILE:HG13	1.99	0.45
68:BZ:12:LEU:HB2	68:BZ:81:MET:HB3	1.98	0.45
85:Bs:78:LEU:HA	85:Bs:81:HIS:HD2	1.81	0.45
86:Bt:118:HIS:CD2	86:Bt:119:ARG:HG2	2.52	0.45
1:A2:303:A:H1'	21:Ah:73:THR:HB	1.99	0.45
1:A2:1806:G:H2'	1:A2:1807:A:H8	1.82	0.45
15:Ab:192:LEU:HB3	15:Ab:227:ARG:HG2	1.99	0.45
16:Ac:135:GLU:HB3	16:Ac:187:LYS:HB2	1.98	0.45
20:Ag:73:GLN:HA	20:Ag:76:GLN:HB2	1.98	0.45
36:Aw:60:LYS:HG3	36:Aw:116:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:158:A:N1	40:B5:276:C:O2'	2.39	0.45
40:B5:1298:A:H62	40:B5:1457:G:HO2'	1.63	0.45
1:A2:682:PSU:O2'	1:A2:1161:U:OP1	2.33	0.45
1:A2:753:G:H2'	1:A2:755:G:H5''	1.99	0.45
1:A2:755:G:H1	1:A2:791:C:H42	1.64	0.45
1:A2:1537:G:H2'	1:A2:1538:A:C8	2.52	0.45
14:Aa:28:LYS:HB3	14:Aa:48:LEU:HD11	1.99	0.45
40:B5:1647:C:O3'	59:BQ:143:ARG:NH1	2.37	0.45
40:B5:1959:U:H5''	85:Bs:57:LYS:HG3	1.98	0.45
40:B5:2325:C:H2'	40:B5:2326:G:H8	1.82	0.45
40:B5:2511:G:OP1	60:BR:128:LYS:NZ	2.50	0.45
40:B5:3380:A:H1'	40:B5:3517:A2M:N6	2.31	0.45
40:B5:4020:A:H2'	40:B5:4021:G:C8	2.51	0.45
40:B5:4628:G:H2'	40:B5:4629:G:C8	2.52	0.45
52:BJ:43:LEU:HG	52:BJ:117:ILE:HD11	1.98	0.45
72:Bd:92:ARG:HA	72:Bd:102:LEU:HD23	1.98	0.45
73:Be:90:MET:HG3	84:Br:33:LYS:HA	1.99	0.45
1:A2:382:C:H5''	21:Ah:54:LYS:HE3	1.98	0.45
1:A2:1353:G:N7	92:A2:2141:HOH:O	2.36	0.45
1:A2:1763:C:H2'	1:A2:1764:G:C8	2.52	0.45
7:AF:25:PRO:HA	7:AF:293:ALA:HB2	1.98	0.45
25:Al:89:VAL:HG11	25:Al:109:VAL:HG11	1.99	0.45
40:B5:1700:G:H1	40:B5:1710:U:H3	1.64	0.45
40:B5:1891:G:N2	40:B5:1970:C:O2	2.42	0.45
40:B5:2110:U:OP1	84:Br:37:SER:OG	2.29	0.45
40:B5:4057:A:H2'	40:B5:4058:PSU:H6	1.82	0.45
56:BN:73:ARG:HB2	56:BN:92:LEU:HD12	1.99	0.45
87:Bv:59:PRO:HB2	87:Bv:171:HIS:CE1	2.52	0.45
1:A2:98:C:OP2	1:A2:427:A:O2'	2.32	0.44
1:A2:385:U:O4	21:Ah:5:ARG:NH2	2.38	0.44
1:A2:678:G:H21	1:A2:1029:A:H62	1.65	0.44
1:A2:1041:G:H2'	1:A2:1042:G:C8	2.52	0.44
1:A2:1679:A2M:OP2	18:Ae:63:LYS:NZ	2.39	0.44
16:Ac:154:ASP:N	16:Ac:154:ASP:OD1	2.51	0.44
22:Ai:110:LEU:HB2	22:Ai:147:PHE:HB3	1.98	0.44
26:Am:37:ILE:HG23	26:Am:50:ILE:HG21	2.00	0.44
40:B5:229:G:H5''	67:BY:11:ARG:HG3	1.99	0.44
40:B5:260:C:H2'	40:B5:261:G:H8	1.83	0.44
40:B5:461:G:H2'	40:B5:462:G:C8	2.52	0.44
40:B5:751:G:H2'	40:B5:752:G:C8	2.51	0.44
40:B5:793:C:N3	40:B5:794:G:N1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:1303:G:H4'	56:BN:203:TYR:HB2	1.99	0.44
40:B5:2328:U:O2	40:B5:2336:G:N2	2.33	0.44
40:B5:2423:U:H4'	68:BZ:74:VAL:O	2.17	0.44
40:B5:4609:G:H5''	55:BM:91:TRP:CE2	2.51	0.44
47:BE:59:TYR:HB3	47:BE:63:ALA:HB3	1.99	0.44
47:BE:225:LEU:HD21	47:BE:227:LYS:HE2	1.99	0.44
52:BJ:99:PHE:HB2	52:BJ:159:LYS:HE3	1.99	0.44
87:Bv:37:SER:HB2	87:Bv:202:ARG:HB2	1.99	0.44
1:A2:371:G:N7	92:A2:2142:HOH:O	2.36	0.44
10:AJ:48:C:C2	10:AJ:59:G:H1'	2.52	0.44
17:Ad:45:ILE:HA	17:Ad:61:VAL:HG11	1.99	0.44
25:Al:131:LYS:HE3	25:Al:132:LYS:HE2	1.99	0.44
40:B5:86:U:HO2'	69:Ba:65:ARG:HH21	1.62	0.44
40:B5:318:A:H2'	40:B5:319:A:C8	2.52	0.44
40:B5:394:G:N2	40:B5:397:G:OP2	2.40	0.44
40:B5:3871:C:H2'	40:B5:3872:G:H8	1.82	0.44
42:B8:13:G:O2'	58:BP:121:LYS:O	2.36	0.44
45:BC:15:GLY:HA2	45:BC:174:LEU:HD23	1.98	0.44
66:BX:73:HIS:CD2	66:BX:115:LYS:HD3	2.52	0.44
80:Bl:30:LYS:HB2	80:Bl:33:ASN:HB2	1.99	0.44
85:Bs:5:ASP:HB2	85:Bs:8:THR:HG22	1.99	0.44
1:A2:74:G:H22	19:Af:171:THR:H	1.64	0.44
1:A2:159:A2M:H8	1:A2:159:A2M:O5'	2.17	0.44
1:A2:1232:C:O2'	1:A2:1254:A:N6	2.50	0.44
1:A2:1299:G:H4'	28:Ao:78:THR:HA	2.00	0.44
5:AD:115:ARG:HE	12:AU:47:GLY:HA2	1.82	0.44
21:Ah:80:ASP:OD1	21:Ah:81:VAL:N	2.46	0.44
22:Ai:142:VAL:HG12	22:Ai:144:ILE:H	1.83	0.44
33:At:41:ARG:O	33:At:45:GLU:HG2	2.18	0.44
40:B5:1489:A2M:N3	78:Bj:11:ARG:HB2	2.33	0.44
40:B5:3694:A:N6	40:B5:3767:G:OP2	2.34	0.44
40:B5:4511:A:N6	50:BH:60:TRP:O	2.39	0.44
46:BD:264:LYS:NZ	46:BD:265:ARG:O	2.46	0.44
1:A2:1209:A:O2'	1:A2:1836:A:N7	2.41	0.44
7:AF:184:LEU:HD23	16:Ac:227:LYS:HD2	1.98	0.44
13:AZ:177:MET:SD	13:AZ:180:ARG:NH2	2.91	0.44
14:Aa:125:VAL:HG12	14:Aa:172:MET:HE3	1.99	0.44
29:Ap:19:ALA:HB2	29:Ap:75:GLY:HA3	1.99	0.44
36:Aw:123:VAL:HG12	36:Aw:124:LYS:HG3	1.99	0.44
40:B5:345:C:H2'	40:B5:346:G:C8	2.53	0.44
40:B5:652:C:H2'	40:B5:653:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:1381:G:N2	40:B5:1413:C:OP2	2.44	0.44
40:B5:1785:G:H2'	40:B5:1786:C:C6	2.53	0.44
42:B8:102:G:OP2	42:B8:104:A:O2'	2.33	0.44
45:BC:76:ILE:HD12	45:BC:77:PRO:HD2	2.00	0.44
1:A2:1059:A:OP1	11:AT:37:U:O2'	2.35	0.44
15:Ab:199:PRO:O	15:Ab:202:THR:OG1	2.34	0.44
16:Ac:163:PRO:O	16:Ac:167:TYR:HB2	2.17	0.44
17:Ad:148:ARG:NH2	19:Af:205:GLU:OE1	2.42	0.44
22:Ai:120:ALA:O	22:Ai:125:HIS:ND1	2.38	0.44
40:B5:417:G:H2'	42:B8:16:G:N2	2.32	0.44
40:B5:461:G:H2'	40:B5:462:G:H8	1.83	0.44
40:B5:1250:C:H2'	40:B5:1251:A:C8	2.52	0.44
40:B5:1688:A:H2'	40:B5:1689:G:C8	2.53	0.44
40:B5:1924:G:H21	40:B5:1924:G:P	2.41	0.44
40:B5:2667:OMC:HM22	40:B5:2668:A:H5'	2.00	0.44
45:BC:218:VAL:HA	45:BC:229:LEU:HG	1.99	0.44
46:BD:128:ASP:O	46:BD:164:LYS:NZ	2.46	0.44
55:BM:126:GLU:HB3	57:BO:181:ALA:HB1	1.99	0.44
57:BO:37:ARG:HG3	57:BO:108:ILE:HG13	2.00	0.44
61:BS:95:ARG:NH2	61:BS:112:ASP:OD2	2.42	0.44
64:BV:87:SER:HA	64:BV:97:TYR:HB3	1.99	0.44
85:Bs:55:MET:HG2	85:Bs:87:GLY:HA2	2.00	0.44
86:Bt:80:LEU:HA	86:Bt:83:LYS:HG2	2.00	0.44
1:A2:1038:G:H4'	1:A2:1846:A:H4'	1.99	0.44
7:AF:32:LEU:HD21	7:AF:92:LEU:HD11	2.00	0.44
31:Ar:124:ARG:HB2	31:Ar:131:VAL:HG12	1.98	0.44
33:At:20:ILE:HG13	33:At:116:ILE:HG13	2.00	0.44
40:B5:788:G:H2'	40:B5:789:G:H8	1.81	0.44
40:B5:3974:OMG:H5''	40:B5:3975:U:O4'	2.18	0.44
40:B5:3989:C:OP2	40:B5:4010:G:N1	2.42	0.44
40:B5:4408:C:O2'	40:B5:4743:C:OP1	2.31	0.44
40:B5:4714:G:O2'	40:B5:4716:A:N6	2.47	0.44
50:BH:40:HIS:ND1	50:BH:41:ILE:HG13	2.33	0.44
68:BZ:41:ALA:HB2	68:BZ:77:TYR:HE1	1.83	0.44
69:Ba:39:V5N:O2	69:Ba:40:HIS:N	2.51	0.44
73:Be:100:ALA:HB3	73:Be:103:VAL:HG23	1.99	0.44
1:A2:1513:C:H5''	8:AG:8:TRP:HZ3	1.83	0.44
15:Ab:256:TRP:CG	35:Av:68:ARG:HD2	2.53	0.44
20:Ag:135:PHE:CG	20:Ag:136:PRO:HA	2.53	0.44
21:Ah:66:SER:HA	21:Ah:73:THR:HA	1.99	0.44
22:Ai:53:ILE:HD13	22:Ai:81:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:66:A:O2'	40:B5:326:C:O2	2.31	0.44
40:B5:322:C:N4	92:B5:5658:HOH:O	2.51	0.44
40:B5:1907:G:H2'	40:B5:1908:G:C8	2.53	0.44
40:B5:2252:U:H4'	40:B5:2271:A:H4'	2.00	0.44
65:BW:96:GLN:OE1	65:BW:101:ARG:NH1	2.50	0.44
1:A2:239:C:H2'	1:A2:240:G:H8	1.82	0.44
1:A2:1657:G:H1	1:A2:1669:U:H3	1.65	0.44
4:AC:81:LYS:HG2	4:AC:82:LYS:H	1.83	0.44
40:B5:443:G:H5''	74:Bf:54:LYS:HB3	2.00	0.44
40:B5:1082:C:H2'	40:B5:1083:C:O4'	2.18	0.44
40:B5:2360:A:H5'	75:Bg:62:LYS:HD3	2.00	0.44
40:B5:3360:G:H2'	40:B5:3361:A:C8	2.53	0.44
40:B5:3639:G:N2	53:BK:4388:GLU:HB3	2.32	0.44
40:B5:4731:G:H2'	40:B5:4732:G:C8	2.53	0.44
44:BB:19:ARG:HB2	44:BB:234:ARG:NH2	2.31	0.44
50:BH:18:ILE:HG12	50:BH:27:VAL:HG22	2.00	0.44
1:A2:1754:C:H2'	1:A2:1755:G:C8	2.53	0.44
4:AC:79:LYS:HG3	4:AC:81:LYS:H	1.83	0.44
19:Af:213:LEU:HG	19:Af:217:MET:HE2	1.99	0.44
24:Ak:89:ARG:NH1	24:Ak:91:ASP:OD1	2.51	0.44
40:B5:2326:G:H1	40:B5:2338:U:H3	1.66	0.44
40:B5:4270:G:C2	44:BB:252:ALA:HB1	2.53	0.44
46:BD:116:ASP:OD1	46:BD:116:ASP:N	2.51	0.44
1:A2:28:U:H2'	1:A2:29:G:C8	2.53	0.43
1:A2:853:G:O2'	24:Ak:97:ARG:NH1	2.51	0.43
1:A2:910:G:H2'	1:A2:911:G:C8	2.53	0.43
7:AF:109:LEU:HD21	7:AF:125:ARG:CZ	2.48	0.43
14:Aa:92:GLN:NE2	14:Aa:229:MET:SD	2.91	0.43
22:Ai:162:ARG:HE	37:Ax:31:GLY:HA2	1.83	0.43
23:Aj:37:ASP:OD1	23:Aj:37:ASP:N	2.51	0.43
40:B5:1934:G:O6	40:B5:1939:G:N2	2.51	0.43
40:B5:2244:A2M:HM'2	40:B5:2245:G:O5'	2.17	0.43
40:B5:3399:C:H4'	43:BA:8:GLN:HA	2.00	0.43
47:BE:49:ASN:ND2	47:BE:57:GLY:HA3	2.33	0.43
49:BG:138:ALA:HB2	49:BG:194:VAL:HG11	2.00	0.43
64:BV:89:ARG:HB2	64:BV:95:PHE:CE2	2.53	0.43
1:A2:51:U:H2'	1:A2:52:G:C8	2.53	0.43
1:A2:99:A2M:H8	1:A2:99:A2M:O5'	2.18	0.43
1:A2:753:G:H1	1:A2:792:C:H42	1.65	0.43
26:Am:99:ARG:NH2	26:Am:119:GLU:OE2	2.51	0.43
40:B5:303:C:OP2	56:BN:68:ARG:NH2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:478:G:H2'	40:B5:479:G:C8	2.53	0.43
40:B5:1276:C:H2'	40:B5:1277:A:C8	2.53	0.43
40:B5:2007:C:OP1	74:Bf:15:LYS:NZ	2.47	0.43
40:B5:2178:C:H2'	40:B5:2179:G:H8	1.83	0.43
40:B5:3657:OMU:HM22	82:Bo:50:GLY:HA3	2.00	0.43
40:B5:4314:A:O2'	40:B5:4720:G:N7	2.48	0.43
40:B5:4599:G:H2'	40:B5:4600:G:H8	1.82	0.43
42:B8:12:G:OP1	58:BP:3:ARG:NH2	2.51	0.43
45:BC:45:ARG:O	45:BC:48:ASN:ND2	2.50	0.43
52:BJ:146:ARG:HG2	52:BJ:147:ARG:HG3	2.00	0.43
1:A2:64:A:O5'	19:Af:136:LYS:NZ	2.46	0.43
1:A2:158:A:H2'	1:A2:159:A2M:O4'	2.19	0.43
1:A2:695:G:H1	1:A2:733:U:H3	1.64	0.43
15:Ab:169:TYR:OH	15:Ab:175:GLY:O	2.37	0.43
16:Ac:64:ARG:NH1	23:Aj:73:ASN:OD1	2.50	0.43
18:Ae:47:LYS:NZ	29:Ap:115:TYR:O	2.49	0.43
31:Ar:44:VAL:HG11	31:Ar:71:MET:HG3	1.99	0.43
40:B5:723:G:H5''	48:BF:75:ARG:HD2	2.00	0.43
40:B5:801:C:H2'	40:B5:802:C:C6	2.53	0.43
40:B5:1931:U:O2'	40:B5:1941:A:OP1	2.33	0.43
40:B5:2719:OMG:C8	83:Bp:16:THR:HG22	2.53	0.43
40:B5:4645:C:N4	40:B5:4646:G:O6	2.51	0.43
45:BC:350:ARG:HG2	45:BC:353:ARG:HH12	1.82	0.43
77:Bi:55:ARG:O	77:Bi:59:GLU:HG2	2.19	0.43
1:A2:193:C:H2'	1:A2:194:C:C6	2.54	0.43
1:A2:400:C:H5	1:A2:681:G:H5''	1.83	0.43
1:A2:642:A:O2'	1:A2:646:C:OP1	2.36	0.43
1:A2:864:PSU:O2'	35:Av:78:ARG:NH1	2.50	0.43
1:A2:907:U:H2'	1:A2:908:G:H8	1.83	0.43
1:A2:1495:U:H4'	1:A2:1496:G:H5''	1.99	0.43
25:Al:25:ALA:O	25:Al:30:GLY:N	2.43	0.43
40:B5:1005:G:OP1	62:BT:142:ARG:NH1	2.51	0.43
40:B5:1712:U:H2'	40:B5:1713:C:C6	2.53	0.43
40:B5:2592:C:H2'	40:B5:2593:G:H8	1.82	0.43
40:B5:4135:C:H2'	40:B5:4136:A:C8	2.54	0.43
49:BG:109:GLU:O	49:BG:112:GLN:NE2	2.51	0.43
52:BJ:63:ARG:HH21	82:Bo:105:GLN:HA	1.83	0.43
66:BX:141:ALA:HB3	66:BX:144:TYR:HD1	1.83	0.43
1:A2:206:G:H2'	1:A2:207:G:H8	1.83	0.43
1:A2:508:G:OP2	37:Ax:104:ARG:NH2	2.52	0.43
4:AC:129:GLY:HA3	25:Al:40:LYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AE:87:ARG:HB3	6:AE:91:ALA:HB3	1.99	0.43
16:Ac:18:LYS:HE2	16:Ac:39:VAL:HB	2.00	0.43
19:Af:44:GLU:H	19:Af:44:GLU:CD	2.27	0.43
40:B5:2232:A:H5'	72:Bd:70:LYS:HE2	2.00	0.43
40:B5:2688:A:H61	40:B5:3575:C:N4	2.16	0.43
40:B5:3432:C:H2'	40:B5:3478:A:H61	1.84	0.43
40:B5:3805:A:N1	40:B5:3917:C:N4	2.66	0.43
40:B5:4204:C:H2'	40:B5:4205:U:C6	2.53	0.43
44:BB:17:LEU:HD21	44:BB:235:TRP:HH2	1.83	0.43
46:BD:37:VAL:HG12	46:BD:50:ARG:HD3	2.00	0.43
50:BH:44:GLU:HB3	50:BH:58:ASP:HB2	2.00	0.43
60:BR:12:SER:OG	60:BR:17:CYS:O	2.29	0.43
61:BS:127:MET:HA	62:BT:153:PRO:HD2	2.00	0.43
68:BZ:103:ASP:OD1	68:BZ:103:ASP:N	2.49	0.43
76:Bh:82:ASP:N	76:Bh:82:ASP:OD1	2.50	0.43
1:A2:1300:A:OP1	28:Ao:59:ARG:NE	2.52	0.43
1:A2:1652:A:N6	92:A2:2173:HOH:O	2.51	0.43
7:AF:32:LEU:HB2	7:AF:71:ILE:HD11	2.01	0.43
7:AF:152:SER:HB2	7:AF:168:CYS:SG	2.59	0.43
14:Aa:28:LYS:NZ	27:An:51:GLU:OE1	2.35	0.43
18:Ae:28:VAL:O	18:Ae:42:LYS:NZ	2.51	0.43
40:B5:92:C:C2	69:Ba:55:LYS:HD3	2.53	0.43
40:B5:642:G:H2'	40:B5:643:A:H8	1.84	0.43
40:B5:2383:C:H2'	40:B5:2384:G:C8	2.53	0.43
40:B5:3450:A2M:H8	40:B5:3450:A2M:O5'	2.18	0.43
40:B5:3975:U:OP1	82:Bo:63:THR:OG1	2.29	0.43
40:B5:4699:G:H2'	40:B5:4700:G:C8	2.53	0.43
40:B5:4805:U:H2'	40:B5:4806:U:C6	2.53	0.43
44:BB:80:GLU:OE1	44:BB:323:TYR:OH	2.28	0.43
48:BF:82:VAL:HG22	61:BS:62:VAL:HA	2.00	0.43
61:BS:86:SER:N	61:BS:89:GLY:O	2.50	0.43
1:A2:120:U:H2'	1:A2:121:OMU:H6	2.00	0.43
1:A2:1649:G:O2'	1:A2:1675:G:O6	2.35	0.43
7:AF:101:PHE:CD2	7:AF:136:GLY:HA2	2.53	0.43
10:AJ:67:G:H2'	10:AJ:68:A:C8	2.54	0.43
12:AU:99:ILE:HD11	12:AU:106:ILE:HD11	2.00	0.43
40:B5:1068:U:H2'	40:B5:1069:G:C8	2.53	0.43
40:B5:1648:U:OP1	59:BQ:143:ARG:NH2	2.52	0.43
40:B5:1726:A:N3	40:B5:3956:U:O2'	2.52	0.43
40:B5:3822:G:H2'	40:B5:3823:G:H8	1.84	0.43
42:B8:96:C:H5''	76:Bh:66:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BA:204:MET:HB3	43:BA:208:GLU:HG3	2.01	0.43
55:BM:101:LYS:HA	55:BM:104:MET:HG3	2.00	0.43
73:Be:104:SER:O	73:Be:108:ARG:HG3	2.19	0.43
1:A2:1320:U:H2'	1:A2:1321:G:C8	2.54	0.43
1:A2:1746:A:O3'	19:Af:31:ARG:NH1	2.52	0.43
1:A2:1757:C:H2'	1:A2:1758:G:C8	2.54	0.43
12:AU:121:LEU:HD13	12:AU:133:ARG:HD2	2.01	0.43
21:Ah:3:ILE:O	21:Ah:30:GLY:N	2.49	0.43
29:Ap:16:LYS:HG3	29:Ap:17:LYS:H	1.84	0.43
40:B5:456:C:H2'	40:B5:457:G:C8	2.53	0.43
40:B5:624:G:H2'	40:B5:625:G:H8	1.84	0.43
40:B5:652:C:H2'	40:B5:653:G:C8	2.54	0.43
40:B5:685:C:H2'	40:B5:686:A:C8	2.54	0.43
40:B5:1081:C:H2'	40:B5:1082:C:C6	2.53	0.43
40:B5:1632:PSU:H4'	40:B5:1635:G:N1	2.34	0.43
40:B5:2317:G:O2'	40:B5:2318:G:H5'	2.19	0.43
40:B5:3829:C:H2'	40:B5:3830:C:C6	2.54	0.43
55:BM:47:ARG:NH2	55:BM:68:ALA:O	2.48	0.43
58:BP:60:PHE:CE1	58:BP:82:ARG:HB2	2.54	0.43
68:BZ:29:ILE:HG22	68:BZ:32:GLY:H	1.84	0.43
85:Bs:102:LEU:HD11	85:Bs:187:LEU:HD12	2.01	0.43
1:A2:387:C:H5'	21:Ah:7:ASN:HD22	1.84	0.43
1:A2:869:G:OP2	1:A2:869:G:N2	2.37	0.43
6:AE:3:LYS:NZ	6:AE:8:ASN:OD1	2.52	0.43
7:AF:191:HIS:CG	7:AF:195:LEU:HD11	2.52	0.43
14:Aa:30:TRP:CG	27:An:19:PRO:HB3	2.54	0.43
19:Af:164:LYS:HG2	19:Af:165:GLU:H	1.84	0.43
21:Ah:116:HIS:O	21:Ah:152:ARG:NH2	2.52	0.43
29:Ap:16:LYS:HA	29:Ap:16:LYS:HD2	1.79	0.43
40:B5:109:G:OP2	54:BL:74:ARG:NH2	2.52	0.43
40:B5:1079:C:H2'	40:B5:1080:G:H8	1.84	0.43
40:B5:1859:C:H3'	40:B5:1860:C:H5''	2.01	0.43
40:B5:2552:C:H5''	60:BR:43:LYS:HD2	2.01	0.43
40:B5:2594:G:H2'	40:B5:2595:G:C8	2.53	0.43
40:B5:3331:A:H2'	40:B5:3332:G:C8	2.54	0.43
40:B5:3572:U:H2'	40:B5:3573:OMC:O4'	2.19	0.43
40:B5:3954:U:H2'	40:B5:3955:G:C8	2.54	0.43
40:B5:4219:A:P	81:Bm:102:ARG:HH21	2.42	0.43
40:B5:4381:A:H3'	40:B5:4382:PSU:H4'	2.01	0.43
47:BE:182:LEU:HD12	47:BE:186:ARG:HA	2.00	0.43
65:BW:89:ASP:O	65:BW:93:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:BZ:22:LYS:NZ	68:BZ:129:TRP:O	2.45	0.43
1:A2:1129:C:H2'	1:A2:1130:G:C8	2.53	0.43
1:A2:1416:C:H2'	1:A2:1417:C:C6	2.54	0.43
1:A2:1550:U:OP1	8:AG:34:TYR:OH	2.34	0.43
1:A2:1858:G:OP2	27:An:146:ARG:NH1	2.50	0.43
40:B5:231:U:O2	67:BY:103:LYS:NZ	2.49	0.43
40:B5:1412:G:O2'	59:BQ:75:ARG:NH2	2.49	0.43
40:B5:2321:C:H2'	40:B5:2322:G:O4'	2.18	0.43
44:BB:31:SER:O	44:BB:348:ARG:NH1	2.46	0.43
44:BB:57:VAL:HG22	44:BB:73:VAL:HG22	2.01	0.43
1:A2:660:G:H21	36:Aw:17:ARG:NH2	2.17	0.42
1:A2:830:C:OP1	17:Ad:21:ASP:HB2	2.19	0.42
1:A2:1532:A:H4'	1:A2:1606:G:H4'	2.00	0.42
7:AF:64:HIS:HB3	7:AF:83:TRP:HB2	2.00	0.42
12:AU:32:GLN:O	22:Ai:116:LYS:NZ	2.50	0.42
22:Ai:32:ILE:HG12	22:Ai:37:LEU:HB2	2.01	0.42
33:At:50:VAL:HG12	33:At:91:LEU:HD22	2.01	0.42
40:B5:4060:C:O2'	70:Bb:36:ASP:OD1	2.37	0.42
49:BG:88:ASP:OD2	49:BG:90:GLN:NE2	2.47	0.42
50:BH:48:LEU:HD11	50:BH:56:ARG:HH11	1.83	0.42
61:BS:154:LEU:HB3	61:BS:157:ARG:HD3	2.00	0.42
1:A2:420:G:N2	1:A2:662:U:O2	2.52	0.42
4:AC:126:CYS:HB2	4:AC:130:VAL:HB	2.00	0.42
10:AJ:5:U:O2	10:AJ:69:G:N2	2.52	0.42
11:AT:47:C:N4	11:AT:58:A:N3	2.66	0.42
15:Ab:102:LEU:HB3	15:Ab:130:ILE:HD11	2.01	0.42
17:Ad:94:LYS:NZ	37:Ax:19:GLN:HE21	2.17	0.42
21:Ah:76:THR:OG1	21:Ah:77:ARG:N	2.52	0.42
22:Ai:63:LEU:HD11	22:Ai:69:ARG:HH21	1.83	0.42
25:Al:89:VAL:HG23	25:Al:91:LEU:HB2	2.01	0.42
30:Aq:77:GLU:OE2	30:Aq:81:ARG:NH2	2.52	0.42
31:Ar:63:GLU:HG2	31:Ar:66:ARG:HH22	1.84	0.42
31:Ar:132:ARG:HB2	31:Ar:134:GLN:NE2	2.34	0.42
40:B5:1061:G:H2'	40:B5:1062:G:H8	1.84	0.42
40:B5:1105:C:O2	70:Bb:91:ARG:NE	2.42	0.42
40:B5:1217:G:H2'	40:B5:1218:A:C8	2.54	0.42
40:B5:1984:G:O6	40:B5:3602:C:O2'	2.37	0.42
40:B5:3954:U:H2'	40:B5:3955:G:H8	1.83	0.42
40:B5:4138:OMG:N3	40:B5:4193:5MC:HM52	2.34	0.42
40:B5:4506:C:OP1	57:BO:116:LYS:NZ	2.52	0.42
40:B5:4684:G:H22	74:Bf:3:GLY:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BB:317:LEU:HD22	44:BB:382:VAL:HG13	2.00	0.42
60:BR:106:LEU:HD13	60:BR:138:LEU:HD21	2.01	0.42
60:BR:167:LYS:HE2	60:BR:167:LYS:HB3	1.88	0.42
86:Bt:116:MET:HA	86:Bt:118:HIS:CE1	2.55	0.42
1:A2:1392:OMC:O3'	33:At:83:ARG:NH2	2.41	0.42
1:A2:1837:G:OP1	1:A2:1840:U:H4'	2.19	0.42
38:Ay:102:LYS:HD2	38:Ay:107:VAL:HG12	2.01	0.42
40:B5:478:G:H2'	40:B5:479:G:H8	1.84	0.42
40:B5:1831:A:N6	92:B5:5622:HOH:O	2.46	0.42
40:B5:1991:G:O2'	40:B5:1996:A:N1	2.46	0.42
40:B5:3781:A:H5'	87:Bv:207:LYS:HZ2	1.84	0.42
40:B5:4283:C:H2'	40:B5:4284:G:C8	2.54	0.42
51:BI:46:PHE:HB2	51:BI:139:ARG:HH11	1.84	0.42
68:BZ:102:ARG:HA	68:BZ:102:ARG:HD2	1.80	0.42
73:Be:67:LYS:HG2	73:Be:68:HIS:CD2	2.55	0.42
85:Bs:121:VAL:HG22	85:Bs:182:PRO:HB3	2.01	0.42
86:Bt:101:SER:HA	86:Bt:141:CYS:HA	2.01	0.42
1:A2:564:G:O2'	1:A2:565:A:H8	2.02	0.42
5:AD:111:GLN:HB3	5:AD:115:ARG:NH1	2.35	0.42
20:Ag:160:LYS:HA	20:Ag:163:GLN:HB2	1.99	0.42
37:Ax:56:PHE:HB2	37:Ax:74:MET:HB2	2.00	0.42
40:B5:500:G:H2'	40:B5:500:G:N3	2.33	0.42
40:B5:667:C:H2'	40:B5:668:G:C8	2.54	0.42
40:B5:1225:G:H5'	45:BC:323:ARG:HB2	2.00	0.42
40:B5:1955:C:H2'	40:B5:1956:A:H8	1.84	0.42
40:B5:1994:G:O5'	57:BO:130:LYS:NZ	2.52	0.42
40:B5:2036:A:H3'	40:B5:2037:G:H5'	2.01	0.42
40:B5:3958:A:N1	62:BT:3:ASN:ND2	2.52	0.42
40:B5:4500:U:OP1	74:Bf:100:ARG:NH2	2.50	0.42
40:B5:4638:G:N2	40:B5:4661:C:O2	2.53	0.42
40:B5:4741:U:H2'	40:B5:4742:U:C6	2.54	0.42
86:Bt:15:LEU:HD22	86:Bt:16:ARG:H	1.84	0.42
1:A2:653:U:H2'	1:A2:654:A:H8	1.84	0.42
1:A2:1453:A:O2'	1:A2:1476:G:N2	2.53	0.42
1:A2:1455:A:H3'	30:Aq:5:ARG:NH2	2.34	0.42
6:AE:60:ASP:OD1	6:AE:60:ASP:N	2.52	0.42
14:Aa:108:ASP:OD1	14:Aa:108:ASP:N	2.52	0.42
19:Af:20:ASP:HB3	19:Af:23:LYS:HD3	2.01	0.42
30:Aq:87:GLU:OE1	30:Aq:87:GLU:N	2.35	0.42
37:Ax:87:PRO:HD2	37:Ax:90:ARG:HD2	2.01	0.42
40:B5:1727:A:H2'	51:BI:22:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:3781:A:H5'	87:Bv:207:LYS:NZ	2.34	0.42
40:B5:3894:C:OP1	68:BZ:59:LYS:NZ	2.34	0.42
40:B5:3895:C:H2'	40:B5:3896:G:H8	1.85	0.42
44:BB:29:VAL:HG13	44:BB:348:ARG:HD3	2.01	0.42
44:BB:86:VAL:HG12	44:BB:201:LEU:HD23	2.02	0.42
46:BD:208:MET:HG2	46:BD:223:PHE:CE2	2.55	0.42
68:BZ:30:ASP:O	68:BZ:39:SER:OG	2.28	0.42
1:A2:411:G:N7	92:A2:2140:HOH:O	2.36	0.42
1:A2:617:A:H1'	5:AD:86:VAL:HG23	2.01	0.42
1:A2:875:G:H2'	1:A2:876:A:H8	1.83	0.42
1:A2:1366:G:H2'	1:A2:1367:G:C8	2.55	0.42
1:A2:1580:A:O2'	1:A2:1582:C:OP2	2.31	0.42
15:Ab:206:SER:HB3	15:Ab:224:THR:HG21	2.02	0.42
16:Ac:8:LYS:HE3	33:At:59:LYS:HD2	2.01	0.42
40:B5:53:C:H2'	40:B5:54:G:C8	2.54	0.42
40:B5:385:A:H4'	40:B5:386:A:H5'	2.00	0.42
40:B5:488:G:H1	40:B5:663:C:H42	1.68	0.42
40:B5:4037:G:H5'	40:B5:4039:PSU:C6	2.55	0.42
40:B5:4367:C:OP1	64:BV:48:ARG:NH1	2.49	0.42
43:BA:48:ILE:HD13	83:Bp:65:ALA:HB2	2.02	0.42
56:BN:143:ARG:NH1	76:Bh:95:LEU:HD23	2.34	0.42
87:Bv:187:VAL:HG11	87:Bv:204:LEU:HD11	2.01	0.42
1:A2:747:C:H4'	1:A2:748:U:H5'	2.02	0.42
1:A2:825:C:H1'	22:Ai:144:ILE:HG21	2.01	0.42
1:A2:1032:A2M:HM'2	1:A2:1033:C:H5'	2.01	0.42
6:AE:33:ASP:OD1	6:AE:33:ASP:N	2.53	0.42
14:Aa:48:LEU:O	27:An:51:GLU:HG3	2.19	0.42
14:Aa:86:LEU:HB3	14:Aa:98:THR:HB	2.01	0.42
14:Aa:218:LEU:C	14:Aa:219:LYS:HD2	2.45	0.42
40:B5:85:G:O2'	40:B5:97:G:O6	2.26	0.42
40:B5:417:G:H1'	42:B8:17:A:H61	1.85	0.42
40:B5:670:C:H2'	40:B5:671:G:H8	1.84	0.42
40:B5:670:C:H2'	40:B5:671:G:C8	2.55	0.42
40:B5:819:C:H2'	40:B5:820:G:C8	2.55	0.42
40:B5:1208:C:H2'	40:B5:1209:G:C8	2.55	0.42
40:B5:1784:U:H2'	40:B5:1785:G:C8	2.55	0.42
40:B5:1922:A:H4'	40:B5:1923:A:C8	2.55	0.42
40:B5:2359:G:OP2	75:Bg:37:LYS:NZ	2.51	0.42
40:B5:2360:A:O2'	75:Bg:66:ARG:NH1	2.52	0.42
40:B5:3517:A2M:HM'1	40:B5:4283:C:H1'	2.02	0.42
40:B5:4151:G:OP2	51:BI:7:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:4445:U:H1'	40:B5:4446:A:H5''	2.00	0.42
42:B8:71:A:N1	42:B8:84:A:O2'	2.43	0.42
48:BF:135:VAL:HG23	48:BF:139:ILE:HD13	2.00	0.42
49:BG:81:ASN:ND2	49:BG:238:GLY:HA3	2.35	0.42
59:BQ:67:ILE:HG12	59:BQ:98:LEU:HD11	2.00	0.42
1:A2:62:G:H1'	1:A2:172:OMU:HM23	2.00	0.42
1:A2:220:U:H2'	1:A2:221:A:H8	1.85	0.42
1:A2:380:C:O2	21:Ah:5:ARG:NE	2.53	0.42
1:A2:1338:4AC:O5'	1:A2:1338:4AC:H6	2.20	0.42
18:Ae:80:GLY:HA2	18:Ae:83:ASN:ND2	2.35	0.42
21:Ah:194:GLU:HG2	24:Ak:10:TYR:CE2	2.55	0.42
25:Al:52:LEU:HD13	25:Al:65:VAL:HG11	2.01	0.42
40:B5:19:G:P	76:Bh:93:ARG:HE	2.42	0.42
40:B5:259:C:H2'	40:B5:260:C:C6	2.55	0.42
40:B5:460:C:H2'	40:B5:461:G:H8	1.85	0.42
40:B5:1733:A:H5''	40:B5:3960:A:N6	2.35	0.42
40:B5:3419:A:O2'	43:BA:236:GLY:N	2.53	0.42
40:B5:3630:G:H8	44:BB:254:ILE:HD11	1.84	0.42
77:Bi:50:PHE:O	77:Bi:55:ARG:NH1	2.52	0.42
87:Bv:59:PRO:HG2	87:Bv:63:PHE:HE2	1.85	0.42
1:A2:155:G:H4'	19:Af:15:LEU:HD22	2.00	0.42
1:A2:661:C:P	36:Aw:17:ARG:HH21	2.43	0.42
1:A2:920:A:OP2	26:Am:64:ARG:NH2	2.53	0.42
1:A2:1427:U:P	29:Ap:69:ARG:HH21	2.43	0.42
22:Ai:42:GLU:HG2	22:Ai:45:ARG:HH22	1.84	0.42
26:Am:37:ILE:HG22	26:Am:75:LEU:HD21	2.02	0.42
28:Ao:100:LYS:HG2	28:Ao:101:THR:HG23	2.01	0.42
40:B5:1288:C:H2'	40:B5:1289:A:C8	2.55	0.42
40:B5:2360:A:N3	40:B5:2382:C:O2'	2.52	0.42
40:B5:2630:A2M:H1'	40:B5:2630:A2M:HM'2	1.66	0.42
40:B5:4480:A:H61	40:B5:4704:U:H3	1.67	0.42
40:B5:4715:U:H1'	44:BB:343:ARG:HH12	1.85	0.42
41:B7:49:A:H3'	46:BD:225:GLN:HE21	1.85	0.42
46:BD:279:ARG:HG2	46:BD:283:LYS:HE3	2.00	0.42
56:BN:146:PRO:HB2	76:Bh:104:THR:HG23	2.01	0.42
57:BO:51:LYS:NZ	57:BO:144:GLU:OE1	2.40	0.42
86:Bt:53:TRP:HD1	86:Bt:56:LEU:HD12	1.85	0.42
87:Bv:114:GLU:N	87:Bv:138:LEU:O	2.46	0.42
1:A2:212:C:H2'	1:A2:213:G:C8	2.55	0.42
1:A2:544:C:H2'	1:A2:545:G:C8	2.55	0.42
1:A2:1155:U:O4	15:Ab:227:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1759:G:H2'	1:A2:1760:G:H8	1.85	0.42
7:AF:107:ASP:OD1	7:AF:107:ASP:N	2.52	0.42
