



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:38 AM UTC

PDB ID : 8T2Z / pdb_00008t2z
EMDB ID : EMD-40992
Title : Hypomethylated yeast 80S bound with cycloheximide, P-site tRNA, and A-site tRNA, messenger RNA, POST
Authors : Zhao, Y.; Li, H.
Deposited on : 2023-06-07
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

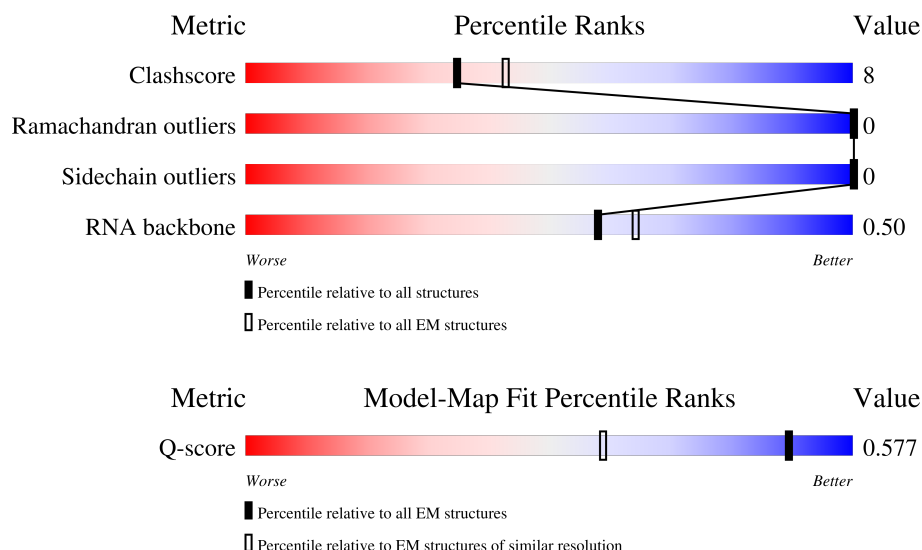
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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	BA	252	
2	BB	255	
3	BC	254	

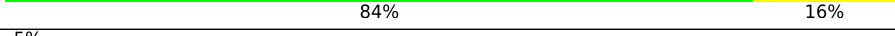
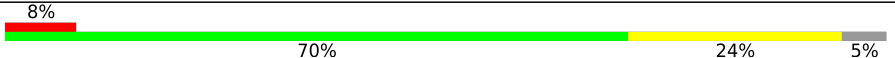
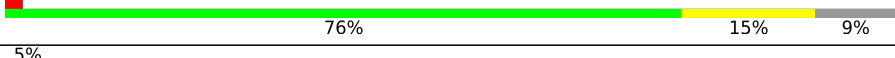
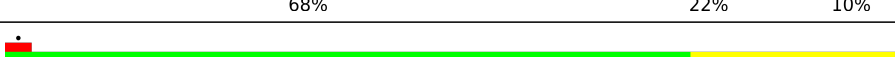
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Mol	Chain	Length	Quality of chain
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	

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Mol	Chain	Length	Quality of chain
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	
34	B5	1798	
35	AA	254	
36	AB	387	
37	AC	362	
38	A1	3395	
39	A3	121	
40	A4	158	
41	AD	297	
42	AE	176	
43	AF	244	
44	AG	256	
45	AH	191	
46	AI	221	
47	AJ	174	
48	AL	199	
49	AM	138	
50	AN	204	
51	AO	199	
52	AP	184	
53	AQ	186	

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Mol	Chain	Length	Quality of chain
54	AR	189	
55	AS	178	
56	AT	160	
57	AU	121	
58	AV	137	
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	

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Mol	Chain	Length	Quality of chain
79	tP	75	 43% 36% 21%
80	tA	76	 5% 46% 43% 11%
81	MR	12	 92% 8%

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 202314 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called RPS1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 3 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	BH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 10 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 13 is a protein called RPS22A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 16 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 19 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 20 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	BQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 28 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	71	Total	C	N	O	0	0
			574	366	108	100		

- Molecule 29 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	75	Total	C	N	O	S	0	0
			605	386	116	99	4		

- Molecule 33 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	124	Total	C	N	O	S	0	0
			935	587	165	181	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1757	Total	C	N	O	P	1	0
			37463	16754	6635	12317	1757		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 37 is a protein called RPL4A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3161	Total	C	N	O	P	0	0
			67606	30202	12171	22072	3161		

- Molecule 39 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8 S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	167	Total	C	N	O	S	0	0
			1303	840	234	228	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	120	LYS	ASN	conflict	UNP Q02326

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	217	Total	C	N	O	S	0	0
			1759	1114	333	305	7		

- Molecule 47 is a protein called RPL11A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	AL	193	Total	C	N	O		
			1543	962	315	266	0	0

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AM	136	Total	C	N	O	S		
			1053	675	199	177	2	0	0

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AN	203	Total	C	N	O	S		
			1720	1077	361	281	1	0	0

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AO	197	Total	C	N	O	S		
			1555	1003	289	262	1	197	0

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AP	175	Total	C	N	O		
			1388	862	277	249	0	0

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	185	Total	C	N	O	S		
			1441	908	290	241	2	0	0

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AR	188	Total	C	N	O		
			1521	935	326	260	0	0

- Molecule 55 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AU	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 59 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 60 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AY	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 64 is a protein called RPL29 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Ab	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 67 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 73 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	Ak	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	tP	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
tP	10	A	G	conflict	GB 176433

- Molecule 80 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	tA	76	Total	C	N	O	P	0	0
			1628	726	302	524	76		

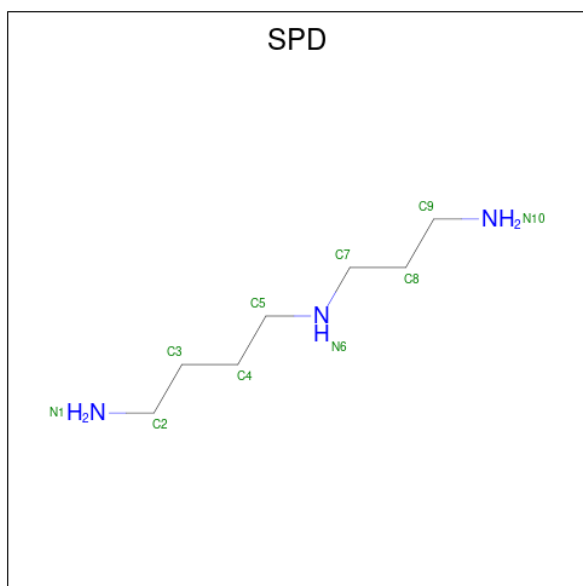
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
tA	10	A	G	conflict	GB 176433
tA	17	A	-	insertion	GB 176433

- Molecule 81 is a RNA chain called messenger RNA.

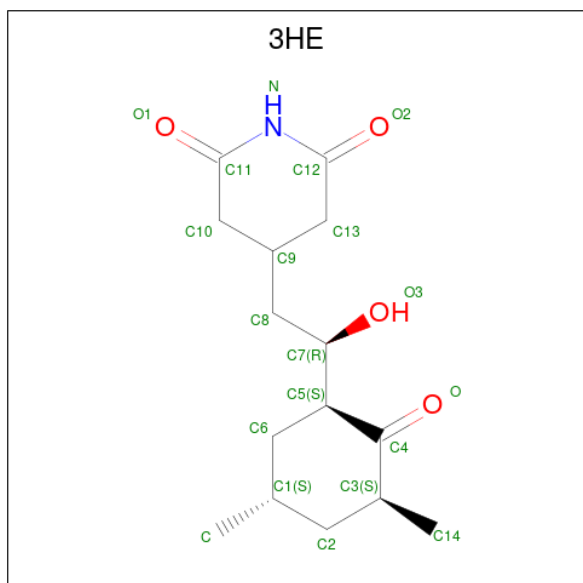
Mol	Chain	Residues	Atoms					AltConf	Trace
81	MR	12	Total	C	N	O	P	0	0
			262	118	54	78	12		

- Molecule 82 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
82	A1	1	Total	C	N	0
			10	7	3	

- Molecule 83 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: $C_{15}H_{23}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
83	A1	1	Total	C	N	O	0
			20	15	1	4	

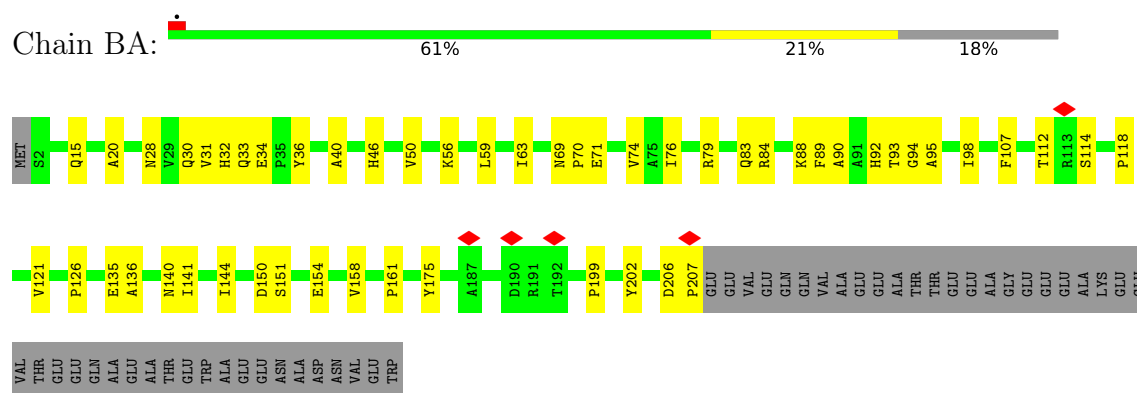
- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Ao	1	Total	Zn	0
			1	1	

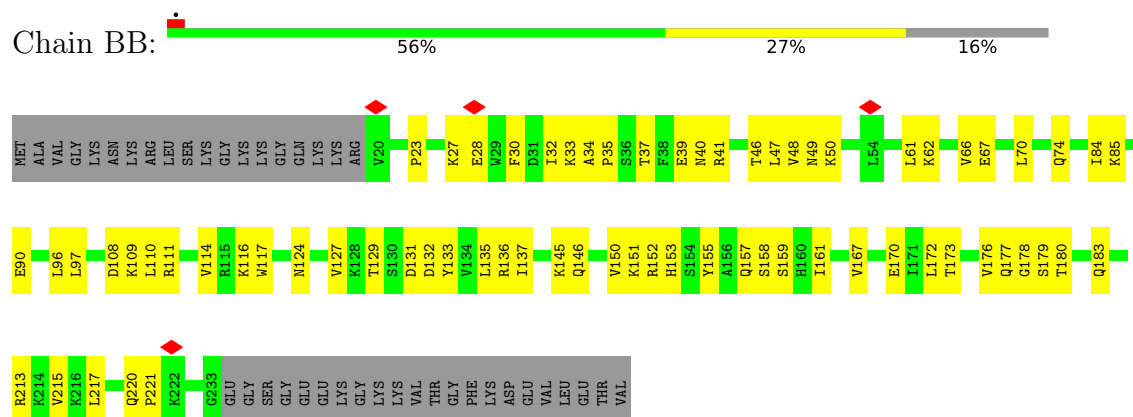
3 Residue-property plots

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

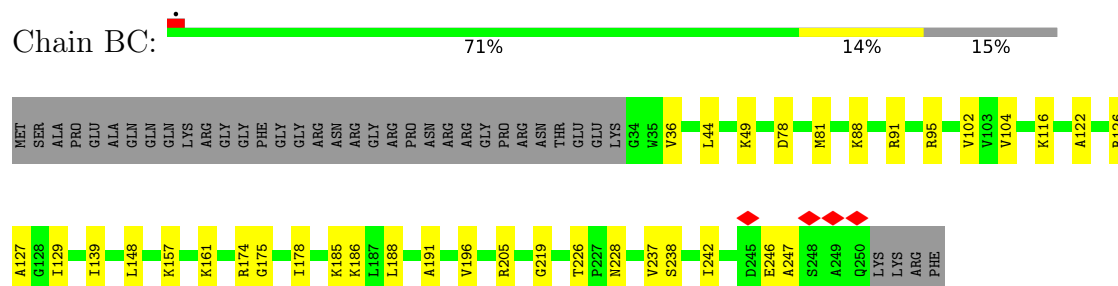
- Molecule 1: 40S ribosomal protein S0-A



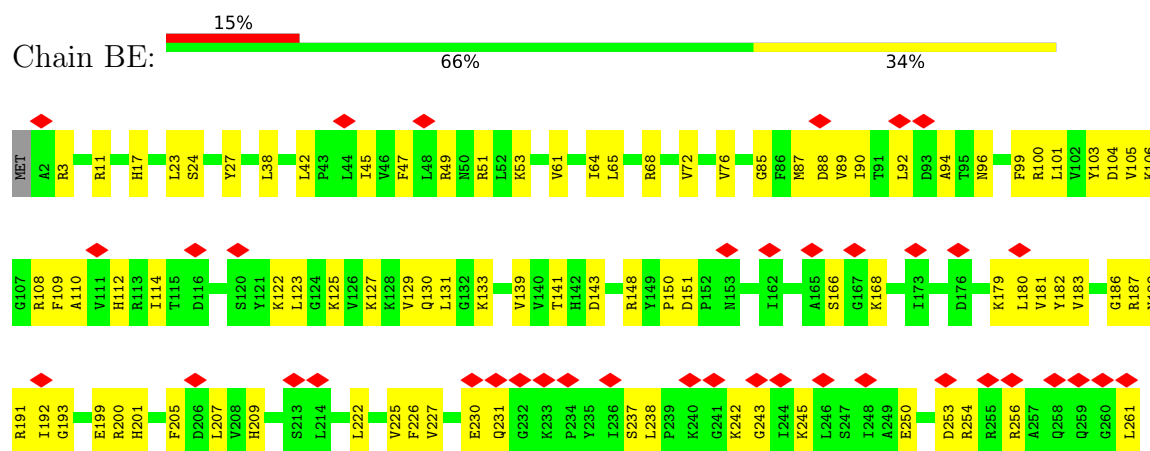
- Molecule 2: RPS1A isoform 1



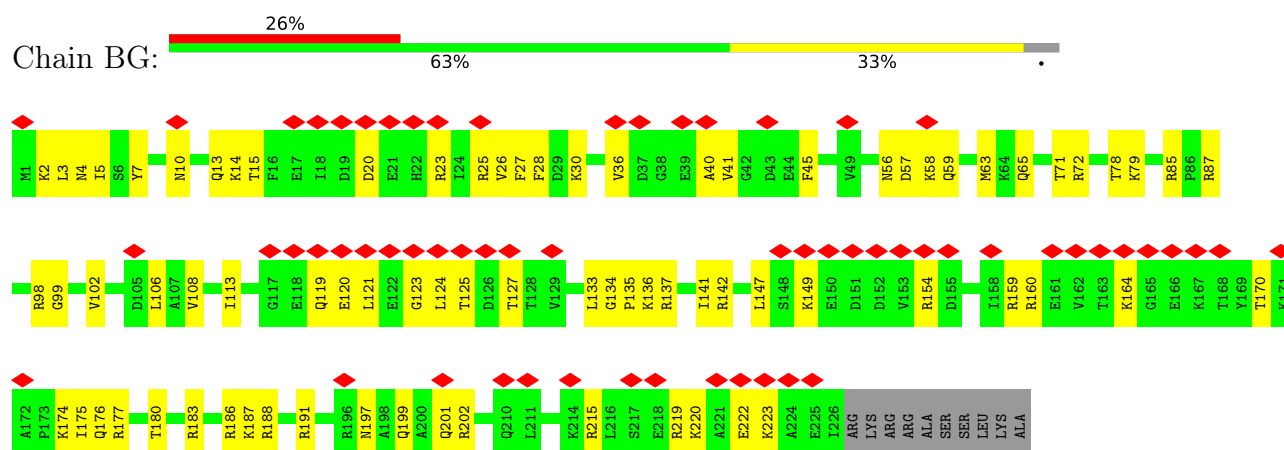
- Molecule 3: RPS2 isoform 1



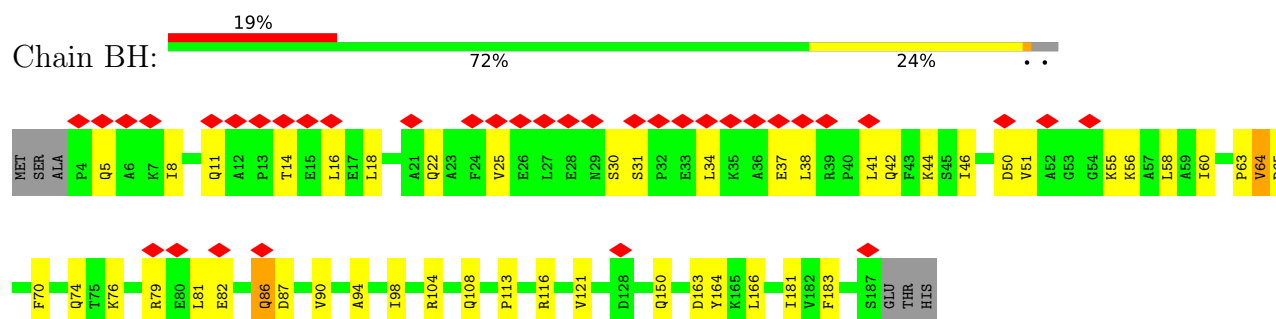
- Molecule 4: 40S ribosomal protein S4-A



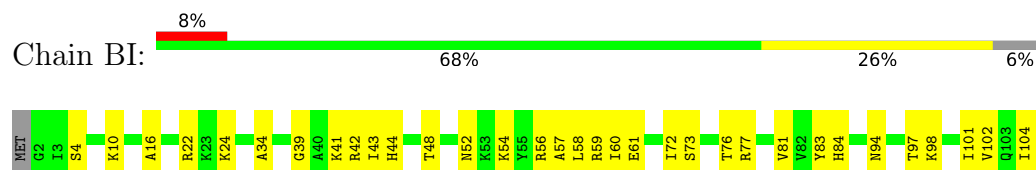
- Molecule 5: 40S ribosomal protein S6-A

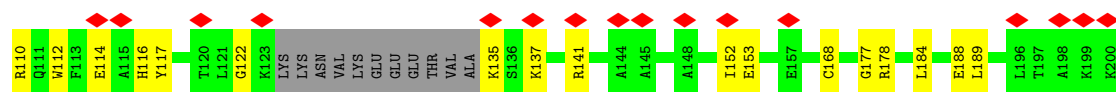


- Molecule 6: 40S ribosomal protein S7-A

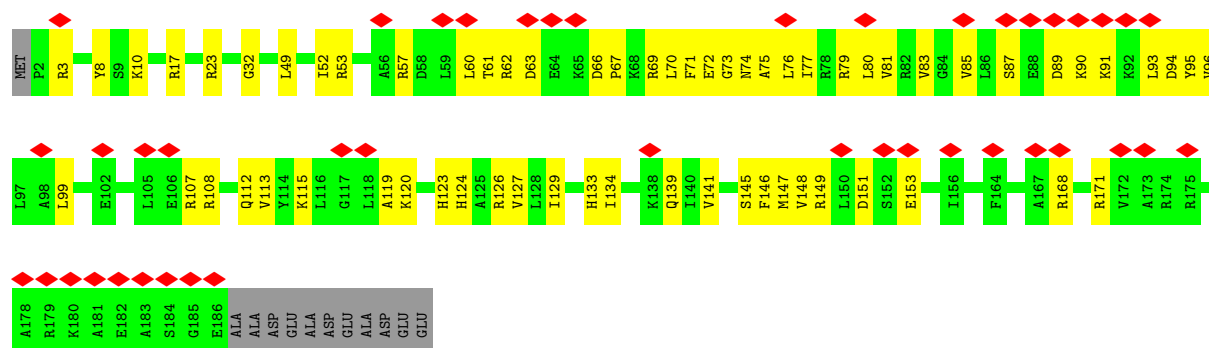


- Molecule 7: 40S ribosomal protein S8-A

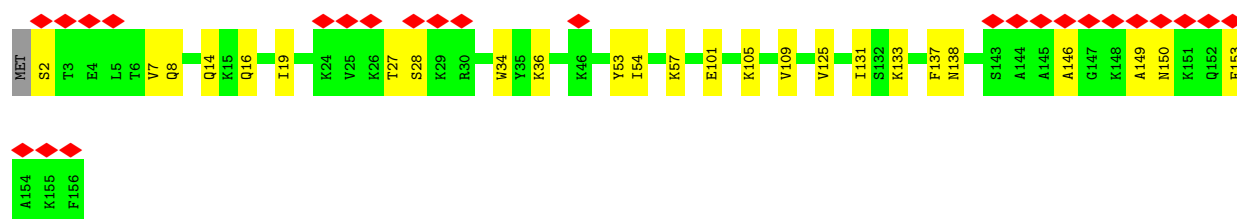
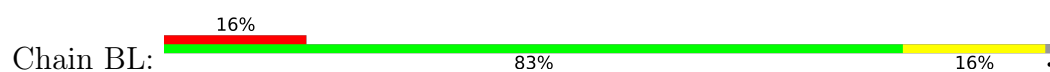




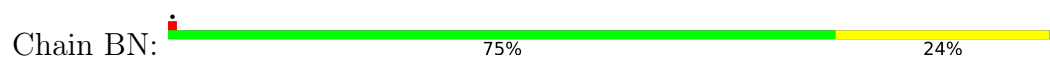
• Molecule 8: 40S ribosomal protein S9-A



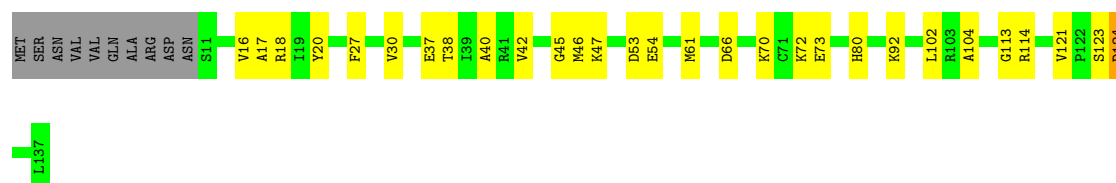
• Molecule 9: 40S ribosomal protein S11-A



• Molecule 10: 40S ribosomal protein S13

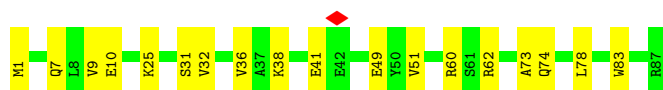


• Molecule 11: 40S ribosomal protein S14-A



- Molecule 12: 40S ribosomal protein S21-A

Chain BV:  79% 21%



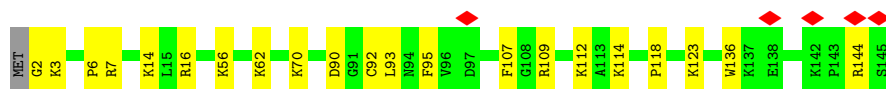
- Molecule 13: RPS22A isoform 1

Chain BW:  79% 20%



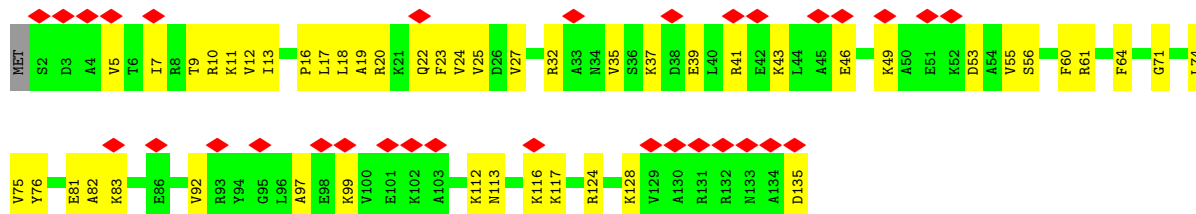
- Molecule 14: 40S ribosomal protein S23-A

Chain BX:  85% 14%



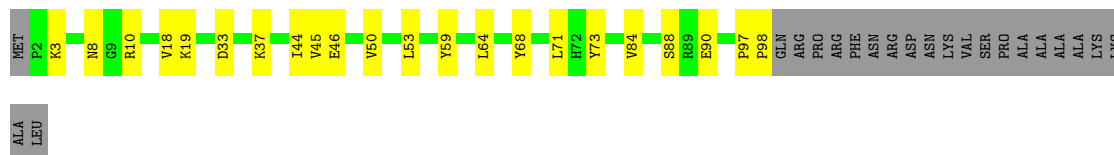
- Molecule 15: 40S ribosomal protein S24-A