22:Ai:88:ASP:OD1	22:Ai:89:GLU:N	2.53	0.42
40:B5:28:C:OP2	56:BN:193:ARG:NH1	2.43	0.42
40:B5:186:G:N2	40:B5:187:U:O2'	2.53	0.42
40:B5:300:A:H2'	40:B5:301:G:C8	2.55	0.42
40:B5:1224:C:O2'	45:BC:321:ASN:OD1	2.31	0.42
40:B5:1285:U:H2'	40:B5:1286:A:C8	2.55	0.42
40:B5:1318:G:OP2	45:BC:120:LYS:NZ	2.48	0.42
40:B5:2012:C:H5''	48:BF:211:LYS:HB3	2.02	0.42
40:B5:3780:C:O3'	87:Bv:207:LYS:NZ	2.53	0.42
44:BB:41:VAL:HA	44:BB:187:GLY:HA3	2.01	0.42
44:BB:229:LYS:HG3	44:BB:272:LYS:HD3	2.02	0.42
84:Br:28:GLU:HG3	84:Br:43:LEU:HG	2.02	0.42
1:A2:755:G:H22	1:A2:791:C:H42	1.67	0.41
1:A2:980:C:H2'	1:A2:981:A:C8	2.54	0.41
1:A2:1229:A:H2'	1:A2:1230:G:C8	2.54	0.41
7:AF:108:VAL:HA	7:AF:124:SER:HA	2.02	0.41
7:AF:278:SER:HB2	7:AF:281:ALA:HB3	2.01	0.41
10:AJ:35:A:H2'	10:AJ:36:U:O4'	2.20	0.41
29:Ap:112:LEU:HD22	29:Ap:119:LEU:HD13	2.02	0.41
40:B5:2169:G:OP1	73:Be:108:ARG:NH2	2.52	0.41
40:B5:2332:C:H4'	40:B5:2333:U:C5	2.55	0.41
61:BS:93:MET:HE1	61:BS:117:HIS:CE1	2.55	0.41
64:BV:13:LYS:NZ	64:BV:59:ASP:OD1	2.53	0.41
1:A2:653:U:H2'	1:A2:654:A:C8	2.55	0.41
1:A2:1061:A:O2'	1:A2:1063:A:N7	2.47	0.41
1:A2:1285:A:H2'	25:Al:91:LEU:HD21	2.02	0.41
1:A2:1731:U:H2'	1:A2:1732:A:C8	2.55	0.41
13:AZ:206:ASP:OD1	13:AZ:206:ASP:N	2.36	0.41
15:Ab:85:SER:OG	34:Au:25:GLY:O	2.36	0.41
40:B5:653:G:H2'	40:B5:654:G:C8	2.54	0.41
40:B5:1763:G:H2'	40:B5:1764:A:C8	2.56	0.41
40:B5:3630:G:C8	44:BB:254:ILE:HD11	2.55	0.41
44:BB:82:PRO:HG3	44:BB:171:LEU:HD21	2.02	0.41
58:BP:94:MET:HE1	58:BP:146:ILE:HB	2.01	0.41
61:BS:30:MET:HE2	61:BS:30:MET:HB3	1.95	0.41
85:Bs:32:ALA:HB1	85:Bs:35:VAL:HG21	2.02	0.41
87:Bv:39:LYS:HE2	87:Bv:40:ASN:ND2	2.35	0.41
1:A2:531:U:H2'	1:A2:532:A:C8	2.53	0.41
1:A2:1712:U:H2'	1:A2:1713:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1852:MA6:H102	1:A2:1853:C:O2'	2.20	0.41
7:AF:39:THR:HG22	7:AF:60:ARG:HG2	2.02	0.41
28:Ao:18:ARG:HD2	31:Ar:88:LYS:HG2	2.02	0.41
31:Ar:26:ILE:HG13	31:Ar:45:LEU:HD21	2.01	0.41
40:B5:1532:G:N2	83:Bp:17:ARG:HD2	2.35	0.41
40:B5:1717:C:H2'	40:B5:1718:PSU:C6	2.55	0.41
40:B5:3780:C:H2'	40:B5:3781:A:C8	2.55	0.41
40:B5:4669:C:H5''	47:BE:269:GLN:HG2	2.02	0.41
44:BB:217:ILE:HD13	44:BB:284:ILE:HD11	2.02	0.41
51:BI:42:LYS:HB2	51:BI:45:GLU:HG3	2.01	0.41
60:BR:105:LEU:HD12	60:BR:135:LYS:HE3	2.02	0.41
76:Bh:8:ASP:N	76:Bh:8:ASP:OD1	2.52	0.41
1:A2:613:U:H4'	5:AD:89:GLN:NE2	2.35	0.41
7:AF:73:SER:H	7:AF:117:ASN:HD21	1.67	0.41
11:AT:61:C:H4'	87:Bv:44:GLN:HG2	2.03	0.41
12:AU:75:LEU:HG	12:AU:79:LYS:HE2	2.03	0.41
13:AZ:58:LEU:HD11	13:AZ:178:LEU:HB2	2.02	0.41
15:Ab:81:ILE:HG23	15:Ab:86:LEU:HB2	2.02	0.41
19:Af:176:ILE:HG21	19:Af:179:LEU:HD22	2.01	0.41
23:Aj:14:LEU:HD22	23:Aj:35:LEU:HD21	2.02	0.41
40:B5:1653:C:H2'	40:B5:1654:A:O4'	2.20	0.41
40:B5:1687:U:H2'	40:B5:1688:A:C8	2.56	0.41
40:B5:2289:C:OP2	92:B5:5426:HOH:O	2.22	0.41
48:BF:240:ASN:O	48:BF:244:ARG:HG2	2.21	0.41
52:BJ:57:VAL:HG12	52:BJ:60:PHE:H	1.86	0.41
58:BP:6:LEU:HD12	58:BP:116:HIS:CG	2.55	0.41
70:Bb:101:HIS:O	70:Bb:109:ARG:NH1	2.39	0.41
1:A2:476:C:O2'	1:A2:508:G:N3	2.46	0.41
1:A2:485:A2M:HM'2	1:A2:486:A:C8	2.56	0.41
1:A2:1093:G:H2'	1:A2:1094:A:C8	2.55	0.41
1:A2:1285:A:C4	25:Al:91:LEU:HD11	2.56	0.41
1:A2:1747:U:P	19:Af:31:ARG:HH12	2.43	0.41
7:AF:171:ASP:OD1	7:AF:171:ASP:N	2.53	0.41
10:AJ:47:U:H2'	10:AJ:49:C:O3'	2.21	0.41
15:Ab:108:LYS:HB2	15:Ab:233:LEU:HD13	2.01	0.41
26:Am:106:ARG:HD3	26:Am:106:ARG:HA	1.89	0.41
29:Ap:89:SER:HB3	29:Ap:112:LEU:HD13	2.03	0.41
30:Aq:99:ASP:OD1	30:Aq:102:THR:N	2.44	0.41
36:Aw:40:PRO:HA	36:Aw:79:LYS:HD2	2.03	0.41
40:B5:408:A:O2'	40:B5:411:G:OP2	2.24	0.41
40:B5:694:G:H2'	40:B5:695:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:2269:U:H5''	60:BR:3:MET:SD	2.60	0.41
40:B5:2387:G:H4'	40:B5:2389:G:C8	2.55	0.41
40:B5:2544:U:H2'	40:B5:2545:C:C6	2.56	0.41
40:B5:4213:A:O2'	40:B5:4256:A:N3	2.45	0.41
40:B5:4335:A:N1	40:B5:4367:C:O2'	2.52	0.41
42:B8:65:A:O2'	76:Bh:10:ARG:NH2	2.54	0.41
43:BA:14:SER:HA	43:BA:17:ARG:HE	1.85	0.41
52:BJ:44:THR:HA	52:BJ:82:ILE:HD11	2.03	0.41
63:BU:84:LYS:HB2	63:BU:110:TYR:CE2	2.55	0.41
71:Bc:28:VAL:HG21	71:Bc:37:MET:HG3	2.02	0.41
76:Bh:87:LYS:HE3	76:Bh:87:LYS:HB3	1.80	0.41
1:A2:529:A:H2'	1:A2:530:A:C8	2.55	0.41
1:A2:981:A:H2'	1:A2:982:A:C8	2.56	0.41
1:A2:1190:A:H2'	1:A2:1191:A:C8	2.56	0.41
4:AC:107:LYS:HB3	4:AC:117:LEU:HD11	2.03	0.41
15:Ab:252:THR:OG1	15:Ab:254:ASP:OD1	2.30	0.41
18:Ae:73:THR:O	18:Ae:89:THR:HG21	2.21	0.41
20:Ag:51:ILE:HD11	20:Ag:176:VAL:HG22	2.01	0.41
21:Ah:130:THR:HG23	21:Ah:133:GLU:H	1.86	0.41
37:Ax:78:SER:OG	37:Ax:80:ASP:OD1	2.36	0.41
40:B5:827:C:H2'	40:B5:828:A:C8	2.56	0.41
40:B5:866:A:H8	48:BF:22:ARG:HD3	1.86	0.41
40:B5:1926:C:H2'	40:B5:1927:G:H8	1.86	0.41
40:B5:2245:G:O2'	75:Bg:10:ARG:O	2.39	0.41
40:B5:3701:G:H2'	40:B5:3702:G:C8	2.56	0.41
40:B5:4090:U:O2'	82:Bo:26:TYR:OH	2.34	0.41
40:B5:4162:G:O6	40:B5:4168:A:O2'	2.34	0.41
41:B7:24:C:H2'	41:B7:25:G:O4'	2.20	0.41
45:BC:37:VAL:HG13	45:BC:237:ILE:HD11	2.01	0.41
59:BQ:155:ALA:O	59:BQ:158:THR:OG1	2.30	0.41
62:BT:93:ILE:HA	62:BT:96:ILE:HG12	2.03	0.41
85:Bs:30:VAL:HG12	85:Bs:189:ILE:HG12	2.03	0.41
1:A2:38:A:H5''	22:Ai:5:ARG:HB3	2.03	0.41
1:A2:1260:A:H1'	1:A2:1265:C:N4	2.35	0.41
1:A2:1496:G:C8	8:AG:41:GLN:HG2	2.55	0.41
1:A2:1764:G:H2'	1:A2:1765:G:C8	2.55	0.41
7:AF:207:CYS:SG	7:AF:219:TRP:HB2	2.61	0.41
15:Ab:232:THR:HG22	15:Ab:235:ASN:H	1.85	0.41
17:Ad:42:LEU:HB2	17:Ad:109:PHE:CD2	2.56	0.41
21:Ah:8:TRP:CE3	21:Ah:20:PRO:HB3	2.55	0.41
33:At:26:SER:HB3	33:At:32:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Aw:22:TRP:O	36:Aw:28:LYS:HD2	2.21	0.41
40:B5:78:U:H5''	56:BN:185:GLY:HA2	2.01	0.41
40:B5:323:C:H2'	40:B5:324:A:C8	2.56	0.41
40:B5:460:C:H2'	40:B5:461:G:C8	2.56	0.41
40:B5:484:G:H5''	40:B5:485:U:H2'	2.03	0.41
40:B5:766:C:H2'	40:B5:767:G:C8	2.55	0.41
40:B5:2425:A:O2'	40:B5:2496:C:O2'	2.33	0.41
40:B5:4281:A:H2'	40:B5:4282:OMC:C6	2.55	0.41
40:B5:4462:C:H2'	40:B5:4463:A:C8	2.55	0.41
42:B8:63:U:O2'	76:Bh:52:LYS:NZ	2.34	0.41
55:BM:9:VAL:HG21	55:BM:66:HIS:HB3	2.02	0.41
56:BN:94:PHE:CE2	56:BN:96:ARG:HB2	2.56	0.41
59:BQ:49:LYS:HE2	59:BQ:49:LYS:HB3	1.91	0.41
71:Bc:14:ILE:HD13	71:Bc:72:HIS:CE1	2.56	0.41
82:Bo:33:LEU:HA	82:Bo:38:LYS:HG2	2.02	0.41
85:Bs:93:GLU:HG2	85:Bs:94:ASP:H	1.86	0.41
1:A2:442:C:O2'	19:Af:92:ARG:NH2	2.54	0.41
1:A2:477:A:N7	92:A2:2144:HOH:O	2.37	0.41
10:Aj:66:A:H2'	10:Aj:67:G:C8	2.55	0.41
38:Ay:68:ILE:HB	38:Ay:109:TYR:HB2	2.02	0.41
40:B5:1070:U:O2	46:BD:286:SER:OG	2.38	0.41
40:B5:1438:C:H4'	40:B5:1439:G:O4'	2.21	0.41
40:B5:2363:C:H2'	40:B5:2364:G:H8	1.86	0.41
40:B5:2515:C:OP1	83:Bp:44:LYS:NZ	2.51	0.41
40:B5:3422:U:O2'	40:B5:3549:A:N3	2.41	0.41
40:B5:4339:C:H2'	40:B5:4340:U:C6	2.56	0.41
44:BB:39:LYS:HG2	44:BB:40:PRO:HD2	2.03	0.41
47:BE:151:THR:OG1	47:BE:203:LYS:NZ	2.47	0.41
59:BQ:155:ALA:HB3	59:BQ:158:THR:HG23	2.03	0.41
66:BX:64:SER:HB2	76:Bh:69:LEU:HD13	2.01	0.41
71:Bc:9:LYS:HB3	71:Bc:17:ARG:NH2	2.36	0.41
1:A2:3:C:O2	22:Ai:18:ARG:NH2	2.40	0.41
1:A2:65:C:C5	19:Af:174:PRO:HB3	2.56	0.41
1:A2:67:C:H41	19:Af:163:ASN:HA	1.86	0.41
1:A2:328:G:H2'	1:A2:330:G:C8	2.56	0.41
1:A2:361:A:H4'	1:A2:362:U:H3'	2.03	0.41
1:A2:507:G:OP1	37:Ax:108:LYS:NZ	2.36	0.41
1:A2:881:G:H2'	1:A2:882:G:H8	1.86	0.41
1:A2:1011:G:H2'	1:A2:1012:A:C8	2.56	0.41
1:A2:1031:A:H2'	1:A2:1032:A2M:C8	2.49	0.41
1:A2:1085:A:OP1	1:A2:1859:G:O2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1702:C:H5'	9:AH:3432:C:N4	2.36	0.41
1:A2:1737:G:H2'	1:A2:1738:G:C8	2.55	0.41
11:AT:49:C:H2'	11:AT:50:G:H8	1.86	0.41
13:AZ:73:ASP:HB3	13:AZ:120:ARG:HB2	2.02	0.41
19:Af:93:LYS:HE2	19:Af:93:LYS:HB2	1.95	0.41
20:Ag:43:LEU:HB3	20:Ag:72:PHE:CE1	2.55	0.41
26:Am:91:LEU:HB3	26:Am:122:ILE:HG12	2.02	0.41
29:Ap:77:HIS:O	29:Ap:81:ILE:HG12	2.21	0.41
37:Ax:114:MET:HE3	37:Ax:126:GLY:HA3	2.03	0.41
39:Az:2:ARG:HD3	39:Az:5:TRP:NE1	2.36	0.41
40:B5:239:C:H2'	40:B5:240:G:C8	2.56	0.41
40:B5:1015:U:O2	40:B5:1086:G:N2	2.43	0.41
40:B5:1449:U:H2'	40:B5:1450:G:C8	2.56	0.41
40:B5:1524:U:H5	83:Bp:2:ALA:HB2	1.84	0.41
40:B5:1714:A:H2'	40:B5:1715:A:O4'	2.21	0.41
40:B5:2001:C:N4	92:B5:5674:HOH:O	2.52	0.41
40:B5:3464:A:H2'	40:B5:3465:A:C8	2.55	0.41
42:B8:58:G:N7	78:Bj:63:ARG:NH2	2.50	0.41
45:BC:157:LYS:HE2	45:BC:157:LYS:HB3	1.81	0.41
45:BC:212:ASN:HD22	45:BC:255:SER:HB3	1.85	0.41
51:BI:193:ASP:OD2	51:BI:198:LYS:HE3	2.21	0.41
56:BN:43:THR:OG1	56:BN:131:GLU:OE2	2.27	0.41
59:BQ:175:GLU:HA	69:Ba:51:GLY:C	2.45	0.41
61:BS:45:TRP:HA	61:BS:48:VAL:HG22	2.03	0.41
65:BW:4:GLU:HB2	65:BW:13:ILE:HB	2.02	0.41
1:A2:919:U:O2'	35:Av:56:HIS:O	2.39	0.41
16:Ac:48:ILE:HG13	16:Ac:86:LEU:HG	2.02	0.41
22:Ai:158:ASP:N	22:Ai:158:ASP:OD1	2.53	0.41
40:B5:699:G:OP1	73:Be:5:ARG:NH2	2.51	0.41
40:B5:748:C:H42	40:B5:807:G:H1	1.69	0.41
40:B5:1093:C:H2'	40:B5:1094:A:C8	2.56	0.41
40:B5:2208:OMC:HM21	40:B5:2671:U:H2'	2.02	0.41
40:B5:3351:G:H22	40:B5:3356:A:H1'	1.86	0.41
40:B5:4324:G:H2'	40:B5:4325:PSU:C6	2.55	0.41
40:B5:4492:G:H22	40:B5:4694:A:H2	1.67	0.41
44:BB:54:THR:OG1	44:BB:55:HIS:N	2.53	0.41
77:Bi:73:ILE:O	77:Bi:77:VAL:HG22	2.21	0.41
1:A2:17:C:H2'	1:A2:18:C:C6	2.55	0.40
22:Ai:140:GLN:NE2	37:Ax:64:PHE:O	2.44	0.40
30:Aq:72:LYS:O	30:Aq:76:GLU:HG2	2.21	0.40
40:B5:18:C:H4'	56:BN:138:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:2142:G:H5'	84:Br:15:SER:HB2	2.03	0.40
40:B5:3388:A:H2'	40:B5:3389:U:C6	2.56	0.40
40:B5:3602:C:H2'	40:B5:3603:A:C8	2.56	0.40
40:B5:4053:A:H4'	59:BQ:186:TYR:CG	2.55	0.40
40:B5:4166:PSU:O4	40:B5:4166:PSU:H2'	2.21	0.40
43:BA:137:ILE:HD11	43:BA:149:LYS:HB2	2.03	0.40
44:BB:238:LYS:HE2	44:BB:238:LYS:HB2	1.92	0.40
51:BI:99:ILE:HG22	51:BI:123:GLN:HB2	2.03	0.40
59:BQ:111:SER:O	59:BQ:115:LYS:HB2	2.21	0.40
1:A2:529:A:H2'	1:A2:530:A:H8	1.85	0.40
1:A2:1116:U:H1'	1:A2:1117:C:H2'	2.02	0.40
1:A2:1278:C:H2'	1:A2:1279:A:H8	1.87	0.40
1:A2:1493:U:O2'	1:A2:1496:G:OP1	2.30	0.40
6:AE:24:THR:HG21	6:AE:71:LEU:HD22	2.04	0.40
8:AG:56:ASP:OXT	33:At:79:ARG:NH1	2.54	0.40
13:AZ:77:ILE:HG13	13:AZ:99:ILE:HB	2.03	0.40
14:Aa:27:LYS:HA	14:Aa:51:ARG:NH1	2.36	0.40
17:Ad:124:CYS:HB3	17:Ad:141:THR:HB	2.02	0.40
20:Ag:37:LYS:O	20:Ag:41:ARG:HG3	2.20	0.40
21:Ah:106:SER:HB3	21:Ah:171:LEU:HG	2.03	0.40
21:Ah:165:GLN:HE22	21:Ah:195:LEU:HD11	1.85	0.40
34:Au:14:PRO:HB2	34:Au:23:ILE:HG23	2.03	0.40
37:Ax:23:MET:N	37:Ax:23:MET:SD	2.94	0.40
40:B5:286:U:H2'	40:B5:287:U:C6	2.55	0.40
40:B5:1320:C:OP1	45:BC:275:SER:N	2.50	0.40
40:B5:1468:U:H4'	54:BL:4:SER:HB2	2.04	0.40
40:B5:1642:U:H2'	40:B5:1643:G:C8	2.56	0.40
40:B5:2127:G:OP1	69:Ba:7:LYS:NZ	2.38	0.40
40:B5:2604:U:H4'	40:B5:2605:G:O4'	2.21	0.40
40:B5:3672:U:H2'	40:B5:3673:G:C8	2.56	0.40
40:B5:3954:U:OP2	62:BT:4:THR:OG1	2.38	0.40
41:B7:75:G:H5''	61:BS:49:SER:O	2.22	0.40
41:B7:110:G:H2'	41:B7:111:C:C6	2.56	0.40
43:BA:30:ARG:HG3	43:BA:76:PHE:HZ	1.87	0.40
63:BU:80:LYS:HE2	63:BU:110:TYR:CZ	2.57	0.40
69:Ba:26:ARG:HA	69:Ba:26:ARG:HD3	1.91	0.40
1:A2:904:A:H2'	1:A2:905:A:C8	2.57	0.40
1:A2:1285:A:C5	25:Al:91:LEU:HD11	2.57	0.40
14:Aa:147:ASN:OD1	14:Aa:148:ASN:N	2.54	0.40
40:B5:175:C:H2'	40:B5:176:G:H8	1.86	0.40
40:B5:1672:G:N3	40:B5:3960:A:H2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:1959:U:H2'	40:B5:1960:G:H8	1.86	0.40
40:B5:3331:A:H2'	40:B5:3332:G:H8	1.85	0.40
69:Ba:13:GLY:O	73:Be:39:ARG:NE	2.51	0.40
69:Ba:71:PRO:HG2	69:Ba:108:TYR:HA	2.04	0.40
71:Bc:45:LEU:HD21	71:Bc:108:MET:HE3	2.03	0.40
1:A2:701:G:H1	1:A2:727:C:H42	1.69	0.40
1:A2:908:G:H2'	1:A2:909:A:C8	2.57	0.40
4:AC:121:CYS:HA	4:AC:122:PRO:HD3	1.92	0.40
7:AF:192:THR:HG23	16:Ac:218:LEU:HD22	2.03	0.40
19:Af:67:VAL:HB	19:Af:99:GLY:HA2	2.04	0.40
21:Ah:57:ALA:HB2	21:Ah:183:GLY:HA2	2.04	0.40
29:Ap:117:ARG:HE	29:Ap:121:VAL:HG21	1.87	0.40
40:B5:61:A:H5''	56:BN:164:LEU:HD21	2.03	0.40
40:B5:1968:A:H2'	40:B5:1969:A:C8	2.56	0.40
40:B5:2239:A:N7	40:B5:2657:C:H2'	2.36	0.40
40:B5:3684:A:H2'	40:B5:3685:G:H8	1.86	0.40
41:B7:74:A:N1	41:B7:100:A:H5''	2.37	0.40
42:B8:67:U:H2'	42:B8:68:G:C8	2.56	0.40
42:B8:130:C:H2'	42:B8:131:G:C8	2.57	0.40
56:BN:120:TRP:HE1	56:BN:123:GLU:HB3	1.86	0.40
66:BX:148:ASP:O	66:BX:152:LYS:HG2	2.21	0.40
67:BY:4:ASN:ND2	92:BY:201:HOH:O	2.53	0.40
81:Bm:98:M3L:HM13	81:Bm:98:M3L:HD2	1.88	0.40
84:Br:28:GLU:OE2	84:Br:31:ASN:ND2	2.52	0.40
1:A2:330:G:H2'	1:A2:331:G:O4'	2.22	0.40
1:A2:1599:G:OP1	38:Ay:80:ARG:NH1	2.55	0.40
1:A2:1625:U:H2'	1:A2:1626:PSU:O4'	2.22	0.40
8:AG:21:CYS:HB3	8:AG:26:ASN:H	1.87	0.40
11:AT:13:U:H2'	11:AT:14:A:H8	1.85	0.40
15:Ab:128:VAL:HG11	15:Ab:155:ILE:HG12	2.04	0.40
15:Ab:253:PRO:HA	15:Ab:256:TRP:CE2	2.56	0.40
23:Aj:58:VAL:HG21	23:Aj:69:TRP:HB3	2.04	0.40
24:Ak:93:LEU:HB3	24:Ak:102:PHE:HB3	2.04	0.40
24:Ak:154:GLN:HA	26:Am:133:ARG:HD2	2.04	0.40
25:Al:41:ALA:HB1	25:Al:47:ALA:HB2	2.04	0.40
25:Al:72:HIS:CD2	25:Al:74:ILE:HD11	2.57	0.40
29:Ap:76:GLY:H	29:Ap:79:ALA:HB3	1.87	0.40
37:Ax:51:THR:OG1	37:Ax:53:ASP:OD1	2.31	0.40
40:B5:38:A:H5''	69:Ba:35:ALA:HB2	2.03	0.40
40:B5:736:C:H2'	40:B5:737:G:H8	1.86	0.40
40:B5:1061:G:H2'	40:B5:1062:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B5:1760:G:H4'	40:B5:1761:U:H5''	2.04	0.40
40:B5:1933:C:H2'	40:B5:1934:G:C8	2.56	0.40
40:B5:2613:C:H2'	40:B5:2614:G:C8	2.56	0.40
56:BN:124:ASP:OD1	56:BN:126:THR:N	2.46	0.40
58:BP:54:LYS:HA	58:BP:83:TRP:CD1	2.57	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	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
5	AD	43/133 (32%)	43 (100%)	0	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AU	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
13	AZ	219/295 (74%)	215 (98%)	4 (2%)	0	100	100
14	Aa	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
15	Ab	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
16	Ac	223/281 (79%)	221 (99%)	1 (0%)	1 (0%)	30	61
17	Ad	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
18	Ae	189/204 (93%)	185 (98%)	4 (2%)	0	100	100
19	Af	235/249 (94%)	235 (100%)	0	0	100	100
20	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
22	Ai	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
23	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
24	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
25	Al	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
26	Am	148/151 (98%)	148 (100%)	0	0	100	100
27	An	134/151 (89%)	133 (99%)	1 (1%)	0	100	100
28	Ao	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
29	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
30	Aq	132/135 (98%)	132 (100%)	0	0	100	100
31	Ar	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
32	As	140/145 (97%)	140 (100%)	0	0	100	100
33	At	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
34	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
35	Av	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
36	Aw	138/143 (96%)	138 (100%)	0	0	100	100
37	Ax	123/130 (95%)	123 (100%)	0	0	100	100
38	Ay	71/124 (57%)	69 (97%)	2 (3%)	0	100	100
39	Az	23/25 (92%)	23 (100%)	0	0	100	100
43	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
44	BB	395/403 (98%)	393 (100%)	2 (0%)	0	100	100
45	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
46	BD	291/297 (98%)	288 (99%)	3 (1%)	0	100	100
47	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
48	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
49	BG	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
50	BH	188/192 (98%)	188 (100%)	0	0	100	100
51	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
52	BJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
53	BK	37/1071 (4%)	32 (86%)	4 (11%)	1 (3%)	4	20
54	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BM	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
56	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
57	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
58	BP	157/184 (85%)	154 (98%)	3 (2%)	0	100	100
59	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
60	BR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
61	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
62	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
63	BU	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
64	BV	137/140 (98%)	137 (100%)	0	0	100	100
65	BW	119/157 (76%)	117 (98%)	2 (2%)	0	100	100
66	BX	120/156 (77%)	119 (99%)	1 (1%)	0	100	100
67	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
68	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
69	Ba	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
70	Bb	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
71	Bc	106/115 (92%)	106 (100%)	0	0	100	100
72	Bd	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
73	Be	128/135 (95%)	128 (100%)	0	0	100	100
74	Bf	108/110 (98%)	108 (100%)	0	0	100	100
75	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
76	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
77	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
78	Bj	84/97 (87%)	84 (100%)	0	0	100	100
79	Bk	67/70 (96%)	67 (100%)	0	0	100	100
80	Bl	48/51 (94%)	48 (100%)	0	0	100	100
81	Bm	49/128 (38%)	49 (100%)	0	0	100	100
82	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
83	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
84	Br	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
85	Bs	194/318 (61%)	187 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
87	Bv	210/217 (97%)	204 (97%)	6 (3%)	0	100	100
All	All	12026/15056 (80%)	11848 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Ac	211	VAL
53	BK	4388	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	61	77
3	AB	56/62 (90%)	55 (98%)	1 (2%)	51	73
4	AC	67/140 (48%)	67 (100%)	0	100	100
5	AD	38/106 (36%)	37 (97%)	1 (3%)	40	68
6	AE	88/98 (90%)	86 (98%)	2 (2%)	44	70
7	AF	272/275 (99%)	267 (98%)	5 (2%)	51	73
8	AG	48/49 (98%)	48 (100%)	0	100	100
12	AU	92/121 (76%)	89 (97%)	3 (3%)	33	63
13	AZ	182/243 (75%)	179 (98%)	3 (2%)	55	75
14	Aa	195/231 (84%)	193 (99%)	2 (1%)	68	79
15	Ab	185/223 (83%)	182 (98%)	3 (2%)	55	75
16	Ac	189/232 (82%)	187 (99%)	2 (1%)	65	78
17	Ad	224/225 (100%)	222 (99%)	2 (1%)	70	80
18	Ae	161/170 (95%)	161 (100%)	0	100	100
19	Af	207/218 (95%)	207 (100%)	0	100	100
20	Ag	170/360 (47%)	168 (99%)	2 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	83
22	Ai	161/168 (96%)	158 (98%)	3 (2%)	50	73
23	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	78
24	Ak	139/142 (98%)	139 (100%)	0	100	100
25	Al	104/108 (96%)	101 (97%)	3 (3%)	37	66
26	Am	130/131 (99%)	129 (99%)	1 (1%)	73	81
27	An	106/119 (89%)	105 (99%)	1 (1%)	70	80
28	Ao	114/130 (88%)	114 (100%)	0	100	100
29	Ap	117/140 (84%)	117 (100%)	0	100	100
30	Aq	120/121 (99%)	118 (98%)	2 (2%)	53	74
31	Ar	127/131 (97%)	125 (98%)	2 (2%)	55	75
32	As	112/114 (98%)	112 (100%)	0	100	100
33	At	94/107 (88%)	92 (98%)	2 (2%)	47	71
34	Au	67/67 (100%)	65 (97%)	2 (3%)	36	65
35	Av	112/113 (99%)	111 (99%)	1 (1%)	70	80
36	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	73
37	Ax	107/112 (96%)	106 (99%)	1 (1%)	70	80
38	Ay	64/102 (63%)	63 (98%)	1 (2%)	55	75
39	Az	24/24 (100%)	24 (100%)	0	100	100
43	BA	194/198 (98%)	193 (100%)	1 (0%)	81	85
44	BB	344/347 (99%)	341 (99%)	3 (1%)	70	80
45	BC	302/337 (90%)	302 (100%)	0	100	100
46	BD	247/250 (99%)	247 (100%)	0	100	100
47	BE	216/251 (86%)	213 (99%)	3 (1%)	59	76
48	BF	197/215 (92%)	197 (100%)	0	100	100
49	BG	198/223 (89%)	196 (99%)	2 (1%)	68	79
50	BH	169/171 (99%)	169 (100%)	0	100	100
51	BI	180/181 (99%)	178 (99%)	2 (1%)	65	78
52	BJ	143/149 (96%)	143 (100%)	0	100	100
53	BK	34/936 (4%)	31 (91%)	3 (9%)	9	33
54	BL	175/176 (99%)	172 (98%)	3 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	BM	117/161 (73%)	116 (99%)	1 (1%)	70	80
56	BN	171/172 (99%)	171 (100%)	0	100	100
57	BO	171/173 (99%)	171 (100%)	0	100	100
58	BP	140/163 (86%)	139 (99%)	1 (1%)	76	82
59	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	78
60	BR	159/175 (91%)	158 (99%)	1 (1%)	78	83
61	BS	154/154 (100%)	153 (99%)	1 (1%)	78	83
62	BT	139/140 (99%)	138 (99%)	1 (1%)	76	82
63	BU	88/113 (78%)	88 (100%)	0	100	100
64	BV	106/107 (99%)	106 (100%)	0	100	100
65	BW	100/126 (79%)	100 (100%)	0	100	100
66	BX	110/134 (82%)	109 (99%)	1 (1%)	70	80
67	BY	124/135 (92%)	122 (98%)	2 (2%)	55	75
68	BZ	117/118 (99%)	117 (100%)	0	100	100
69	Ba	118/119 (99%)	118 (100%)	0	100	100
70	Bb	87/183 (48%)	87 (100%)	0	100	100
71	Bc	92/98 (94%)	92 (100%)	0	100	100
72	Bd	98/110 (89%)	98 (100%)	0	100	100
73	Be	116/121 (96%)	116 (100%)	0	100	100
74	Bf	89/89 (100%)	89 (100%)	0	100	100
75	Bg	98/100 (98%)	98 (100%)	0	100	100
76	Bh	109/110 (99%)	106 (97%)	3 (3%)	38	66
77	Bi	86/89 (97%)	85 (99%)	1 (1%)	63	78
78	Bj	73/80 (91%)	73 (100%)	0	100	100
79	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	75
80	Bl	47/48 (98%)	46 (98%)	1 (2%)	47	71
81	Bm	47/115 (41%)	47 (100%)	0	100	100
82	Bo	92/93 (99%)	92 (100%)	0	100	100
83	Bp	74/75 (99%)	72 (97%)	2 (3%)	39	67
84	Br	109/120 (91%)	109 (100%)	0	100	100
85	Bs	164/258 (64%)	161 (98%)	3 (2%)	51	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	Bt	128/137 (93%)	124 (97%)	4 (3%)	35	64
87	Bv	191/195 (98%)	187 (98%)	4 (2%)	47	71
All	All	10465/12763 (82%)	10369 (99%)	96 (1%)	68	80