Chain BY:  24% 64% 36%



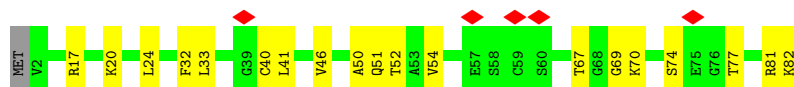
- Molecule 16: RPS26B isoform 1

Chain Ba:  63% 18% 18%

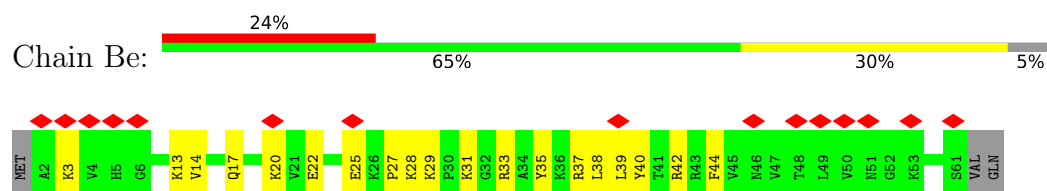


- Molecule 17: 40S ribosomal protein S27-A

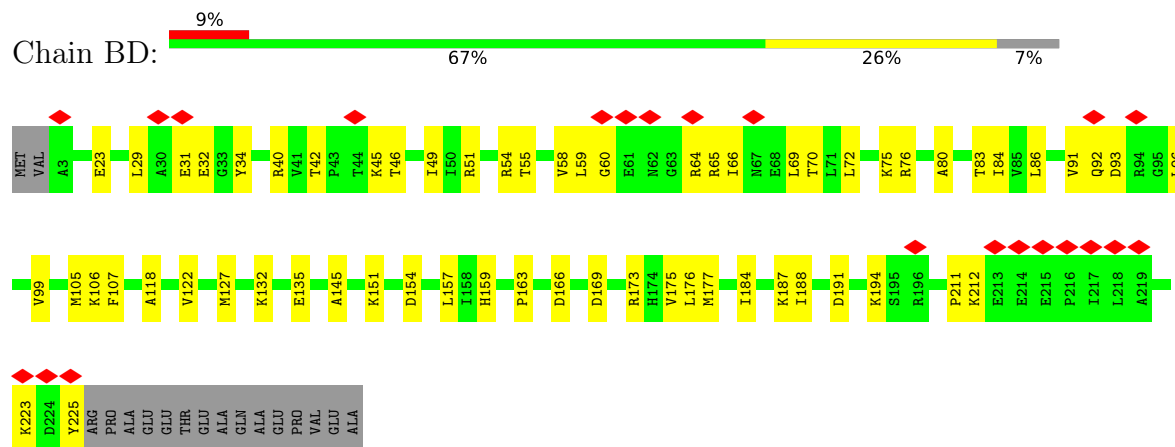
Chain Bb:  6% 76% 23%



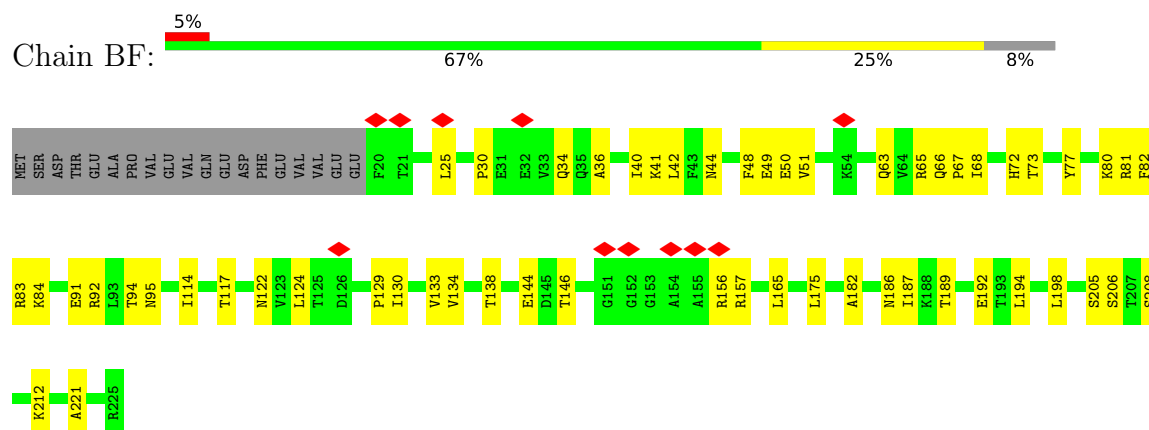
- Molecule 18: 40S ribosomal protein S30-A



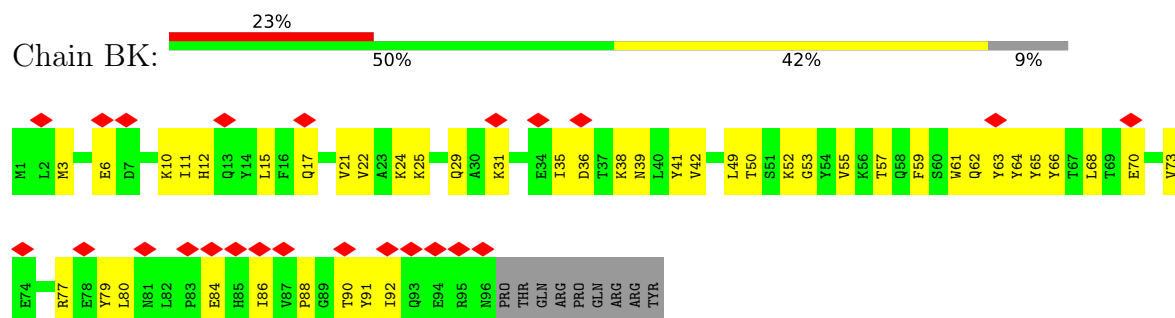
- Molecule 19: RPS3 isoform 1



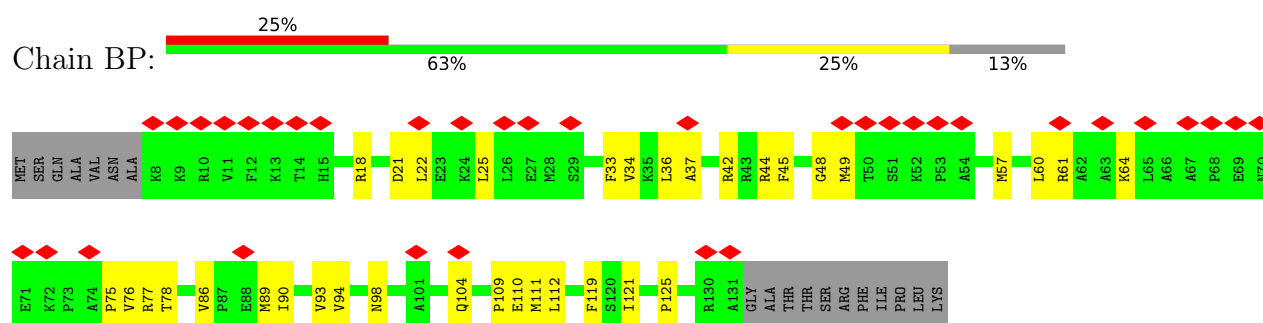
- Molecule 20: Rps5p



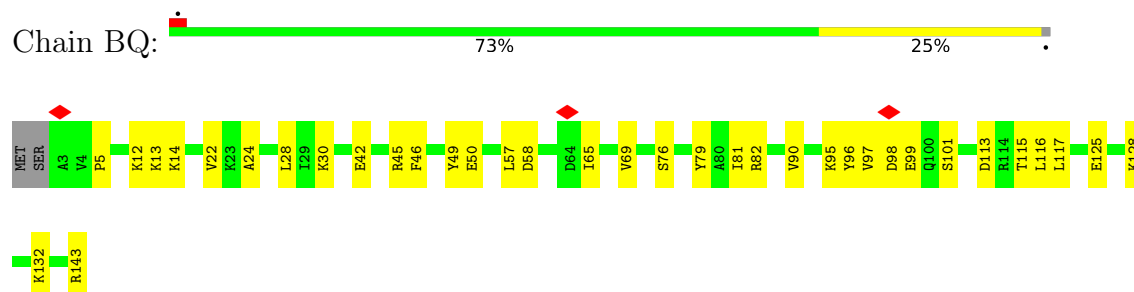
- Molecule 21: 40S ribosomal protein S10-A



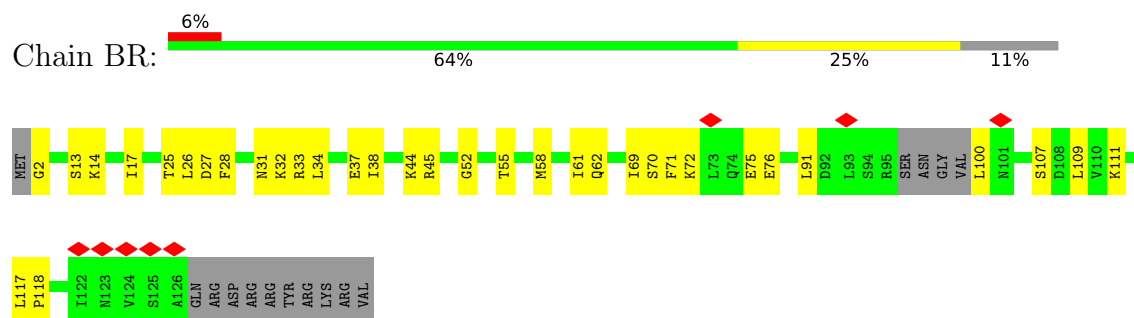
- Molecule 22: RPS15 isoform 1



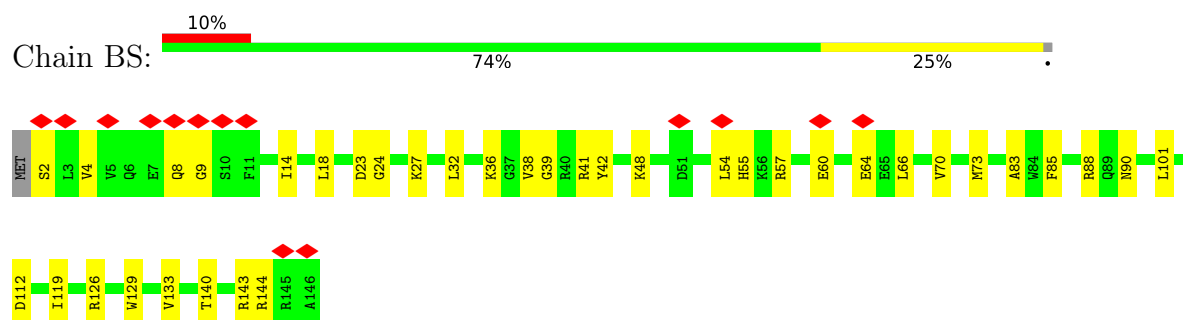
- Molecule 23: 40S ribosomal protein S16-A



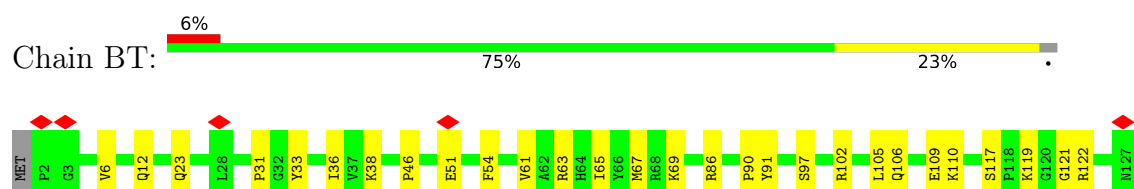
- Molecule 24: 40S ribosomal protein S17-A