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	74	THR
3	AB	14	VAL
5	AD	120	VAL
6	AE	40	VAL
6	AE	75	VAL
7	AF	107	ASP
7	AF	143	GLN
7	AF	159	ASN
7	AF	235	ILE
7	AF	266	ILE
12	AU	55	THR
12	AU	73	VAL
12	AU	90	LEU
13	AZ	87	VAL
13	AZ	121	LEU
13	AZ	206	ASP
14	Aa	170	GLU
14	Aa	178	THR
15	Ab	79	GLU
15	Ab	121	ARG
15	Ab	248	TYR
16	Ac	46	THR
16	Ac	105	LEU
17	Ad	139	LEU
17	Ad	236	ILE
20	Ag	53	VAL
20	Ag	109	ARG
21	Ah	46	VAL
22	Ai	41	ARG
22	Ai	55	LYS
22	Ai	152	ASP
23	Aj	40	VAL
25	Al	75	ASN
25	Al	91	LEU

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Mol	Chain	Res	Type
25	Al	104	VAL
26	Am	80	LEU
27	An	100	THR
30	Aq	16	ILE
30	Aq	73	LEU
31	Ar	94	LYS
31	Ar	103	LEU
33	At	54	VAL
33	At	68	THR
34	Au	42	VAL
34	Au	61	ARG
35	Av	105	THR
36	Aw	105	PHE
36	Aw	125	VAL
37	Ax	98	GLU
38	Ay	44	LEU
43	BA	246	LEU
44	BB	248	LEU
44	BB	340	THR
44	BB	344	VAL
47	BE	107	THR
47	BE	109	VAL
47	BE	223	LYS
49	BG	28	VAL
49	BG	106	THR
51	BI	38	ARG
51	BI	43	VAL
53	BK	4372	VAL
53	BK	4377	LYS
53	BK	4386	LEU
54	BL	63	THR
54	BL	115	GLN
54	BL	200	LYS
55	BM	126	GLU
58	BP	140	MET
59	BQ	82	VAL
59	BQ	115	LYS
60	BR	106	LEU
61	BS	6	THR
62	BT	76	VAL
66	BX	39	LYS
67	BY	88	GLU

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Mol	Chain	Res	Type
67	BY	120	GLU
76	Bh	8	ASP
76	Bh	87	LYS
76	Bh	88	THR
77	Bi	35	LYS
79	Bk	36	VAL
80	Bl	47	THR
83	Bp	3	LYS
83	Bp	52	VAL
85	Bs	44	ARG
85	Bs	61	MET
85	Bs	78	LEU
86	Bt	12	VAL
86	Bt	15	LEU
86	Bt	35	LEU
86	Bt	73	VAL
87	Bv	58	THR
87	Bv	60	ARG
87	Bv	96	ASN
87	Bv	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	19	HIS
2	AA	29	ASN
2	AA	51	GLN
5	AD	89	GLN
5	AD	111	GLN
6	AE	72	HIS
7	AF	62	HIS
7	AF	159	ASN
7	AF	296	GLN
8	AG	37	ASN
12	AU	32	GLN
12	AU	51	GLN
12	AU	52	HIS
12	AU	100	ASN
12	AU	117	ASN
13	AZ	113	GLN
14	Aa	92	GLN
14	Aa	101	HIS

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Mol	Chain	Res	Type
14	Aa	160	GLN
14	Aa	186	ASN
15	Ab	115	GLN
15	Ab	178	HIS
17	Ad	98	ASN
17	Ad	142	HIS
17	Ad	197	ASN
18	Ae	65	GLN
18	Ae	118	ASN
19	Af	81	HIS
20	Ag	68	GLN
20	Ag	91	HIS
20	Ag	112	ASN
21	Ah	7	ASN
21	Ah	165	GLN
21	Ah	167	GLN
23	Aj	66	HIS
23	Aj	77	GLN
24	Ak	11	GLN
24	Ak	19	ASN
24	Ak	39	ASN
25	Al	28	HIS
26	Am	5	HIS
26	Am	13	GLN
26	Am	36	GLN
26	Am	69	ASN
27	An	113	GLN
28	Ao	103	ASN
29	Ap	11	GLN
29	Ap	80	GLN
29	Ap	86	GLN
29	Ap	97	GLN
30	Aq	29	HIS
30	Aq	121	GLN
32	As	12	GLN
34	Au	2	GLN
35	Av	91	ASN
36	Aw	23	HIS
36	Aw	39	ASN
36	Aw	61	GLN
36	Aw	92	ASN
36	Aw	110	HIS

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Mol	Chain	Res	Type
37	Ax	19	GLN
37	Ax	63	HIS
37	Ax	85	ASN
37	Ax	89	HIS
38	Ay	112	ASN
43	BA	50	HIS
43	BA	83	HIS
43	BA	140	ASN
44	BB	184	GLN
44	BB	186	ASN
45	BC	48	ASN
45	BC	61	GLN
45	BC	187	GLN
45	BC	203	GLN
45	BC	212	ASN
45	BC	276	ASN
45	BC	329	ASN
45	BC	347	HIS
46	BD	122	GLN
46	BD	131	ASN
46	BD	202	GLN
46	BD	222	GLN
46	BD	291	GLN
47	BE	131	HIS
48	BF	57	HIS
48	BF	115	GLN
48	BF	205	ASN
49	BG	43	GLN
49	BG	64	GLN
49	BG	81	ASN
50	BH	140	GLN
51	BI	59	GLN
51	BI	163	GLN
51	BI	166	HIS
52	BJ	42	GLN
52	BJ	104	ASN
55	BM	34	ASN
55	BM	48	GLN
55	BM	125	ASN
56	BN	15	GLN
57	BO	167	HIS
57	BO	180	GLN

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Mol	Chain	Res	Type
58	BP	75	GLN
58	BP	120	ASN
58	BP	137	ASN
59	BQ	57	ASN
60	BR	39	GLN
60	BR	40	GLN
60	BR	118	HIS
61	BS	125	GLN
61	BS	173	ASN
62	BT	131	GLN
63	BU	17	GLN
63	BU	38	ASN
65	BW	63	GLN
65	BW	120	GLN
66	BX	111	GLN
67	BY	14	ASN
67	BY	18	HIS
67	BY	56	GLN
68	BZ	127	ASN
69	Ba	34	ASN
69	Ba	62	HIS
69	Ba	66	ASN
70	Bb	50	ASN
71	Bc	33	GLN
71	Bc	72	HIS
72	Bd	28	ASN
74	Bf	56	ASN
75	Bg	112	GLN
75	Bg	114	GLN
76	Bh	98	HIS
78	Bj	13	ASN
78	Bj	57	ASN
78	Bj	66	HIS
80	Bl	4	HIS
80	Bl	25	GLN
82	Bo	102	GLN
83	Bp	92	GLN
84	Br	4	HIS
84	Br	6	GLN
85	Bs	34	ASN
85	Bs	41	GLN
85	Bs	58	ASN

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Mol	Chain	Res	Type
85	Bs	127	ASN
86	Bt	70	GLN
86	Bt	100	HIS
87	Bv	96	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1765/1870 (94%)	244 (13%)	2 (0%)
10	AJ	75/76 (98%)	14 (18%)	0
11	AT	74/75 (98%)	12 (16%)	0
40	B5	3752/4808 (78%)	475 (12%)	2 (0%)
41	B7	118/120 (98%)	8 (6%)	0
42	B8	155/158 (98%)	15 (9%)	0
9	AH	9/217 (4%)	1 (11%)	0
All	All	5948/7324 (81%)	769 (12%)	4 (0%)

All (769) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	4	C
1	A2	26	U
1	A2	33	G
1	A2	41	G
1	A2	44	U
1	A2	46	A
1	A2	56	G
1	A2	58	C
1	A2	67	C
1	A2	68	A
1	A2	73	C
1	A2	74	G
1	A2	76	U
1	A2	77	A
1	A2	79	A
1	A2	103	A
1	A2	113	G
1	A2	115	U
1	A2	126	G

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Mol	Chain	Res	Type
1	A2	129	C
1	A2	130	G
1	A2	143	U
1	A2	147	A
1	A2	155	G
1	A2	158	A
1	A2	168	C
1	A2	178	C
1	A2	180	G
1	A2	184	G
1	A2	188	C
1	A2	189	U
1	A2	190	G
1	A2	192	C
1	A2	204	G
1	A2	226	A
1	A2	227	U
1	A2	228	C
1	A2	283	G
1	A2	287	U
1	A2	288	U
1	A2	303	A
1	A2	306	U
1	A2	308	G
1	A2	310	G
1	A2	313	G
1	A2	321	G
1	A2	324	C
1	A2	325	U
1	A2	327	C
1	A2	328	G
1	A2	333	G
1	A2	334	G
1	A2	348	G
1	A2	363	C
1	A2	365	A
1	A2	369	U
1	A2	370	C
1	A2	386	G
1	A2	387	C
1	A2	401	C
1	A2	410	C

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Mol	Chain	Res	Type
1	A2	417	U
1	A2	449	A
1	A2	450	A
1	A2	451	C
1	A2	465	A
1	A2	472	G
1	A2	473	C
1	A2	474	A
1	A2	475	G
1	A2	477	A
1	A2	483	G
1	A2	488	U
1	A2	493	C
1	A2	494	A
1	A2	502	C
1	A2	509	A
1	A2	535	G
1	A2	537	A
1	A2	544	C
1	A2	545	G
1	A2	556	A
1	A2	557	U
1	A2	565	A
1	A2	577	A2M
1	A2	588	A
1	A2	590	G
1	A2	592	U
1	A2	607	G
1	A2	609	C
1	A2	615	C
1	A2	629	A
1	A2	632	U
1	A2	644	A
1	A2	645	OMG
1	A2	656	A
1	A2	661	C
1	A2	669	A2M
1	A2	670	A
1	A2	672	A
1	A2	673	A
1	A2	674	G
1	A2	689	U

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Mol	Chain	Res	Type
1	A2	697	G
1	A2	746	C
1	A2	747	C
1	A2	749	C
1	A2	754	C
1	A2	755	G
1	A2	757	C
1	A2	759	C
1	A2	789	G
1	A2	800	U
1	A2	809	A
1	A2	812	A
1	A2	822	G
1	A2	823	PSU
1	A2	831	A
1	A2	832	G
1	A2	837	G
1	A2	838	A
1	A2	839	G
1	A2	840	C
1	A2	841	C
1	A2	842	G
1	A2	848	A
1	A2	870	A
1	A2	871	A
1	A2	872	U
1	A2	873	A
1	A2	879	G
1	A2	892	G
1	A2	902	G
1	A2	914	A
1	A2	915	U
1	A2	921	A
1	A2	923	A
1	A2	931	C
1	A2	934	G
1	A2	944	U
1	A2	956	A
1	A2	957	G
1	A2	964	A
1	A2	971	G
1	A2	972	G

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Mol	Chain	Res	Type
1	A2	986	G
1	A2	991	A
1	A2	993	A
1	A2	1000	G
1	A2	1003	U
1	A2	1024	A
1	A2	1062	U
1	A2	1063	A
1	A2	1084	A
1	A2	1086	C
1	A2	1116	U
1	A2	1117	C
1	A2	1118	C
1	A2	1119	C
1	A2	1122	G
1	A2	1134	A
1	A2	1145	A
1	A2	1154	C
1	A2	1155	U
1	A2	1196	A
1	A2	1216	C
1	A2	1243	U
1	A2	1249	B8N
1	A2	1250	C
1	A2	1252	A
1	A2	1254	A
1	A2	1257	G
1	A2	1258	G
1	A2	1260	A
1	A2	1272	C
1	A2	1275	G
1	A2	1276	G
1	A2	1303	G
1	A2	1304	C
1	A2	1316	U
1	A2	1343	U
1	A2	1359	U
1	A2	1372	U
1	A2	1373	U
1	A2	1379	A
1	A2	1398	U
1	A2	1406	A

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Mol	Chain	Res	Type
1	A2	1407	G
1	A2	1419	C
1	A2	1420	C
1	A2	1422	A
1	A2	1424	C
1	A2	1436	C
1	A2	1448	OMG
1	A2	1455	A
1	A2	1463	U
1	A2	1464	U
1	A2	1481	A
1	A2	1490	A
1	A2	1491	OMG
1	A2	1495	U
1	A2	1498	G
1	A2	1522	C
1	A2	1523	A
1	A2	1534	A
1	A2	1545	C
1	A2	1553	G
1	A2	1554	C
1	A2	1579	U
1	A2	1580	A
1	A2	1581	A
1	A2	1589	A
1	A2	1602	A
1	A2	1605	G
1	A2	1622	U
1	A2	1624	A
1	A2	1647	C
1	A2	1655	G
1	A2	1662	A
1	A2	1666	G
1	A2	1681	G
1	A2	1699	C
1	A2	1700	A
1	A2	1722	U
1	A2	1723	G
1	A2	1730	U
1	A2	1749	G
1	A2	1783	G
1	A2	1784	C

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Mol	Chain	Res	Type
1	A2	1785	G
1	A2	1825	A
1	A2	1830	G
1	A2	1836	A
1	A2	1837	G
1	A2	1839	U
1	A2	1850	G
1	A2	1852	MA6
1	A2	1862	G
1	A2	1863	G
1	A2	1864	A
1	A2	1865	U
1	A2	1866	C
9	AH	3430	C
10	AJ	5	U
10	AJ	9	A
10	AJ	17	A
10	AJ	18	G
10	AJ	19	G
10	AJ	20	C
10	AJ	21	A
10	AJ	22	G
10	AJ	36	U
10	AJ	46	G
10	AJ	48	C
10	AJ	49	C
10	AJ	73	A
10	AJ	74	C
11	AT	9	G
11	AT	16	G
11	AT	17	G
11	AT	18	G
11	AT	19	U
11	AT	20	A
11	AT	45	G
11	AT	46	U
11	AT	47	C
11	AT	48	C
11	AT	58	A
11	AT	75	A
40	B5	25	A
40	B5	39	A

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Mol	Chain	Res	Type
40	B5	42	A
40	B5	59	A
40	B5	64	A
40	B5	65	A
40	B5	72	C
40	B5	74	G
40	B5	85	G
40	B5	91	G
40	B5	98	A
40	B5	108	A
40	B5	109	G
40	B5	110	C
40	B5	119	G
40	B5	132	G
40	B5	134	G
40	B5	135	G
40	B5	140	G
40	B5	142	G
40	B5	159	C
40	B5	200	U
40	B5	201	C
40	B5	209	U
40	B5	210	C
40	B5	218	A
40	B5	219	G
40	B5	220	C
40	B5	233	U
40	B5	234	G
40	B5	265	C
40	B5	266	C
40	B5	297	U
40	B5	309	C
40	B5	310	G
40	B5	315	G
40	B5	316	U
40	B5	322	C
40	B5	326	C
40	B5	334	A
40	B5	340	C
40	B5	363	A
40	B5	386	A
40	B5	387	G

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Mol	Chain	Res	Type
40	B5	409	G
40	B5	410	A
40	B5	449	C
40	B5	450	G
40	B5	452	A
40	B5	453	G
40	B5	454	U
40	B5	467	U
40	B5	468	U
40	B5	482	U
40	B5	483	G
40	B5	493	U
40	B5	499	C
40	B5	500	G
40	B5	501	G
40	B5	502	U
40	B5	503	C
40	B5	504	U
40	B5	505	C
40	B5	506	G
40	B5	515	U
40	B5	517	C
40	B5	635	G
40	B5	681	U
40	B5	691	G
40	B5	698	C
40	B5	724	G
40	B5	725	G
40	B5	732	C
40	B5	734	G
40	B5	739	G
40	B5	758	C
40	B5	760	C
40	B5	790	G
40	B5	791	C
40	B5	792	G
40	B5	794	G
40	B5	795	A
40	B5	797	C
40	B5	798	C
40	B5	799	C
40	B5	810	U

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Mol	Chain	Res	Type
40	B5	812	A
40	B5	814	A
40	B5	815	G
40	B5	824	C
40	B5	825	G
40	B5	831	A
40	B5	832	G
40	B5	835	G
40	B5	843	A
40	B5	844	A
40	B5	845	U
40	B5	856	A
40	B5	859	G
40	B5	860	A
40	B5	861	G
40	B5	866	A
40	B5	867	C
40	B5	868	C
40	B5	870	G
40	B5	879	C
40	B5	884	U
40	B5	891	U
40	B5	985	G
40	B5	987	C
40	B5	1072	C
40	B5	1073	C
40	B5	1082	C
40	B5	1083	C
40	B5	1091	G
40	B5	1102	G
40	B5	1105	C
40	B5	1106	U
40	B5	1124	A
40	B5	1127	G
40	B5	1129	G
40	B5	1133	C
40	B5	1202	C
40	B5	1214	A
40	B5	1215	G
40	B5	1216	C
40	B5	1217	G
40	B5	1228	G

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Mol	Chain	Res	Type
40	B5	1231	G
40	B5	1238	A
40	B5	1239	U
40	B5	1240	G
40	B5	1246	U
40	B5	1247	A
40	B5	1270	A2M
40	B5	1298	A
40	B5	1299	G
40	B5	1303	G
40	B5	1309	C
40	B5	1310	G
40	B5	1311	C
40	B5	1312	A
40	B5	1323	C
40	B5	1331	A
40	B5	1341	A
40	B5	1351	G
40	B5	1362	C
40	B5	1367	G
40	B5	1375	A
40	B5	1391	C
40	B5	1393	C
40	B5	1401	C
40	B5	1412	G
40	B5	1452	A
40	B5	1453	G
40	B5	1457	G
40	B5	1459	G
40	B5	1480	A
40	B5	1489	A2M
40	B5	1502	A
40	B5	1521	C
40	B5	1533	U
40	B5	1546	U
40	B5	1551	U
40	B5	1568	A
40	B5	1579	G
40	B5	1580	OMG
40	B5	1586	A
40	B5	1588	G
40	B5	1589	A

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Mol	Chain	Res	Type
40	B5	1609	G
40	B5	1616	C
40	B5	1631	C
40	B5	1632	PSU
40	B5	1646	G
40	B5	1653	C
40	B5	1657	C
40	B5	1658	C
40	B5	1694	C
40	B5	1695	U
40	B5	1700	G
40	B5	1704	A
40	B5	1705	A
40	B5	1707	C
40	B5	1720	PSU
40	B5	1726	A
40	B5	1743	A
40	B5	1745	G
40	B5	1754	G
40	B5	1767	C
40	B5	1774	G
40	B5	1775	G
40	B5	1776	A
40	B5	1781	G
40	B5	1794	G
40	B5	1808	G
40	B5	1831	A
40	B5	1832	C
40	B5	1836	A
40	B5	1857	U
40	B5	1859	C
40	B5	1860	C
40	B5	1861	G
40	B5	1870	C
40	B5	1871	A
40	B5	1879	G
40	B5	1887	G
40	B5	1890	G
40	B5	1898	U
40	B5	1899	A
40	B5	1900	G
40	B5	1913	U

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Mol	Chain	Res	Type
40	B5	1914	G
40	B5	1922	A
40	B5	1923	A
40	B5	1924	G
40	B5	1925	U
40	B5	1926	C
40	B5	1936	U
40	B5	1940	G
40	B5	1942	G
40	B5	1943	U
40	B5	1963	G
40	B5	1965	A
40	B5	1985	G
40	B5	1987	U
40	B5	1994	G
40	B5	1995	G
40	B5	2008	A
40	B5	2023	U
40	B5	2024	G
40	B5	2032	G
40	B5	2034	A
40	B5	2037	G
40	B5	2041	G
40	B5	2043	A
40	B5	2044	A
40	B5	2045	G
40	B5	2046	A
40	B5	2101	C
40	B5	2132	C
40	B5	2143	A
40	B5	2144	G
40	B5	2156	A
40	B5	2157	G
40	B5	2191	G
40	B5	2194	OMC
40	B5	2203	A
40	B5	2207	OMG
40	B5	2238	A
40	B5	2240	G
40	B5	2242	G
40	B5	2264	G
40	B5	2268	U

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Mol	Chain	Res	Type
40	B5	2269	U
40	B5	2296	A
40	B5	2318	G
40	B5	2331	C
40	B5	2332	C
40	B5	2338	U
40	B5	2346	G
40	B5	2349	G
40	B5	2356	A
40	B5	2372	A
40	B5	2380	A
40	B5	2386	A
40	B5	2387	G
40	B5	2388	U
40	B5	2390	G
40	B5	2397	U
40	B5	2409	G
40	B5	2416	A
40	B5	2429	G
40	B5	2430	A
40	B5	2444	A
40	B5	2483	G
40	B5	2496	C
40	B5	2503	A
40	B5	2504	U
40	B5	2512	C
40	B5	2530	U
40	B5	2537	G
40	B5	2538	A
40	B5	2539	A
40	B5	2551	U
40	B5	2552	C
40	B5	2554	G
40	B5	2564	G
40	B5	2586	A
40	B5	2606	U
40	B5	2612	U
40	B5	2630	A2M
40	B5	2631	U
40	B5	2633	U
40	B5	2641	A
40	B5	2649	A

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Mol	Chain	Res	Type
40	B5	2657	C
40	B5	2669	U
40	B5	2670	G
40	B5	2672	U
40	B5	2698	G
40	B5	2745	G
40	B5	3329	G
40	B5	3350	C
40	B5	3358	G
40	B5	3367	A
40	B5	3380	A
40	B5	3385	A
40	B5	3394	A
40	B5	3405	C
40	B5	3428	C
40	B5	3441	U
40	B5	3442	G
40	B5	3444	A
40	B5	3445	U
40	B5	3478	A
40	B5	3493	C
40	B5	3498	A
40	B5	3506	A
40	B5	3507	A
40	B5	3508	G
40	B5	3509	G
40	B5	3510	U
40	B5	3516	A
40	B5	3541	G
40	B5	3542	C
40	B5	3543	G
40	B5	3546	U
40	B5	3549	A
40	B5	3551	G
40	B5	3570	U
40	B5	3572	U
40	B5	3600	G
40	B5	3609	A
40	B5	3610	C
40	B5	3611	G
40	B5	3629	G
40	B5	3633	A

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Mol	Chain	Res	Type
40	B5	3638	A
40	B5	3639	G
40	B5	3640	A
40	B5	3647	U
40	B5	3670	G
40	B5	3688	G
40	B5	3689	U
40	B5	3704	A
40	B5	3783	U
40	B5	3784	A
40	B5	3792	C
40	B5	3793	G
40	B5	3804	G
40	B5	3812	G
40	B5	3824	C
40	B5	3825	G
40	B5	3832	G
40	B5	3833	A
40	B5	3834	G
40	B5	3847	C
40	B5	3849	G
40	B5	3855	A
40	B5	3875	C
40	B5	3890	G
40	B5	3892	G
40	B5	3916	A
40	B5	3929	G
40	B5	3930	G
40	B5	3937	G
40	B5	3949	A
40	B5	3971	G
40	B5	3975	U
40	B5	3979	A
40	B5	3980	A
40	B5	3997	A
40	B5	4000	G
40	B5	4001	A
40	B5	4012	G
40	B5	4014	A
40	B5	4017	A
40	B5	4019	A
40	B5	4027	A

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Mol	Chain	Res	Type
40	B5	4043	G
40	B5	4051	G
40	B5	4052	OMU
40	B5	4060	C
40	B5	4076	G
40	B5	4078	C
40	B5	4096	C
40	B5	4100	U
40	B5	4119	G
40	B5	4123	G
40	B5	4124	A
40	B5	4126	A
40	B5	4133	C
40	B5	4137	G
40	B5	4140	A
40	B5	4144	C
40	B5	4168	A
40	B5	4183	U
40	B5	4194	G
40	B5	4198	U
40	B5	4210	A
40	B5	4221	G
40	B5	4222	C
40	B5	4258	U
40	B5	4259	A
40	B5	4270	G
40	B5	4277	U
40	B5	4278	PSU
40	B5	4294	A
40	B5	4295	G
40	B5	4306	C
40	B5	4313	G
40	B5	4321	G
40	B5	4336	A2M
40	B5	4346	G
40	B5	4382	PSU
40	B5	4383	OMG
40	B5	4402	A
40	B5	4416	C
40	B5	4418	A
40	B5	4437	A
40	B5	4446	A

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Mol	Chain	Res	Type
40	B5	4454	A
40	B5	4455	U
40	B5	4465	G
40	B5	4475	A
40	B5	4476	C
40	B5	4477	G
40	B5	4478	G
40	B5	4484	C
40	B5	4486	G
40	B5	4487	A
40	B5	4488	A
40	B5	4489	G
40	B5	4490	G
40	B5	4492	G
40	B5	4498	G
40	B5	4501	G
40	B5	4504	C
40	B5	4506	C
40	B5	4508	G
40	B5	4512	G
40	B5	4518	C
40	B5	4609	G
40	B5	4610	C
40	B5	4614	G
40	B5	4621	U
40	B5	4622	C
40	B5	4634	U
40	B5	4638	G
40	B5	4639	C
40	B5	4640	G
40	B5	4642	G
40	B5	4644	C
40	B5	4645	C
40	B5	4646	G
40	B5	4647	G
40	B5	4649	A
40	B5	4651	G
40	B5	4658	G
40	B5	4674	C
40	B5	4682	A
40	B5	4686	U
40	B5	4705	A

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Mol	Chain	Res	Type
40	B5	4715	U
40	B5	4728	U
40	B5	4729	C
40	B5	4753	A
40	B5	4756	G
40	B5	4764	C
40	B5	4780	G
40	B5	4789	C
40	B5	4793	C
40	B5	4801	G
40	B5	4808	U
41	B7	7	G
41	B7	53	U
41	B7	54	A
41	B7	63	C
41	B7	64	G
41	B7	102	U
41	B7	110	G
41	B7	120	U
42	B8	23	C
42	B8	34	U
42	B8	35	C
42	B8	59	A
42	B8	62	A
42	B8	63	U
42	B8	81	C
42	B8	84	A
42	B8	87	G
42	B8	94	G
42	B8	103	A
42	B8	105	C
42	B8	110	U
42	B8	114	G
42	B8	127	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	745	G
1	A2	871	A
40	B5	4294	A
40	B5	4445	U

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

227 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
40	A2M	B5	4269	40,88	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
40	PSU	B5	3502	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
40	OMC	B5	1820	40,88	19,22,23	0.80	0	26,31,34	0.79	0
1	6MZ	A2	1833	1,88	22,25,26	1.47	4 (18%)	30,36,39	2.17	8 (26%)
40	PSU	B5	1801	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
40	OMU	B5	3657	40	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
1	OMG	A2	1329	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
40	PSU	B5	4322	40	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
40	A2M	B5	3492	40	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
42	PSU	B8	69	42	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	1032	1	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
40	PSU	B5	2351	40	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1047	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	3585	40,88	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	1632	40	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
40	PSU	B5	4166	40	18,21,22	1.39	3 (16%)	22,30,33	1.80	4 (18%)
40	OMG	B5	4383	40	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
40	PSU	B5	4169	40	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	A2	602	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
40	OMC	B5	3619	40	19,22,23	0.82	0	26,31,34	0.86	0
40	OMG	B5	4240	40	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	A2	815	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
40	OMU	B5	2680	40	19,22,23	1.21	2 (10%)	26,31,34	1.71	5 (19%)
41	GTP	B7	1	41	30,34,34	0.50	0	46,54,54	0.56	0
40	OMC	B5	2667	40	19,22,23	0.81	0	26,31,34	0.82	0
1	PSU	A2	93	1	18,21,22	1.37	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
40	OMC	B5	2194	40,88	19,22,23	0.82	0	26,31,34	0.92	1 (3%)
40	PSU	B5	3652	40,88	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	119	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	3447	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
69	V5N	Ba	39	69	9,11,12	2.09	2 (22%)	9,14,16	1.69	2 (22%)
1	OMU	A2	1443	1,88	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
40	OMC	B5	2265	40,88	19,22,23	0.82	0	26,31,34	0.89	1 (3%)
40	PSU	B5	4749	40	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	4058	40	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	1679	1	22,25,26	1.46	4 (18%)	31,36,39	2.18	10 (32%)
1	PSU	A2	1057	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A2	684	1	23,26,27	1.19	3 (13%)	33,38,41	1.91	6 (18%)
1	OMG	A2	510	1,88	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
40	OMC	B5	3573	40	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	PSU	A2	1178	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
42	PSU	B8	55	42	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
40	PSU	B5	3462	40	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	3496	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	577	1	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
1	A2M	A2	469	1	22,25,26	1.48	4 (18%)	31,36,39	2.12	9 (29%)
40	PSU	B5	4099	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
40	PSU	B5	4435	40	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
40	PSU	B5	3371	40	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
40	PSU	B5	4045	40	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
40	OMC	B5	3540	40	19,22,23	0.81	0	26,31,34	0.79	0
1	PSU	A2	687	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
40	A2M	B5	400	40	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
1	4AC	A2	1843	1	21,24,25	1.13	2 (9%)	29,34,37	1.28	3 (10%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
1	A2M	A2	159	1	22,25,26	1.47	4 (18%)	31,36,39	2.16	10 (32%)
40	PSU	B5	3576	40	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
40	OMG	B5	1260	40	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
40	OMG	B5	1580	40	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
11	5MU	AT	53	11	19,22,23	1.42	6 (31%)	28,32,35	2.07	7 (25%)
81	M3L	Bm	98	81	10,11,12	0.84	0	9,14,16	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A2	34	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	4740	40	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	A2	1392	1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	OMC	A2	463	1	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.89	1 (3%)
40	OMG	B5	2719	40	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)
1	A2M	A2	485	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
1	MA6	A2	1852	1	23,26,27	1.53	5 (21%)	34,38,41	2.39	10 (29%)
40	PSU	B5	3490	40	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	A2	1448	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
40	OMG	B5	2267	40	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
44	HIC	BB	245	44	10,11,12	0.62	0	8,14,16	0.38	0
40	OMC	B5	1284	40	19,22,23	0.81	0	26,31,34	0.79	0
40	5MC	B5	4193	40	18,22,23	0.99	2 (11%)	26,32,35	1.19	2 (7%)
1	OMU	A2	1327	1	19,22,23	1.18	2 (10%)	26,31,34	1.72	5 (19%)
40	OMG	B5	2207	40	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
40	OMU	B5	2258	40	19,22,23	1.22	3 (15%)	26,31,34	1.74	5 (19%)
1	PSU	A2	36	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	MA6	A2	1851	1	23,26,27	1.52	5 (21%)	34,38,41	2.21	12 (35%)
40	PSU	B5	1799	40	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
40	UR3	B5	4276	40	19,22,23	0.97	0	26,32,35	1.42	1 (3%)
40	OMG	B5	3524	40	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	109	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	A2	174	1,88	19,22,23	0.82	0	26,31,34	0.82	0
40	PSU	B5	3554	40	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
32	NMM	As	67	32	9,11,12	0.59	0	6,12,14	0.40	0
1	PSU	A2	650	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	A2	868	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
40	OMG	B5	4364	40	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	1233	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
40	OMU	B5	3973	40	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
40	PSU	B5	1720	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	A2	355	1	19,22,23	1.22	2 (10%)	26,31,34	1.72	4 (15%)
1	PSU	A2	1046	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	1721	40	18,21,22	1.35	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
40	OMG	B5	3942	40	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
40	PSU	B5	1718	40	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
40	A2M	B5	2630	40,88	22,25,26	1.45	4 (18%)	31,36,39	2.16	11 (35%)
40	PSU	B5	4177	40	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
40	PSU	B5	4217	40	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	1289	1	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
1	4AC	A2	1338	1	21,24,25	1.07	2 (9%)	29,34,37	1.26	3 (10%)
40	PSU	B5	4298	40	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	4382	40	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1626	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	105	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
40	OMC	B5	2704	40	19,22,23	0.82	0	26,31,34	0.82	0
40	PSU	B5	4188	40	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
40	PSU	B5	4149	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	6MZ	B5	3966	40	22,25,26	1.43	4 (18%)	30,36,39	2.18	9 (30%)
11	PSU	AT	54	11	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
40	PSU	B5	4711	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
40	A2M	B5	1270	40	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
1	OMU	A2	429	1	19,22,23	1.22	4 (21%)	26,31,34	1.69	5 (19%)
1	PSU	A2	1644	1,88	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
40	PSU	B5	3500	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	A2	1491	1,88	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	573	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
84	SAC	Br	2	84	7,8,9	0.53	0	8,9,11	0.85	1 (12%)
1	PSU	A2	867	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
40	PSU	B5	1537	40	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
40	OMG	B5	3476	40	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
40	PSU	B5	3583	40	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
40	OMG	B5	3631	40	23,26,27	1.19	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	A2	682	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	A2	628	1	19,22,23	1.19	2 (10%)	26,31,34	1.73	5 (19%)
40	A2M	B5	2244	40	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
40	OMG	B5	3676	40	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
40	A2M	B5	2206	40,88	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
1	PSU	A2	864	1	18,21,22	1.35	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
40	OMG	B5	4116	40	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	1245	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
40	PSU	B5	4419	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	A2	518	1	19,22,23	0.82	0	26,31,34	0.83	0
40	OMG	B5	3974	40	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
40	PSU	B5	4246	40	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
10	5MU	AJ	54	10	19,22,23	1.42	6 (31%)	28,32,35	1.99	6 (21%)
1	PSU	A2	1082	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	A2	1005	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
40	OMG	B5	3359	40	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
10	PSU	AJ	55	10	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
40	OMU	B5	4052	40	19,22,23	1.23	4 (21%)	26,31,34	1.67	4 (15%)
40	UY1	B5	3550	40	19,22,23	1.38	3 (15%)	22,31,34	1.83	4 (18%)
82	MLZ	B _o	53	82	8,9,10	0.49	0	4,9,11	0.08	0
40	OMC	B5	2647	40	19,22,23	0.82	0	26,31,34	0.82	0
1	A2M	A2	591	1	22,25,26	1.48	4 (18%)	31,36,39	2.21	7 (22%)
1	A2M	A2	27	1,88	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
1	OMU	A2	116	1	19,22,23	1.20	2 (10%)	26,31,34	1.69	4 (15%)
34	AME	A _u	1	34	9,10,11	0.49	0	9,11,13	0.87	1 (11%)
1	PSU	A2	967	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	669	1,88	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
1	OMG	A2	645	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
40	PSU	B5	1491	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	PSU	B5	3369	40	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
40	PSU	B5	4278	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	A2	166	1	22,25,26	1.48	4 (18%)	31,36,39	2.14	10 (32%)
1	PSU	A2	1175	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
40	1MA	B5	1266	40,88	21,25,26	1.37	4 (19%)	31,37,40	1.69	5 (16%)
40	PSU	B5	4042	40	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
70	MLZ	B _b	5	70	8,9,10	0.49	0	4,9,11	0.11	0
40	A2M	B5	1479	40	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
1	PSU	A2	1348	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
40	PSU	B5	4325	40	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A2	437	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	A2M	B5	1489	40,88	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
40	A2M	B5	3599	40	22,25,26	1.46	4 (18%)	31,36,39	2.09	9 (29%)
40	A2M	B5	3450	40	22,25,26	1.46	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	A2	823	1	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
40	A2M	B5	3562	40	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	A2M	B5	4317	40	22,25,26	1.46	4 (18%)	31,36,39	2.10	10 (32%)
40	A2M	B5	4336	40	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
40	PSU	B5	1683	40	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
40	PSU	B5	4267	40,88	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
40	A2M	B5	3456	40	22,25,26	1.47	4 (18%)	31,36,39	2.12	10 (32%)
40	A2M	B5	3517	40	22,25,26	1.43	4 (18%)	31,36,39	2.23	11 (35%)
40	OMC	B5	3601	40	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	PSU	A2	1239	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
40	OMC	B5	4202	40	19,22,23	0.81	0	26,31,34	0.79	0
40	OMG	B5	4138	40	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	B8N	A2	1249	1	24,29,30	1.30	3 (12%)	29,42,45	1.28	3 (10%)
40	OMG	B5	4245	40,10	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	A2M	A2	513	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
40	PSU	B5	4039	40	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
40	OMG	B5	1477	40	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
36	HY3	Aw	62	36	6,8,9	2.14	1 (16%)	5,10,12	1.08	1 (20%)
40	OMG	B5	4369	40	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	G7M	A2	1640	1,11	23,26,27	2.31	5 (21%)	35,39,42	2.95	10 (28%)
31	SAC	Ar	2	31	7,8,9	0.53	0	8,9,11	0.87	1 (12%)
40	PSU	B5	4107	40	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	A2	99	1,88	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
43	V5N	BA	216	43	9,11,12	2.06	2 (22%)	9,14,16	1.72	2 (22%)
1	PSU	A2	1693	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	802	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
13	SAC	AZ	2	13	7,8,9	0.52	0	8,9,11	0.87	1 (12%)
1	PSU	A2	652	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
40	PSU	B5	4203	40	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A2	210	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
40	OMC	B5	3433	40	19,22,23	0.80	0	26,31,34	0.74	0
40	PSU	B5	2475	40	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	218	1	18,21,22	1.32	2 (11%)	22,30,33	1.88	3 (13%)
40	PSU	B5	1638	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
40	OMU	B5	4244	40	19,22,23	1.20	2 (10%)	26,31,34	1.72	5 (19%)
40	OMC	B5	2208	40	19,22,23	0.80	0	26,31,34	0.77	0
40	PSU	B5	4374	40	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
45	AYA	BC	2	45	6,7,8	0.71	0	5,8,10	0.43	0
40	A2M	B5	2658	40,88	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
40	PSU	B5	3427	40	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	1384	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
40	A2M	B5	1810	40,88	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
40	PSU	B5	3616	40	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
40	OMC	B5	4282	40	19,22,23	0.82	0	26,31,34	0.85	0
1	OMU	A2	121	1	19,22,23	1.22	2 (10%)	26,31,34	1.69	4 (15%)
40	PSU	B5	1731	40	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
40	PSU	B5	3494	40	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
40	A2M	B5	3557	40	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
1	OMU	A2	172	1	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
40	OMU	B5	4366	40	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
40	A2M	B5	398	40	22,25,26	1.46	4 (18%)	31,36,39	2.19	10 (32%)
42	OMG	B8	75	42	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
40	PSU	B5	3466	40	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
40	5MC	B5	3514	40,88	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)