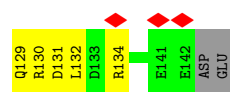


- Molecule 25: 40S ribosomal protein S18-A

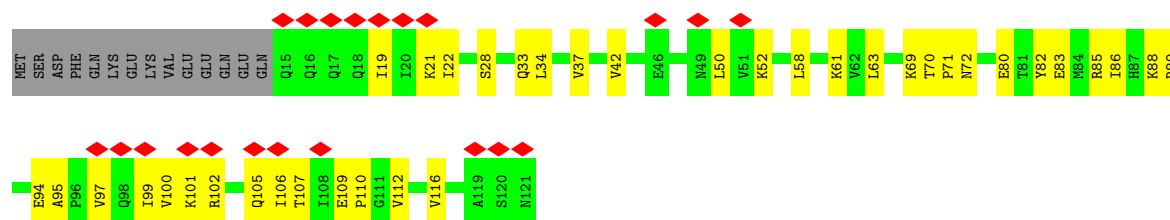


- Molecule 26: 40S ribosomal protein S19-A

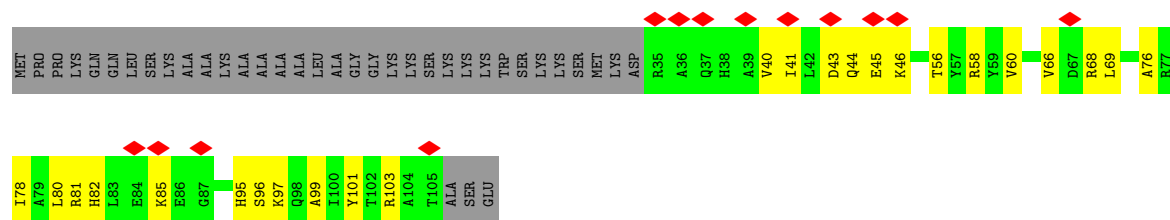
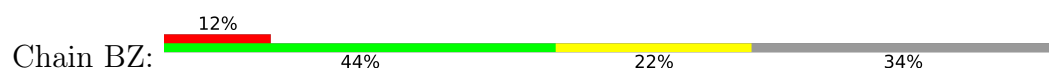




• Molecule 27: RPS20 isoform 1



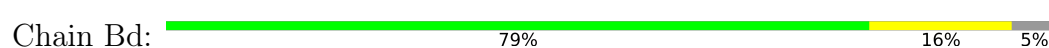
• Molecule 28: RPS25A isoform 1



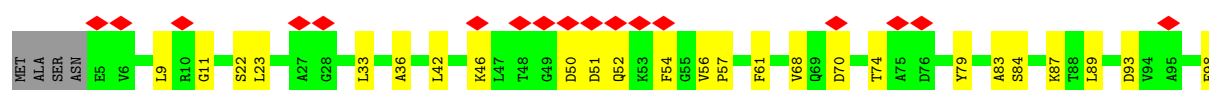
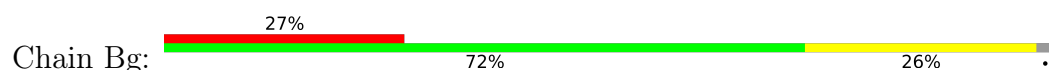
• Molecule 29: RPS28A isoform 1

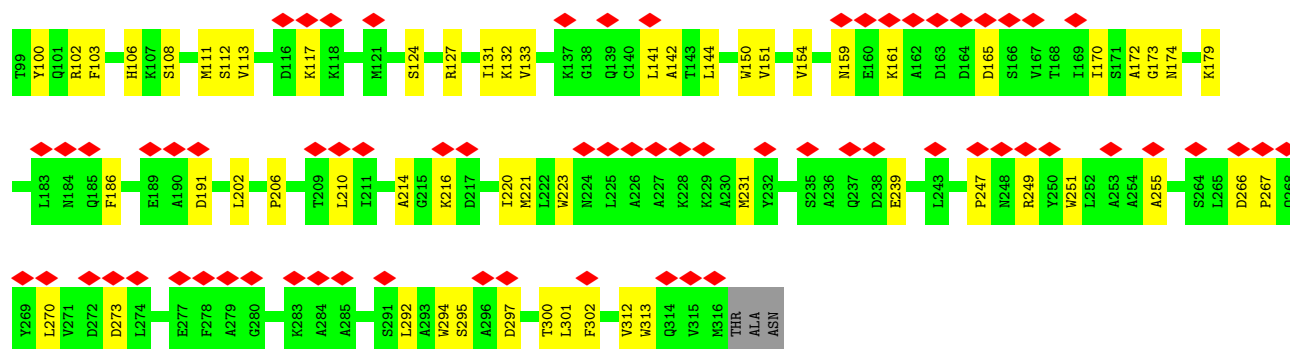


• Molecule 30: RPS29A isoform 1

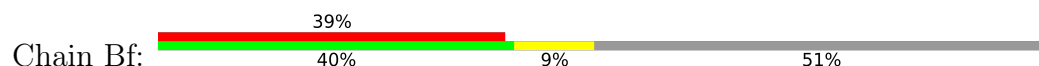


• Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein

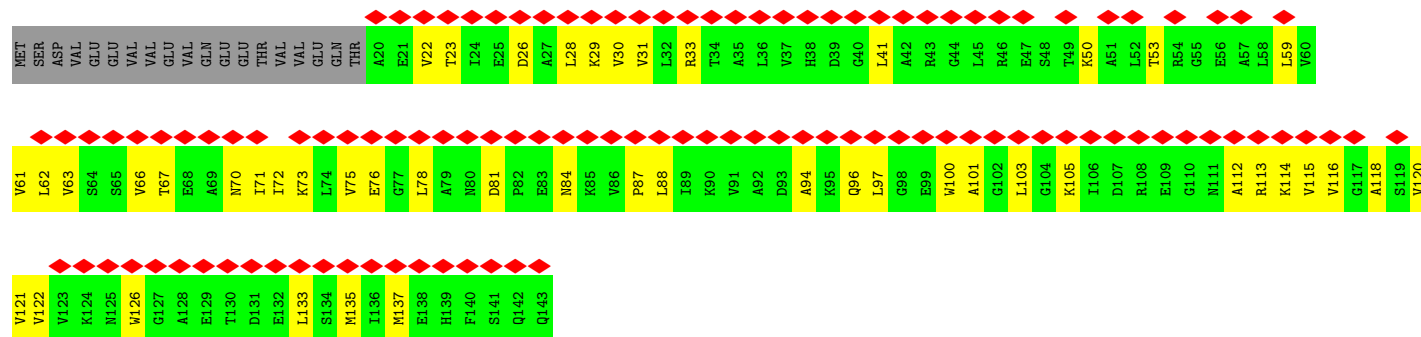
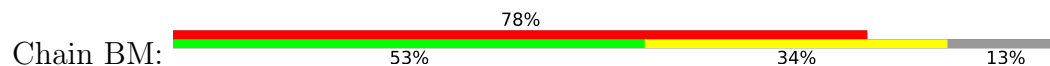




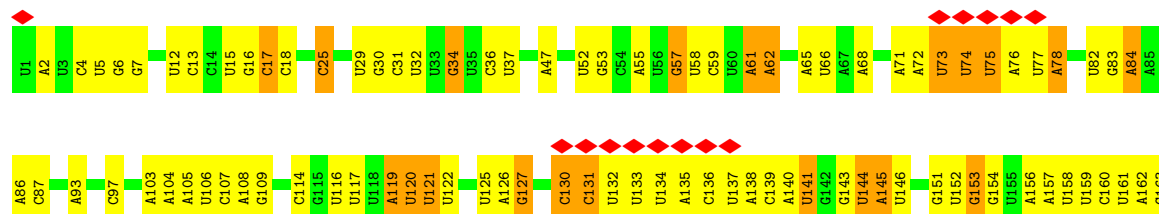
• Molecule 32: Ubiquitin-40S ribosomal protein S31



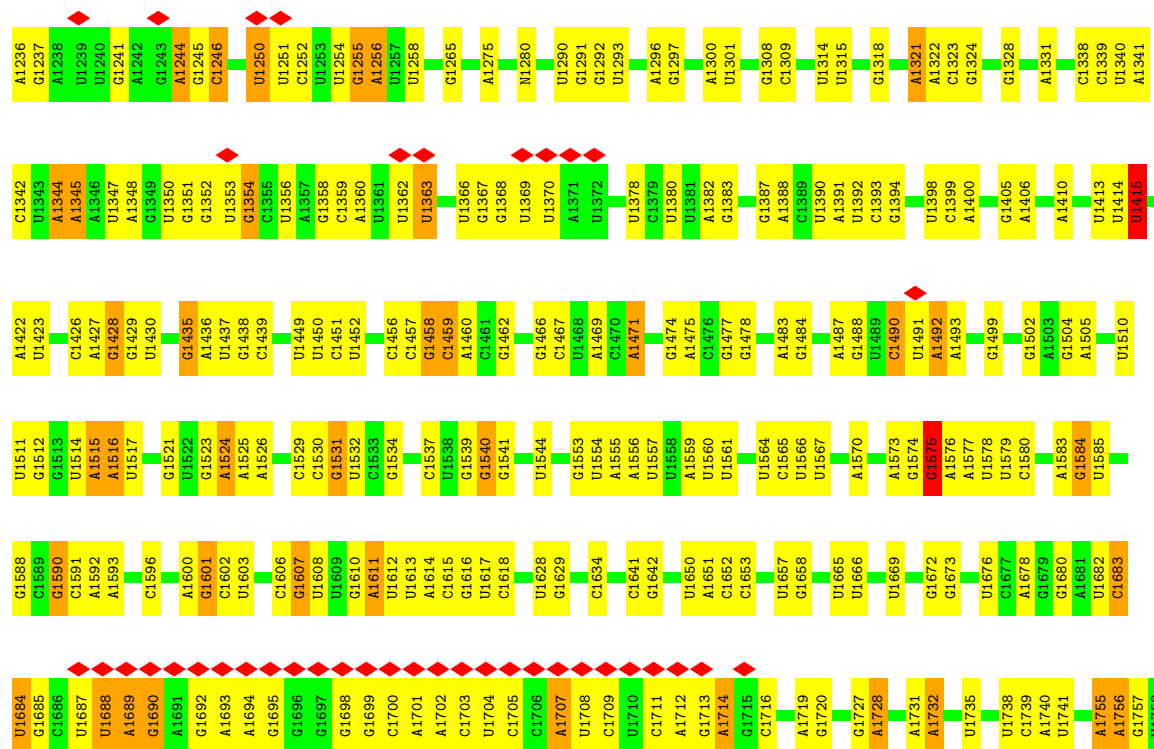
• Molecule 33: 40S ribosomal protein S12



• Molecule 34: 18S rRNA

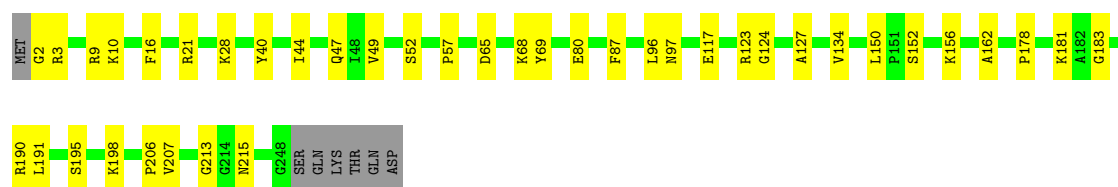






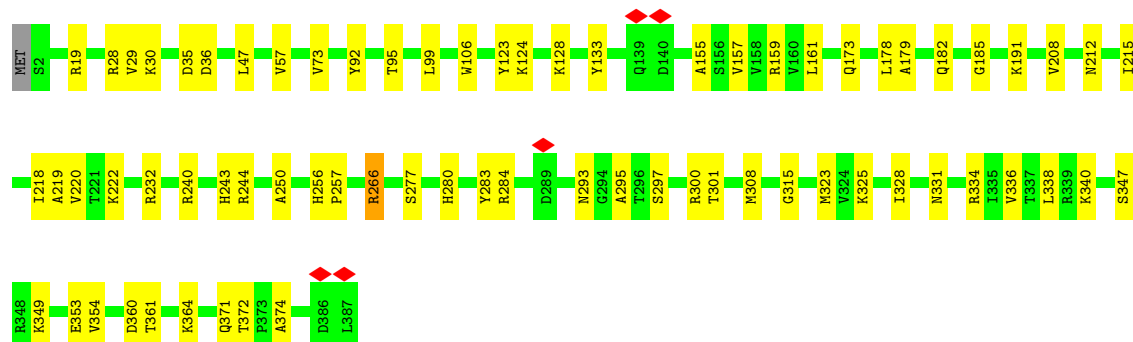
• Molecule 35: 60S ribosomal protein L2-A