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
40	A2M	B5	4269	40,88	-	0/9/27/28	0/3/3/3
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3502	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	1820	40,88	-	1/9/27/28	0/2/2/2
1	6MZ	A2	1833	1,88	-	0/9/27/28	0/3/3/3
40	PSU	B5	1801	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMU	B5	3657	40	-	1/9/27/28	0/2/2/2
1	OMG	A2	1329	1	-	0/9/27/28	0/3/3/3
40	PSU	B5	4322	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	3492	40	-	0/9/27/28	0/3/3/3
42	PSU	B8	69	42	-	0/7/25/26	0/2/2/2
1	A2M	A2	1032	1	-	1/9/27/28	0/3/3/3
40	PSU	B5	2351	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3585	40,88	-	0/7/25/26	0/2/2/2
40	PSU	B5	1632	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4166	40	-	2/7/25/26	0/2/2/2
40	OMG	B5	4383	40	-	0/9/27/28	0/3/3/3
40	PSU	B5	4169	40	-	0/7/25/26	0/2/2/2
1	OMG	A2	602	1	-	0/9/27/28	0/3/3/3
40	OMC	B5	3619	40	-	2/9/27/28	0/2/2/2
40	OMG	B5	4240	40	-	0/9/27/28	0/3/3/3
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
40	OMU	B5	2680	40	-	1/9/27/28	0/2/2/2
41	GTP	B7	1	41	-	0/22/38/38	0/3/3/3
40	OMC	B5	2667	40	-	0/9/27/28	0/2/2/2
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	2194	40,88	-	2/9/27/28	0/2/2/2
40	PSU	B5	3652	40,88	-	0/7/25/26	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3447	40	-	0/7/25/26	0/2/2/2
69	V5N	Ba	39	69	-	1/9/10/12	0/1/1/1
1	OMU	A2	1443	1,88	-	0/9/27/28	0/2/2/2
40	OMC	B5	2265	40,88	-	0/9/27/28	0/2/2/2
40	PSU	B5	4749	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4058	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	1679	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	684	1	-	3/9/27/28	0/3/3/3
1	OMG	A2	510	1,88	-	1/9/27/28	0/3/3/3
40	OMC	B5	3573	40	-	1/9/27/28	0/2/2/2
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
42	PSU	B8	55	42	-	0/7/25/26	0/2/2/2
40	PSU	B5	3462	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3496	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	577	1	-	2/9/27/28	0/3/3/3
1	A2M	A2	469	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PSU	B5	4099	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4435	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3371	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4045	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	3540	40	-	0/9/27/28	0/2/2/2
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	400	40	-	0/9/27/28	0/3/3/3
1	4AC	A2	1843	1	-	4/11/29/30	0/2/2/2
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	159	1	-	0/9/27/28	0/3/3/3
40	PSU	B5	3576	40	-	1/7/25/26	0/2/2/2
40	OMG	B5	1260	40	-	1/9/27/28	0/3/3/3
40	OMG	B5	1580	40	-	0/9/27/28	0/3/3/3
11	5MU	AT	53	11	-	1/7/25/26	0/2/2/2
81	M3L	Bm	98	81	-	0/9/10/12	-
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4740	40	-	0/7/25/26	0/2/2/2
1	OMC	A2	1392	1	-	0/9/27/28	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
1	OMC	A2	1704	1	-	3/9/27/28	0/2/2/2
40	OMG	B5	2719	40	-	0/9/27/28	0/3/3/3
1	A2M	A2	485	1	-	0/9/27/28	0/3/3/3
1	MA6	A2	1852	1	-	1/11/29/30	0/3/3/3
40	PSU	B5	3490	40	-	0/7/25/26	0/2/2/2
1	OMG	A2	1448	1	-	3/9/27/28	0/3/3/3
40	OMG	B5	2267	40	-	1/9/27/28	0/3/3/3
44	HIC	BB	245	44	-	2/5/6/8	0/1/1/1
40	OMC	B5	1284	40	-	1/9/27/28	0/2/2/2
40	5MC	B5	4193	40	-	4/7/25/26	0/2/2/2
1	OMU	A2	1327	1	-	0/9/27/28	0/2/2/2
40	OMG	B5	2207	40	-	2/9/27/28	0/3/3/3
40	OMU	B5	2258	40	-	0/9/27/28	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
1	MA6	A2	1851	1	-	0/11/29/30	0/3/3/3
40	PSU	B5	1799	40	-	0/7/25/26	0/2/2/2
40	UR3	B5	4276	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3524	40	-	0/9/27/28	0/3/3/3
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	174	1,88	-	0/9/27/28	0/2/2/2
40	PSU	B5	3554	40	-	0/7/25/26	0/2/2/2
32	NMM	As	67	32	-	0/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	868	1	-	3/9/27/28	0/3/3/3
40	OMG	B5	4364	40	-	0/9/27/28	0/3/3/3
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
40	OMU	B5	3973	40	-	0/9/27/28	0/2/2/2
40	PSU	B5	1720	40	-	2/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	1721	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3942	40	-	0/9/27/28	0/3/3/3
40	PSU	B5	1718	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	2630	40,88	-	4/9/27/28	0/3/3/3
40	PSU	B5	4177	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4217	40	-	0/7/25/26	0/2/2/2
1	OMU	A2	1289	1	-	1/9/27/28	0/2/2/2
1	4AC	A2	1338	1	-	2/11/29/30	0/2/2/2
40	PSU	B5	4298	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4382	40	-	4/7/25/26	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	2704	40	-	0/9/27/28	0/2/2/2
40	PSU	B5	4188	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4149	40	-	0/7/25/26	0/2/2/2
40	6MZ	B5	3966	40	-	0/9/27/28	0/3/3/3
11	PSU	AT	54	11	-	0/7/25/26	0/2/2/2
40	PSU	B5	4711	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	1270	40	-	0/9/27/28	0/3/3/3
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
1	PSU	A2	1644	1,88	-	0/7/25/26	0/2/2/2
40	PSU	B5	3500	40	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	1,88	-	1/9/27/28	0/3/3/3
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
84	SAC	Br	2	84	-	0/7/8/10	-
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	1537	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3476	40	-	1/9/27/28	0/3/3/3
40	PSU	B5	3583	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	3631	40	-	1/9/27/28	0/3/3/3
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	628	1	-	0/9/27/28	0/2/2/2
40	A2M	B5	2244	40	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	B5	3676	40	-	1/9/27/28	0/3/3/3
40	A2M	B5	2206	40,88	-	0/9/27/28	0/3/3/3
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	4116	40	-	0/9/27/28	0/3/3/3
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4419	40	-	0/7/25/26	0/2/2/2
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
40	OMG	B5	3974	40	-	0/9/27/28	0/3/3/3
40	PSU	B5	4246	40	-	1/7/25/26	0/2/2/2
10	5MU	AJ	54	10	-	0/7/25/26	0/2/2/2
1	PSU	A2	1082	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	3359	40	-	0/9/27/28	0/3/3/3
10	PSU	AJ	55	10	-	0/7/25/26	0/2/2/2
40	OMU	B5	4052	40	-	1/9/27/28	0/2/2/2
40	UY1	B5	3550	40	-	2/9/27/28	0/2/2/2
82	MLZ	B _o	53	82	-	0/7/8/10	-
40	OMC	B5	2647	40	-	0/9/27/28	0/2/2/2
1	A2M	A2	591	1	-	4/9/27/28	0/3/3/3
1	A2M	A2	27	1,88	-	2/9/27/28	0/3/3/3
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
34	AME	A _u	1	34	-	2/9/10/12	-
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	1,88	-	2/9/27/28	0/3/3/3
1	OMG	A2	645	1	-	3/9/27/28	0/3/3/3
40	PSU	B5	1491	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3369	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4278	40	-	3/7/25/26	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
40	1MA	B5	1266	40,88	-	0/7/25/26	0/3/3/3
40	PSU	B5	4042	40	-	0/7/25/26	0/2/2/2
70	MLZ	B _b	5	70	-	0/7/8/10	-
40	A2M	B5	1479	40	-	0/9/27/28	0/3/3/3
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4325	40	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	1/9/27/28	0/3/3/3
40	A2M	B5	1489	40,88	-	2/9/27/28	0/3/3/3
40	A2M	B5	3599	40	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	A2M	B5	3450	40	-	2/9/27/28	0/3/3/3
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	3562	40	-	0/9/27/28	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	4317	40	-	0/9/27/28	0/3/3/3
40	A2M	B5	4336	40	-	1/9/27/28	0/3/3/3
40	PSU	B5	1683	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4267	40,88	-	0/7/25/26	0/2/2/2
40	A2M	B5	3456	40	-	0/9/27/28	0/3/3/3
40	A2M	B5	3517	40	-	2/9/27/28	0/3/3/3
40	OMC	B5	3601	40	-	0/9/27/28	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	4202	40	-	0/9/27/28	0/2/2/2
40	OMG	B5	4138	40	-	0/9/27/28	0/3/3/3
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
40	OMG	B5	4245	40,10	-	0/9/27/28	0/3/3/3
1	A2M	A2	513	1	-	2/9/27/28	0/3/3/3
40	PSU	B5	4039	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	1477	40	-	0/9/27/28	0/3/3/3
36	HY3	Aw	62	36	-	0/1/12/14	0/1/1/1
40	OMG	B5	4369	40	-	1/9/27/28	0/3/3/3
1	G7M	A2	1640	1,11	-	0/7/25/26	0/3/3/3
31	SAC	Ar	2	31	-	0/7/8/10	-
40	PSU	B5	4107	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	99	1,88	-	1/9/27/28	0/3/3/3
43	V5N	BA	216	43	-	2/9/10/12	0/1/1/1
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
13	SAC	AZ	2	13	-	2/7/8/10	-
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4203	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	3433	40	-	4/9/27/28	0/2/2/2
40	PSU	B5	2475	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	1638	40	-	0/7/25/26	0/2/2/2
40	OMU	B5	4244	40	-	0/9/27/28	0/2/2/2
40	OMC	B5	2208	40	-	0/9/27/28	0/2/2/2
40	PSU	B5	4374	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	AYA	BC	2	45	-	3/4/6/8	-
40	A2M	B5	2658	40,88	-	0/9/27/28	0/3/3/3
40	PSU	B5	3427	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/9/27/28	0/3/3/3
40	A2M	B5	1810	40,88	-	0/9/27/28	0/3/3/3
40	PSU	B5	3616	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	4282	40	-	1/9/27/28	0/2/2/2
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
40	PSU	B5	1731	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3494	40	-	2/7/25/26	0/2/2/2
40	A2M	B5	3557	40	-	0/9/27/28	0/3/3/3
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
40	OMU	B5	4366	40	-	1/9/27/28	0/2/2/2
40	A2M	B5	398	40	-	3/9/27/28	0/3/3/3
42	OMG	B8	75	42	-	0/9/27/28	0/3/3/3
40	PSU	B5	3466	40	-	0/7/25/26	0/2/2/2
40	5MC	B5	3514	40,88	-	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)
1	A2	1640	G7M	C8-N7	7.33	1.46	1.33
69	Ba	39	V5N	CG-ND1	-4.91	1.33	1.37
36	Aw	62	HY3	C3-CA	-4.90	1.50	1.55
43	BA	216	V5N	CG-ND1	-4.77	1.33	1.37
1	A2	1640	G7M	C5-N7	-4.68	1.33	1.39
1	A2	591	A2M	C5-C4	4.65	1.47	1.39
1	A2	1833	6MZ	C5-C4	4.64	1.47	1.39
1	A2	469	A2M	C5-C4	4.57	1.47	1.39
1	A2	1852	MA6	C5-C4	4.57	1.47	1.39
1	A2	166	A2M	C5-C4	4.54	1.47	1.39
40	B5	400	A2M	C5-C4	4.51	1.47	1.39
40	B5	3456	A2M	C5-C4	4.51	1.47	1.39
40	B5	2658	A2M	C5-C4	4.50	1.47	1.39
1	A2	159	A2M	C5-C4	4.50	1.47	1.39
40	B5	4336	A2M	C5-C4	4.50	1.47	1.39
40	B5	3450	A2M	C5-C4	4.49	1.47	1.39
1	A2	1851	MA6	C5-C4	4.49	1.47	1.39
40	B5	4317	A2M	C5-C4	4.49	1.47	1.39
40	B5	3557	A2M	C5-C4	4.49	1.47	1.39
1	A2	513	A2M	C5-C4	4.49	1.47	1.39
1	A2	99	A2M	C5-C4	4.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3599	A2M	C5-C4	4.48	1.47	1.39
40	B5	2244	A2M	C5-C4	4.47	1.47	1.39
1	A2	577	A2M	C5-C4	4.47	1.47	1.39
40	B5	2206	A2M	C5-C4	4.46	1.47	1.39
40	B5	1479	A2M	C5-C4	4.46	1.47	1.39
40	B5	3492	A2M	C5-C4	4.46	1.47	1.39
1	A2	485	A2M	C5-C4	4.45	1.47	1.39
40	B5	1810	A2M	C5-C4	4.45	1.47	1.39
40	B5	3562	A2M	C5-C4	4.45	1.47	1.39
1	A2	1032	A2M	C5-C4	4.45	1.47	1.39
1	A2	27	A2M	C5-C4	4.45	1.47	1.39
1	A2	1679	A2M	C5-C4	4.45	1.47	1.39
40	B5	3966	6MZ	C5-C4	4.44	1.47	1.39
40	B5	1270	A2M	C5-C4	4.43	1.47	1.39
1	A2	669	A2M	C5-C4	4.43	1.47	1.39
40	B5	1489	A2M	C5-C4	4.42	1.47	1.39
40	B5	4269	A2M	C5-C4	4.42	1.47	1.39
40	B5	398	A2M	C5-C4	4.42	1.47	1.39
40	B5	2630	A2M	C5-C4	4.42	1.47	1.39
1	A2	1384	A2M	C5-C4	4.42	1.47	1.39
40	B5	3517	A2M	C5-C4	4.37	1.47	1.39
1	A2	1640	G7M	C8-N9	3.98	1.46	1.35
1	A2	1640	G7M	C5-C4	3.75	1.47	1.38
40	B5	3550	UY1	C6-C5	3.65	1.39	1.35
11	AT	54	PSU	C6-C5	3.30	1.39	1.35
1	A2	867	PSU	C6-C5	3.27	1.39	1.35
10	AJ	55	PSU	C6-C5	3.27	1.39	1.35
1	A2	93	PSU	C6-C5	3.25	1.39	1.35
1	A2	210	PSU	C6-C5	3.25	1.39	1.35
40	B5	4166	PSU	C6-C5	3.24	1.39	1.35
40	B5	3466	PSU	C6-C5	3.23	1.39	1.35
40	B5	3583	PSU	C6-C5	3.20	1.39	1.35
1	A2	967	PSU	C6-C5	3.20	1.39	1.35
40	B5	1632	PSU	C6-C5	3.20	1.39	1.35
40	B5	3494	PSU	C6-C5	3.19	1.39	1.35
40	B5	3576	PSU	C6-C5	3.19	1.39	1.35
1	A2	1245	PSU	C6-C5	3.18	1.39	1.35
1	A2	823	PSU	C6-C5	3.18	1.39	1.35
40	B5	4188	PSU	C6-C5	3.18	1.39	1.35
40	B5	3490	PSU	C6-C5	3.18	1.39	1.35
40	B5	3427	PSU	C6-C5	3.18	1.39	1.35
1	A2	105	PSU	C6-C5	3.17	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4099	PSU	C6-C5	3.17	1.39	1.35
1	A2	119	PSU	C6-C5	3.17	1.39	1.35
1	A2	1348	PSU	C6-C5	3.17	1.39	1.35
1	A2	652	PSU	C6-C5	3.16	1.39	1.35
40	B5	3447	PSU	C6-C5	3.16	1.39	1.35
1	A2	34	PSU	C6-C5	3.16	1.39	1.35
40	B5	4382	PSU	C6-C5	3.15	1.39	1.35
1	A2	815	PSU	C6-C5	3.15	1.39	1.35
1	A2	1368	PSU	C6-C5	3.15	1.39	1.35
40	B5	4740	PSU	C6-C5	3.15	1.39	1.35
40	B5	1720	PSU	C6-C5	3.15	1.39	1.35
1	A2	816	PSU	C6-C5	3.14	1.39	1.35
1	A2	573	PSU	C6-C5	3.14	1.39	1.35
40	B5	4058	PSU	C6-C5	3.14	1.39	1.35
1	A2	1005	PSU	C6-C5	3.14	1.39	1.35
40	B5	1721	PSU	C6-C5	3.14	1.39	1.35
40	B5	3676	OMG	C5-C4	3.14	1.47	1.38
1	A2	407	PSU	C6-C5	3.14	1.39	1.35
40	B5	3502	PSU	C6-C5	3.14	1.39	1.35
42	B8	69	PSU	C6-C5	3.14	1.39	1.35
40	B5	1683	PSU	C6-C5	3.13	1.39	1.35
40	B5	1731	PSU	C6-C5	3.13	1.39	1.35
1	A2	1178	PSU	C6-C5	3.13	1.39	1.35
1	A2	868	OMG	C5-C4	3.13	1.47	1.38
1	A2	1047	PSU	C6-C5	3.13	1.39	1.35
1	A2	1057	PSU	C6-C5	3.13	1.39	1.35
40	B5	3496	PSU	C6-C5	3.13	1.39	1.35
40	B5	4711	PSU	C6-C5	3.13	1.39	1.35
40	B5	4169	PSU	C6-C5	3.12	1.39	1.35
1	A2	109	PSU	C6-C5	3.12	1.39	1.35
40	B5	4322	PSU	C6-C5	3.12	1.39	1.35
1	A2	610	PSU	C6-C5	3.12	1.39	1.35
40	B5	4107	PSU	C6-C5	3.12	1.39	1.35
40	B5	3500	PSU	C6-C5	3.12	1.39	1.35
40	B5	1266	1MA	C6-N6	3.11	1.35	1.28
1	A2	687	PSU	C6-C5	3.11	1.38	1.35
40	B5	4749	PSU	C6-C5	3.11	1.38	1.35
40	B5	4278	PSU	C6-C5	3.11	1.38	1.35
40	B5	3462	PSU	C6-C5	3.11	1.38	1.35
40	B5	3554	PSU	C6-C5	3.11	1.38	1.35
1	A2	802	PSU	C6-C5	3.11	1.38	1.35
40	B5	4419	PSU	C6-C5	3.11	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	437	OMG	C5-C4	3.10	1.47	1.38
1	A2	1693	PSU	C6-C5	3.10	1.38	1.35
40	B5	4374	PSU	C6-C5	3.10	1.38	1.35
1	A2	1239	PSU	C6-C5	3.10	1.38	1.35
40	B5	1537	PSU	C6-C5	3.10	1.38	1.35
40	B5	1638	PSU	C6-C5	3.10	1.38	1.35
1	A2	1491	OMG	C5-C4	3.09	1.47	1.38
40	B5	4149	PSU	C6-C5	3.09	1.38	1.35
40	B5	1491	PSU	C6-C5	3.09	1.38	1.35
40	B5	4364	OMG	C5-C4	3.09	1.47	1.38
1	A2	1249	B8N	C4-N3	-3.09	1.34	1.40
1	A2	36	PSU	C6-C5	3.09	1.38	1.35
1	A2	650	PSU	C6-C5	3.09	1.38	1.35
40	B5	3585	PSU	C6-C5	3.09	1.38	1.35
1	A2	510	OMG	C5-C4	3.08	1.47	1.38
1	A2	1448	OMG	C5-C4	3.08	1.47	1.38
40	B5	1799	PSU	C6-C5	3.08	1.38	1.35
1	A2	1843	4AC	C4-N4	-3.08	1.35	1.39
40	B5	1266	1MA	C5-C4	3.08	1.47	1.38
40	B5	4039	PSU	C6-C5	3.08	1.38	1.35
40	B5	4267	PSU	C6-C5	3.08	1.38	1.35
1	A2	602	OMG	C5-C4	3.08	1.47	1.38
40	B5	3524	OMG	C5-C4	3.08	1.47	1.38
1	A2	1175	PSU	C6-C5	3.08	1.38	1.35
1	A2	1644	PSU	C6-C5	3.07	1.38	1.35
40	B5	2475	PSU	C6-C5	3.07	1.38	1.35
1	A2	864	PSU	C6-C5	3.07	1.38	1.35
40	B5	4203	PSU	C6-C5	3.07	1.38	1.35
40	B5	4325	PSU	C6-C5	3.07	1.38	1.35
40	B5	3942	OMG	C5-C4	3.07	1.47	1.38
1	A2	1329	OMG	C5-C4	3.07	1.47	1.38
1	A2	218	PSU	C6-C5	3.07	1.38	1.35
1	A2	1446	PSU	C6-C5	3.07	1.38	1.35
40	B5	2267	OMG	C5-C4	3.07	1.47	1.38
1	A2	684	OMG	C5-C4	3.07	1.47	1.38
1	A2	1082	PSU	C6-C5	3.06	1.38	1.35
42	B8	75	OMG	C5-C4	3.06	1.47	1.38
40	B5	1801	PSU	C6-C5	3.06	1.38	1.35
40	B5	1580	OMG	C5-C4	3.06	1.47	1.38
40	B5	1718	PSU	C6-C5	3.06	1.38	1.35
40	B5	4435	PSU	C6-C5	3.06	1.38	1.35
40	B5	4116	OMG	C5-C4	3.06	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4217	PSU	C6-C5	3.06	1.38	1.35
40	B5	4246	PSU	C6-C5	3.06	1.38	1.35
40	B5	3476	OMG	C5-C4	3.05	1.47	1.38
1	A2	645	OMG	C5-C4	3.05	1.47	1.38
40	B5	4383	OMG	C5-C4	3.05	1.47	1.38
1	A2	1233	PSU	C6-C5	3.05	1.38	1.35
40	B5	3616	PSU	C6-C5	3.05	1.38	1.35
40	B5	4045	PSU	C6-C5	3.05	1.38	1.35
40	B5	4177	PSU	C6-C5	3.04	1.38	1.35
40	B5	2351	PSU	C6-C5	3.04	1.38	1.35
40	B5	4369	OMG	C5-C4	3.04	1.47	1.38
1	A2	1626	PSU	C6-C5	3.04	1.38	1.35
40	B5	4245	OMG	C5-C4	3.04	1.47	1.38
40	B5	3369	PSU	C6-C5	3.04	1.38	1.35
42	B8	55	PSU	C6-C5	3.04	1.38	1.35
40	B5	4042	PSU	C6-C5	3.04	1.38	1.35
40	B5	2207	OMG	C5-C4	3.04	1.47	1.38
40	B5	4138	OMG	C5-C4	3.04	1.47	1.38
1	A2	682	PSU	C6-C5	3.04	1.38	1.35
40	B5	2719	OMG	C5-C4	3.04	1.47	1.38
40	B5	4240	OMG	C5-C4	3.04	1.47	1.38
1	A2	1249	B8N	C6-C5	3.04	1.39	1.34
1	A2	1046	PSU	C6-C5	3.03	1.38	1.35
40	B5	3371	PSU	C6-C5	3.03	1.38	1.35
40	B5	3359	OMG	C5-C4	3.03	1.47	1.38
40	B5	3974	OMG	C5-C4	3.02	1.47	1.38
40	B5	1477	OMG	C5-C4	3.01	1.47	1.38
40	B5	1260	OMG	C5-C4	3.01	1.47	1.38
40	B5	3652	PSU	C6-C5	3.00	1.38	1.35
40	B5	4298	PSU	C6-C5	2.99	1.38	1.35
40	B5	3631	OMG	C5-C4	2.99	1.47	1.38
43	BA	216	V5N	CD2-NE2	-2.86	1.33	1.37
69	Ba	39	V5N	CD2-NE2	-2.84	1.33	1.37
40	B5	4193	5MC	C6-C5	2.83	1.39	1.34
1	A2	1338	4AC	C4-N4	-2.82	1.35	1.39
40	B5	3616	PSU	C4-N3	-2.79	1.33	1.38
40	B5	3369	PSU	C4-N3	-2.77	1.33	1.38
1	A2	1851	MA6	C5-C6	2.76	1.48	1.41
40	B5	3652	PSU	C4-N3	-2.76	1.33	1.38
40	B5	1799	PSU	C4-N3	-2.76	1.33	1.38
40	B5	4267	PSU	C4-N3	-2.76	1.33	1.38
1	A2	1852	MA6	C6-N6	2.76	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3514	5MC	C6-C5	2.75	1.39	1.34
1	A2	1239	PSU	C4-N3	-2.75	1.33	1.38
40	B5	3490	PSU	C4-N3	-2.75	1.33	1.38
40	B5	4045	PSU	C4-N3	-2.75	1.33	1.38
1	A2	815	PSU	C4-N3	-2.74	1.33	1.38
1	A2	166	A2M	C5-C6	2.74	1.48	1.41
40	B5	3585	PSU	C4-N3	-2.73	1.33	1.38
11	AT	53	5MU	C6-C5	2.73	1.39	1.34
1	A2	1693	PSU	C4-N3	-2.73	1.33	1.38
40	B5	2351	PSU	C4-N3	-2.73	1.33	1.38
40	B5	4149	PSU	C4-N3	-2.73	1.33	1.38
40	B5	4188	PSU	C4-N3	-2.72	1.33	1.38
42	B8	55	PSU	C4-N3	-2.72	1.33	1.38
1	A2	1446	PSU	C4-N3	-2.72	1.33	1.38
10	AJ	54	5MU	C6-C5	2.72	1.39	1.34
40	B5	1683	PSU	C4-N3	-2.72	1.33	1.38
40	B5	1491	PSU	C4-N3	-2.72	1.33	1.38
40	B5	1638	PSU	C4-N3	-2.72	1.33	1.38
40	B5	4107	PSU	C4-N3	-2.72	1.33	1.38
1	A2	1046	PSU	C4-N3	-2.71	1.33	1.38
40	B5	3492	A2M	C5-C6	2.71	1.48	1.41
40	B5	3502	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1644	PSU	C4-N3	-2.71	1.33	1.38
40	B5	1801	PSU	C4-N3	-2.70	1.33	1.38
40	B5	1721	PSU	C4-N3	-2.70	1.33	1.38
40	B5	4177	PSU	C4-N3	-2.70	1.33	1.38
1	A2	682	PSU	C4-N3	-2.70	1.33	1.38
40	B5	4298	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1233	PSU	C4-N3	-2.70	1.33	1.38
40	B5	398	A2M	C5-C6	2.70	1.48	1.41
1	A2	1852	MA6	C5-C6	2.70	1.48	1.41
40	B5	4203	PSU	C4-N3	-2.70	1.33	1.38
40	B5	4269	A2M	C5-C6	2.69	1.48	1.41
1	A2	867	PSU	C4-N3	-2.69	1.33	1.38
1	A2	652	PSU	C4-N3	-2.69	1.33	1.38
40	B5	3500	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4382	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4711	PSU	C4-N3	-2.69	1.33	1.38
40	B5	3371	PSU	C4-N3	-2.69	1.33	1.38
1	A2	1626	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4042	PSU	C4-N3	-2.69	1.33	1.38
40	B5	4740	PSU	C4-N3	-2.69	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4278	PSU	C4-N3	-2.69	1.33	1.38
40	B5	1479	A2M	C5-C6	2.69	1.48	1.41
40	B5	4317	A2M	C5-C6	2.69	1.48	1.41
40	B5	3496	PSU	C4-N3	-2.69	1.33	1.38
1	A2	802	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1178	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4217	PSU	C4-N3	-2.68	1.33	1.38
1	A2	34	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1851	MA6	C6-N6	2.68	1.44	1.36
40	B5	4325	PSU	C4-N3	-2.68	1.33	1.38
1	A2	469	A2M	C5-C6	2.68	1.48	1.41
40	B5	4039	PSU	C4-N3	-2.68	1.33	1.38
40	B5	4374	PSU	C4-N3	-2.68	1.33	1.38
1	A2	669	A2M	C5-C6	2.67	1.48	1.41
40	B5	4099	PSU	C4-N3	-2.67	1.33	1.38
1	A2	93	PSU	C4-N3	-2.67	1.33	1.38
40	B5	4435	PSU	C4-N3	-2.67	1.33	1.38
1	A2	513	A2M	C5-C6	2.67	1.48	1.41
40	B5	3456	A2M	C5-C6	2.67	1.48	1.41
40	B5	4322	PSU	C4-N3	-2.67	1.33	1.38
40	B5	4749	PSU	C4-N3	-2.67	1.33	1.38
40	B5	3562	A2M	C5-C6	2.67	1.48	1.41
40	B5	3450	A2M	C5-C6	2.67	1.48	1.41
40	B5	3583	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1047	PSU	C4-N3	-2.67	1.33	1.38
40	B5	3447	PSU	C4-N3	-2.67	1.33	1.38
1	A2	407	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1175	PSU	C4-N3	-2.67	1.33	1.38
1	A2	159	A2M	C5-C6	2.67	1.48	1.41
1	A2	1384	A2M	C5-C6	2.67	1.48	1.41
1	A2	573	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1057	PSU	C4-N3	-2.67	1.33	1.38
1	A2	27	A2M	C5-C6	2.67	1.48	1.41
40	B5	400	A2M	C5-C6	2.66	1.48	1.41
40	B5	3427	PSU	C4-N3	-2.66	1.33	1.38
40	B5	3554	PSU	C4-N3	-2.66	1.33	1.38
40	B5	1718	PSU	C4-N3	-2.66	1.33	1.38
1	A2	99	A2M	C5-C6	2.66	1.48	1.41
40	B5	1537	PSU	C4-N3	-2.66	1.33	1.38
1	A2	687	PSU	C4-N3	-2.66	1.33	1.38
1	A2	967	PSU	C4-N3	-2.66	1.33	1.38
1	A2	1679	A2M	C5-C6	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3557	A2M	C5-C6	2.66	1.48	1.41
1	A2	610	PSU	C4-N3	-2.66	1.33	1.38
40	B5	1632	PSU	C4-N3	-2.66	1.33	1.38
10	AJ	55	PSU	C4-N3	-2.66	1.33	1.38
40	B5	2658	A2M	C5-C6	2.66	1.48	1.41
40	B5	3576	PSU	C4-N3	-2.66	1.33	1.38
1	A2	591	A2M	C5-C6	2.66	1.48	1.41
40	B5	3599	A2M	C5-C6	2.66	1.48	1.41
1	A2	1368	PSU	C4-N3	-2.66	1.33	1.38
40	B5	3494	PSU	C4-N3	-2.66	1.33	1.38
40	B5	4419	PSU	C4-N3	-2.66	1.33	1.38
1	A2	485	A2M	C5-C6	2.66	1.48	1.41
1	A2	864	PSU	C4-N3	-2.65	1.33	1.38
1	A2	1005	PSU	C4-N3	-2.65	1.33	1.38
42	B8	69	PSU	C4-N3	-2.65	1.33	1.38
40	B5	3550	UY1	C2-N1	2.65	1.40	1.36
40	B5	1720	PSU	C4-N3	-2.65	1.33	1.38
1	A2	816	PSU	C4-N3	-2.65	1.33	1.38
1	A2	650	PSU	C4-N3	-2.65	1.33	1.38
40	B5	1489	A2M	C5-C6	2.65	1.48	1.41
40	B5	1731	PSU	C4-N3	-2.65	1.33	1.38
1	A2	1348	PSU	C4-N3	-2.65	1.33	1.38
1	A2	577	A2M	C5-C6	2.65	1.48	1.41
40	B5	4336	A2M	C5-C6	2.65	1.48	1.41
40	B5	3466	PSU	C4-N3	-2.65	1.33	1.38
40	B5	3462	PSU	C4-N3	-2.65	1.33	1.38
1	A2	109	PSU	C4-N3	-2.64	1.33	1.38
1	A2	1082	PSU	C4-N3	-2.64	1.33	1.38
1	A2	36	PSU	C4-N3	-2.64	1.33	1.38
40	B5	4058	PSU	C4-N3	-2.64	1.33	1.38
11	AT	54	PSU	C4-N3	-2.63	1.33	1.38
40	B5	1810	A2M	C5-C6	2.63	1.48	1.41
1	A2	105	PSU	C4-N3	-2.63	1.34	1.38
40	B5	2206	A2M	C5-C6	2.63	1.48	1.41
40	B5	2475	PSU	C4-N3	-2.63	1.34	1.38
1	A2	1245	PSU	C4-N3	-2.62	1.34	1.38
1	A2	1032	A2M	C5-C6	2.62	1.48	1.41
40	B5	2244	A2M	C5-C6	2.62	1.48	1.41
1	A2	210	PSU	C4-N3	-2.62	1.34	1.38
40	B5	2630	A2M	C5-C6	2.62	1.48	1.41
40	B5	4169	PSU	C4-N3	-2.61	1.34	1.38
40	B5	1270	A2M	C5-C6	2.61	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	53	5MU	C4-N3	-2.60	1.34	1.38
10	AJ	54	5MU	C4-N3	-2.60	1.34	1.38
1	A2	119	PSU	C4-N3	-2.60	1.34	1.38
1	A2	218	PSU	C4-N3	-2.60	1.34	1.38
40	B5	4166	PSU	C4-N3	-2.59	1.34	1.38
40	B5	3657	OMU	C4-N3	-2.58	1.33	1.38
1	A2	823	PSU	C4-N3	-2.58	1.34	1.38
40	B5	4246	PSU	C4-N3	-2.58	1.34	1.38
40	B5	1260	OMG	C6-N1	-2.57	1.34	1.38
40	B5	3517	A2M	C5-C6	2.57	1.48	1.41
1	A2	1491	OMG	C6-N1	-2.57	1.34	1.38
1	A2	602	OMG	C6-N1	-2.56	1.34	1.38
40	B5	4138	OMG	C6-N1	-2.56	1.34	1.38
40	B5	4244	OMU	C4-N3	-2.56	1.34	1.38
40	B5	2680	OMU	C4-N3	-2.55	1.34	1.38
40	B5	4116	OMG	C6-N1	-2.54	1.34	1.38
40	B5	3524	OMG	C6-N1	-2.54	1.34	1.38
40	B5	2719	OMG	C6-N1	-2.54	1.34	1.38
40	B5	3359	OMG	C6-N1	-2.54	1.34	1.38
1	A2	355	OMU	C4-N3	-2.53	1.34	1.38
40	B5	3973	OMU	C4-N3	-2.53	1.34	1.38
40	B5	3631	OMG	C6-N1	-2.53	1.34	1.38
1	A2	868	OMG	C6-N1	-2.52	1.34	1.38
40	B5	4052	OMU	C4-N3	-2.52	1.34	1.38
1	A2	1805	OMU	C4-N3	-2.52	1.34	1.38
1	A2	510	OMG	C6-N1	-2.52	1.34	1.38
1	A2	1443	OMU	C4-N3	-2.52	1.34	1.38
40	B5	3942	OMG	C6-N1	-2.52	1.34	1.38
1	A2	121	OMU	C4-N3	-2.51	1.34	1.38
40	B5	2207	OMG	C6-N1	-2.50	1.34	1.38
1	A2	1329	OMG	C6-N1	-2.50	1.34	1.38
1	A2	628	OMU	C4-N3	-2.50	1.34	1.38
40	B5	4383	OMG	C6-N1	-2.50	1.34	1.38
40	B5	3476	OMG	C6-N1	-2.50	1.34	1.38
40	B5	2258	OMU	C4-N3	-2.50	1.34	1.38
40	B5	3676	OMG	C6-N1	-2.49	1.34	1.38
1	A2	645	OMG	C6-N1	-2.49	1.34	1.38
40	B5	1477	OMG	C6-N1	-2.49	1.34	1.38
42	B8	75	OMG	C6-N1	-2.48	1.34	1.38
40	B5	1580	OMG	C6-N1	-2.48	1.34	1.38
1	A2	684	OMG	C6-N1	-2.48	1.34	1.38
1	A2	116	OMU	C4-N3	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4369	OMG	C6-N1	-2.48	1.34	1.38
40	B5	4245	OMG	C6-N1	-2.48	1.34	1.38
1	A2	429	OMU	C4-N3	-2.48	1.34	1.38
40	B5	3966	6MZ	C5-C6	2.48	1.48	1.41
1	A2	437	OMG	C6-N1	-2.47	1.34	1.38
1	A2	1289	OMU	C4-N3	-2.47	1.34	1.38
40	B5	4240	OMG	C6-N1	-2.47	1.34	1.38
40	B5	3974	OMG	C6-N1	-2.47	1.34	1.38
1	A2	1851	MA6	C8-N7	2.47	1.36	1.31
1	A2	1327	OMU	C4-N3	-2.46	1.34	1.38
40	B5	4366	OMU	C4-N3	-2.46	1.34	1.38
1	A2	1448	OMG	C6-N1	-2.46	1.34	1.38
1	A2	166	A2M	C8-N7	2.45	1.36	1.31
1	A2	172	OMU	C4-N3	-2.45	1.34	1.38
40	B5	3456	A2M	C8-N7	2.45	1.36	1.31
11	AT	53	5MU	C2-N1	2.44	1.42	1.38
1	A2	1249	B8N	C2-N3	-2.44	1.34	1.38
40	B5	1489	A2M	C8-N7	2.43	1.36	1.31
40	B5	2267	OMG	C6-N1	-2.43	1.34	1.38
1	A2	1384	A2M	C8-N7	2.42	1.36	1.31
40	B5	3562	A2M	C8-N7	2.42	1.36	1.31
40	B5	4364	OMG	C6-N1	-2.42	1.34	1.38
40	B5	1810	A2M	C8-N7	2.41	1.36	1.31
40	B5	4317	A2M	C8-N7	2.41	1.36	1.31
1	A2	159	A2M	C8-N7	2.41	1.36	1.31
40	B5	3450	A2M	C8-N7	2.40	1.36	1.31
1	A2	27	A2M	C8-N7	2.40	1.36	1.31
40	B5	3492	A2M	C8-N7	2.40	1.36	1.31
40	B5	1270	A2M	C8-N7	2.40	1.36	1.31
1	A2	1833	6MZ	C5-N7	-2.39	1.34	1.39
40	B5	2206	A2M	C8-N7	2.39	1.36	1.31
40	B5	4336	A2M	C8-N7	2.39	1.36	1.31
1	A2	1679	A2M	C8-N7	2.39	1.36	1.31
1	A2	99	A2M	C8-N7	2.39	1.36	1.31
10	AJ	54	5MU	C4-C5	2.39	1.48	1.44
40	B5	2630	A2M	C8-N7	2.39	1.36	1.31
1	A2	469	A2M	C8-N7	2.38	1.36	1.31
40	B5	398	A2M	C8-N7	2.38	1.36	1.31
1	A2	513	A2M	C8-N7	2.38	1.36	1.31
1	A2	577	A2M	C8-N7	2.38	1.36	1.31
40	B5	400	A2M	C8-N7	2.38	1.36	1.31
1	A2	1032	A2M	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	2244	A2M	C8-N7	2.37	1.36	1.31
40	B5	4269	A2M	C8-N7	2.37	1.36	1.31
1	A2	1640	G7M	C6-N1	-2.37	1.34	1.38
40	B5	1479	A2M	C8-N7	2.37	1.36	1.31
40	B5	3599	A2M	C8-N7	2.37	1.36	1.31
1	A2	669	A2M	C8-N7	2.36	1.36	1.31
1	A2	1833	6MZ	C5-C6	2.36	1.48	1.41
40	B5	3517	A2M	C8-N7	2.34	1.36	1.31
40	B5	3557	A2M	C8-N7	2.33	1.36	1.31
40	B5	2658	A2M	C8-N7	2.33	1.36	1.31
11	AT	53	5MU	C4-C5	2.31	1.48	1.44
40	B5	3966	6MZ	C8-N7	2.31	1.36	1.31
1	A2	485	A2M	C8-N7	2.31	1.36	1.31
1	A2	591	A2M	C5-N7	-2.30	1.34	1.39
40	B5	3514	5MC	C6-N1	-2.29	1.34	1.38
1	A2	591	A2M	C8-N7	2.29	1.35	1.31
10	AJ	54	5MU	C2-N1	2.28	1.42	1.38
10	AJ	54	5MU	C6-N1	-2.26	1.34	1.38
40	B5	1270	A2M	C5-N7	-2.26	1.34	1.39
40	B5	4193	5MC	C6-N1	-2.25	1.34	1.38
1	A2	1032	A2M	C5-N7	-2.25	1.34	1.39
1	A2	1833	6MZ	C8-N7	2.24	1.35	1.31
1	A2	485	A2M	C5-N7	-2.24	1.34	1.39
1	A2	602	OMG	C5-N7	-2.24	1.34	1.39
40	B5	3966	6MZ	C5-N7	-2.23	1.34	1.39
1	A2	577	A2M	C5-N7	-2.23	1.34	1.39
40	B5	2658	A2M	C5-N7	-2.23	1.34	1.39
40	B5	4138	OMG	C5-N7	-2.23	1.34	1.39
1	A2	429	OMU	C2-N1	2.23	1.42	1.38
40	B5	3557	A2M	C5-N7	-2.22	1.34	1.39
1	A2	99	A2M	C5-N7	-2.22	1.34	1.39
1	A2	1384	A2M	C5-N7	-2.22	1.34	1.39
1	A2	1852	MA6	C5-N7	-2.22	1.34	1.39
1	A2	469	A2M	C5-N7	-2.22	1.34	1.39
40	B5	400	A2M	C5-N7	-2.22	1.34	1.39
40	B5	1810	A2M	C5-N7	-2.22	1.34	1.39
1	A2	510	OMG	C5-N7	-2.21	1.34	1.39
1	A2	1852	MA6	C8-N7	2.21	1.35	1.31
40	B5	3524	OMG	C5-N7	-2.21	1.34	1.39
40	B5	3562	A2M	C5-N7	-2.21	1.34	1.39
40	B5	1266	1MA	C2-N3	2.21	1.34	1.30
40	B5	1479	A2M	C5-N7	-2.21	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3550	UY1	C6-N1	-2.21	1.32	1.36
1	A2	355	OMU	C2-N3	-2.21	1.34	1.38
40	B5	2206	A2M	C5-N7	-2.20	1.34	1.39
40	B5	2630	A2M	C5-N7	-2.20	1.34	1.39
40	B5	4269	A2M	C5-N7	-2.20	1.34	1.39
40	B5	1266	1MA	C5-N7	-2.20	1.34	1.39
1	A2	27	A2M	C5-N7	-2.20	1.34	1.39
40	B5	2719	OMG	C5-N7	-2.20	1.34	1.39
40	B5	4369	OMG	C5-N7	-2.19	1.34	1.39
40	B5	4336	A2M	C5-N7	-2.19	1.34	1.39
40	B5	2244	A2M	C5-N7	-2.19	1.34	1.39
40	B5	4240	OMG	C5-N7	-2.19	1.34	1.39
40	B5	1260	OMG	C5-N7	-2.18	1.34	1.39
40	B5	2267	OMG	C5-N7	-2.18	1.34	1.39
40	B5	3492	A2M	C5-N7	-2.18	1.34	1.39
40	B5	1489	A2M	C5-N7	-2.18	1.34	1.39
1	A2	628	OMU	C2-N3	-2.18	1.34	1.38
40	B5	3599	A2M	C5-N7	-2.18	1.34	1.39
1	A2	121	OMU	C2-N3	-2.18	1.34	1.38
1	A2	1491	OMG	C5-N7	-2.18	1.34	1.39
1	A2	513	A2M	C5-N7	-2.18	1.34	1.39
1	A2	669	A2M	C5-N7	-2.17	1.34	1.39
40	B5	3657	OMU	C2-N3	-2.17	1.34	1.38
40	B5	4052	OMU	C2-N3	-2.17	1.34	1.38
40	B5	4116	OMG	C5-N7	-2.17	1.34	1.39
40	B5	398	A2M	C5-N7	-2.17	1.34	1.39
1	A2	1679	A2M	C5-N7	-2.17	1.34	1.39
1	A2	645	OMG	C5-N7	-2.17	1.34	1.39
42	B8	75	OMG	C5-N7	-2.17	1.34	1.39
40	B5	3942	OMG	C5-N7	-2.17	1.34	1.39
40	B5	2680	OMU	C2-N3	-2.17	1.34	1.38
1	A2	1329	OMG	C5-N7	-2.17	1.34	1.39
1	A2	684	OMG	C5-N7	-2.16	1.34	1.39
1	A2	1843	4AC	C7-N4	-2.16	1.33	1.37
1	A2	159	A2M	C5-N7	-2.16	1.34	1.39
40	B5	4317	A2M	C5-N7	-2.16	1.34	1.39
1	A2	166	A2M	C5-N7	-2.16	1.34	1.39
40	B5	4245	OMG	C5-N7	-2.16	1.34	1.39
40	B5	4366	OMU	C2-N3	-2.16	1.34	1.38
40	B5	3973	OMU	C2-N3	-2.16	1.34	1.38
40	B5	3476	OMG	C5-N7	-2.16	1.34	1.39
1	A2	437	OMG	C5-N7	-2.16	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	3631	OMG	C5-N7	-2.15	1.34	1.39
40	B5	4244	OMU	C2-N3	-2.15	1.34	1.38
11	AT	53	5MU	C6-N1	-2.15	1.34	1.38
40	B5	4383	OMG	C5-N7	-2.15	1.34	1.39
40	B5	1477	OMG	C5-N7	-2.15	1.34	1.39
40	B5	4364	OMG	C5-N7	-2.15	1.34	1.39
40	B5	3517	A2M	C5-N7	-2.15	1.35	1.39
1	A2	1443	OMU	C2-N1	2.14	1.41	1.38
1	A2	1805	OMU	C2-N3	-2.14	1.34	1.38
1	A2	1289	OMU	C2-N1	2.14	1.41	1.38
1	A2	1327	OMU	C2-N3	-2.14	1.34	1.38
40	B5	1580	OMG	C5-N7	-2.14	1.34	1.39
40	B5	3450	A2M	C5-N7	-2.14	1.35	1.39
1	A2	172	OMU	C2-N3	-2.14	1.34	1.38
40	B5	3456	A2M	C5-N7	-2.14	1.35	1.39
40	B5	3974	OMG	C5-N7	-2.14	1.34	1.39
40	B5	2258	OMU	C2-N1	2.13	1.41	1.38
40	B5	3676	OMG	C5-N7	-2.13	1.35	1.39
40	B5	2207	OMG	C5-N7	-2.12	1.35	1.39
40	B5	3359	OMG	C5-N7	-2.12	1.35	1.39
1	A2	116	OMU	C2-N3	-2.12	1.34	1.38
1	A2	1448	OMG	C5-N7	-2.12	1.35	1.39
1	A2	1805	OMU	C2-N1	2.11	1.41	1.38
1	A2	1851	MA6	C5-N7	-2.11	1.35	1.39
1	A2	868	OMG	C5-N7	-2.11	1.35	1.39
1	A2	1443	OMU	C2-N3	-2.10	1.34	1.38
1	A2	429	OMU	C2-N3	-2.09	1.34	1.38
1	A2	1289	OMU	C2-N3	-2.08	1.34	1.38
40	B5	4052	OMU	C2-N1	2.05	1.41	1.38
40	B5	4366	OMU	C5-C4	-2.03	1.39	1.43
40	B5	3973	OMU	C2-N1	2.03	1.41	1.38
1	A2	429	OMU	C5-C4	-2.03	1.39	1.43
1	A2	1338	4AC	C7-N4	-2.02	1.33	1.37
40	B5	4052	OMU	C5-C4	-2.02	1.39	1.43
10	AJ	54	5MU	C2-N3	-2.02	1.34	1.38
40	B5	2258	OMU	C5-C4	-2.02	1.39	1.43
40	B5	4166	PSU	C4-C5	2.02	1.49	1.44
11	AT	53	5MU	C2-N3	-2.01	1.34	1.38

All (977) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1640	G7M	CN7-N7-C8	-7.77	112.86	124.84
1	A2	591	A2M	C5-C4-N3	-7.00	117.61	126.75
1	A2	1852	MA6	C5-C4-N3	-6.95	117.68	126.75
1	A2	1833	6MZ	C5-C4-N3	-6.78	117.90	126.75
1	A2	1640	G7M	N9-C8-N7	-6.59	95.91	112.21
1	A2	1640	G7M	C8-N7-C5	6.52	115.93	107.78
1	A2	1640	G7M	N9-C4-N3	6.43	138.85	125.94
1	A2	469	A2M	C5-C4-N3	-6.38	118.43	126.75
40	B5	2658	A2M	C5-C4-N3	-6.35	118.47	126.75
40	B5	1489	A2M	C5-C4-N3	-6.27	118.57	126.75
40	B5	1479	A2M	C5-C4-N3	-6.24	118.61	126.75
40	B5	3557	A2M	C5-C4-N3	-6.24	118.61	126.75
40	B5	400	A2M	C5-C4-N3	-6.22	118.63	126.75
1	A2	513	A2M	C5-C4-N3	-6.21	118.64	126.75
40	B5	3966	6MZ	C5-C4-N3	-6.21	118.64	126.75
40	B5	4336	A2M	C5-C4-N3	-6.21	118.64	126.75
40	B5	3599	A2M	C5-C4-N3	-6.21	118.65	126.75
40	B5	2719	OMG	C5-C4-N3	-6.21	118.39	128.46
1	A2	1032	A2M	C5-C4-N3	-6.20	118.66	126.75
40	B5	4138	OMG	C5-C4-N3	-6.20	118.40	128.46
1	A2	99	A2M	C5-C4-N3	-6.20	118.66	126.75
1	A2	669	A2M	C5-C4-N3	-6.20	118.66	126.75
40	B5	3369	PSU	N1-C2-N3	6.20	122.16	115.13
1	A2	159	A2M	C5-C4-N3	-6.19	118.68	126.75
1	A2	485	A2M	C5-C4-N3	-6.18	118.68	126.75
40	B5	2206	A2M	C5-C4-N3	-6.18	118.68	126.75
40	B5	3562	A2M	C5-C4-N3	-6.17	118.70	126.75
40	B5	3456	A2M	C5-C4-N3	-6.17	118.71	126.75
1	A2	27	A2M	C5-C4-N3	-6.16	118.71	126.75
1	A2	166	A2M	C5-C4-N3	-6.16	118.71	126.75
40	B5	398	A2M	C5-C4-N3	-6.15	118.73	126.75
40	B5	4317	A2M	C5-C4-N3	-6.14	118.73	126.75
1	A2	602	OMG	C5-C4-N3	-6.14	118.50	128.46
40	B5	3942	OMG	C5-C4-N3	-6.14	118.50	128.46
40	B5	3524	OMG	C5-C4-N3	-6.14	118.50	128.46
40	B5	1270	A2M	C5-C4-N3	-6.13	118.75	126.75
1	A2	868	OMG	C5-C4-N3	-6.13	118.52	128.46
40	B5	4269	A2M	C5-C4-N3	-6.13	118.76	126.75
40	B5	3616	PSU	N1-C2-N3	6.12	122.07	115.13
40	B5	3676	OMG	C5-C4-N3	-6.11	118.54	128.46
1	A2	1491	OMG	C5-C4-N3	-6.11	118.54	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	1580	OMG	C5-C4-N3	-6.11	118.56	128.46
1	A2	1384	A2M	C5-C4-N3	-6.10	118.79	126.75
1	A2	1329	OMG	C5-C4-N3	-6.10	118.56	128.46
40	B5	2244	A2M	C5-C4-N3	-6.10	118.80	126.75
40	B5	4369	OMG	C5-C4-N3	-6.10	118.57	128.46
1	A2	577	A2M	C5-C4-N3	-6.10	118.80	126.75
40	B5	4045	PSU	N1-C2-N3	6.10	122.04	115.13
1	A2	510	OMG	C5-C4-N3	-6.09	118.59	128.46
1	A2	1679	A2M	C5-C4-N3	-6.08	118.81	126.75
40	B5	4116	OMG	C5-C4-N3	-6.08	118.60	128.46
42	B8	75	OMG	C5-C4-N3	-6.08	118.60	128.46
40	B5	3450	A2M	C5-C4-N3	-6.08	118.82	126.75
1	A2	1448	OMG	C5-C4-N3	-6.07	118.61	128.46
40	B5	4383	OMG	C5-C4-N3	-6.07	118.61	128.46
40	B5	4435	PSU	N1-C2-N3	6.07	122.01	115.13
1	A2	645	OMG	C5-C4-N3	-6.07	118.61	128.46
40	B5	4188	PSU	N1-C2-N3	6.07	122.01	115.13
40	B5	1720	PSU	N1-C2-N3	6.07	122.01	115.13
40	B5	2207	OMG	C5-C4-N3	-6.07	118.62	128.46
40	B5	1477	OMG	C5-C4-N3	-6.06	118.62	128.46
1	A2	1057	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	1446	PSU	N1-C2-N3	6.06	122.00	115.13
40	B5	4042	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	815	PSU	N1-C2-N3	6.06	121.99	115.13
1	A2	1233	PSU	N1-C2-N3	6.05	121.98	115.13
40	B5	4278	PSU	N1-C2-N3	6.04	121.98	115.13
40	B5	3494	PSU	N1-C2-N3	6.04	121.98	115.13
40	B5	3492	A2M	C5-C4-N3	-6.04	118.87	126.75
1	A2	437	OMG	C5-C4-N3	-6.04	118.66	128.46
40	B5	1491	PSU	N1-C2-N3	6.04	121.97	115.13
40	B5	3359	OMG	C5-C4-N3	-6.04	118.67	128.46
40	B5	3476	OMG	C5-C4-N3	-6.04	118.67	128.46
40	B5	3500	PSU	N1-C2-N3	6.03	121.97	115.13
40	B5	2267	OMG	C5-C4-N3	-6.03	118.67	128.46
40	B5	3554	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	1239	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	682	PSU	N1-C2-N3	6.03	121.96	115.13
40	B5	1810	A2M	C5-C4-N3	-6.03	118.89	126.75
40	B5	3490	PSU	N1-C2-N3	6.03	121.96	115.13
40	B5	4364	OMG	C5-C4-N3	-6.02	118.69	128.46
40	B5	3447	PSU	N1-C2-N3	6.02	121.95	115.13
40	B5	3583	PSU	N1-C2-N3	6.02	121.95	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3652	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	3427	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4740	PSU	N1-C2-N3	6.01	121.94	115.13
42	B8	55	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	1260	OMG	C5-C4-N3	-6.01	118.71	128.46
40	B5	1638	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4325	PSU	N1-C2-N3	6.01	121.94	115.13
10	AJ	55	PSU	N1-C2-N3	6.01	121.94	115.13
1	A2	34	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4267	PSU	N1-C2-N3	6.01	121.94	115.13
40	B5	4711	PSU	N1-C2-N3	6.01	121.93	115.13
40	B5	1731	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	3496	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	650	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	610	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	4419	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	3517	A2M	C5-C4-N3	-6.00	118.92	126.75
1	A2	407	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	1693	PSU	N1-C2-N3	6.00	121.93	115.13
40	B5	4099	PSU	N1-C2-N3	6.00	121.92	115.13
40	B5	3502	PSU	N1-C2-N3	6.00	121.92	115.13
40	B5	3462	PSU	N1-C2-N3	6.00	121.92	115.13
40	B5	3585	PSU	N1-C2-N3	6.00	121.92	115.13
1	A2	1626	PSU	N1-C2-N3	5.99	121.92	115.13
40	B5	1799	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	36	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	652	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	1047	PSU	N1-C2-N3	5.99	121.92	115.13
40	B5	2351	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	4149	PSU	N1-C2-N3	5.99	121.91	115.13
1	A2	684	OMG	C5-C4-N3	-5.99	118.75	128.46
1	A2	105	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	1718	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	4217	PSU	N1-C2-N3	5.99	121.91	115.13
40	B5	3576	PSU	N1-C2-N3	5.98	121.91	115.13
1	A2	573	PSU	N1-C2-N3	5.98	121.91	115.13
1	A2	1046	PSU	N1-C2-N3	5.98	121.91	115.13
40	B5	1801	PSU	N1-C2-N3	5.98	121.90	115.13
1	A2	119	PSU	N1-C2-N3	5.97	121.89	115.13
40	B5	4246	PSU	N1-C2-N3	5.97	121.89	115.13
1	A2	1644	PSU	N1-C2-N3	5.96	121.89	115.13
40	B5	4240	OMG	C5-C4-N3	-5.96	118.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1245	PSU	N1-C2-N3	5.96	121.89	115.13
40	B5	3466	PSU	N1-C2-N3	5.96	121.89	115.13
40	B5	4169	PSU	N1-C2-N3	5.96	121.89	115.13
40	B5	4203	PSU	N1-C2-N3	5.96	121.88	115.13
40	B5	4374	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	210	PSU	N1-C2-N3	5.96	121.88	115.13
40	B5	2630	A2M	C5-C4-N3	-5.96	118.98	126.75
40	B5	4039	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	1368	PSU	N1-C2-N3	5.95	121.88	115.13
1	A2	864	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	967	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	93	PSU	N1-C2-N3	5.95	121.87	115.13
40	B5	4322	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	218	PSU	N1-C2-N3	5.95	121.87	115.13
1	A2	1178	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	867	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	1348	PSU	N1-C2-N3	5.94	121.86	115.13
40	B5	3974	OMG	C5-C4-N3	-5.94	118.83	128.46
40	B5	4298	PSU	N1-C2-N3	5.94	121.86	115.13
40	B5	4749	PSU	N1-C2-N3	5.94	121.86	115.13
40	B5	4245	OMG	C5-C4-N3	-5.93	118.83	128.46
40	B5	4177	PSU	N1-C2-N3	5.93	121.85	115.13
40	B5	1721	PSU	N1-C2-N3	5.93	121.85	115.13
40	B5	4107	PSU	N1-C2-N3	5.93	121.85	115.13
40	B5	3631	OMG	C5-C4-N3	-5.93	118.84	128.46
40	B5	4382	PSU	N1-C2-N3	5.93	121.84	115.13
40	B5	2475	PSU	N1-C2-N3	5.92	121.84	115.13
1	A2	823	PSU	N1-C2-N3	5.92	121.84	115.13
40	B5	4058	PSU	N1-C2-N3	5.92	121.84	115.13
40	B5	4276	UR3	C4-N3-C2	-5.92	118.99	124.56
1	A2	816	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	802	PSU	N1-C2-N3	5.91	121.83	115.13
42	B8	69	PSU	N1-C2-N3	5.91	121.83	115.13
40	B5	1537	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	1175	PSU	N1-C2-N3	5.91	121.82	115.13
1	A2	1005	PSU	N1-C2-N3	5.91	121.82	115.13
40	B5	1683	PSU	N1-C2-N3	5.89	121.81	115.13
1	A2	109	PSU	N1-C2-N3	5.89	121.80	115.13
40	B5	1632	PSU	N1-C2-N3	5.88	121.80	115.13
40	B5	3371	PSU	N1-C2-N3	5.88	121.79	115.13
1	A2	687	PSU	N1-C2-N3	5.86	121.76	115.13
1	A2	1082	PSU	N1-C2-N3	5.85	121.76	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1851	MA6	C5-C4-N3	-5.83	119.14	126.75
11	AT	54	PSU	N1-C2-N3	5.77	121.67	115.13
40	B5	4166	PSU	N1-C2-N3	5.60	121.48	115.13
1	A2	591	A2M	N3-C4-N9	5.52	136.17	127.08
1	A2	1852	MA6	N3-C4-N9	5.43	136.03	127.08
1	A2	1833	6MZ	N3-C4-N9	5.42	136.02	127.08
40	B5	1266	1MA	C5-C4-N3	-5.42	119.17	127.26
1	A2	1640	G7M	C5-C4-N3	-5.38	117.83	128.15
40	B5	3550	UY1	C4-N3-C2	-5.21	118.83	126.34
40	B5	2719	OMG	C2-N3-C4	4.99	121.20	112.30
1	A2	469	A2M	N3-C4-N9	4.98	135.29	127.08
11	AT	53	5MU	C4-N3-C2	-4.97	120.92	127.35
10	AJ	54	5MU	C4-N3-C2	-4.94	120.95	127.35
40	B5	2207	OMG	C2-N3-C4	4.92	121.06	112.30
40	B5	2658	A2M	N3-C4-N9	4.90	135.15	127.08
1	A2	602	OMG	C2-N3-C4	4.89	121.02	112.30
40	B5	4138	OMG	C2-N3-C4	4.89	121.02	112.30
40	B5	1479	A2M	N3-C4-N9	4.88	135.12	127.08
40	B5	4116	OMG	C2-N3-C4	4.88	121.00	112.30
1	A2	1329	OMG	C2-N3-C4	4.88	120.99	112.30
40	B5	3942	OMG	C2-N3-C4	4.88	120.99	112.30
40	B5	1260	OMG	C2-N3-C4	4.87	120.98	112.30
40	B5	3524	OMG	C2-N3-C4	4.87	120.98	112.30
40	B5	1580	OMG	C2-N3-C4	4.87	120.97	112.30
1	A2	1491	OMG	C2-N3-C4	4.87	120.97	112.30
1	A2	1852	MA6	C2-N3-C4	4.87	123.25	111.75
40	B5	3966	6MZ	N3-C4-N9	4.86	135.09	127.08
1	A2	1448	OMG	C2-N3-C4	4.86	120.96	112.30
40	B5	1477	OMG	C2-N3-C4	4.86	120.96	112.30
42	B8	75	OMG	C2-N3-C4	4.86	120.95	112.30
40	B5	3676	OMG	C2-N3-C4	4.86	120.95	112.30
40	B5	3359	OMG	C2-N3-C4	4.85	120.95	112.30
40	B5	3599	A2M	N3-C4-N9	4.85	135.08	127.08
40	B5	4383	OMG	C2-N3-C4	4.85	120.94	112.30
1	A2	485	A2M	N3-C4-N9	4.85	135.07	127.08
1	A2	437	OMG	C2-N3-C4	4.85	120.94	112.30
1	A2	868	OMG	C2-N3-C4	4.85	120.94	112.30
1	A2	510	OMG	C2-N3-C4	4.85	120.94	112.30
40	B5	3557	A2M	N3-C4-N9	4.85	135.06	127.08
40	B5	3476	OMG	C2-N3-C4	4.84	120.93	112.30
40	B5	400	A2M	N3-C4-N9	4.84	135.06	127.08
40	B5	2267	OMG	C2-N3-C4	4.84	120.92	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4369	OMG	C2-N3-C4	4.84	120.92	112.30
40	B5	3974	OMG	C2-N3-C4	4.84	120.92	112.30
1	A2	645	OMG	C2-N3-C4	4.84	120.92	112.30
1	A2	513	A2M	N3-C4-N9	4.84	135.05	127.08
40	B5	4240	OMG	C2-N3-C4	4.84	120.92	112.30
1	A2	99	A2M	N3-C4-N9	4.83	135.05	127.08
40	B5	4364	OMG	C2-N3-C4	4.83	120.91	112.30
1	A2	684	OMG	C2-N3-C4	4.83	120.91	112.30
40	B5	4245	OMG	C2-N3-C4	4.83	120.90	112.30
1	A2	159	A2M	N3-C4-N9	4.81	135.00	127.08
40	B5	4336	A2M	N3-C4-N9	4.81	135.00	127.08
40	B5	2206	A2M	N3-C4-N9	4.80	135.00	127.08
10	AJ	54	5MU	N3-C2-N1	4.80	121.26	114.89
40	B5	3631	OMG	C2-N3-C4	4.80	120.84	112.30
1	A2	577	A2M	N3-C4-N9	4.79	134.98	127.08
1	A2	27	A2M	N3-C4-N9	4.79	134.98	127.08
1	A2	1679	A2M	N3-C4-N9	4.79	134.97	127.08
40	B5	3517	A2M	N3-C4-N9	4.79	134.97	127.08
1	A2	1032	A2M	N3-C4-N9	4.78	134.97	127.08
1	A2	669	A2M	N3-C4-N9	4.78	134.96	127.08
40	B5	3562	A2M	N3-C4-N9	4.78	134.95	127.08
40	B5	3456	A2M	N3-C4-N9	4.78	134.95	127.08
1	A2	1338	4AC	N4-C4-N3	4.77	121.85	113.85
1	A2	1384	A2M	N3-C4-N9	4.76	134.93	127.08
11	AT	53	5MU	N3-C2-N1	4.76	121.21	114.89
1	A2	166	A2M	N3-C4-N9	4.76	134.93	127.08
40	B5	4317	A2M	N3-C4-N9	4.76	134.93	127.08
40	B5	398	A2M	N3-C4-N9	4.76	134.92	127.08
40	B5	4269	A2M	N3-C4-N9	4.74	134.89	127.08
40	B5	1270	A2M	N3-C4-N9	4.74	134.89	127.08
40	B5	1266	1MA	C2-N3-C4	4.73	121.71	112.41
40	B5	1489	A2M	N3-C4-N9	4.73	134.88	127.08
40	B5	2244	A2M	N3-C4-N9	4.72	134.86	127.08
40	B5	2719	OMG	N9-C4-N3	4.72	135.42	125.94
40	B5	3450	A2M	N3-C4-N9	4.71	134.84	127.08
40	B5	3492	A2M	N3-C4-N9	4.69	134.80	127.08
40	B5	2630	A2M	N3-C4-N9	4.68	134.79	127.08
40	B5	1810	A2M	N3-C4-N9	4.68	134.79	127.08
1	A2	628	OMU	C4-N3-C2	-4.65	120.44	126.58
40	B5	4138	OMG	N9-C4-N3	4.65	135.27	125.94
40	B5	3524	OMG	N9-C4-N3	4.63	135.23	125.94
1	A2	602	OMG	N9-C4-N3	4.62	135.22	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3942	OMG	N9-C4-N3	4.61	135.20	125.94
1	A2	1491	OMG	N9-C4-N3	4.61	135.19	125.94
40	B5	3676	OMG	N9-C4-N3	4.61	135.19	125.94
1	A2	510	OMG	N9-C4-N3	4.59	135.16	125.94
1	A2	1843	4AC	N4-C4-N3	4.58	121.54	113.85
1	A2	1327	OMU	C4-N3-C2	-4.58	120.54	126.58
40	B5	4369	OMG	N9-C4-N3	4.58	135.13	125.94
40	B5	1580	OMG	N9-C4-N3	4.57	135.12	125.94
1	A2	868	OMG	N9-C4-N3	4.57	135.12	125.94
1	A2	1329	OMG	N9-C4-N3	4.56	135.10	125.94
11	AT	53	5MU	C5-C4-N3	4.56	119.21	115.31
42	B8	75	OMG	N9-C4-N3	4.56	135.09	125.94
40	B5	3476	OMG	N9-C4-N3	4.55	135.07	125.94
1	A2	684	OMG	N9-C4-N3	4.54	135.05	125.94
40	B5	4383	OMG	N9-C4-N3	4.53	135.04	125.94
1	A2	355	OMU	C4-N3-C2	-4.53	120.60	126.58
1	A2	1448	OMG	N9-C4-N3	4.52	135.02	125.94
40	B5	4116	OMG	N9-C4-N3	4.52	135.02	125.94
40	B5	4244	OMU	C4-N3-C2	-4.51	120.63	126.58
1	A2	645	OMG	N9-C4-N3	4.51	135.00	125.94
1	A2	437	OMG	N9-C4-N3	4.51	134.99	125.94
40	B5	2680	OMU	C4-N3-C2	-4.50	120.65	126.58
40	B5	3359	OMG	N9-C4-N3	4.48	134.94	125.94
40	B5	1477	OMG	N9-C4-N3	4.48	134.93	125.94
40	B5	2267	OMG	N9-C4-N3	4.48	134.93	125.94
40	B5	2207	OMG	N9-C4-N3	4.47	134.92	125.94
40	B5	4364	OMG	N9-C4-N3	4.47	134.91	125.94
1	A2	172	OMU	C4-N3-C2	-4.47	120.69	126.58
40	B5	4366	OMU	C4-N3-C2	-4.46	120.70	126.58
40	B5	4240	OMG	N9-C4-N3	4.45	134.88	125.94
40	B5	3657	OMU	C4-N3-C2	-4.45	120.71	126.58
40	B5	4245	OMG	N9-C4-N3	4.44	134.86	125.94
40	B5	1260	OMG	N9-C4-N3	4.44	134.85	125.94
1	A2	116	OMU	C4-N3-C2	-4.41	120.77	126.58
40	B5	3631	OMG	N9-C4-N3	4.39	134.76	125.94
1	A2	1851	MA6	N1-C6-N6	4.38	121.88	117.08
1	A2	121	OMU	C4-N3-C2	-4.37	120.81	126.58
1	A2	1851	MA6	N3-C4-N9	4.37	134.29	127.08
1	A2	1851	MA6	C2-N1-C6	4.36	122.06	111.75
40	B5	3974	OMG	N9-C4-N3	4.36	134.69	125.94
40	B5	4244	OMU	N3-C2-N1	4.35	120.67	114.89
40	B5	3973	OMU	C4-N3-C2	-4.35	120.84	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	2258	OMU	C4-N3-C2	-4.31	120.90	126.58
40	B5	4052	OMU	C4-N3-C2	-4.29	120.92	126.58
1	A2	1852	MA6	C2-N1-C6	4.29	121.88	111.75
1	A2	1289	OMU	C4-N3-C2	-4.27	120.95	126.58
1	A2	1640	G7M	C8-N9-C4	4.26	117.93	107.16
1	A2	1805	OMU	C4-N3-C2	-4.25	120.97	126.58
1	A2	429	OMU	C4-N3-C2	-4.25	120.97	126.58
1	A2	1640	G7M	C2-N3-C4	4.25	119.87	112.30
1	A2	1443	OMU	C4-N3-C2	-4.24	120.99	126.58
10	AJ	54	5MU	C5-C4-N3	4.23	118.92	115.31
1	A2	355	OMU	N3-C2-N1	4.20	120.46	114.89
40	B5	3550	UY1	N1-C2-N3	4.19	119.88	115.13
40	B5	2258	OMU	N3-C2-N1	4.18	120.43	114.89
40	B5	3657	OMU	N3-C2-N1	4.17	120.42	114.89
1	A2	591	A2M	C2-N3-C4	4.16	121.58	111.75
1	A2	628	OMU	N3-C2-N1	4.15	120.39	114.89
1	A2	1640	G7M	C1'-N9-C8	-4.14	112.75	126.74
40	B5	4366	OMU	N3-C2-N1	4.13	120.38	114.89
1	A2	1327	OMU	N3-C2-N1	4.12	120.36	114.89
40	B5	2680	OMU	N3-C2-N1	4.10	120.33	114.89
1	A2	1443	OMU	N3-C2-N1	4.10	120.33	114.89
1	A2	172	OMU	N3-C2-N1	4.09	120.32	114.89
11	AT	53	5MU	O4-C4-C5	-4.09	120.16	124.90
1	A2	116	OMU	N3-C2-N1	4.09	120.32	114.89
1	A2	121	OMU	N3-C2-N1	4.07	120.30	114.89
40	B5	3616	PSU	C4-N3-C2	-4.05	120.51	126.34
40	B5	3973	OMU	N3-C2-N1	4.04	120.25	114.89
1	A2	1805	OMU	N3-C2-N1	4.03	120.24	114.89
40	B5	398	A2M	C2'-C1'-N9	-4.03	106.74	113.53
1	A2	1852	MA6	N1-C2-N3	-4.03	122.30	128.60
1	A2	429	OMU	N3-C2-N1	4.02	120.22	114.89
40	B5	4042	PSU	C4-N3-C2	-4.01	120.56	126.34
40	B5	4188	PSU	C4-N3-C2	-4.01	120.57	126.34
40	B5	1799	PSU	C4-N3-C2	-4.00	120.57	126.34
40	B5	4711	PSU	C4-N3-C2	-4.00	120.57	126.34
40	B5	4099	PSU	C4-N3-C2	-3.99	120.59	126.34
40	B5	3490	PSU	C4-N3-C2	-3.99	120.59	126.34
40	B5	4203	PSU	C4-N3-C2	-3.98	120.61	126.34
40	B5	3652	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A2	1446	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A2	1233	PSU	C4-N3-C2	-3.97	120.62	126.34
1	A2	1239	PSU	C4-N3-C2	-3.96	120.63	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3369	PSU	C4-N3-C2	-3.96	120.63	126.34
40	B5	4045	PSU	C4-N3-C2	-3.96	120.63	126.34
40	B5	4052	OMU	N3-C2-N1	3.96	120.15	114.89
40	B5	4149	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	1175	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	407	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	1644	PSU	C4-N3-C2	-3.96	120.64	126.34
40	B5	1801	PSU	C4-N3-C2	-3.95	120.64	126.34
42	B8	69	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A2	1289	OMU	N3-C2-N1	3.95	120.13	114.89
40	B5	4298	PSU	C4-N3-C2	-3.94	120.66	126.34
40	B5	4193	5MC	C5-C6-N1	-3.94	119.28	123.34
40	B5	1731	PSU	C4-N3-C2	-3.94	120.66	126.34
42	B8	55	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	218	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	682	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	650	PSU	C4-N3-C2	-3.94	120.66	126.34
40	B5	4435	PSU	C4-N3-C2	-3.94	120.66	126.34
40	B5	1489	A2M	C2-N3-C4	3.94	121.05	111.75
40	B5	2351	PSU	C4-N3-C2	-3.94	120.67	126.34
40	B5	1718	PSU	C4-N3-C2	-3.94	120.67	126.34
40	B5	3496	PSU	C4-N3-C2	-3.93	120.67	126.34
40	B5	3502	PSU	C4-N3-C2	-3.93	120.67	126.34
40	B5	3447	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A2	1046	PSU	C4-N3-C2	-3.93	120.68	126.34
40	B5	4267	PSU	C4-N3-C2	-3.93	120.68	126.34
1	A2	573	PSU	C4-N3-C2	-3.92	120.68	126.34
1	A2	93	PSU	C4-N3-C2	-3.92	120.69	126.34
40	B5	3500	PSU	C4-N3-C2	-3.92	120.69	126.34
40	B5	4039	PSU	C4-N3-C2	-3.92	120.69	126.34
40	B5	1491	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	1693	PSU	C4-N3-C2	-3.91	120.70	126.34
40	B5	1721	PSU	C4-N3-C2	-3.91	120.70	126.34
40	B5	4749	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	119	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A2	1348	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A2	1057	PSU	C4-N3-C2	-3.90	120.72	126.34
40	B5	4177	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	469	A2M	C2-N3-C4	3.90	120.97	111.75
1	A2	1626	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	105	PSU	C4-N3-C2	-3.90	120.72	126.34
40	B5	4374	PSU	C4-N3-C2	-3.90	120.72	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	652	PSU	C4-N3-C2	-3.90	120.73	126.34
1	A2	36	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A2	34	PSU	C4-N3-C2	-3.89	120.73	126.34
40	B5	4322	PSU	C4-N3-C2	-3.89	120.73	126.34
40	B5	4419	PSU	C4-N3-C2	-3.89	120.73	126.34
40	B5	1638	PSU	C4-N3-C2	-3.89	120.74	126.34
40	B5	3583	PSU	C4-N3-C2	-3.89	120.74	126.34
40	B5	4246	PSU	C4-N3-C2	-3.89	120.74	126.34
40	B5	4058	PSU	C4-N3-C2	-3.88	120.74	126.34
10	AJ	55	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A2	27	A2M	C2-N3-C4	3.88	120.92	111.75
40	B5	2658	A2M	C2-N3-C4	3.88	120.92	111.75
1	A2	1047	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A2	864	PSU	C4-N3-C2	-3.88	120.75	126.34
40	B5	4278	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	1368	PSU	C4-N3-C2	-3.88	120.75	126.34
40	B5	4325	PSU	C4-N3-C2	-3.87	120.76	126.34
1	A2	1178	PSU	C4-N3-C2	-3.87	120.76	126.34
40	B5	1479	A2M	C2-N3-C4	3.87	120.90	111.75
40	B5	1720	PSU	C4-N3-C2	-3.87	120.76	126.34
40	B5	398	A2M	C2-N3-C4	3.87	120.89	111.75
40	B5	3427	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A2	816	PSU	C4-N3-C2	-3.86	120.77	126.34
40	B5	3585	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A2	1679	A2M	C2-N3-C4	3.86	120.88	111.75
1	A2	1245	PSU	C4-N3-C2	-3.86	120.77	126.34
40	B5	3462	PSU	C4-N3-C2	-3.86	120.77	126.34
1	A2	166	A2M	C2-N3-C4	3.86	120.87	111.75
40	B5	3554	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A2	513	A2M	C2-N3-C4	3.86	120.87	111.75
40	B5	4269	A2M	C2-N3-C4	3.86	120.87	111.75
40	B5	4217	PSU	C4-N3-C2	-3.86	120.78	126.34
40	B5	4336	A2M	C2-N3-C4	3.86	120.86	111.75
1	A2	99	A2M	C2-N3-C4	3.85	120.86	111.75
40	B5	1683	PSU	C4-N3-C2	-3.85	120.79	126.34
1	A2	1032	A2M	C2-N3-C4	3.85	120.85	111.75
40	B5	2206	A2M	C2-N3-C4	3.85	120.85	111.75
40	B5	3599	A2M	C2-N3-C4	3.85	120.85	111.75
40	B5	3517	A2M	C2-N3-C4	3.85	120.85	111.75
40	B5	3466	PSU	C4-N3-C2	-3.85	120.79	126.34
40	B5	400	A2M	C2-N3-C4	3.85	120.85	111.75
40	B5	3562	A2M	C2-N3-C4	3.85	120.85	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	967	PSU	C4-N3-C2	-3.85	120.80	126.34
1	A2	159	A2M	C2-N3-C4	3.85	120.83	111.75
1	A2	815	PSU	C4-N3-C2	-3.84	120.80	126.34
40	B5	3557	A2M	C2-N3-C4	3.84	120.83	111.75
1	A2	1384	A2M	C2-N3-C4	3.84	120.81	111.75
40	B5	3456	A2M	C2-N3-C4	3.83	120.81	111.75
40	B5	2244	A2M	C2-N3-C4	3.83	120.81	111.75
40	B5	1810	A2M	C2-N3-C4	3.83	120.81	111.75
1	A2	485	A2M	C2-N3-C4	3.83	120.80	111.75
1	A2	669	A2M	C2-N3-C4	3.83	120.80	111.75
1	A2	109	PSU	C4-N3-C2	-3.83	120.82	126.34
40	B5	2630	A2M	C2-N3-C4	3.83	120.80	111.75
40	B5	4317	A2M	C2-N3-C4	3.83	120.79	111.75
40	B5	4740	PSU	C4-N3-C2	-3.83	120.83	126.34
40	B5	3966	6MZ	C2-N3-C4	3.83	120.79	111.75
40	B5	3492	A2M	C2-N3-C4	3.82	120.78	111.75
1	A2	210	PSU	C4-N3-C2	-3.82	120.83	126.34
40	B5	3371	PSU	C4-N3-C2	-3.82	120.83	126.34
40	B5	3576	PSU	C4-N3-C2	-3.82	120.83	126.34
1	A2	610	PSU	C4-N3-C2	-3.82	120.83	126.34
40	B5	1537	PSU	C4-N3-C2	-3.82	120.84	126.34
11	AT	54	PSU	C4-N3-C2	-3.81	120.84	126.34
1	A2	867	PSU	C4-N3-C2	-3.81	120.84	126.34
1	A2	577	A2M	C2-N3-C4	3.81	120.75	111.75
40	B5	1270	A2M	C2-N3-C4	3.81	120.75	111.75
1	A2	1005	PSU	C4-N3-C2	-3.81	120.86	126.34
40	B5	4169	PSU	C4-N3-C2	-3.80	120.86	126.34
40	B5	3450	A2M	C2-N3-C4	3.80	120.72	111.75
40	B5	4107	PSU	C4-N3-C2	-3.80	120.87	126.34
1	A2	1679	A2M	C2'-C1'-N9	-3.79	107.14	113.53
1	A2	687	PSU	C4-N3-C2	-3.79	120.88	126.34
40	B5	2475	PSU	C4-N3-C2	-3.79	120.88	126.34
1	A2	1833	6MZ	C2-N3-C4	3.78	120.69	111.75
40	B5	3494	PSU	C4-N3-C2	-3.78	120.89	126.34
1	A2	802	PSU	C4-N3-C2	-3.77	120.90	126.34
1	A2	1851	MA6	C2-N3-C4	3.77	120.65	111.75
40	B5	4382	PSU	C4-N3-C2	-3.75	120.94	126.34
1	A2	823	PSU	C4-N3-C2	-3.71	120.99	126.34
1	A2	513	A2M	C2'-C1'-N9	-3.71	107.28	113.53
40	B5	1632	PSU	C4-N3-C2	-3.70	121.01	126.34
1	A2	1082	PSU	C4-N3-C2	-3.69	121.02	126.34
1	A2	628	OMU	C5-C4-N3	3.68	120.34	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AJ	54	5MU	O4-C4-C5	-3.66	120.66	124.90
40	B5	1810	A2M	C2'-C1'-N9	-3.64	107.40	113.53
1	A2	1327	OMU	C5-C4-N3	3.60	120.22	114.84
40	B5	3514	5MC	C5-C6-N1	-3.59	119.64	123.34
40	B5	2680	OMU	C5-C4-N3	3.59	120.21	114.84
1	A2	1640	G7M	CN7-N7-C5	3.58	131.21	126.77
1	A2	355	OMU	C5-C4-N3	3.57	120.19	114.84
1	A2	116	OMU	C5-C4-N3	3.57	120.19	114.84
40	B5	4366	OMU	C5-C4-N3	3.57	120.17	114.84
1	A2	172	OMU	C5-C4-N3	3.56	120.17	114.84
40	B5	4435	PSU	O2-C2-N1	-3.55	118.88	122.79
40	B5	3657	OMU	C5-C4-N3	3.55	120.15	114.84
1	A2	121	OMU	C5-C4-N3	3.54	120.14	114.84
40	B5	4052	OMU	C5-C4-N3	3.54	120.14	114.84
1	A2	1851	MA6	C4-C5-N7	-3.54	106.31	110.62
40	B5	3973	OMU	C5-C4-N3	3.54	120.13	114.84
1	A2	1289	OMU	C5-C4-N3	3.53	120.12	114.84
1	A2	429	OMU	C5-C4-N3	3.52	120.11	114.84
10	AJ	54	5MU	C5-C6-N1	-3.49	119.75	123.34
1	A2	652	PSU	O2-C2-N1	-3.48	118.96	122.79
1	A2	1852	MA6	N1-C6-N6	3.48	120.89	117.08
40	B5	3554	PSU	O2-C2-N1	-3.47	118.97	122.79
42	B8	55	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A2	1368	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A2	1805	OMU	C5-C4-N3	3.46	120.02	114.84
40	B5	4244	OMU	C5-C4-N3	3.46	120.02	114.84
40	B5	3616	PSU	O2-C2-N1	-3.46	118.98	122.79
40	B5	4278	PSU	O2-C2-N1	-3.46	118.98	122.79
40	B5	1489	A2M	C4-C5-N7	-3.45	106.41	110.62
1	A2	210	PSU	O2-C2-N1	-3.45	118.99	122.79
40	B5	1638	PSU	O2-C2-N1	-3.45	118.99	122.79
1	A2	823	PSU	O2-C2-N1	-3.44	119.00	122.79
40	B5	3496	PSU	O2-C2-N1	-3.44	119.00	122.79
40	B5	1731	PSU	O2-C2-N1	-3.43	119.01	122.79
40	B5	3369	PSU	O2-C2-N1	-3.43	119.01	122.79
1	A2	1057	PSU	O2-C2-N1	-3.43	119.01	122.79
1	A2	99	A2M	C2'-C1'-N9	-3.43	107.75	113.53
1	A2	650	PSU	O2-C2-N1	-3.43	119.01	122.79
40	B5	1801	PSU	O2-C2-N1	-3.43	119.02	122.79
40	B5	1718	PSU	O2-C2-N1	-3.43	119.02	122.79
40	B5	4749	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	1446	PSU	O2-C2-N1	-3.42	119.03	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3585	PSU	O2-C2-N1	-3.42	119.03	122.79
40	B5	2475	PSU	O2-C2-N1	-3.42	119.03	122.79
40	B5	3427	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	1443	OMU	C5-C4-N3	3.41	119.94	114.84
40	B5	2258	OMU	C5-C4-N3	3.41	119.94	114.84
40	B5	1720	PSU	O2-C2-N1	-3.41	119.04	122.79
10	AJ	55	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A2	815	PSU	O2-C2-N1	-3.41	119.04	122.79
40	B5	4267	PSU	O2-C2-N1	-3.40	119.04	122.79
40	B5	1491	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	3490	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A2	1852	MA6	C4-C5-N7	-3.40	106.48	110.62
1	A2	1233	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	4169	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	3966	6MZ	C9-N6-C6	-3.40	119.95	122.87
1	A2	1047	PSU	O2-C2-N1	-3.40	119.05	122.79
40	B5	3517	A2M	C2'-C1'-N9	-3.39	107.82	113.53
1	A2	1626	PSU	O2-C2-N1	-3.39	119.06	122.79
40	B5	3462	PSU	O2-C2-N1	-3.39	119.06	122.79
40	B5	4188	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A2	407	PSU	O2-C2-N1	-3.38	119.06	122.79
1	A2	1005	PSU	O2-C2-N1	-3.38	119.07	122.79
43	BA	216	V5N	CD2-CG-ND1	3.38	110.15	105.71
40	B5	4325	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	3494	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1082	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	3447	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1245	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1644	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4374	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4149	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4419	PSU	O2-C2-N1	-3.38	119.07	122.79
40	B5	4382	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	119	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1046	PSU	O2-C2-N1	-3.37	119.08	122.79
40	B5	3502	PSU	O2-C2-N1	-3.37	119.08	122.79
40	B5	4740	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	36	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	573	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1239	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	4322	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	682	PSU	O2-C2-N1	-3.36	119.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4045	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	109	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	3583	PSU	O2-C2-N1	-3.36	119.09	122.79
40	B5	4166	PSU	C4-N3-C2	-3.36	121.50	126.34
40	B5	3466	PSU	O2-C2-N1	-3.36	119.10	122.79
40	B5	4042	PSU	O2-C2-N1	-3.36	119.10	122.79
40	B5	4298	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1178	PSU	O2-C2-N1	-3.35	119.10	122.79
40	B5	4217	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	669	A2M	C4-C5-N7	-3.35	106.54	110.62
69	Ba	39	V5N	CD2-CG-ND1	3.35	110.11	105.71
40	B5	4203	PSU	O2-C2-N1	-3.35	119.10	122.79
40	B5	4246	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	967	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	577	A2M	C2'-C1'-N9	-3.35	107.90	113.53
40	B5	4107	PSU	O2-C2-N1	-3.34	119.11	122.79
40	B5	4039	PSU	O2-C2-N1	-3.34	119.11	122.79
1	A2	1693	PSU	O2-C2-N1	-3.34	119.12	122.79
1	A2	864	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	1175	PSU	O2-C2-N1	-3.33	119.12	122.79
40	B5	1537	PSU	O2-C2-N1	-3.33	119.12	122.79
40	B5	4336	A2M	C4-C5-N7	-3.33	106.56	110.62
1	A2	1384	A2M	C2'-C1'-N9	-3.33	107.93	113.53
1	A2	610	PSU	O2-C2-N1	-3.33	119.13	122.79
40	B5	4099	PSU	O2-C2-N1	-3.33	119.13	122.79
40	B5	3652	PSU	O2-C2-N1	-3.32	119.13	122.79
1	A2	166	A2M	C4-C5-N7	-3.32	106.57	110.62
40	B5	3456	A2M	C4-C5-N7	-3.31	106.58	110.62
1	A2	218	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	159	A2M	C4-C5-N7	-3.31	106.58	110.62
40	B5	3562	A2M	C4-C5-N7	-3.31	106.58	110.62
1	A2	93	PSU	O2-C2-N1	-3.31	119.14	122.79
40	B5	3500	PSU	O2-C2-N1	-3.31	119.14	122.79
40	B5	4269	A2M	C4-C5-N7	-3.31	106.59	110.62
1	A2	513	A2M	C4-C5-N7	-3.31	106.59	110.62
40	B5	1270	A2M	C4-C5-N7	-3.31	106.59	110.62
40	B5	2658	A2M	C4-C5-N7	-3.31	106.59	110.62
40	B5	4177	PSU	O2-C2-N1	-3.31	119.15	122.79
1	A2	1249	B8N	C4-N3-C2	-3.31	121.28	125.46
1	A2	105	PSU	O2-C2-N1	-3.30	119.15	122.79
40	B5	1266	1MA	N9-C4-N3	3.30	134.64	126.94
40	B5	4166	PSU	O2-C2-N1	-3.30	119.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3492	A2M	C4-C5-N7	-3.30	106.60	110.62
1	A2	802	PSU	O2-C2-N1	-3.30	119.16	122.79
40	B5	4058	PSU	O2-C2-N1	-3.30	119.16	122.79
40	B5	2244	A2M	C4-C5-N7	-3.30	106.61	110.62
40	B5	398	A2M	C4-C5-N7	-3.29	106.61	110.62
1	A2	867	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A2	1032	A2M	C4-C5-N7	-3.29	106.61	110.62
42	B8	69	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A2	687	PSU	O2-C2-N1	-3.29	119.17	122.79
40	B5	3371	PSU	O2-C2-N1	-3.29	119.17	122.79
40	B5	4317	A2M	C4-C5-N7	-3.29	106.62	110.62
40	B5	2206	A2M	C4-C5-N7	-3.29	106.62	110.62
40	B5	1721	PSU	O2-C2-N1	-3.28	119.17	122.79
40	B5	3974	OMG	C6-C5-N7	3.28	136.36	130.25
40	B5	2207	OMG	C6-C5-N7	3.28	136.36	130.25
40	B5	1810	A2M	C4-C5-N7	-3.28	106.62	110.62
40	B5	3576	PSU	O2-C2-N1	-3.28	119.18	122.79
40	B5	1799	PSU	O2-C2-N1	-3.28	119.18	122.79
1	A2	1348	PSU	O2-C2-N1	-3.28	119.18	122.79
40	B5	3557	A2M	C4-C5-N7	-3.27	106.63	110.62
40	B5	1260	OMG	C6-C5-N7	3.27	136.32	130.25
1	A2	469	A2M	C4-C5-N7	-3.27	106.64	110.62
40	B5	3450	A2M	C4-C5-N7	-3.27	106.64	110.62
40	B5	2351	PSU	O2-C2-N1	-3.26	119.20	122.79
40	B5	1683	PSU	O2-C2-N1	-3.26	119.20	122.79
1	A2	99	A2M	C4-C5-N7	-3.26	106.64	110.62
1	A2	1679	A2M	C4-C5-N7	-3.26	106.65	110.62
40	B5	400	A2M	C4-C5-N7	-3.26	106.65	110.62
1	A2	34	PSU	O2-C2-N1	-3.26	119.20	122.79
1	A2	27	A2M	C4-C5-N7	-3.26	106.65	110.62
1	A2	485	A2M	C4-C5-N7	-3.25	106.66	110.62
40	B5	4245	OMG	C6-C5-N7	3.25	136.28	130.25
1	A2	27	A2M	C2'-C1'-N9	-3.24	108.07	113.53
40	B5	2244	A2M	C2'-C1'-N9	-3.24	108.08	113.53
40	B5	3599	A2M	C4-C5-N7	-3.24	106.68	110.62
40	B5	3517	A2M	N3-C2-N1	-3.23	123.55	128.60
40	B5	4711	PSU	O2-C2-N1	-3.23	119.23	122.79
1	A2	159	A2M	C2'-C1'-N9	-3.23	108.10	113.53
1	A2	868	OMG	C6-C5-N7	3.22	136.24	130.25
1	A2	1384	A2M	C4-C5-N7	-3.22	106.69	110.62
40	B5	2630	A2M	N3-C2-N1	-3.22	123.57	128.60
11	AT	53	5MU	C5-C6-N1	-3.22	120.03	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	1479	A2M	C4-C5-N7	-3.22	106.70	110.62
40	B5	3631	OMG	C6-C5-N7	3.21	136.22	130.25
40	B5	3966	6MZ	C6-C5-N7	3.21	135.86	132.39
40	B5	1477	OMG	C6-C5-N7	3.21	136.21	130.25
40	B5	3359	OMG	C6-C5-N7	3.20	136.20	130.25
40	B5	4116	OMG	C6-C5-N7	3.20	136.20	130.25
40	B5	4240	OMG	C6-C5-N7	3.20	136.20	130.25
40	B5	4364	OMG	C6-C5-N7	3.19	136.19	130.25
1	A2	577	A2M	C4-C5-N7	-3.19	106.73	110.62
1	A2	1679	A2M	N3-C2-N1	-3.19	123.61	128.60
40	B5	1489	A2M	N3-C2-N1	-3.18	123.62	128.60
40	B5	398	A2M	N3-C2-N1	-3.18	123.63	128.60
40	B5	2630	A2M	C4-C5-N7	-3.18	106.75	110.62
40	B5	1810	A2M	N3-C2-N1	-3.18	123.63	128.60
40	B5	2267	OMG	C6-C5-N7	3.17	136.15	130.25
1	A2	437	OMG	C6-C5-N7	3.17	136.15	130.25
40	B5	3966	6MZ	C4-C5-N7	-3.17	106.75	110.62
1	A2	1448	OMG	C6-C5-N7	3.17	136.14	130.25
40	B5	4383	OMG	C6-C5-N7	3.17	136.14	130.25
1	A2	645	OMG	C6-C5-N7	3.16	136.13	130.25
40	B5	3492	A2M	N3-C2-N1	-3.16	123.66	128.60
1	A2	1384	A2M	N3-C2-N1	-3.16	123.66	128.60
1	A2	816	PSU	O2-C2-N1	-3.15	119.32	122.79
11	AT	54	PSU	O2-C2-N1	-3.15	119.32	122.79
40	B5	3517	A2M	C4-C5-N7	-3.15	106.78	110.62
1	A2	1851	MA6	N1-C2-N3	-3.15	123.68	128.60
1	A2	591	A2M	N3-C2-N1	-3.14	123.69	128.60
1	A2	27	A2M	N3-C2-N1	-3.14	123.69	128.60
40	B5	2244	A2M	N3-C2-N1	-3.14	123.69	128.60
40	B5	2258	OMU	O4-C4-C5	-3.14	119.64	125.16
42	B8	75	OMG	C6-C5-N7	3.14	136.08	130.25
40	B5	4269	A2M	N3-C2-N1	-3.14	123.70	128.60
1	A2	1329	OMG	C6-C5-N7	3.13	136.08	130.25
1	A2	591	A2M	C4-C5-N7	-3.13	106.80	110.62
40	B5	1270	A2M	C2'-C1'-N9	-3.13	108.26	113.53
1	A2	1491	OMG	C6-C5-N7	3.13	136.07	130.25
40	B5	3476	OMG	C6-C5-N7	3.13	136.07	130.25
1	A2	485	A2M	N3-C2-N1	-3.13	123.71	128.60
40	B5	3676	OMG	C6-C5-N7	3.12	136.06	130.25
1	A2	159	A2M	N3-C2-N1	-3.12	123.72	128.60
40	B5	1632	PSU	O2-C2-N1	-3.12	119.36	122.79
40	B5	2206	A2M	N3-C2-N1	-3.12	123.73	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	577	A2M	N3-C2-N1	-3.12	123.73	128.60
1	A2	1032	A2M	N3-C2-N1	-3.11	123.73	128.60
40	B5	3562	A2M	N3-C2-N1	-3.11	123.73	128.60
1	A2	684	OMG	C6-C5-N7	3.11	136.04	130.25
40	B5	4317	A2M	N3-C2-N1	-3.11	123.74	128.60
1	A2	166	A2M	N3-C2-N1	-3.11	123.74	128.60
40	B5	4369	OMG	C6-C5-N7	3.11	136.02	130.25
40	B5	1270	A2M	N3-C2-N1	-3.10	123.75	128.60
1	A2	510	OMG	C6-C5-N7	3.10	136.02	130.25
40	B5	4336	A2M	N3-C2-N1	-3.10	123.76	128.60
1	A2	99	A2M	N3-C2-N1	-3.10	123.76	128.60
40	B5	3450	A2M	N3-C2-N1	-3.09	123.77	128.60
40	B5	3557	A2M	N3-C2-N1	-3.09	123.77	128.60
40	B5	3450	A2M	C2'-C1'-N9	-3.09	108.33	113.53
40	B5	1479	A2M	N3-C2-N1	-3.09	123.77	128.60
40	B5	1580	OMG	C6-C5-N7	3.09	135.99	130.25
40	B5	400	A2M	N3-C2-N1	-3.09	123.78	128.60
40	B5	3599	A2M	N3-C2-N1	-3.09	123.78	128.60
40	B5	3562	A2M	C2'-C1'-N9	-3.08	108.34	113.53
1	A2	1032	A2M	C2'-C1'-N9	-3.08	108.34	113.53
40	B5	3456	A2M	N3-C2-N1	-3.08	123.78	128.60
1	A2	469	A2M	N3-C2-N1	-3.08	123.79	128.60
40	B5	3524	OMG	C6-C5-N7	3.08	135.97	130.25
1	A2	602	OMG	C6-C5-N7	3.07	135.96	130.25
1	A2	166	A2M	C2'-C1'-N9	-3.07	108.36	113.53
40	B5	3966	6MZ	N1-C2-N3	-3.07	123.80	128.60
40	B5	2658	A2M	N3-C2-N1	-3.07	123.81	128.60
1	A2	513	A2M	N3-C2-N1	-3.06	123.81	128.60
40	B5	4138	OMG	C6-C5-N7	3.06	135.94	130.25
40	B5	2719	OMG	C6-C5-N7	3.06	135.94	130.25
1	A2	669	A2M	N3-C2-N1	-3.06	123.82	128.60
40	B5	2630	A2M	C2'-C1'-N9	-3.06	108.38	113.53
1	A2	429	OMU	O4-C4-C5	-3.05	119.80	125.16
40	B5	3942	OMG	C6-C5-N7	3.03	135.89	130.25
40	B5	2680	OMU	O4-C4-C5	-3.02	119.84	125.16
1	A2	1833	6MZ	C4-C5-N7	-3.02	106.94	110.62
1	A2	116	OMU	O4-C4-C5	-3.01	119.86	125.16
1	A2	628	OMU	O4-C4-C5	-3.00	119.89	125.16
1	A2	172	OMU	O4-C4-C5	-2.98	119.91	125.16
40	B5	3456	A2M	C2'-C1'-N9	-2.98	108.51	113.53
40	B5	4366	OMU	O4-C4-C5	-2.97	119.94	125.16
40	B5	3657	OMU	O4-C4-C5	-2.96	119.95	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1327	OMU	O4-C4-C5	-2.95	119.96	125.16
1	A2	1249	B8N	N3-C2-N1	2.95	120.93	116.76
40	B5	3973	OMU	O4-C4-C5	-2.95	119.97	125.16
40	B5	2206	A2M	C2'-C1'-N9	-2.95	108.56	113.53
1	A2	121	OMU	O4-C4-C5	-2.95	119.98	125.16
1	A2	1805	OMU	O4-C4-C5	-2.92	120.03	125.16
1	A2	1289	OMU	O4-C4-C5	-2.92	120.03	125.16
1	A2	1443	OMU	O4-C4-C5	-2.91	120.04	125.16
1	A2	1851	MA6	C5-N7-C8	2.91	107.64	103.51
40	B5	4244	OMU	O4-C4-C5	-2.90	120.06	125.16
40	B5	4052	OMU	O4-C4-C5	-2.90	120.06	125.16
1	A2	355	OMU	O4-C4-C5	-2.88	120.09	125.16
40	B5	4336	A2M	C2'-C1'-N9	-2.87	108.69	113.53
40	B5	3517	A2M	O4'-C1'-N9	2.86	113.69	108.06
40	B5	3517	A2M	C4-N9-C8	2.84	108.80	105.73
1	A2	1852	MA6	C5-N7-C8	2.83	107.53	103.51
40	B5	4269	A2M	C5-N7-C8	2.82	107.51	103.51
40	B5	4317	A2M	C2'-C1'-N9	-2.82	108.79	113.53
40	B5	1489	A2M	C5-N7-C8	2.81	107.50	103.51
1	A2	669	A2M	C5-N7-C8	2.81	107.50	103.51
40	B5	1270	A2M	C5-N7-C8	2.80	107.48	103.51
40	B5	3562	A2M	C5-N7-C8	2.79	107.47	103.51
40	B5	4336	A2M	C5-N7-C8	2.79	107.47	103.51
40	B5	3557	A2M	C2'-C1'-N9	-2.78	108.84	113.53
1	A2	513	A2M	C5-N7-C8	2.78	107.46	103.51
1	A2	1032	A2M	C5-N7-C8	2.78	107.46	103.51
1	A2	166	A2M	C5-N7-C8	2.78	107.46	103.51
1	A2	1679	A2M	C5-N7-C8	2.78	107.45	103.51
1	A2	159	A2M	C5-N7-C8	2.76	107.44	103.51
40	B5	398	A2M	C5-N7-C8	2.76	107.44	103.51
40	B5	3456	A2M	C5-N7-C8	2.76	107.43	103.51
1	A2	99	A2M	C5-N7-C8	2.76	107.43	103.51
40	B5	3492	A2M	C5-N7-C8	2.76	107.42	103.51
40	B5	2658	A2M	C2'-C1'-N9	-2.76	108.89	113.53
1	A2	469	A2M	C5-N7-C8	2.75	107.42	103.51
1	A2	1833	6MZ	N1-C2-N3	-2.75	124.30	128.60
1	A2	485	A2M	C2'-C1'-N9	-2.75	108.89	113.53
1	A2	27	A2M	C5-N7-C8	2.75	107.41	103.51
1	A2	1384	A2M	C5-N7-C8	2.74	107.41	103.51
40	B5	4317	A2M	C5-N7-C8	2.74	107.40	103.51
1	A2	485	A2M	C5-N7-C8	2.74	107.40	103.51
40	B5	2244	A2M	C5-N7-C8	2.74	107.40	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	577	A2M	C5-N7-C8	2.73	107.39	103.51
40	B5	2630	A2M	C4-N9-C8	2.73	108.69	105.73
40	B5	2206	A2M	C5-N7-C8	2.73	107.39	103.51
40	B5	2658	A2M	C5-N7-C8	2.73	107.39	103.51
40	B5	400	A2M	C5-N7-C8	2.73	107.39	103.51
40	B5	1810	A2M	C5-N7-C8	2.72	107.38	103.51
40	B5	2258	OMU	C1'-N1-C2	2.72	122.49	117.57
40	B5	3557	A2M	C5-N7-C8	2.71	107.37	103.51
40	B5	3517	A2M	C5-N7-C8	2.71	107.36	103.51
40	B5	3599	A2M	C5-N7-C8	2.71	107.36	103.51
40	B5	1479	A2M	C5-N7-C8	2.71	107.36	103.51
40	B5	3450	A2M	C5-N7-C8	2.70	107.35	103.51
1	A2	591	A2M	C5-N7-C8	2.69	107.33	103.51
1	A2	1679	A2M	C4-N9-C8	2.68	108.64	105.73
40	B5	3966	6MZ	C5-N7-C8	2.67	107.31	103.51
1	A2	868	OMG	C4-C5-N7	-2.66	106.51	110.72
1	A2	1851	MA6	C5-C6-N6	-2.65	120.68	125.30
40	B5	2630	A2M	C5-N7-C8	2.65	107.28	103.51
40	B5	3599	A2M	C2'-C1'-N9	-2.65	109.07	113.53
40	B5	400	A2M	C2'-C1'-N9	-2.65	109.07	113.53
1	A2	1448	OMG	C4-C5-N7	-2.64	106.54	110.72
40	B5	2207	OMG	C4-C5-N7	-2.64	106.54	110.72
40	B5	3974	OMG	C4-C5-N7	-2.64	106.54	110.72
40	B5	1260	OMG	C4-C5-N7	-2.64	106.55	110.72
40	B5	1810	A2M	C4-N9-C8	2.63	108.58	105.73
40	B5	1477	OMG	C4-C5-N7	-2.63	106.56	110.72
1	A2	1851	MA6	C4-N9-C8	2.63	108.57	105.73
40	B5	3492	A2M	C4-N9-C8	2.62	108.56	105.73
40	B5	4364	OMG	C4-C5-N7	-2.61	106.59	110.72
40	B5	4383	OMG	C4-C5-N7	-2.61	106.59	110.72
1	A2	1640	G7M	O6-C6-C5	-2.61	122.18	128.06
1	A2	645	OMG	C4-C5-N7	-2.60	106.60	110.72
40	B5	3359	OMG	C4-C5-N7	-2.60	106.60	110.72
11	AT	53	5MU	C1'-N1-C2	2.60	122.28	117.57
40	B5	3456	A2M	C4-N9-C8	2.59	108.54	105.73
1	A2	159	A2M	C4-N9-C8	2.59	108.53	105.73
40	B5	2267	OMG	C4-C5-N7	-2.59	106.63	110.72
40	B5	4116	OMG	C4-C5-N7	-2.59	106.63	110.72
40	B5	4245	OMG	C4-C5-N7	-2.58	106.64	110.72
1	A2	513	A2M	C4-N9-C8	2.58	108.52	105.73
1	A2	577	A2M	C4-N9-C8	2.58	108.52	105.73
1	A2	669	A2M	C4-N9-C8	2.58	108.52	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	437	OMG	C4-C5-N7	-2.57	106.65	110.72
40	B5	3676	OMG	C4-C5-N7	-2.57	106.65	110.72
42	B8	75	OMG	C4-C5-N7	-2.57	106.65	110.72
1	A2	1329	OMG	C4-C5-N7	-2.57	106.66	110.72
40	B5	1580	OMG	C4-C5-N7	-2.57	106.66	110.72
1	A2	1384	A2M	C4-N9-C8	2.56	108.51	105.73
1	A2	1338	4AC	C5-C4-N4	-2.56	118.47	122.92
40	B5	3631	OMG	C4-C5-N7	-2.56	106.67	110.72
40	B5	4369	OMG	C4-C5-N7	-2.56	106.67	110.72
40	B5	2206	A2M	C4-N9-C8	2.56	108.50	105.73
40	B5	3562	A2M	C4-N9-C8	2.55	108.50	105.73
40	B5	4269	A2M	C2'-C1'-N9	-2.55	109.23	113.53
1	A2	1833	6MZ	C5-N7-C8	2.55	107.13	103.51
1	A2	1491	OMG	C4-C5-N7	-2.55	106.69	110.72
40	B5	2244	A2M	C4-N9-C8	2.55	108.49	105.73
40	B5	4138	OMG	C4-C5-N7	-2.54	106.69	110.72
40	B5	398	A2M	C4-N9-C8	2.54	108.48	105.73
1	A2	99	A2M	C4-N9-C8	2.54	108.48	105.73
40	B5	3599	A2M	C4-N9-C8	2.54	108.48	105.73
40	B5	4240	OMG	C4-C5-N7	-2.53	106.71	110.72
40	B5	3450	A2M	C4-N9-C8	2.53	108.47	105.73
40	B5	3524	OMG	C4-C5-N7	-2.53	106.72	110.72
40	B5	4317	A2M	C4-N9-C8	2.53	108.47	105.73
40	B5	4269	A2M	C4-N9-C8	2.53	108.47	105.73
40	B5	4336	A2M	C4-N9-C8	2.53	108.47	105.73
1	A2	510	OMG	C4-C5-N7	-2.52	106.73	110.72
40	B5	1270	A2M	C4-N9-C8	2.52	108.46	105.73
40	B5	3476	OMG	C4-C5-N7	-2.52	106.74	110.72
40	B5	3942	OMG	C4-C5-N7	-2.51	106.74	110.72
40	B5	4193	5MC	C5-C4-N3	-2.51	118.96	121.67
40	B5	3514	5MC	C5-C4-N3	-2.51	118.96	121.67
1	A2	485	A2M	C4-N9-C8	2.51	108.45	105.73
1	A2	602	OMG	C4-C5-N7	-2.51	106.75	110.72
40	B5	400	A2M	C4-N9-C8	2.51	108.44	105.73
40	B5	1266	1MA	C4-C5-N7	-2.50	106.76	110.72
1	A2	166	A2M	C4-N9-C8	2.50	108.44	105.73
40	B5	1479	A2M	C4-N9-C8	2.50	108.43	105.73
1	A2	27	A2M	C4-N9-C8	2.49	108.43	105.73
40	B5	2719	OMG	C4-C5-N7	-2.49	106.78	110.72
1	A2	684	OMG	C4-C5-N7	-2.48	106.79	110.72
34	Au	1	AME	O-C-CA	-2.48	118.28	124.78
43	BA	216	V5N	O-C-CA	-2.47	118.30	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3966	6MZ	C4-N9-C8	2.47	108.40	105.73
40	B5	1489	A2M	C4-N9-C8	2.47	108.40	105.73
1	A2	1843	4AC	C6-C5-C4	2.45	119.96	116.96
1	A2	469	A2M	C2'-C1'-N9	-2.44	109.41	113.53
1	A2	1852	MA6	C4-N9-C8	2.44	108.38	105.73
40	B5	4166	PSU	C6-C5-C4	-2.43	116.50	118.20
40	B5	3557	A2M	C4-N9-C8	2.43	108.36	105.73
1	A2	1338	4AC	C6-C5-C4	2.42	119.93	116.96
1	A2	469	A2M	C4-N9-C8	2.42	108.35	105.73
1	A2	1032	A2M	C4-N9-C8	2.42	108.35	105.73
69	Ba	39	V5N	O-C-CA	-2.41	118.45	124.78
40	B5	4244	OMU	O2-C2-N1	-2.41	119.59	122.79
1	A2	1843	4AC	C5-C4-N4	-2.40	118.75	122.92
13	AZ	2	SAC	O-C-CA	-2.36	118.59	124.78
40	B5	3550	UY1	C6-C5-C4	2.36	119.85	118.20
31	Ar	2	SAC	O-C-CA	-2.36	118.61	124.78
40	B5	3550	UY1	O2-C2-N1	-2.36	120.20	122.79
40	B5	2658	A2M	C4-N9-C8	2.35	108.28	105.73
1	A2	628	OMU	O2-C2-N1	-2.35	119.66	122.79
40	B5	1489	A2M	C6-C5-N7	2.31	136.33	132.02
40	B5	2194	OMC	O2-C2-N3	-2.28	118.63	122.33
11	AT	53	5MU	C1'-N1-C6	-2.28	117.33	121.12
84	Br	2	SAC	O-C-CA	-2.27	118.82	124.78
40	B5	3492	A2M	C6-C5-N7	2.26	136.23	132.02
1	A2	1833	6MZ	C4-N9-C8	2.26	108.17	105.73
40	B5	2630	A2M	C2'-C3'-C4'	2.25	106.88	101.99
40	B5	1810	A2M	C6-C5-N7	2.25	136.21	132.02
40	B5	2265	OMC	O2-C2-N3	-2.24	118.68	122.33
40	B5	2630	A2M	C6-C5-N7	2.24	136.19	132.02
40	B5	2719	OMG	O6-C6-C5	-2.23	120.68	126.60
40	B5	4269	A2M	C6-C5-N7	2.23	136.18	132.02
1	A2	1679	A2M	C6-C5-N7	2.23	136.17	132.02
40	B5	3514	5MC	O2-C2-N3	-2.22	118.71	122.33
40	B5	1479	A2M	C2'-C1'-N9	-2.22	109.79	113.53
40	B5	398	A2M	C6-C5-N7	2.22	136.16	132.02
1	A2	1249	B8N	C5-C4-N3	2.22	120.28	116.17
40	B5	2244	A2M	C6-C5-N7	2.22	136.15	132.02
1	A2	166	A2M	C6-C5-N7	2.21	136.15	132.02
1	A2	27	A2M	C6-C5-N7	2.21	136.14	132.02
40	B5	4336	A2M	C6-C5-N7	2.21	136.13	132.02
40	B5	1270	A2M	C6-C5-N7	2.20	136.13	132.02
1	A2	429	OMU	C1'-N1-C2	2.20	121.56	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1851	MA6	N9-C8-N7	-2.20	110.90	113.91
40	B5	3517	A2M	C6-C5-N7	2.20	136.12	132.02
40	B5	3562	A2M	C6-C5-N7	2.20	136.12	132.02
1	A2	1327	OMU	O2-C2-N1	-2.20	119.86	122.79
40	B5	3456	A2M	C6-C5-N7	2.19	136.11	132.02
40	B5	4138	OMG	O6-C6-C5	-2.19	120.78	126.60
40	B5	3450	A2M	C6-C5-N7	2.18	136.09	132.02
1	A2	1704	OMC	O2-C2-N3	-2.18	118.78	122.33
40	B5	4317	A2M	C6-C5-N7	2.18	136.07	132.02
40	B5	1580	OMG	O6-C6-C5	-2.18	120.83	126.60
1	A2	669	A2M	C6-C5-N7	2.18	136.07	132.02
1	A2	1032	A2M	C6-C5-N7	2.18	136.07	132.02
1	A2	513	A2M	C6-C5-N7	2.18	136.07	132.02
40	B5	3517	A2M	N9-C8-N7	-2.17	110.94	113.91
1	A2	159	A2M	C6-C5-N7	2.17	136.06	132.02
1	A2	1384	A2M	C6-C5-N7	2.17	136.06	132.02
40	B5	2206	A2M	C6-C5-N7	2.17	136.06	132.02
1	A2	1491	OMG	O6-C6-C5	-2.16	120.86	126.60
1	A2	463	OMC	O2-C2-N3	-2.16	118.82	122.33
40	B5	4369	OMG	O6-C6-C5	-2.16	120.88	126.60
1	A2	99	A2M	C6-C5-N7	2.16	136.04	132.02
1	A2	684	OMG	O6-C6-C5	-2.15	120.89	126.60
1	A2	1329	OMG	O6-C6-C5	-2.15	120.90	126.60
40	B5	2267	OMG	O6-C6-C5	-2.15	120.90	126.60
1	A2	1833	6MZ	C6-C5-N7	2.15	134.72	132.39
40	B5	2680	OMU	O2-C2-N1	-2.14	119.94	122.79
40	B5	4245	OMG	O6-C6-C5	-2.14	120.92	126.60
40	B5	4364	OMG	O6-C6-C5	-2.14	120.94	126.60
1	A2	577	A2M	C6-C5-N7	2.13	135.99	132.02
1	A2	510	OMG	O6-C6-C5	-2.13	120.95	126.60
40	B5	3631	OMG	O6-C6-C5	-2.13	120.95	126.60
36	Aw	62	HY3	O-C-CA	-2.13	118.90	124.83
1	A2	485	A2M	C6-C5-N7	2.13	135.98	132.02
1	A2	1443	OMU	C1'-N1-C2	2.13	121.42	117.57
40	B5	3599	A2M	C6-C5-N7	2.12	135.98	132.02
40	B5	1477	OMG	O6-C6-C5	-2.12	120.97	126.60
1	A2	602	OMG	O6-C6-C5	-2.12	120.97	126.60
40	B5	400	A2M	C6-C5-N7	2.12	135.97	132.02
40	B5	3476	OMG	O6-C6-C5	-2.12	120.98	126.60
40	B5	3524	OMG	O6-C6-C5	-2.12	120.98	126.60
40	B5	3557	A2M	C6-C5-N7	2.12	135.97	132.02
40	B5	3974	OMG	O6-C6-C5	-2.12	120.98	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	1479	A2M	C6-C5-N7	2.12	135.96	132.02
40	B5	4116	OMG	O6-C6-C5	-2.12	120.99	126.60
40	B5	4240	OMG	O6-C6-C5	-2.11	120.99	126.60
40	B5	4383	OMG	O6-C6-C5	-2.11	121.00	126.60
40	B5	3942	OMG	O6-C6-C5	-2.11	121.00	126.60
1	A2	645	OMG	O6-C6-C5	-2.11	121.01	126.60
40	B5	1260	OMG	O6-C6-C5	-2.10	121.02	126.60
40	B5	1632	PSU	O4'-C1'-C2'	2.10	108.11	105.14
42	B8	75	OMG	O6-C6-C5	-2.10	121.03	126.60
40	B5	3573	OMC	O2-C2-N3	-2.10	118.92	122.33
40	B5	2207	OMG	O6-C6-C5	-2.10	121.04	126.60
40	B5	3359	OMG	O6-C6-C5	-2.09	121.04	126.60
1	A2	1679	A2M	N9-C8-N7	-2.09	111.05	113.91
40	B5	3601	OMC	O2-C2-N3	-2.09	118.93	122.33
40	B5	2658	A2M	C6-C5-N7	2.09	135.91	132.02
1	A2	1392	OMC	O2-C2-N3	-2.09	118.93	122.33
40	B5	2630	A2M	N9-C8-N7	-2.09	111.06	113.91
1	A2	669	A2M	C2'-C1'-N9	-2.09	110.02	113.53
1	A2	469	A2M	C6-C5-N7	2.08	135.90	132.02
1	A2	669	A2M	N9-C8-N7	-2.08	111.07	113.91
40	B5	1799	PSU	C5-C6-N1	-2.08	118.99	122.11
10	AJ	54	5MU	O2-C2-N1	-2.08	120.02	122.79
1	A2	591	A2M	C4-N9-C8	2.08	107.98	105.73
40	B5	4269	A2M	N9-C8-N7	-2.07	111.08	113.91
40	B5	3492	A2M	N9-C8-N7	-2.07	111.08	113.91
1	A2	868	OMG	O6-C6-C5	-2.06	121.13	126.60
1	A2	1448	OMG	O6-C6-C5	-2.06	121.14	126.60
40	B5	1810	A2M	N9-C8-N7	-2.06	111.10	113.91
1	A2	437	OMG	O6-C6-C5	-2.06	121.14	126.60
40	B5	3562	A2M	N9-C8-N7	-2.06	111.10	113.91
40	B5	1270	A2M	N9-C8-N7	-2.05	111.11	113.91
40	B5	3456	A2M	N9-C8-N7	-2.05	111.11	113.91
1	A2	1384	A2M	N9-C8-N7	-2.05	111.11	113.91
40	B5	398	A2M	N9-C8-N7	-2.04	111.12	113.91
40	B5	1266	1MA	C6-C5-N7	2.04	135.91	132.20
1	A2	513	A2M	N9-C8-N7	-2.04	111.12	113.91
1	A2	159	A2M	N9-C8-N7	-2.04	111.12	113.91
40	B5	4188	PSU	C5-C6-N1	-2.04	119.05	122.11
40	B5	4711	PSU	C5-C6-N1	-2.04	119.05	122.11
1	A2	1239	PSU	C5-C6-N1	-2.03	119.06	122.11
1	A2	1852	MA6	C5-C6-N6	-2.03	121.76	125.30
1	A2	577	A2M	N9-C8-N7	-2.03	111.14	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	1489	A2M	N9-C8-N7	-2.03	111.14	113.91
1	A2	1289	OMU	C1'-N1-C2	2.03	121.24	117.57
40	B5	4336	A2M	N9-C8-N7	-2.03	111.14	113.91
1	A2	99	A2M	N9-C8-N7	-2.02	111.15	113.91
1	A2	1644	PSU	C5-C6-N1	-2.02	119.08	122.11
1	A2	166	A2M	N9-C8-N7	-2.01	111.17	113.91
40	B5	2244	A2M	N9-C8-N7	-2.01	111.17	113.91
1	A2	1175	PSU	C5-C6-N1	-2.01	119.10	122.11
40	B5	3676	OMG	O6-C6-C5	-2.00	121.28	126.60
1	A2	1851	MA6	C6-C5-N7	2.00	136.65	133.28
40	B5	2206	A2M	N9-C8-N7	-2.00	111.18	113.91
40	B5	4317	A2M	N9-C8-N7	-2.00	111.18	113.91