Chain AA: 81% 16%

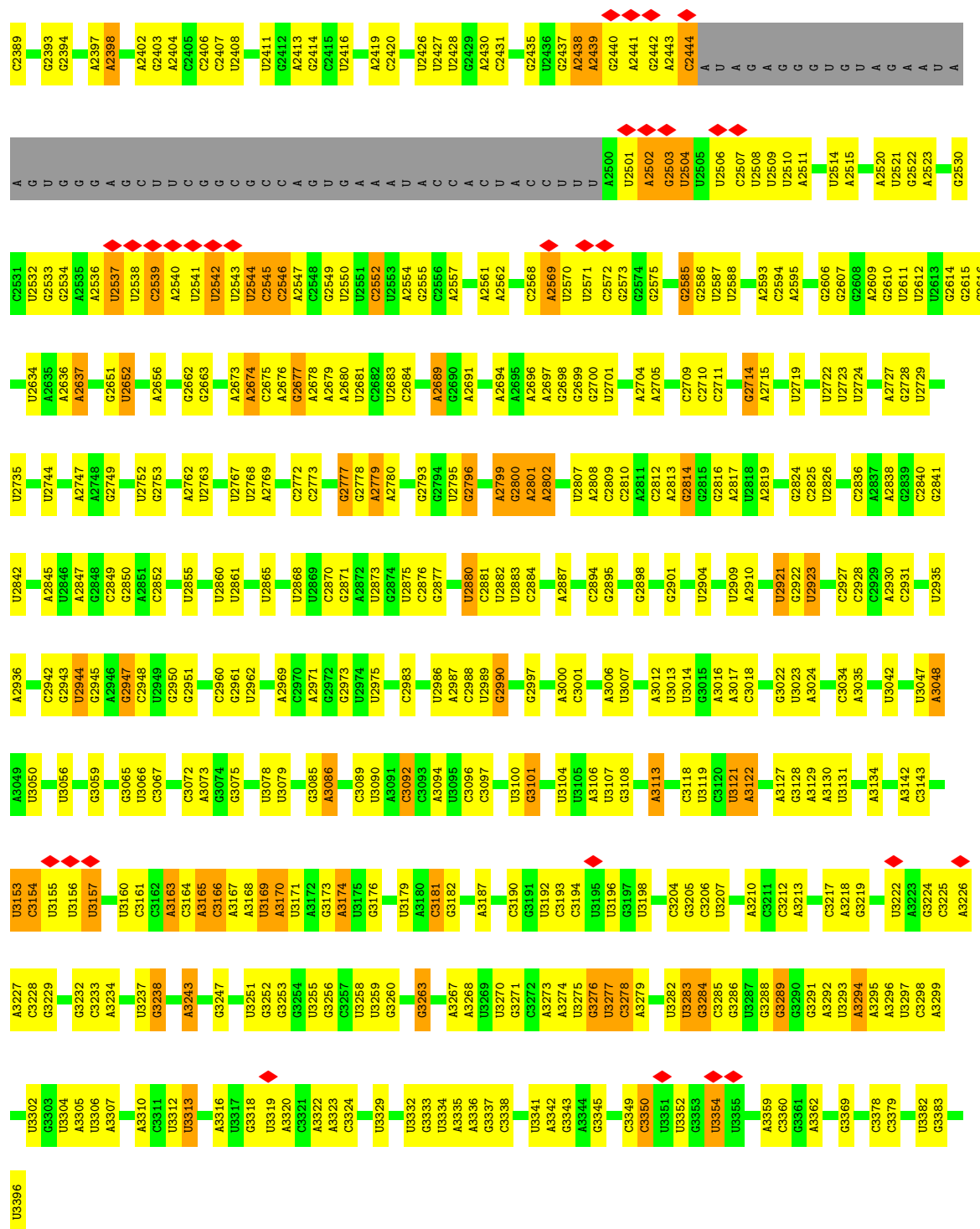


• Molecule 36: 60S ribosomal protein L3

Chain AB: 81% 18%







• Molecule 39: 5s rRNA

Chain A3:





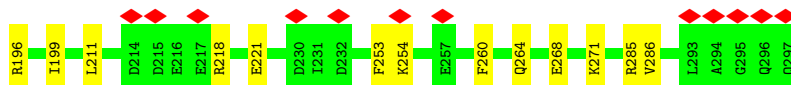
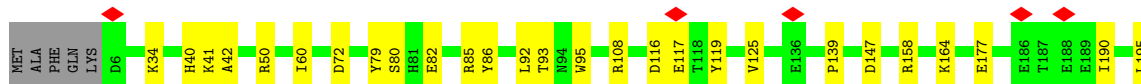
• Molecule 40: 5.8 S rRNA

Chain A4: 



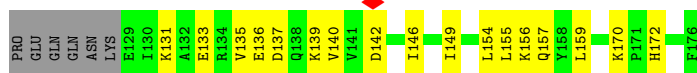
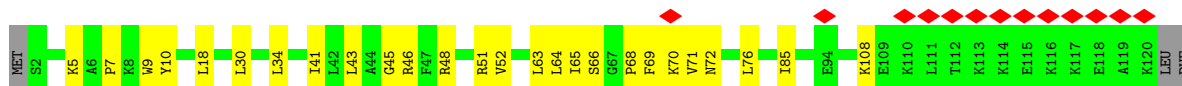
• Molecule 41: RPL5 isoform 1

Chain AD: 



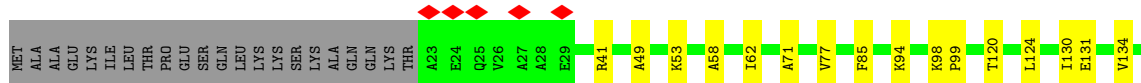
• Molecule 42: 60S ribosomal protein L6-A

Chain AE: 



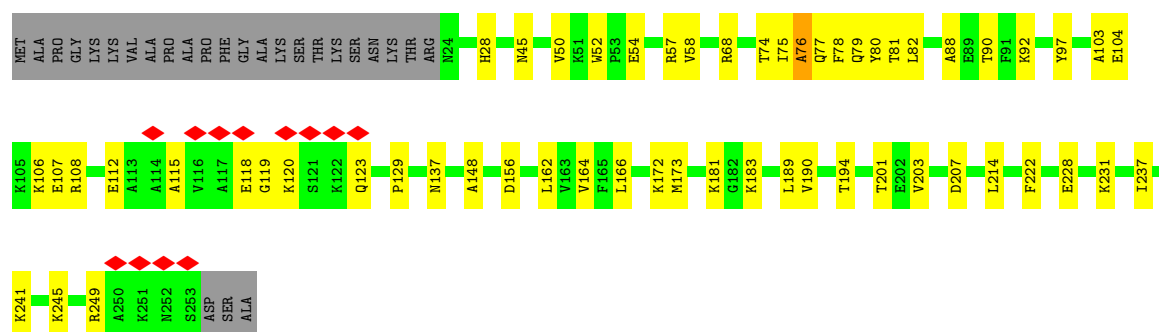
• Molecule 43: 60S ribosomal protein L7-A

Chain AF: 



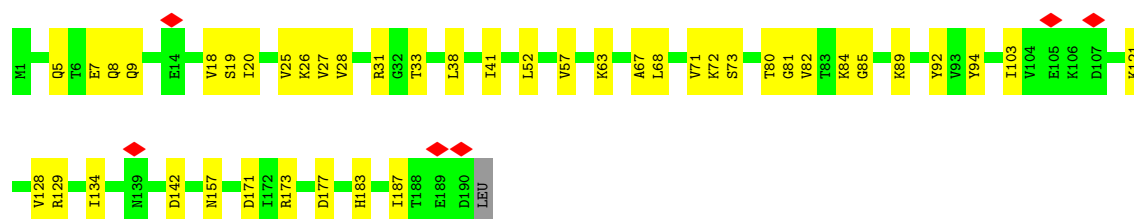
• Molecule 44: 60S ribosomal protein L8-A

Chain AG: 



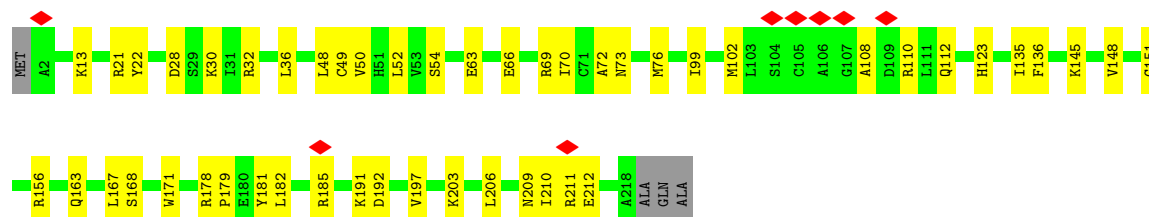
• Molecule 45: 60S ribosomal protein L9-A

Chain AH: 77% 23%



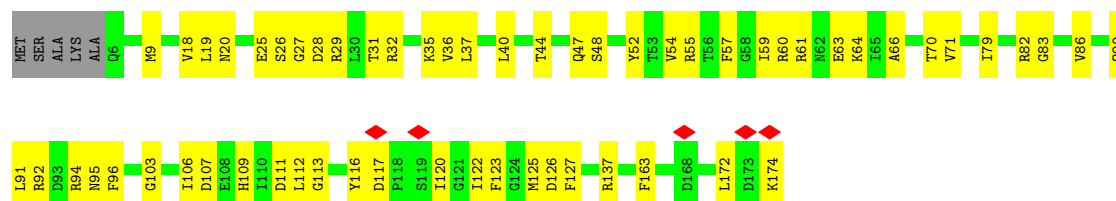
• Molecule 46: RPL10 isoform 1

Chain AI: 76% 22%



• Molecule 47: RPL11A isoform 1

Chain AJ: 63% 34%



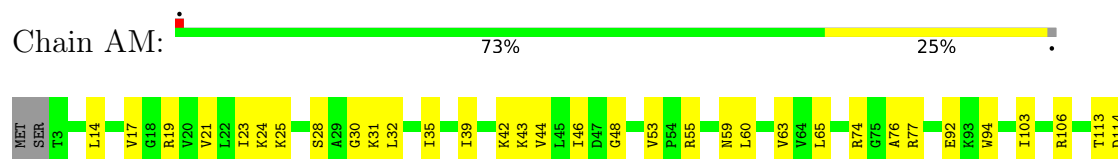
• Molecule 48: 60S ribosomal protein L13-A

Chain AL: 82% 15%

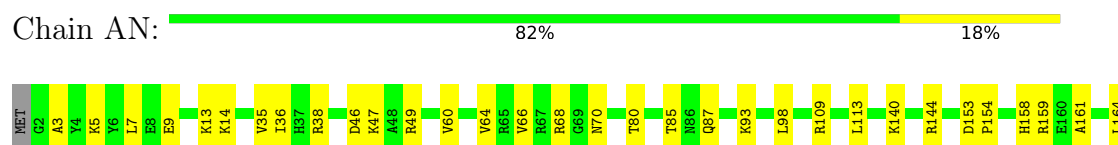




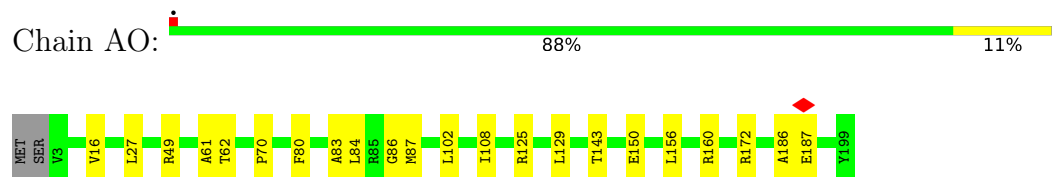
- Molecule 49: 60S ribosomal protein L14-A



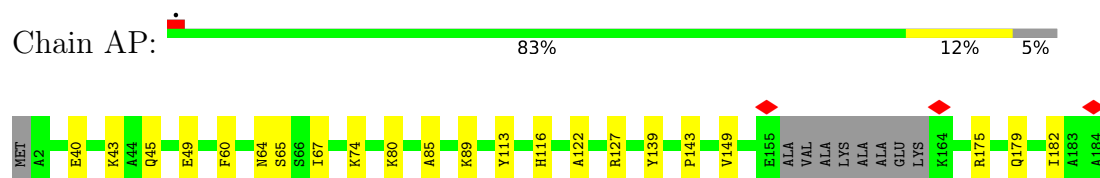
- Molecule 50: 60S ribosomal protein L15-A



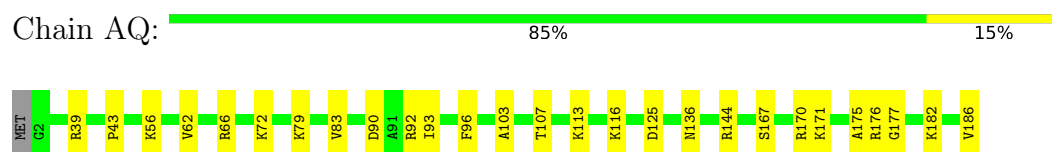
- Molecule 51: 60S ribosomal protein L16-A



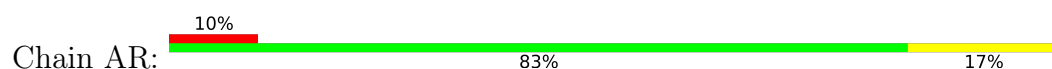
- Molecule 52: 60S ribosomal protein L17-A



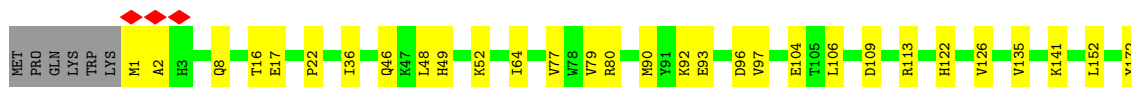
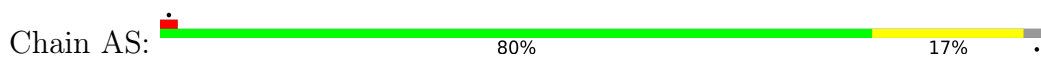
- Molecule 53: 60S ribosomal protein L18-A



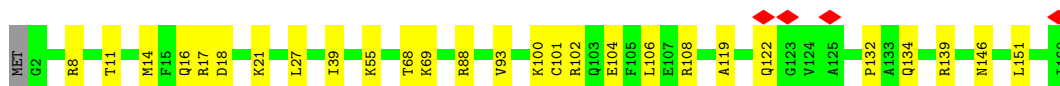
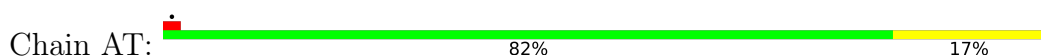
- Molecule 54: 60S ribosomal protein L19-A



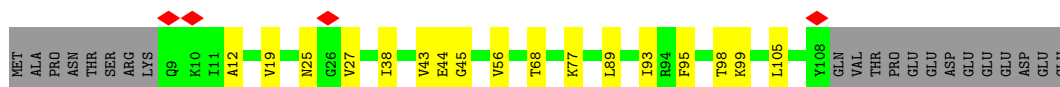
- Molecule 55: 60S ribosomal protein L20



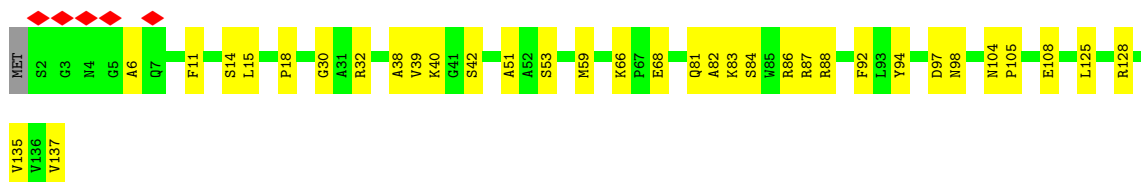
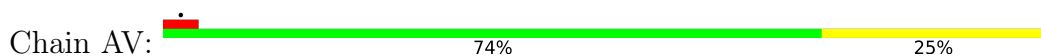
- Molecule 56: 60S ribosomal protein L21-A



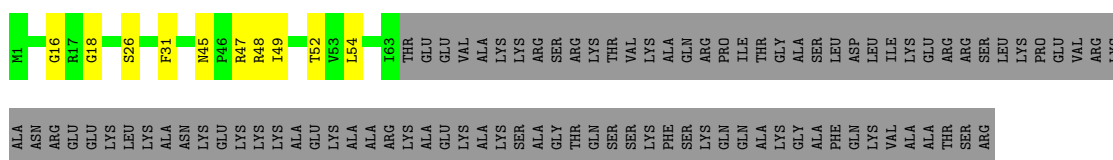
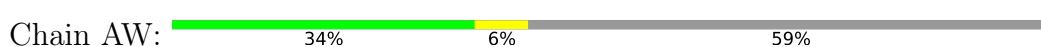
- Molecule 57: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L23-A

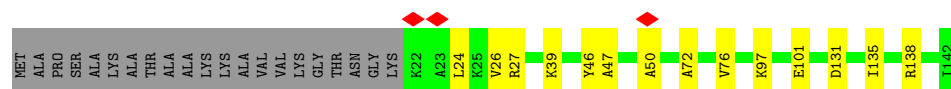


- Molecule 59: RPL24A isoform 1



- Molecule 60: 60S ribosomal protein L25

Chain AX:  75% 10% 15%



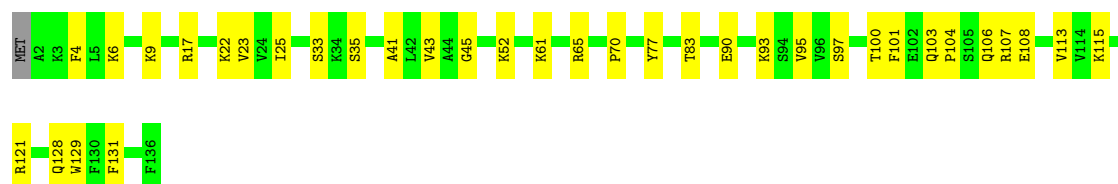
- Molecule 61: 60S ribosomal protein L26-A

Chain AY:  78% 21%



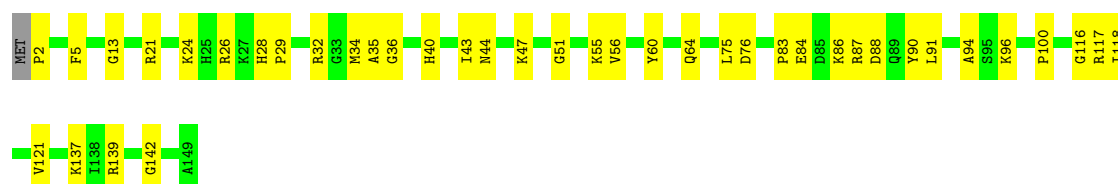
- Molecule 62: 60S ribosomal protein L27-A

Chain AZ:  74% 26%



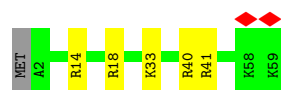
- Molecule 63: 60S ribosomal protein L28

Chain Aa:  72% 27%



- Molecule 64: RPL29 isoform 1

Chain Ab:  90% 8%

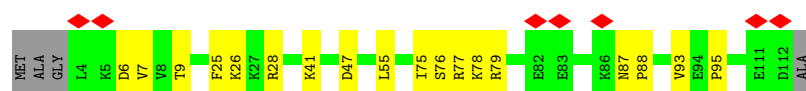
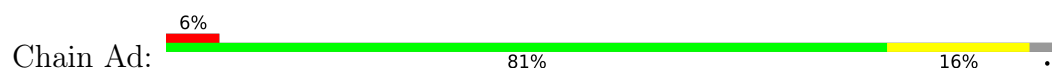


- Molecule 65: 60S ribosomal protein L30

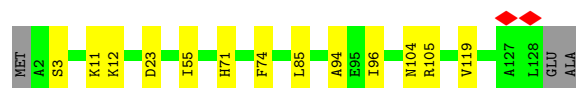
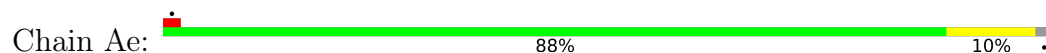
Chain Ac:  69% 24% 8%



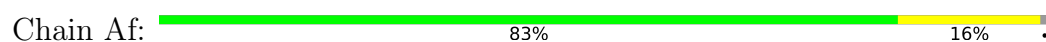
- Molecule 66: 60S ribosomal protein L31-A



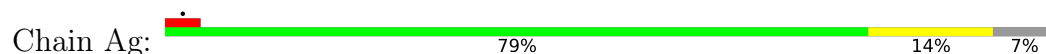
- Molecule 67: RPL32 isoform 1



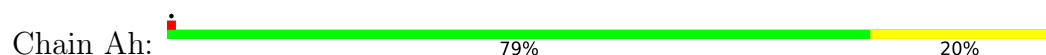
- Molecule 68: 60S ribosomal protein L33-A



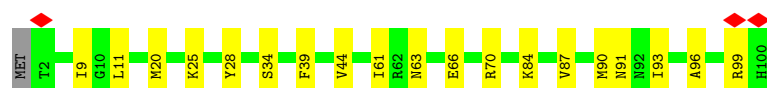
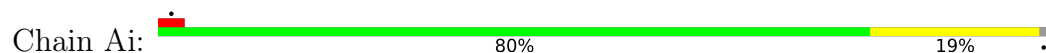
- Molecule 69: 60S ribosomal protein L34-A



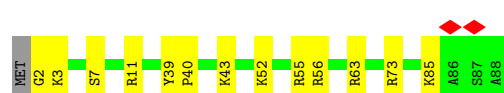
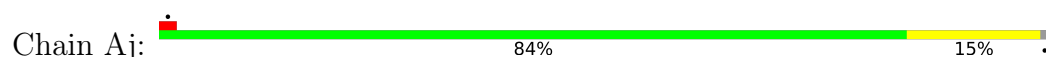
- Molecule 70: 60S ribosomal protein L35-A



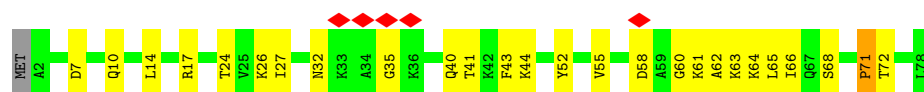
- Molecule 71: 60S ribosomal protein L36-A



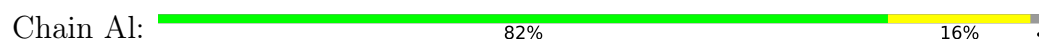
- Molecule 72: 60S ribosomal protein L37-A



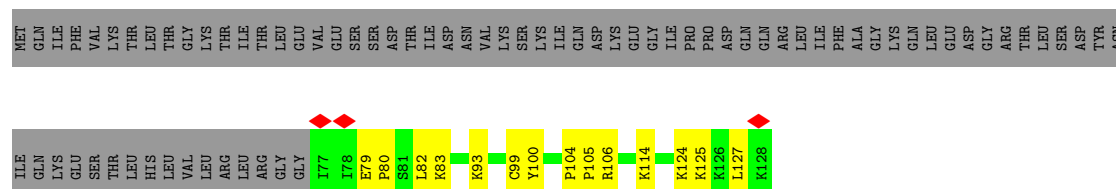
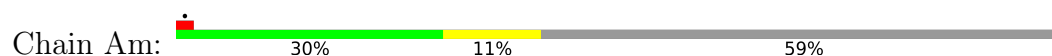
- Molecule 73: RPL38 isoform 1



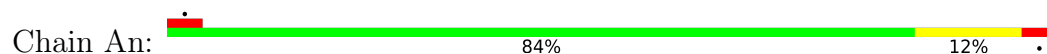
- Molecule 74: 60S ribosomal protein L39



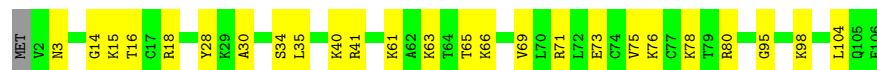
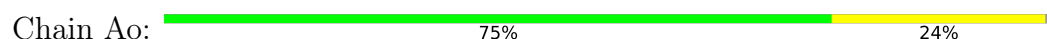
- Molecule 75: Ubiquitin-60S ribosomal protein L40



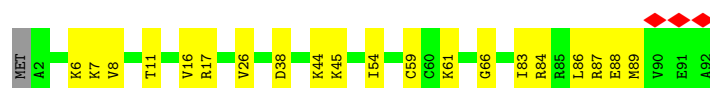
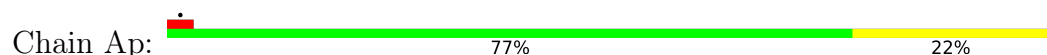
- Molecule 76: 60S ribosomal protein L41-A