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	O4'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	429	OMU	O4'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	684	OMG	C3'-C4'-C5'-O5'
1	A2	1448	OMG	C3'-C4'-C5'-O5'
40	B5	1720	PSU	C3'-C4'-C5'-O5'
40	B5	2207	OMG	O4'-C4'-C5'-O5'
40	B5	2630	A2M	C1'-C2'-O2'-CM'
40	B5	3433	OMC	C2'-C1'-N1-C2
40	B5	3433	OMC	C2'-C1'-N1-C6
40	B5	4166	PSU	C2'-C1'-C5-C4
40	B5	4166	PSU	C2'-C1'-C5-C6
40	B5	4278	PSU	O4'-C4'-C5'-O5'
40	B5	4336	A2M	C4'-C5'-O5'-P
40	B5	4382	PSU	O4'-C1'-C5-C4
40	B5	4382	PSU	O4'-C1'-C5-C6
40	B5	4382	PSU	C3'-C4'-C5'-O5'
1	A2	1249	B8N	N34-C33-C34-O35
1	A2	1338	4AC	N3-C4-N4-C7
1	A2	1338	4AC	C5-C4-N4-C7
1	A2	1843	4AC	N3-C4-N4-C7
1	A2	1843	4AC	C5-C4-N4-C7
1	A2	1843	4AC	O7-C7-N4-C4