- Molecule 77: 60S ribosomal protein L42-A

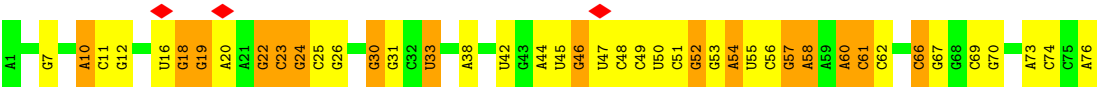


- Molecule 78: 60S ribosomal protein L43-A

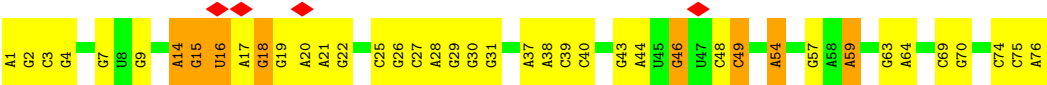


- Molecule 79: P site tRNA





● Molecule 80: A site tRNA



● Molecule 81: messenger RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215904	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.263	Depositor
Minimum map value	-3.940	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.277	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	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: 5MC, HIC, UR3, 3HE, PSU, OMU, G7M, SPD, OMG, 4AC, ZN, B8N, 1MA, MA6

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	BA	0.17	0/1653	0.39	0/2261
2	BB	0.21	0/1735	0.50	0/2335
3	BC	0.17	0/1665	0.35	0/2263
4	BE	0.16	0/2109	0.44	0/2839
5	BG	0.14	0/1844	0.40	0/2464
6	BH	0.18	0/1506	0.51	2/2028 (0.1%)
7	BI	0.17	0/1514	0.40	0/2021
8	BJ	0.18	0/1519	0.49	0/2035
9	BL	0.17	0/1272	0.38	0/1712
10	BN	0.18	0/1215	0.37	0/1638
11	BO	0.23	0/952	0.48	0/1279
12	BV	0.16	0/693	0.31	0/935
13	BW	0.20	0/1038	0.39	0/1395
14	BX	0.17	0/1139	0.36	0/1518
15	BY	0.16	0/1087	0.40	0/1449
16	Ba	0.20	0/782	0.48	0/1047
17	Bb	0.16	0/620	0.39	0/838
18	Be	0.16	0/483	0.51	0/643
19	BD	0.17	0/1759	0.43	0/2368
20	BF	0.15	0/1629	0.35	0/2202
21	BK	0.20	0/837	0.56	0/1131
22	BP	0.15	0/1012	0.42	0/1356
23	BQ	0.16	0/1125	0.37	0/1510
24	BR	0.17	0/957	0.40	0/1283
25	BS	0.15	0/1211	0.45	0/1628
26	BT	0.14	0/1113	0.41	0/1494
27	BU	0.17	0/865	0.44	0/1169
28	BZ	0.18	0/582	0.46	0/782
29	Bc	0.17	0/499	0.52	0/670
30	Bd	0.16	0/452	0.36	0/600
31	Bg	0.14	0/2454	0.39	0/3340
32	Bf	0.11	0/616	0.35	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.16	0/943	0.55	2/1274 (0.2%)
34	B5	0.18	1/41450 (0.0%)	0.32	0/64582
35	AA	0.22	0/1912	0.43	0/2569
36	AB	0.19	0/3139	0.40	0/4219
37	AC	0.20	0/2800	0.44	0/3790
38	A1	0.23	0/74838	0.34	1/116683 (0.0%)
39	A3	0.19	0/2861	0.28	0/4457
40	A4	0.24	0/3724	0.33	0/5798
41	AD	0.16	0/2390	0.38	0/3225
42	AE	0.18	0/1324	0.44	0/1782
43	AF	0.21	0/1821	0.42	0/2451
44	AG	0.20	0/1830	0.44	0/2469
45	AH	0.20	0/1531	0.45	0/2062
46	AI	0.18	0/1796	0.42	0/2409
47	AJ	0.19	0/1374	0.53	0/1842
48	AL	0.23	0/1568	0.45	0/2106
49	AM	0.20	0/1068	0.39	0/1438
50	AN	0.23	0/1757	0.41	0/2354
51	AO	0.21	0/1585	0.38	0/2128
52	AP	0.22	0/1410	0.39	0/1893
53	AQ	0.20	0/1465	0.39	0/1965
54	AR	0.21	0/1538	0.45	0/2050
55	AS	0.19	0/1481	0.38	0/1990
56	AT	0.19	0/1300	0.36	0/1743
57	AU	0.17	0/812	0.38	0/1099
58	AV	0.18	0/1018	0.38	0/1369
59	AW	0.18	0/533	0.37	0/707
60	AX	0.20	0/983	0.41	0/1325
61	AY	0.22	0/1004	0.39	0/1341
62	AZ	0.22	0/1118	0.48	0/1497
63	Aa	0.21	0/1204	0.39	0/1612
64	Ab	0.19	0/473	0.42	0/629
65	Ac	0.20	0/751	0.41	0/1008
66	Ad	0.19	0/904	0.40	0/1213
67	Ae	0.20	0/1041	0.41	0/1394
68	Af	0.21	0/868	0.39	0/1168
69	Ag	0.20	0/890	0.39	0/1189
70	Ah	0.19	0/978	0.38	0/1301
71	Ai	0.21	0/778	0.43	0/1034
72	Aj	0.21	0/696	0.38	0/923
73	Ak	0.24	0/618	0.50	1/826 (0.1%)
74	Al	0.21	0/443	0.43	0/588
75	Am	0.22	0/423	0.47	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.27	0/234	0.70	1/300 (0.3%)
77	Ao	0.19	0/860	0.42	0/1136
78	Ap	0.20	0/701	0.45	0/934
79	tP	0.18	0/1796	0.36	0/2799
80	tA	0.14	0/1821	0.29	0/2838
81	MR	0.16	0/295	0.24	0/458
All	All	0.20	1/216084 (0.0%)	0.37	7/317579 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	BH	0	1
11	BO	0	2
13	BW	0	1
36	AB	0	1
43	AF	0	1
44	AG	0	1
54	AR	0	1
76	An	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O3'-P	6.00	1.62	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BM	126	TRP	CA-C-N	7.05	134.39	121.70
33	BM	126	TRP	C-N-CA	7.05	134.39	121.70
6	BH	86	GLN	CA-C-N	6.48	133.92	121.54
6	BH	86	GLN	C-N-CA	6.48	133.92	121.54
76	An	9	ARG	CG-CD-NE	6.11	125.44	112.00
73	Ak	71	PRO	CA-N-CD	-5.54	104.25	112.00
38	A1	240	U	C2'-C3'-O3'	5.26	117.38	109.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	AB	266	ARG	Sidechain
43	AF	232	ARG	Peptide
44	AG	76	ALA	Peptide
54	AR	131	ALA	Peptide
76	An	9	ARG	Sidechain
6	BH	64	VAL	Peptide
11	BO	123	SER	Peptide
11	BO	124	ASP	Peptide
13	BW	54	ASP	Peptide

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	BA	1612	0	1623	33	0
2	BB	1709	0	1784	48	0
3	BC	1635	0	1723	23	0
4	BE	2068	0	2154	79	0
5	BG	1820	0	1918	66	0
6	BH	1481	0	1572	32	0
7	BI	1489	0	1525	46	0
8	BJ	1494	0	1573	56	0
9	BL	1244	0	1314	21	0
10	BN	1192	0	1255	22	0
11	BO	941	0	979	22	0
12	BV	684	0	672	15	0
13	BW	1021	0	1060	19	0
14	BX	1121	0	1196	16	0
15	BY	1073	0	1132	45	0
16	Ba	769	0	818	15	0
17	Bb	610	0	633	12	0
18	Be	475	0	525	23	0
19	BD	1734	0	1817	50	0
20	BF	1609	0	1675	39	0
21	BK	817	0	804	34	0
22	BP	991	0	1035	27	0
23	BQ	1105	0	1166	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BR	948	0	990	25	0
25	BS	1192	0	1222	32	0
26	BT	1095	0	1114	26	0
27	BU	855	0	917	28	0
28	BZ	574	0	616	19	0
29	Bc	497	0	535	16	0
30	Bd	442	0	432	8	0
31	Bg	2401	0	2356	56	0
32	Bf	605	0	654	12	0
33	BM	935	0	975	34	0
34	B5	37463	0	18841	555	0
35	AA	1878	0	1946	28	0
36	AB	3081	0	3162	45	0
37	AC	2748	0	2859	44	0
38	A1	67606	0	33985	673	0
39	A3	2579	0	1304	31	0
40	A4	3353	0	1695	46	0
41	AD	2341	0	2290	30	0
42	AE	1303	0	1376	36	0
43	AF	1784	0	1862	26	0
44	AG	1798	0	1894	39	0
45	AH	1510	0	1576	30	0
46	AI	1759	0	1799	36	0
47	AJ	1353	0	1383	47	0
48	AL	1543	0	1608	23	0
49	AM	1053	0	1149	23	0
50	AN	1720	0	1779	28	0
51	AO	1555	0	1659	15	0
52	AP	1388	0	1423	15	0
53	AQ	1441	0	1543	24	0
54	AR	1521	0	1617	29	0
55	AS	1445	0	1487	22	0
56	AT	1276	0	1323	22	0
57	AU	796	0	812	11	0
58	AV	1003	0	1048	21	0
59	AW	521	0	551	9	0
60	AX	968	0	1036	12	0
61	AY	993	0	1081	21	0
62	AZ	1092	0	1155	27	0
63	Aa	1173	0	1215	36	0
64	Ab	462	0	491	9	0
65	Ac	743	0	797	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	Ad	890	0	938	13	0
67	Ae	1020	0	1090	8	0
68	Af	850	0	880	14	0
69	Ag	880	0	945	12	0
70	Ah	969	0	1078	18	0
71	Ai	771	0	849	15	0
72	Aj	681	0	687	13	0
73	Ak	612	0	682	17	0
74	Al	436	0	475	7	0
75	Am	417	0	459	13	0
76	An	233	0	283	9	0
77	Ao	847	0	914	18	0
78	Ap	694	0	738	14	0
79	tP	1606	0	816	23	0
80	tA	1628	0	827	26	0
81	MR	262	0	131	0	0
82	A1	10	0	19	1	0
83	A1	20	0	23	0	0
84	Ao	1	0	0	0	0
All	All	202314	0	149344	2779	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 8.