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Mol	Chain	Res	Type	Atoms
1	A2	1843	4AC	CM7-C7-N4-C4
43	BA	216	V5N	O-C-CA-CB
45	BC	2	AYA	CM-CT-N-CA
1	A2	645	OMG	C3'-C4'-C5'-O5'
1	A2	684	OMG	O4'-C4'-C5'-O5'
40	B5	1489	A2M	O4'-C4'-C5'-O5'
40	B5	3517	A2M	O4'-C4'-C5'-O5'
40	B5	3517	A2M	C3'-C4'-C5'-O5'
40	B5	4278	PSU	C3'-C4'-C5'-O5'
45	BC	2	AYA	OT-CT-N-CA
1	A2	1249	B8N	N34-C33-C34-O36
34	Au	1	AME	CT2-CT1-N-CA
34	Au	1	AME	OT-CT1-N-CA
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	577	A2M	O4'-C4'-C5'-O5'
1	A2	577	A2M	C3'-C4'-C5'-O5'
1	A2	669	A2M	C3'-C4'-C5'-O5'
40	B5	2207	OMG	C3'-C4'-C5'-O5'
40	B5	4382	PSU	O4'-C4'-C5'-O5'
40	B5	3550	UY1	C1'-C2'-O2'-CM2
1	A2	1448	OMG	O4'-C4'-C5'-O5'
40	B5	4193	5MC	C2'-C1'-N1-C6
40	B5	398	A2M	O4'-C4'-C5'-O5'
40	B5	1489	A2M	C3'-C4'-C5'-O5'
40	B5	1720	PSU	O4'-C4'-C5'-O5'
40	B5	3450	A2M	O4'-C4'-C5'-O5'
1	A2	513	A2M	C3'-C4'-C5'-O5'
44	BB	245	HIC	CA-CB-CG-ND1
40	B5	3631	OMG	C3'-C2'-O2'-CM2
1	A2	591	A2M	C2'-C1'-N9-C4
40	B5	4193	5MC	O4'-C1'-N1-C6
40	B5	4193	5MC	C2'-C1'-N1-C2
45	BC	2	AYA	C-CA-N-CT
1	A2	645	OMG	C4'-C5'-O5'-P
40	B5	3550	UY1	C4'-C5'-O5'-P
40	B5	2630	A2M	C2'-C1'-N9-C8
13	AZ	2	SAC	C-CA-N-C1A
13	AZ	2	SAC	CB-CA-N-C1A
1	A2	437	OMG	C3'-C2'-O2'-CM2
40	B5	4282	OMC	C3'-C2'-O2'-CM2
40	B5	3676	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	A2	27	A2M	O4'-C4'-C5'-O5'
1	A2	868	OMG	C3'-C4'-C5'-O5'
40	B5	3494	PSU	C3'-C4'-C5'-O5'
1	A2	1249	B8N	C32-C33-C34-O36
1	A2	591	A2M	C2'-C1'-N9-C8
1	A2	868	OMG	C4'-C5'-O5'-P
1	A2	1852	MA6	C4'-C5'-O5'-P
40	B5	3576	PSU	C4'-C5'-O5'-P
40	B5	4246	PSU	C4'-C5'-O5'-P
1	A2	99	A2M	O4'-C4'-C5'-O5'
1	A2	116	OMU	O4'-C4'-C5'-O5'
1	A2	469	A2M	O4'-C4'-C5'-O5'
40	B5	1284	OMC	O4'-C4'-C5'-O5'
40	B5	4193	5MC	O4'-C1'-N1-C2
40	B5	3619	OMC	C4'-C5'-O5'-P
69	Ba	39	V5N	O2-CB-CG-CD2
43	BA	216	V5N	O2-CB-CG-CD2
1	A2	510	OMG	C3'-C2'-O2'-CM2
1	A2	1289	OMU	C3'-C2'-O2'-CM2
1	A2	1491	OMG	C3'-C2'-O2'-CM2
40	B5	2267	OMG	C3'-C2'-O2'-CM2
40	B5	3657	OMU	C3'-C2'-O2'-CM2
40	B5	4052	OMU	C3'-C2'-O2'-CM2
40	B5	4369	OMG	C3'-C2'-O2'-CM2
1	A2	1249	B8N	C32-C33-C34-O35
40	B5	3433	OMC	O4'-C1'-N1-C6
40	B5	4278	PSU	C4'-C5'-O5'-P
44	BB	245	HIC	CA-CB-CG-CD2
1	A2	684	OMG	C3'-C2'-O2'-CM2
40	B5	1820	OMC	C3'-C2'-O2'-CM2
40	B5	2680	OMU	C3'-C2'-O2'-CM2
40	B5	4366	OMU	C3'-C2'-O2'-CM2
40	B5	2630	A2M	C2'-C1'-N9-C4
1	A2	1704	OMC	O4'-C4'-C5'-O5'
1	A2	868	OMG	O4'-C4'-C5'-O5'
1	A2	1032	A2M	O4'-C4'-C5'-O5'
40	B5	398	A2M	C3'-C4'-C5'-O5'
40	B5	3450	A2M	C3'-C4'-C5'-O5'
1	A2	1704	OMC	C1'-C2'-O2'-CM2
1	A2	1704	OMC	C3'-C2'-O2'-CM2
40	B5	3573	OMC	C3'-C2'-O2'-CM2
40	B5	3433	OMC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	A2	591	A2M	C3'-C4'-C5'-O5'
40	B5	2194	OMC	O4'-C4'-C5'-O5'
1	A2	591	A2M	O4'-C1'-N9-C8
40	B5	2630	A2M	O4'-C1'-N9-C8
40	B5	3494	PSU	O4'-C4'-C5'-O5'
11	AT	53	5MU	C2'-C1'-N1-C2
40	B5	398	A2M	C3'-C2'-O2'-CM'
40	B5	1260	OMG	C3'-C2'-O2'-CM2
40	B5	3476	OMG	C3'-C2'-O2'-CM2
40	B5	3619	OMC	C3'-C2'-O2'-CM2
1	A2	27	A2M	C3'-C4'-C5'-O5'
40	B5	2194	OMC	C2'-C1'-N1-C2
1	A2	1448	OMG	C4'-C5'-O5'-P

There are no ring outliers.

97 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	B5	4269	A2M	1	0
1	A2	1833	6MZ	1	0
40	B5	3657	OMU	1	0
1	A2	1329	OMG	1	0
1	A2	1032	A2M	3	0
40	B5	1632	PSU	1	0
40	B5	4166	PSU	1	0
40	B5	4383	OMG	1	0
1	A2	602	OMG	1	0
40	B5	3619	OMC	1	0
41	B7	1	GTP	1	0
40	B5	2667	OMC	1	0
40	B5	2194	OMC	2	0
69	Ba	39	V5N	1	0
1	A2	1443	OMU	1	0
40	B5	4058	PSU	1	0
1	A2	1679	A2M	1	0
1	A2	510	OMG	1	0
40	B5	3573	OMC	2	0
1	A2	577	A2M	1	0
1	A2	469	A2M	1	0
40	B5	400	A2M	1	0
1	A2	1843	4AC	2	0
1	A2	1805	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A2	159	A2M	2	0
40	B5	1260	OMG	1	0
81	Bm	98	M3L	1	0
1	A2	1392	OMC	2	0
1	A2	463	OMC	2	0
1	A2	1704	OMC	1	0
40	B5	2719	OMG	1	0
1	A2	485	A2M	2	0
1	A2	1852	MA6	1	0
1	A2	1448	OMG	1	0
40	B5	1284	OMC	1	0
40	B5	4193	5MC	1	0
40	B5	2207	OMG	1	0
40	B5	2258	OMU	2	0
1	A2	36	PSU	1	0
1	A2	109	PSU	1	0
1	A2	868	OMG	2	0
40	B5	4364	OMG	1	0
1	A2	355	OMU	1	0
40	B5	1718	PSU	2	0
40	B5	2630	A2M	1	0
1	A2	1289	OMU	2	0
1	A2	1338	4AC	3	0
40	B5	4382	PSU	2	0
1	A2	1626	PSU	1	0
40	B5	2704	OMC	1	0
40	B5	1270	A2M	2	0
1	A2	1491	OMG	1	0
40	B5	3476	OMG	1	0
40	B5	3631	OMG	1	0
1	A2	682	PSU	2	0
40	B5	2244	A2M	1	0
40	B5	2206	A2M	1	0
1	A2	864	PSU	1	0
1	A2	518	OMC	1	0
40	B5	3974	OMG	1	0
40	B5	4052	OMU	1	0
40	B5	2647	OMC	1	0
1	A2	27	A2M	1	0
1	A2	116	OMU	1	0
34	Au	1	AME	1	0
1	A2	166	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	B5	4325	PSU	2	0
1	A2	437	OMG	1	0
40	B5	1489	A2M	1	0
40	B5	3450	A2M	2	0
40	B5	3562	A2M	1	0
40	B5	4317	A2M	1	0
40	B5	4336	A2M	1	0
40	B5	4267	PSU	1	0
40	B5	3456	A2M	1	0
40	B5	3517	A2M	2	0
1	A2	1446	PSU	1	0
40	B5	4202	OMC	1	0
40	B5	4138	OMG	2	0
1	A2	1249	B8N	1	0
1	A2	513	A2M	1	0
40	B5	4039	PSU	1	0
1	A2	99	A2M	2	0
40	B5	4203	PSU	2	0
1	A2	210	PSU	1	0
40	B5	2208	OMC	2	0
40	B5	2658	A2M	2	0
1	A2	1384	A2M	1	0
40	B5	1810	A2M	2	0
40	B5	3616	PSU	1	0
40	B5	4282	OMC	3	0
1	A2	121	OMU	2	0
40	B5	3557	A2M	1	0
1	A2	172	OMU	2	0
40	B5	4366	OMU	2	0
40	B5	398	A2M	1	0
42	B8	75	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 624 ligands modelled in this entry, 357 are monoatomic and 266 are unknown - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
91	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.16	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
91	SPD	B5	4901	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	B5	4901	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	1249:B8N	O3'	1250:C	P	3.10

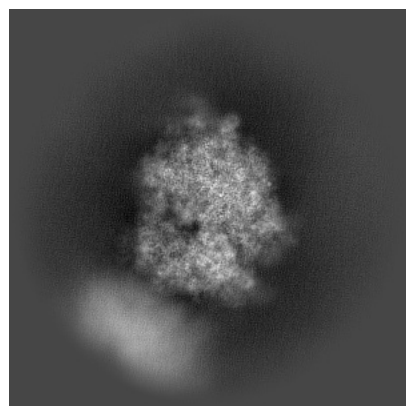
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12759. These allow visual inspection of the internal detail of the map and identification of artifacts.

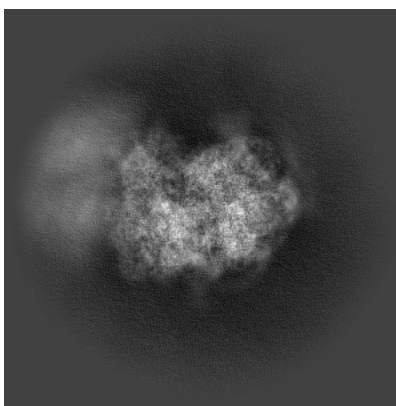
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

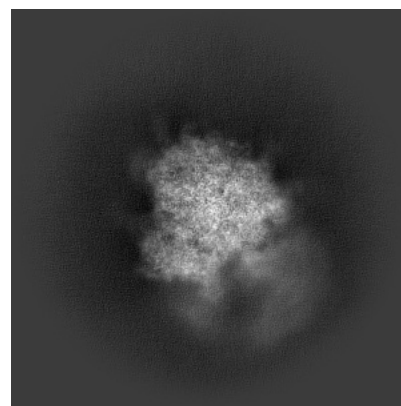
6.1.1 Primary map



X

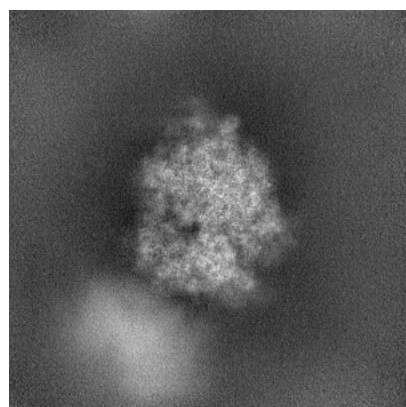


Y

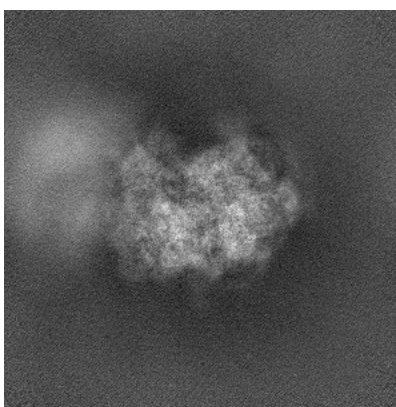


Z

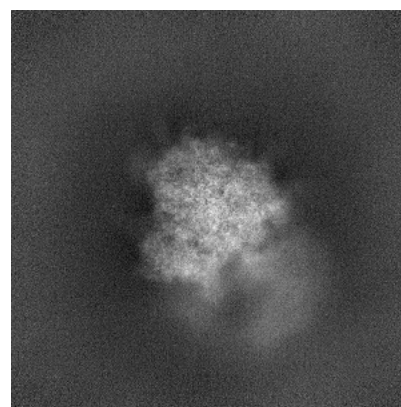
6.1.2 Raw map



X



Y

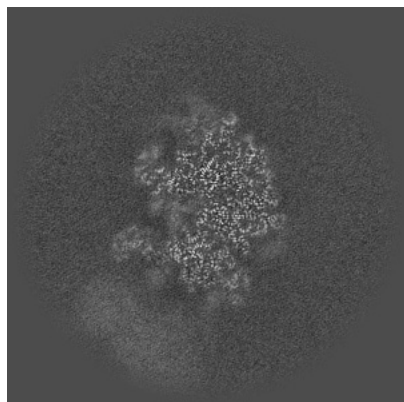


Z

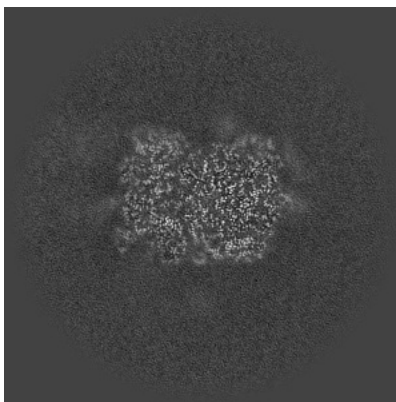
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

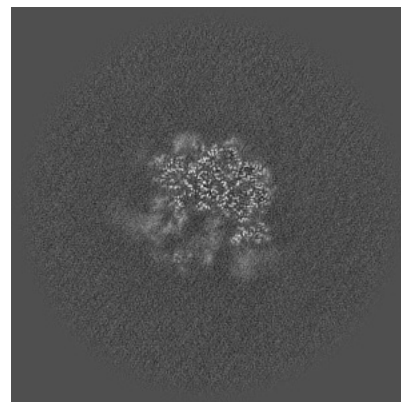
6.2.1 Primary map



X Index: 280

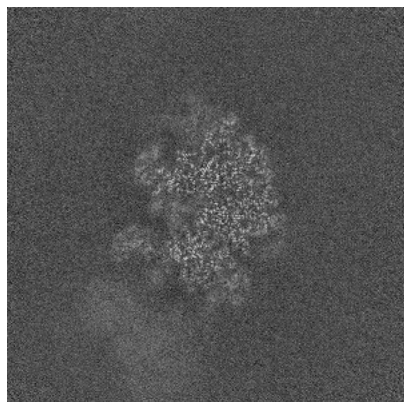


Y Index: 280

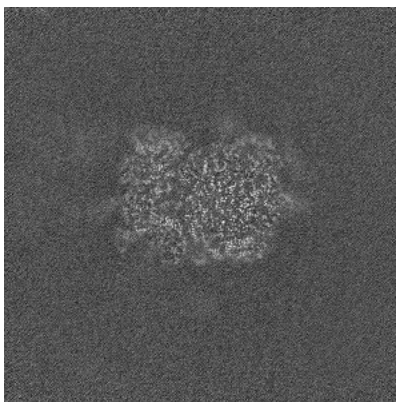


Z Index: 280

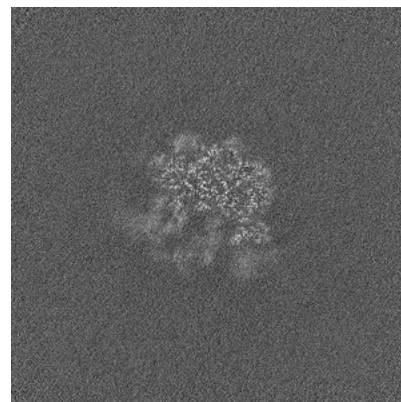
6.2.2 Raw map



X Index: 280



Y Index: 280

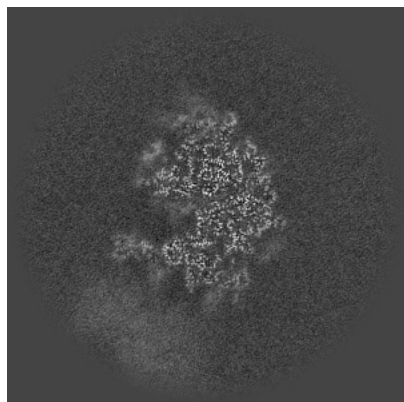


Z Index: 280

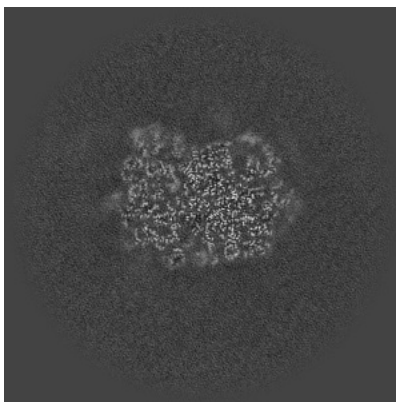
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

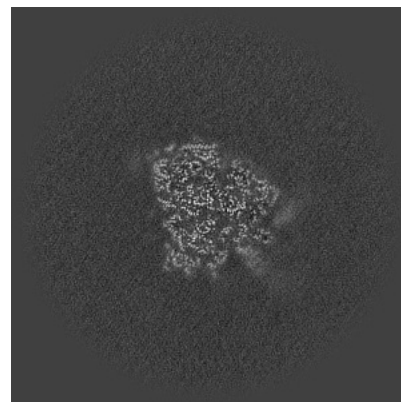
6.3.1 Primary map



X Index: 285

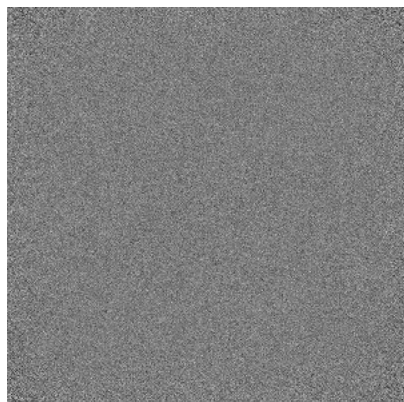


Y Index: 290

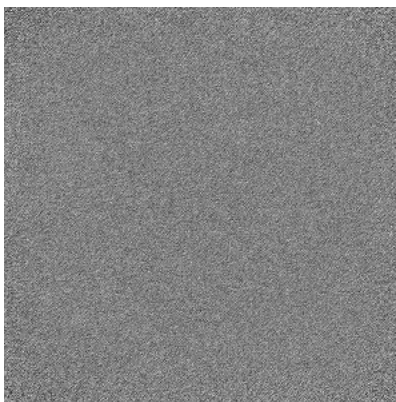


Z Index: 314

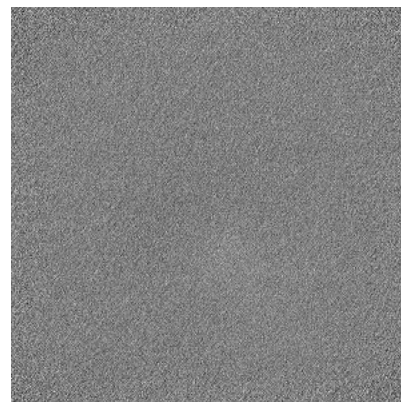
6.3.2 Raw map



X Index: 0



Y Index: 0

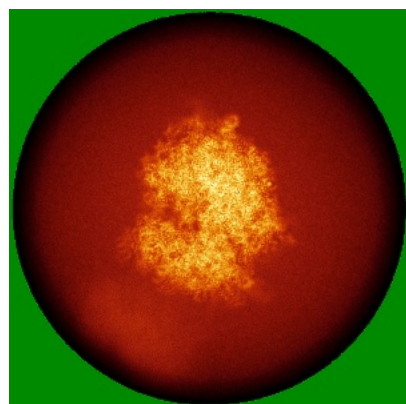


Z Index: 0

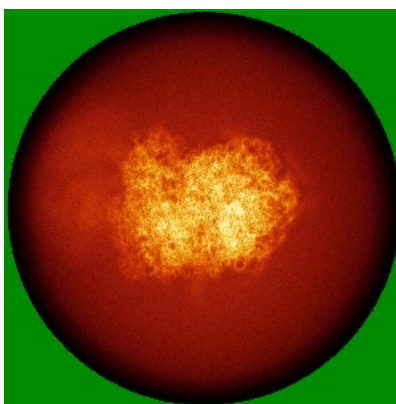
The images above show the largest variance slices of the map in three orthogonal directions.

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

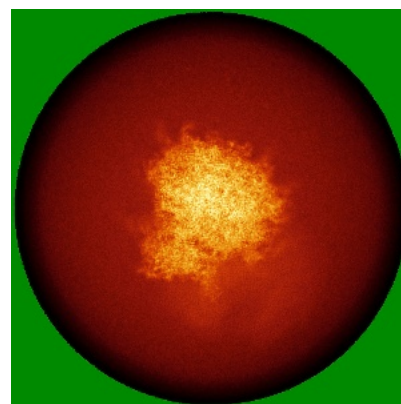
6.4.1 Primary map



X

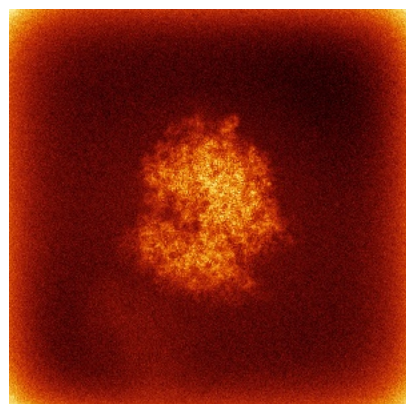


Y

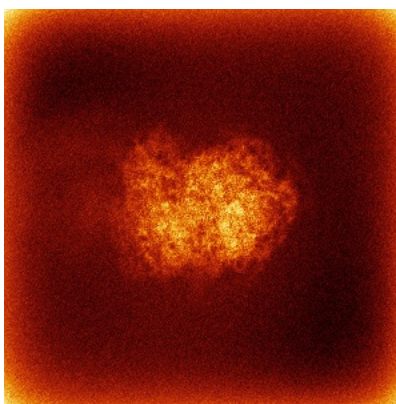


Z

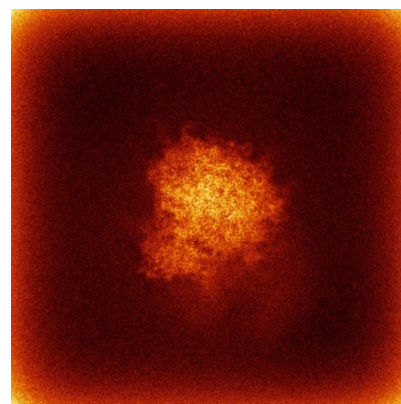
6.4.2 Raw map



X



Y

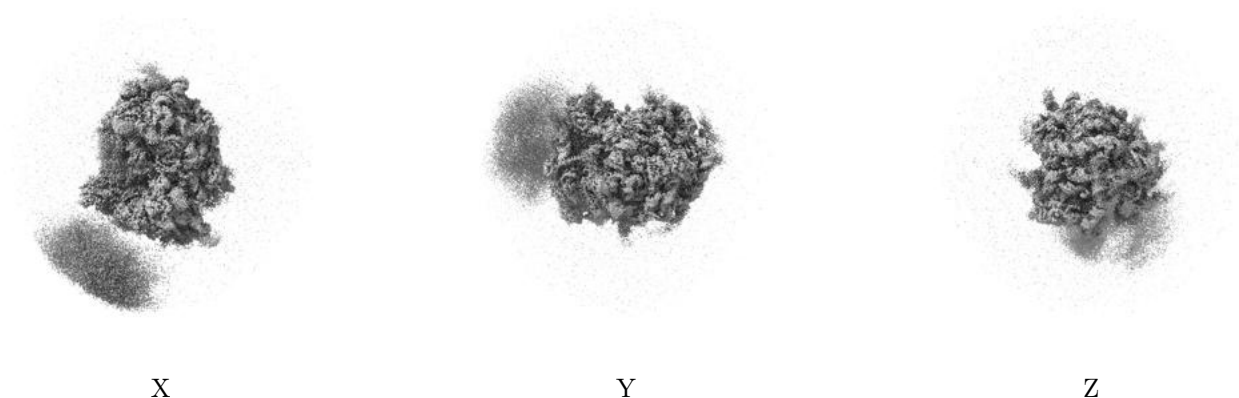


Z

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

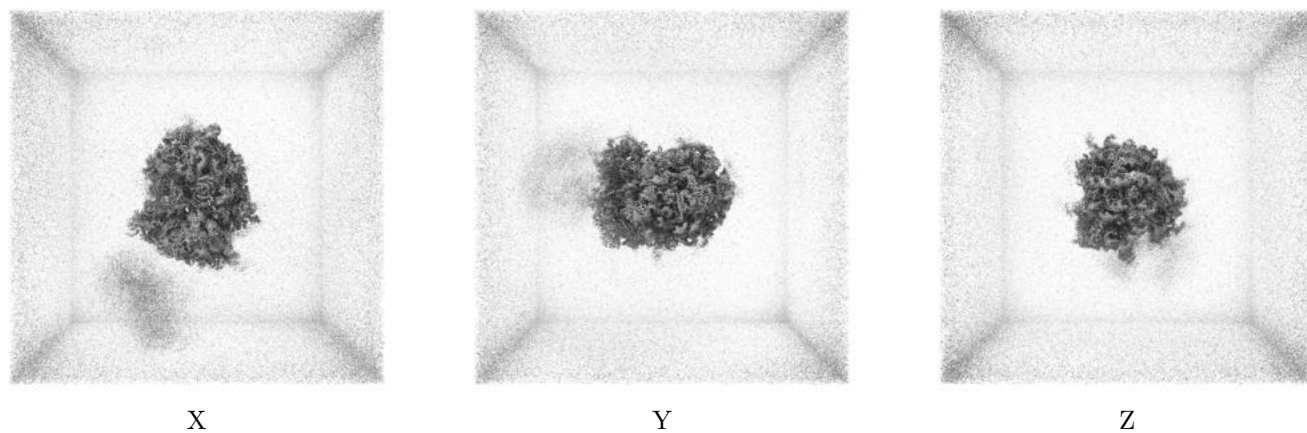
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

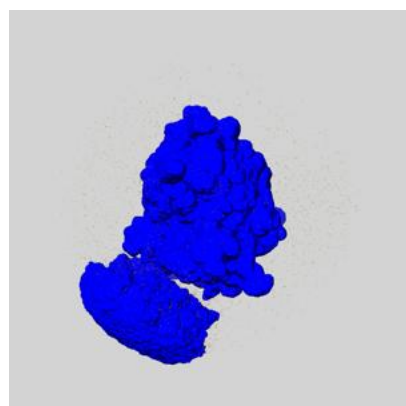
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

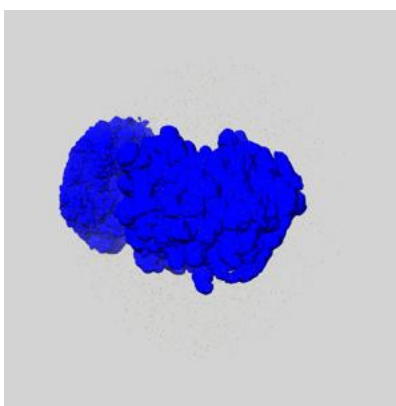
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

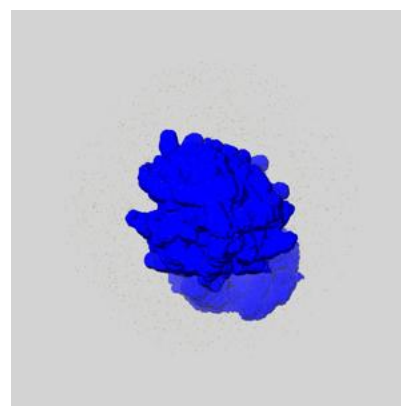
6.6.1 emd_12759_msk_1.map [i](#)



X

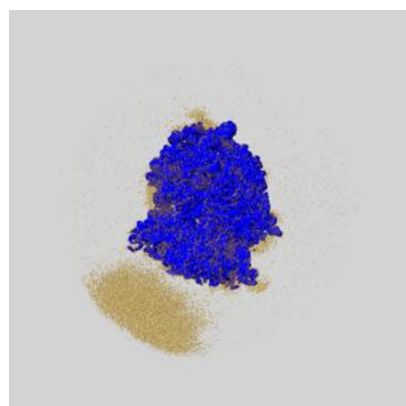


Y

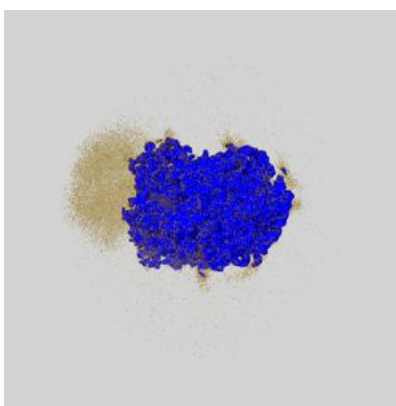


Z

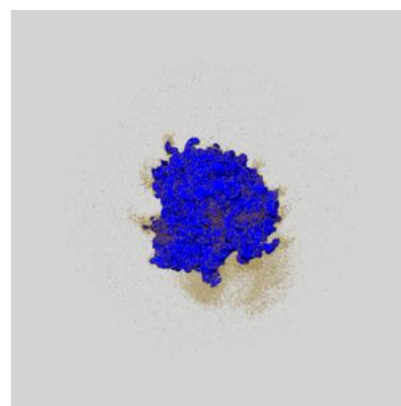
6.6.2 emd_12759_msk_2.map [i](#)



X



Y

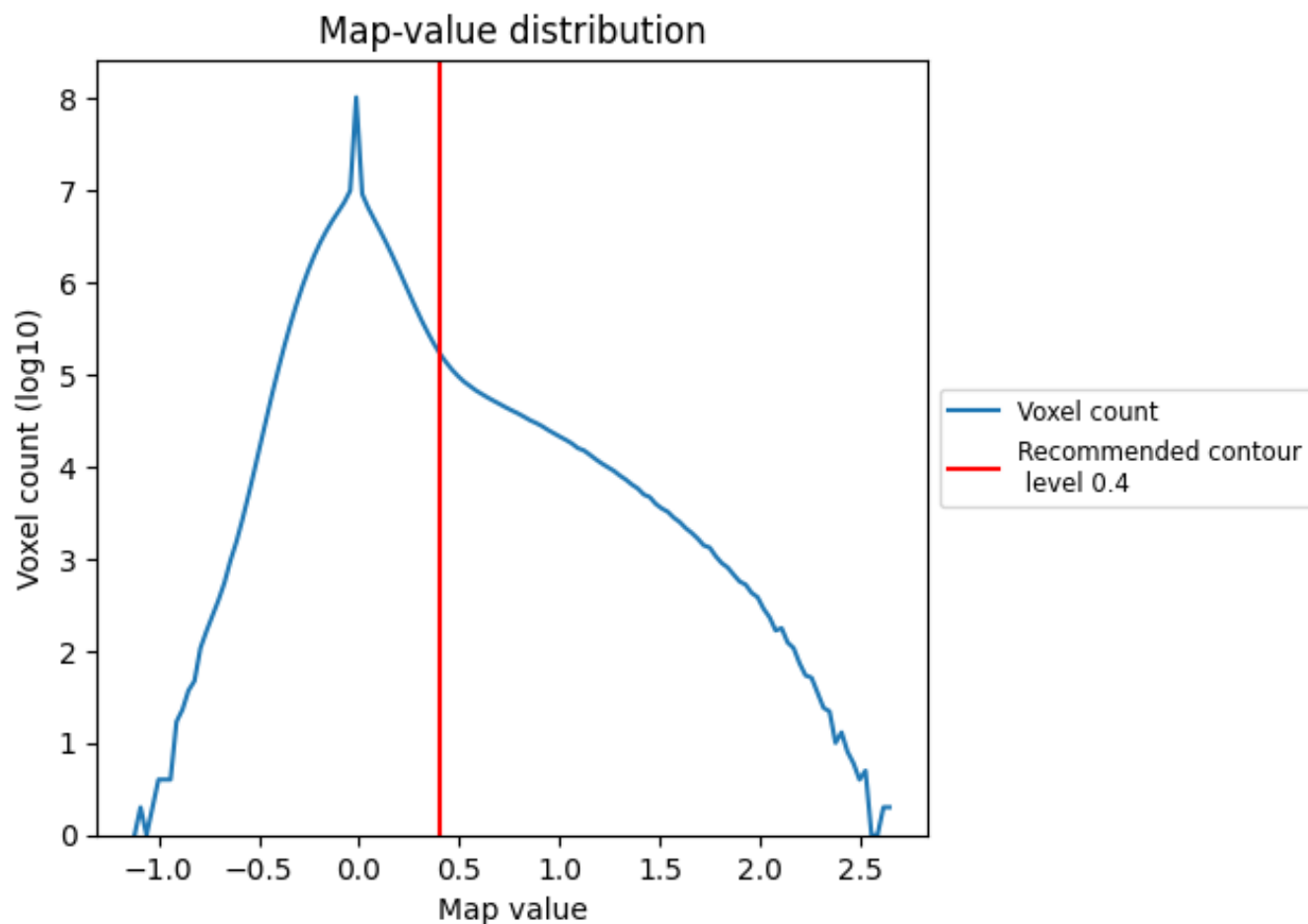


Z

7 Map analysis [i](#)

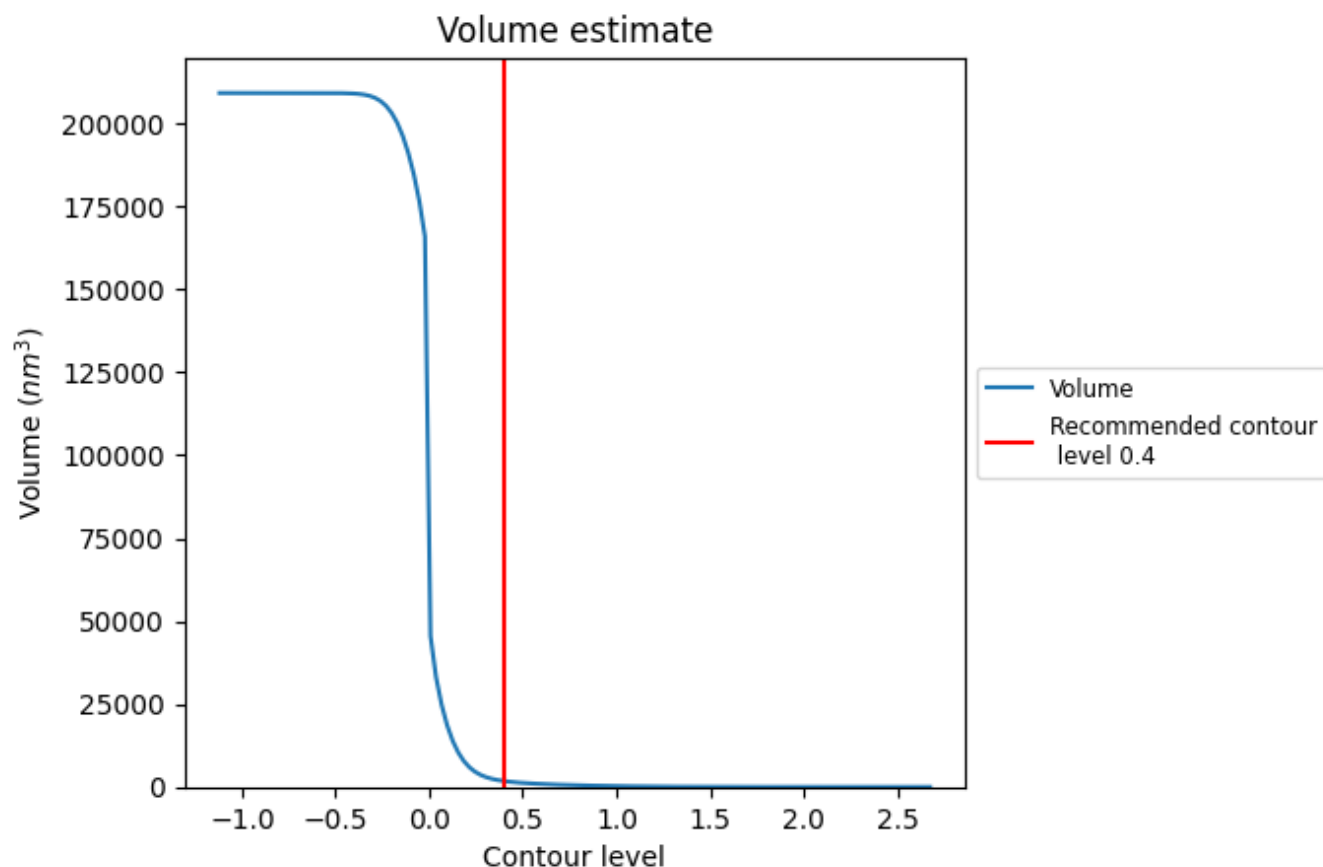
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

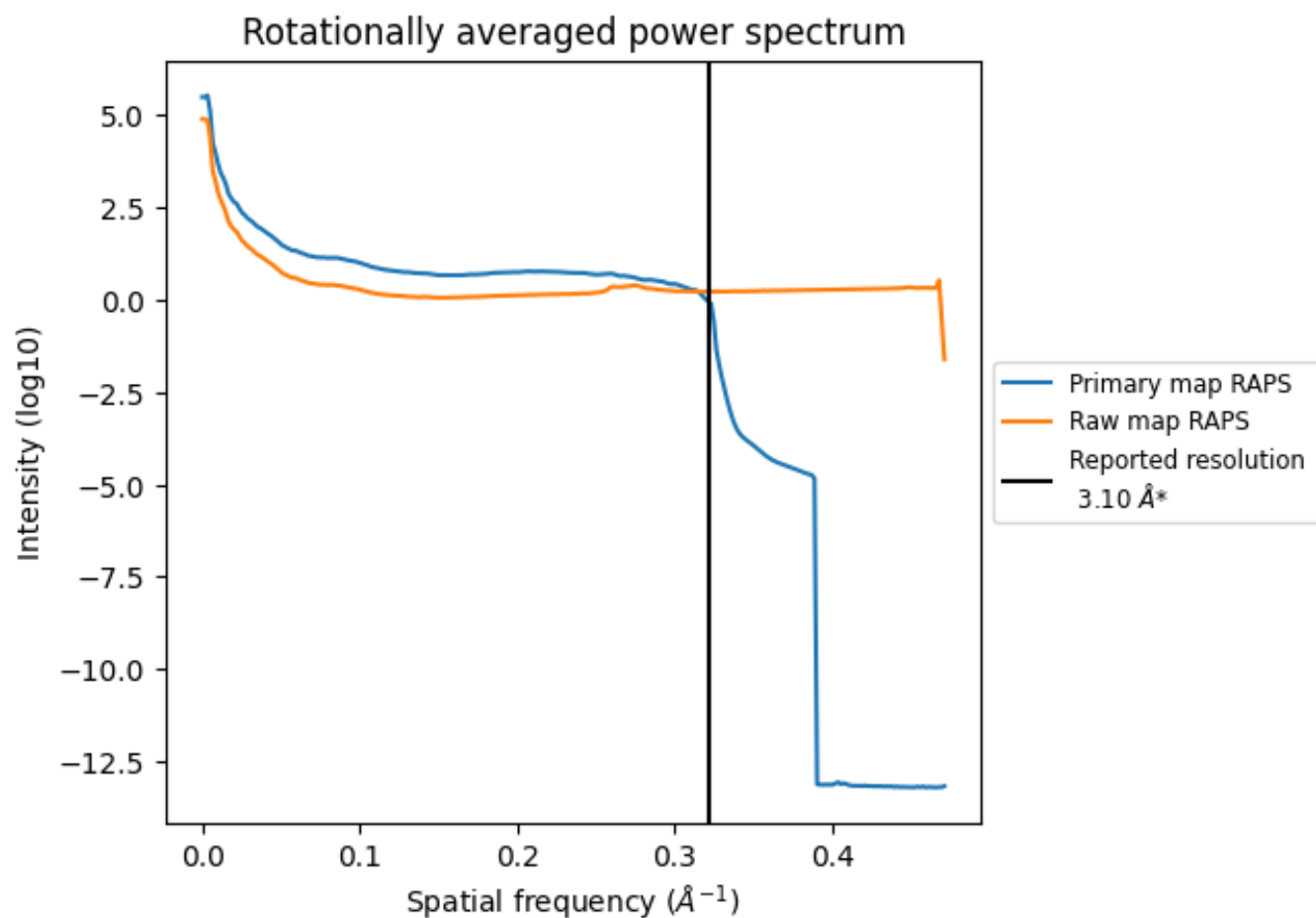
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1771 nm^3 ; this corresponds to an approximate mass of 1600 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

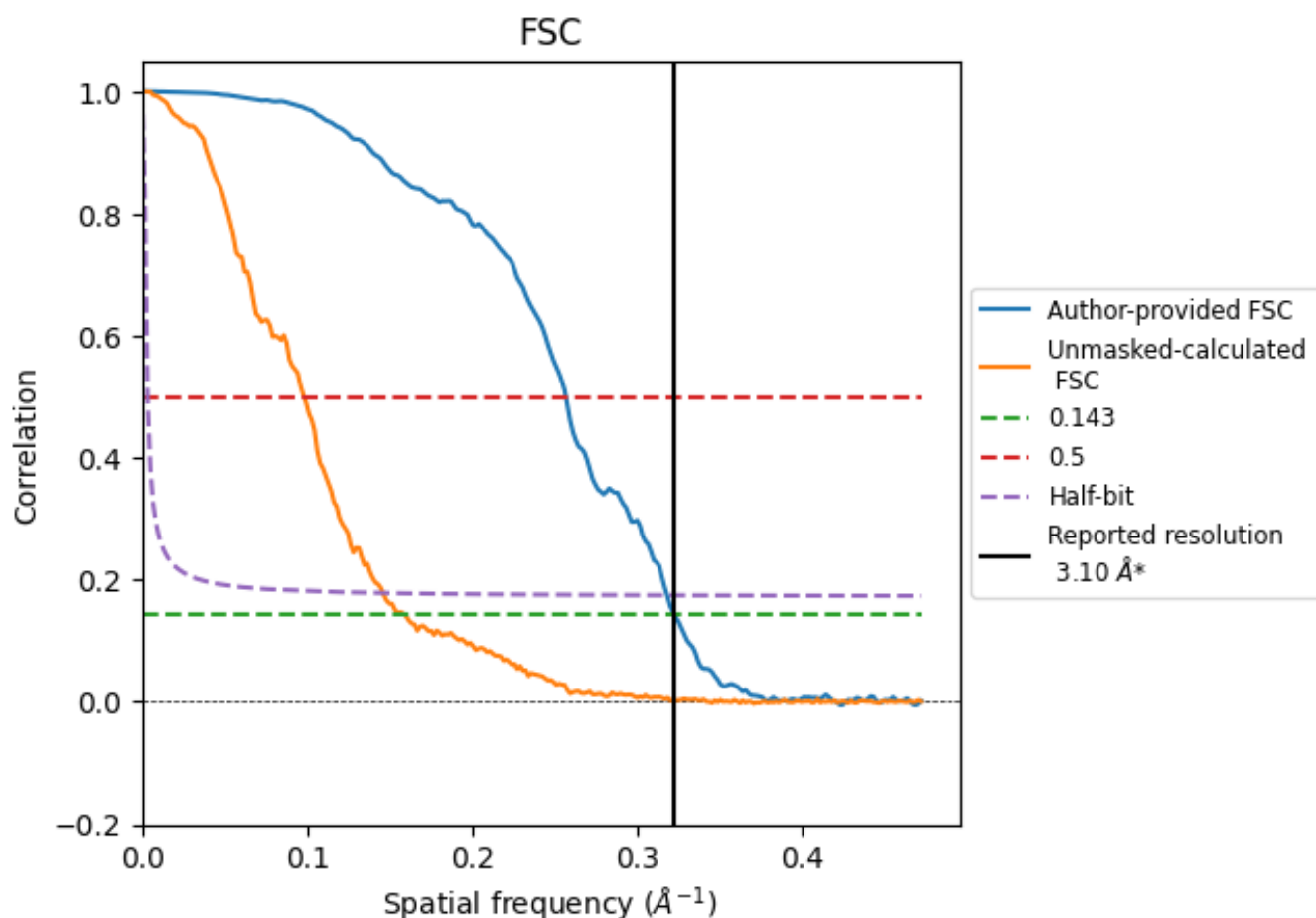


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

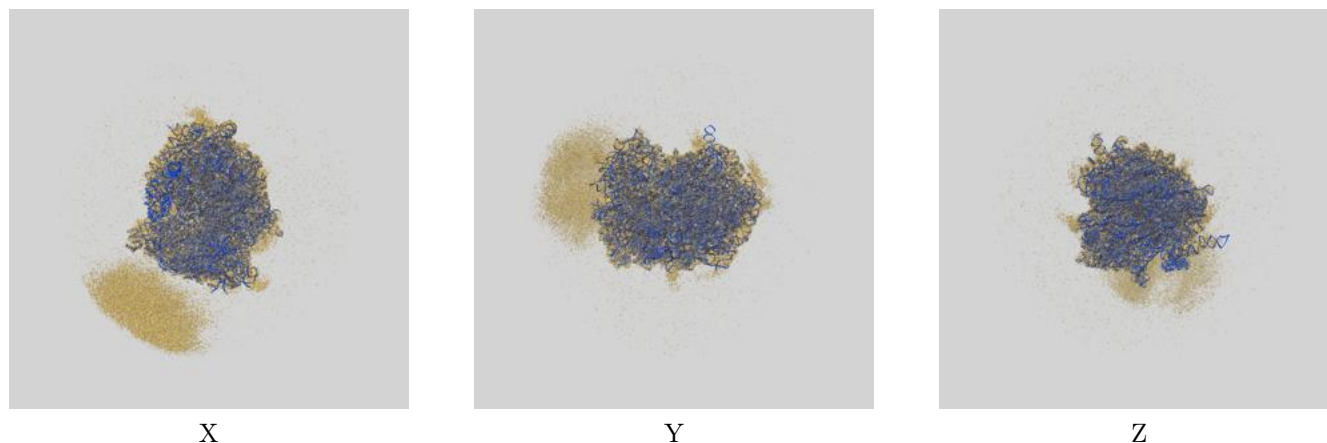
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.89	3.14
Unmasked-calculated*	6.29	10.19	6.85

*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 6.29 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

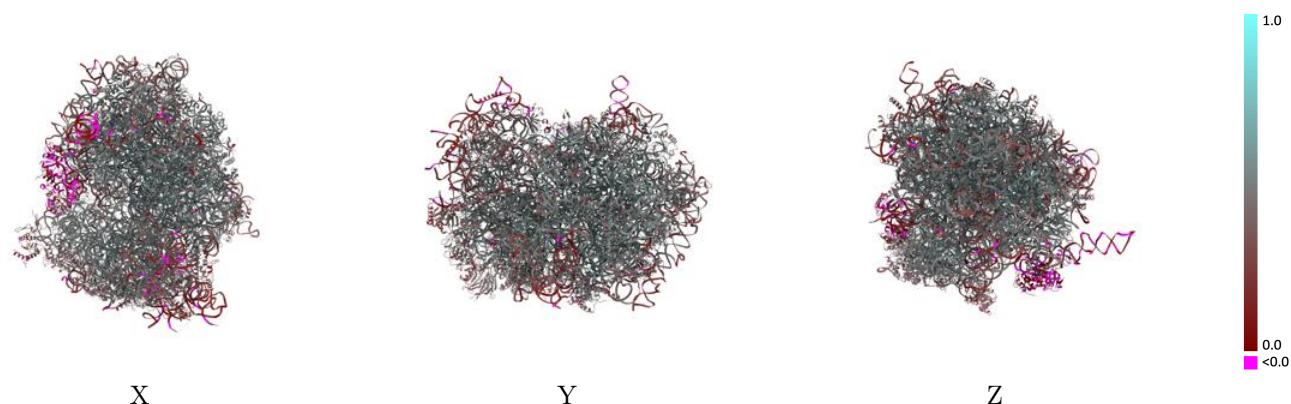
This section contains information regarding the fit between EMDB map EMD-12759 and PDB model 7O81. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



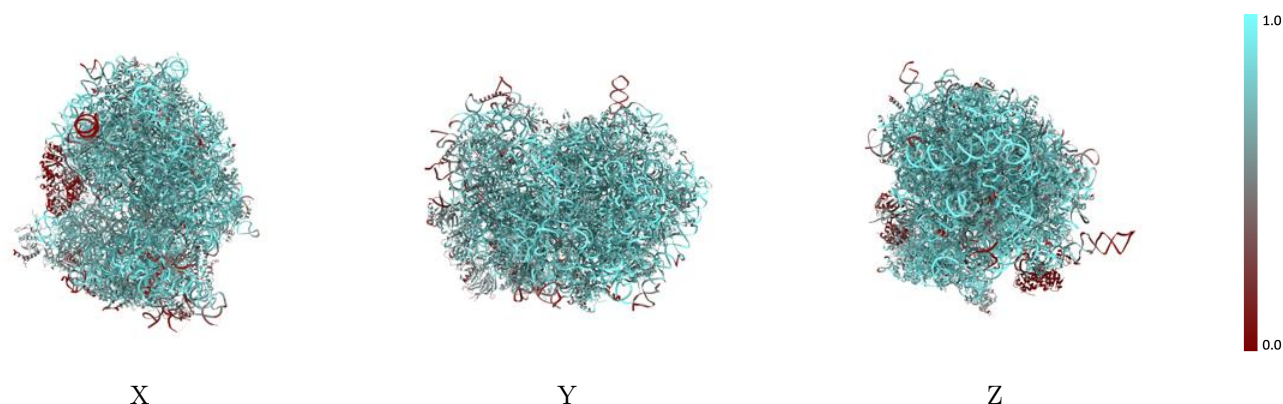
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



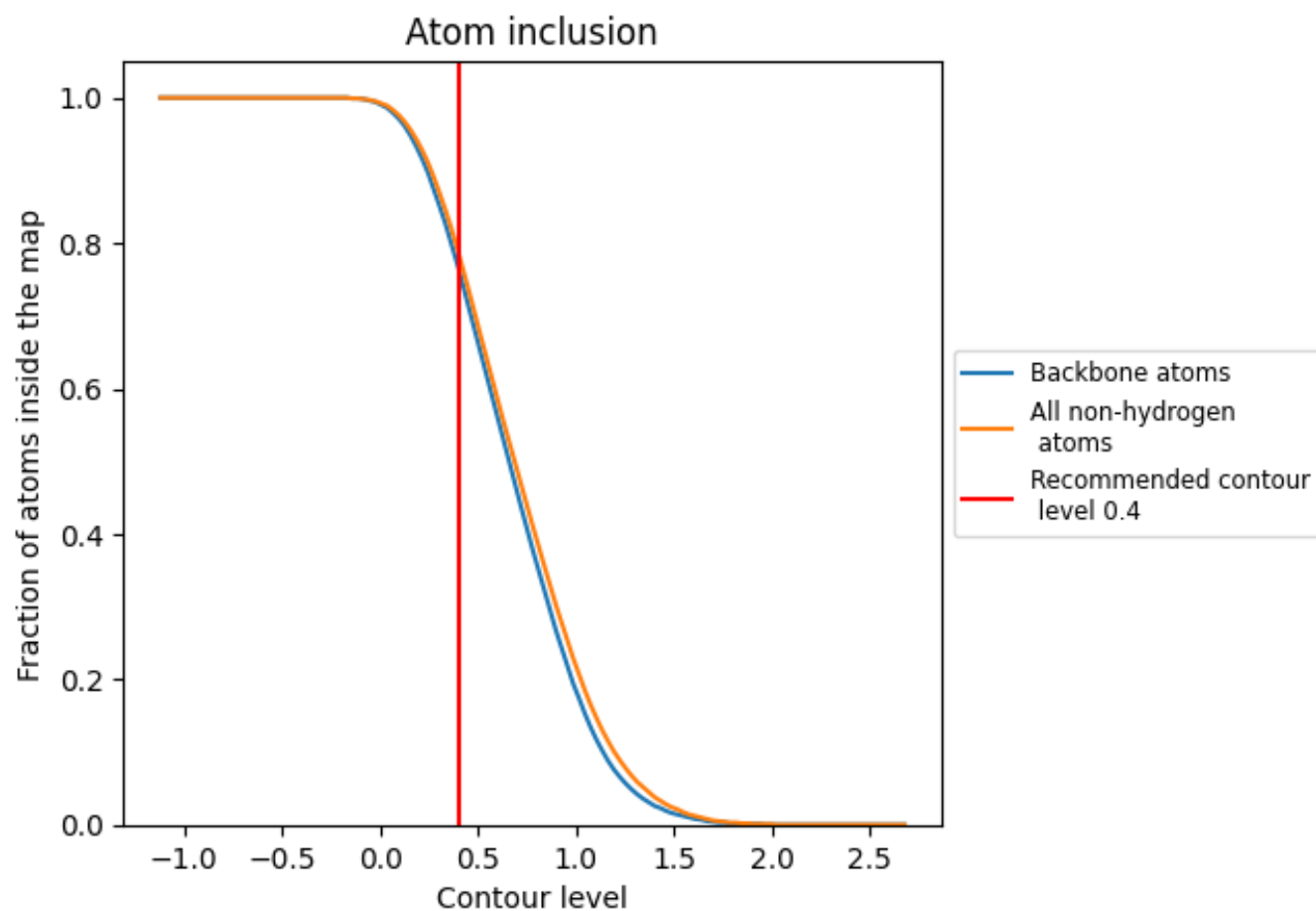
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 79% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.4470
A2	 0.8610	 0.4500
AA	 0.6510	 0.4030
AB	 0.6060	 0.4100
AC	 0.5030	 0.2740
AD	 0.6880	 0.4360
AE	 0.7290	 0.4640
AF	 0.5730	 0.3350
AG	 0.7990	 0.4900
AH	 0.9100	 0.5100
AJ	 0.5190	 0.3100
AT	 0.8180	 0.3800
AU	 0.2870	 0.3270
AZ	 0.6660	 0.4230
Aa	 0.6940	 0.4550
Ab	 0.6920	 0.4640
Ac	 0.6220	 0.4060
Ad	 0.6980	 0.4520
Ae	 0.6660	 0.4080
Af	 0.6690	 0.3720
Ag	 0.5450	 0.3460
Ah	 0.6880	 0.4030
Ai	 0.6760	 0.4340
Aj	 0.6700	 0.4060
Ak	 0.6540	 0.4370
Al	 0.4140	 0.2160
Am	 0.6910	 0.4330
An	 0.6950	 0.4630
Ao	 0.6900	 0.4250
Ap	 0.7050	 0.4220
Aq	 0.5920	 0.3810
Ar	 0.7100	 0.4130
As	 0.7550	 0.4270
At	 0.5940	 0.3480
Au	 0.6760	 0.4520



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Chain	Atom inclusion	Q-score
Av	 0.7530	 0.4940
Aw	 0.7430	 0.4900
Ax	 0.6790	 0.4110
Ay	 0.6730	 0.3960
Az	 0.7250	 0.4940
B5	 0.8740	 0.4620
B7	 0.9670	 0.5200
B8	 0.9050	 0.4870
BA	 0.7610	 0.5240
BB	 0.8050	 0.4950
BC	 0.8020	 0.5040
BD	 0.8140	 0.4660
BE	 0.7020	 0.4330
BF	 0.7910	 0.5060
BG	 0.7210	 0.4440
BH	 0.7530	 0.4680
BI	 0.7520	 0.4850
BJ	 0.7470	 0.4480
BK	 0.3640	 0.3750
BL	 0.7690	 0.4740
BM	 0.7780	 0.4670
BN	 0.8320	 0.5350
BO	 0.8050	 0.5010
BP	 0.7850	 0.5010
BQ	 0.8010	 0.5100
BR	 0.7720	 0.4650
BS	 0.8210	 0.5110
BT	 0.7830	 0.4990
BU	 0.7260	 0.3990
BV	 0.7290	 0.4920
BW	 0.5320	 0.3520
BX	 0.7470	 0.4700
BY	 0.8070	 0.4820
BZ	 0.7620	 0.4560
Ba	 0.8310	 0.5290
Bb	 0.6490	 0.4040
Bc	 0.6530	 0.4050
Bd	 0.7820	 0.4760
Be	 0.7800	 0.5130
Bf	 0.8160	 0.5190
Bg	 0.7340	 0.4710
Bh	 0.7670	 0.4630

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Chain	Atom inclusion	Q-score
Bi	 0.7520	 0.4550
Bj	 0.8540	 0.5300
Bk	 0.6770	 0.4010
Bl	 0.7820	 0.4920
Bm	 0.7830	 0.4980
Bo	 0.7570	 0.4880
Bp	 0.7460	 0.5070
Br	 0.8030	 0.4970
Bs	 0.0690	 0.0450
Bt	 0.0330	 0.0840
Bv	 0.1970	 0.0930