All (2779) 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)
76:An:1:MET:HE3	76:An:6:ARG:HD2	1.47	0.96
39:A3:52:G:H21	47:AJ:9:MET:HE1	1.31	0.94
34:B5:162:A:H3'	34:B5:163:G:H21	1.33	0.91
19:BD:64:ARG:HH22	21:BK:91:TYR:HB2	1.35	0.90
38:A1:162:G:N7	38:A1:259:C:N4	2.19	0.90
38:A1:1213:G:H4'	55:AS:90:MET:HG3	1.55	0.89
38:A1:1018:G:N2	38:A1:1019:G:O2'	2.06	0.89
58:AV:81:GLN:O	58:AV:98:ASN:ND2	2.07	0.88
45:AH:41:ILE:HD11	45:AH:67:ALA:HB1	1.54	0.87
6:BH:98:ILE:HD11	6:BH:121:VAL:HG21	1.58	0.85
5:BG:13:GLN:NE2	34:B5:151:G:N3	2.25	0.84
38:A1:538:G:H1	38:A1:553:U:H3	1.25	0.84
34:B5:849:C:OP2	54:AR:170:ARG:NH2	2.11	0.83
34:B5:1585:U:H3	34:B5:1611:A:H2	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:868:G:H1	34:B5:960:U:H3	1.28	0.82
2:BB:39:GLU:HG3	2:BB:40:ASN:H	1.45	0.82
7:BI:141:ARG:HD3	34:B5:190:C:H42	1.44	0.82
38:A1:1940:G:H21	38:A1:3362:A:H8	1.28	0.82
68:Af:54:ARG:HG2	68:Af:64:ILE:HG22	1.61	0.81
47:AJ:37:LEU:HD23	47:AJ:125:MET:HE2	1.61	0.81
4:BE:100:ARG:HG3	4:BE:114:ILE:HD13	1.63	0.81
20:BF:63:GLN:NE2	20:BF:66:GLN:OE1	2.13	0.81
34:B5:210:A:H62	34:B5:255:U:H3	1.27	0.81
34:B5:477:A:H61	34:B5:511:A:H61	1.26	0.81
5:BG:56:ASN:HD21	34:B5:153:G:H21	1.28	0.80
34:B5:1426:C:O2'	34:B5:1428:G:OP2	1.98	0.80
7:BI:39:GLY:HA2	7:BI:61:GLU:HG3	1.62	0.80
3:BC:237:VAL:HG13	3:BC:242:ILE:HD11	1.63	0.80
34:B5:1339:C:O2'	34:B5:1341:A:N7	2.15	0.79
38:A1:2138:A:HO2'	72:Aj:2:GLY:N	1.80	0.78
31:Bg:150:TRP:HB2	31:Bg:174:ASN:HD22	1.49	0.78
38:A1:284:A:OP2	77:Ao:41:ARG:NH1	2.17	0.78
18:Be:28:LYS:NZ	34:B5:477:A:OP2	2.18	0.77
37:AC:31:ARG:NH1	38:A1:674:G:OP1	2.17	0.77
54:AR:148:ASP:OD1	54:AR:151:ARG:NH1	2.18	0.77
52:AP:40:GLU:H	52:AP:43:LYS:HE3	1.50	0.76
12:BV:38:LYS:HD2	12:BV:49:GLU:HB3	1.68	0.76
34:B5:815:G:O4'	54:AR:162:ARG:NH1	2.19	0.76
42:AE:51:ARG:NH1	49:AM:114:ASP:OD2	2.18	0.76
34:B5:1584:G:N2	34:B5:1611:A:OP2	2.15	0.76
36:AB:372:THR:HG22	36:AB:374:ALA:H	1.49	0.75
13:BW:2:THR:N	34:B5:1034:C:HO2'	1.83	0.75
38:A1:3190:C:OP1	51:AO:172[A]:ARG:NH1	2.19	0.75
23:BQ:13:LYS:HG3	23:BQ:14:LYS:H	1.50	0.75
34:B5:1672:G:H2'	34:B5:1673:G:C8	2.22	0.75
38:A1:13:A:H4'	60:AX:39:LYS:HD3	1.69	0.75
34:B5:648:G:N1	34:B5:686:C:N3	2.29	0.74
46:AI:76:MET:HE1	46:AI:148:VAL:HA	1.70	0.74
34:B5:1690:G:O6	34:B5:1707:A:N6	2.21	0.74
53:AQ:182:LYS:NZ	63:Aa:55:LYS:O	2.20	0.74
19:BD:106:LYS:HG3	19:BD:175:VAL:HG22	1.70	0.74
35:AA:3:ARG:HH11	38:A1:911:C:H42	1.33	0.74
26:BT:69:LYS:HG2	34:B5:1367:G:H5''	1.70	0.74
38:A1:436:A:N1	38:A1:624:G:N2	2.36	0.74
32:Bf:104:SER:O	32:Bf:118:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:424:G:O2'	67:Ae:23:ASP:OD1	2.05	0.73
38:A1:241:G:HO2'	38:A1:242:C:H6	1.36	0.73
40:A4:75:G:OP2	61:AY:74:TYR:OH	2.06	0.73
79:tP:18:G:O2'	79:tP:57:G:N2	2.18	0.73
31:Bg:89:LEU:HB2	31:Bg:103:PHE:HB2	1.69	0.73
20:BF:124:LEU:O	28:BZ:58:ARG:NH2	2.21	0.73
58:AV:87:ARG:HH22	58:AV:137:VAL:HG21	1.53	0.73
34:B5:1669:U:H3	34:B5:1732:A:H62	1.37	0.73
38:A1:1311:G:N2	51:AO:86[A]:GLY:O	2.19	0.73
8:BJ:83:VAL:HA	8:BJ:149:ARG:HA	1.71	0.72
6:BH:11:GLN:NE2	6:BH:44:LYS:O	2.21	0.72
27:BU:101:LYS:O	27:BU:105:GLN:NE2	2.22	0.72
38:A1:1018:G:N2	38:A1:1019:G:HO2'	1.88	0.72
14:BX:70:LYS:NZ	34:B5:567:A:OP1	2.23	0.72
47:AJ:54:VAL:O	47:AJ:55:ARG:HG3	1.90	0.71
70:Ah:102:GLU:HB2	70:Ah:105:ARG:HH21	1.53	0.71
34:B5:871:G:H2'	34:B5:872:G:C8	2.26	0.71
27:BU:58:LEU:HD12	27:BU:88:LYS:HD2	1.70	0.71
46:AI:36:LEU:HD11	46:AI:69:ARG:HH11	1.55	0.71
34:B5:648:G:N2	34:B5:686:C:O2	2.15	0.71
23:BQ:14:LYS:NZ	34:B5:1610:G:N7	2.37	0.71
34:B5:1356:U:H3	34:B5:1367:G:H1	1.39	0.70
36:AB:240:ARG:NH2	38:A1:1907:C:O2	2.25	0.70
80:tA:16:U:H3	80:tA:59:A:H62	1.38	0.70
38:A1:1233:G:O2'	38:A1:1245:A:N1	2.23	0.70
35:AA:80:GLU:HG3	78:Ap:66:GLY:HA2	1.74	0.70
31:Bg:270:LEU:HD21	31:Bg:273:ASP:HB2	1.73	0.70
2:BB:152:ARG:NH2	34:B5:1799:U:O3'	2.22	0.70
5:BG:2:LYS:HB3	5:BG:108:VAL:HG22	1.74	0.69
37:AC:20:LEU:HD11	37:AC:252:GLU:HG3	1.73	0.69
5:BG:154:ARG:NH2	34:B5:75:U:O4	2.25	0.69
21:BK:24:LYS:O	21:BK:39:ASN:ND2	2.25	0.69
80:tA:30:G:H1	80:tA:40:C:H5	1.41	0.69
50:AN:183:THR:HG22	50:AN:187:ARG:HB3	1.73	0.69
11:BO:38:THR:HG21	34:B5:895:G:H21	1.57	0.69
5:BG:164:LYS:NZ	34:B5:71:A:OP2	2.25	0.69
15:BY:124:ARG:NH1	34:B5:151:G:O6	2.25	0.69
34:B5:1213:G:H1	34:B5:1450:U:H5	1.41	0.69
34:B5:1575:G7M:O2'	34:B5:1576:A:O4'	2.10	0.69
38:A1:1814:A:H1'	38:A1:1817:G:H21	1.58	0.69
38:A1:1953:G:H1'	38:A1:1954:G:H3'	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3118:C:O3'	75:Am:106:ARG:NH2	2.24	0.69
78:Ap:86:LEU:HD22	78:Ap:89:MET:HE2	1.75	0.69
4:BE:64:ILE:HD11	15:BY:18:LEU:HD12	1.75	0.69
38:A1:1017:C:H42	38:A1:1034:U:H3	1.38	0.68
38:A1:3034:C:H5	45:AH:121:LYS:H	1.40	0.68
36:AB:244:ARG:NH1	38:A1:2948:C:OP1	2.24	0.68
38:A1:170:G:N1	38:A1:250:U:O2	2.27	0.68
1:BA:107:PHE:HB2	1:BA:135:GLU:HG2	1.76	0.68
3:BC:161:LYS:NZ	34:B5:1086:A:OP2	2.26	0.68
38:A1:1352:A:H2	38:A1:1355:A:H62	1.41	0.68
46:AI:211:ARG:HE	46:AI:212:GLU:HG2	1.58	0.68
55:AS:48:LEU:HD11	56:AT:151:LEU:HD13	1.75	0.68
6:BH:113:PRO:HG2	6:BH:116:ARG:HD3	1.75	0.68
33:BM:105:LYS:H	33:BM:112:ALA:HB2	1.59	0.68
4:BE:179:LYS:NZ	4:BE:230:GLU:OE1	2.25	0.68
24:BR:25:THR:HG23	24:BR:27:ASP:H	1.57	0.68
37:AC:11:LEU:HD21	37:AC:156:LEU:HB2	1.76	0.68
38:A1:776:PSU:H4'	64:Ab:40:ARG:NH2	2.08	0.68
7:BI:16:ALA:HB2	34:B5:354:C:H5''	1.76	0.68
34:B5:924:A:H2'	34:B5:925:G:C8	2.29	0.68
38:A1:776:PSU:H4'	64:Ab:40:ARG:HH22	1.58	0.68
76:An:1:MET:HE3	76:An:6:ARG:CD	2.24	0.67
34:B5:591:A:H2'	34:B5:592:A:C8	2.29	0.67
38:A1:3092:C:O2'	38:A1:3094:A:OP2	2.10	0.67
48:AL:165:SER:H	63:Aa:139:ARG:HH22	1.42	0.67
22:BP:75:PRO:HB3	22:BP:104:GLN:HE22	1.60	0.67
34:B5:1588:G:H1	34:B5:1608:U:H3	1.41	0.67
38:A1:1348:U:OP1	53:AQ:39:ARG:NH1	2.27	0.67
7:BI:81:VAL:HG12	7:BI:102:VAL:HG12	1.76	0.67
38:A1:900:G:H1'	38:A1:1589:A:N6	2.10	0.67
5:BG:26:VAL:O	5:BG:30:LYS:NZ	2.24	0.67
21:BK:11:ILE:HD13	21:BK:35:ILE:HG21	1.76	0.67
38:A1:1661:G:H2'	38:A1:1662:G:C8	2.30	0.67
74:Al:9:ILE:HG22	74:Al:13:MET:HE2	1.77	0.67
2:BB:61:LEU:HD21	2:BB:96:LEU:HD11	1.78	0.66
7:BI:101:ILE:HD12	7:BI:184:LEU:HD11	1.77	0.66
5:BG:56:ASN:ND2	34:B5:153:G:H21	1.93	0.66
34:B5:1458:G:O2'	34:B5:1459:C:OP1	2.12	0.66
38:A1:2213:A:H2'	38:A1:2214:A:C8	2.30	0.66
55:AS:8:GLN:HB3	55:AS:64:ILE:HD11	1.76	0.66
4:BE:129:VAL:HG22	4:BE:139:VAL:HG12	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:65:A:H2	34:B5:84:A:H62	1.43	0.66
38:A1:241:G:H5'	38:A1:241:G:C8	2.30	0.66
1:BA:136:ALA:HB1	1:BA:141:ILE:HB	1.76	0.66
26:BT:119:LYS:NZ	34:B5:1368:G:OP1	2.26	0.66
32:Bf:141:CYS:O	34:B5:1252:C:O2'	2.14	0.66
33:BM:96:GLN:HE21	33:BM:100:TRP:NE1	1.94	0.66
21:BK:12:HIS:HB3	21:BK:80:LEU:HD11	1.78	0.66
34:B5:499:U:O2'	34:B5:501:U:O4	2.13	0.66
38:A1:1062:A:O2'	38:A1:1098:A:OP1	2.12	0.66
41:AD:50:ARG:NH1	41:AD:147:ASP:OD2	2.26	0.66
7:BI:39:GLY:O	7:BI:59:ARG:HB3	1.96	0.66
33:BM:23:THR:HG21	33:BM:26:ASP:HB2	1.78	0.66
38:A1:173:G:H1	38:A1:244:G:H1	1.43	0.66
37:AC:157:GLU:OE2	37:AC:211:GLU:N	2.24	0.65
41:AD:260:PHE:HA	41:AD:264:GLN:HE21	1.60	0.65
4:BE:106:LYS:NZ	34:B5:788:A:OP1	2.25	0.65
24:BR:2:GLY:N	34:B5:1414:U:OP1	2.29	0.65
38:A1:2895:G:O2'	75:Am:100:TYR:O	2.15	0.65
40:A4:63:G:O2'	70:Ah:49:LYS:NZ	2.25	0.65
34:B5:702:G:O2'	34:B5:703:G:O5'	2.14	0.65
38:A1:2205:U:H2'	38:A1:2206:G:C8	2.31	0.65
4:BE:38:LEU:HD22	34:B5:298:C:H5''	1.78	0.65
66:Ad:55:LEU:HB2	66:Ad:95:PRO:HD3	1.78	0.65
5:BG:136:LYS:NZ	5:BG:174:LYS:O	2.26	0.65
21:BK:15:LEU:HG	21:BK:68:LEU:HD12	1.77	0.65
38:A1:2945:G:O2'	38:A1:2948:C:OP2	2.14	0.65
34:B5:513:U:H2'	34:B5:514:G:C8	2.32	0.65
34:B5:1171:A:H2'	34:B5:1172:G:C8	2.32	0.65
38:A1:1149:G:OP2	68:Af:21:ARG:NH2	2.29	0.65
73:Ak:58:ASP:HB3	73:Ak:61:LYS:HG2	1.79	0.65
2:BB:146:GLN:NE2	34:B5:1065:A:N3	2.43	0.65
8:BJ:145:SER:OG	34:B5:474:A:OP1	2.11	0.65
23:BQ:12:LYS:NZ	34:B5:1380:U:OP1	2.28	0.65
34:B5:472:U:O2'	34:B5:769:A:N3	2.26	0.65
34:B5:1474:G:H2'	34:B5:1475:A:H8	1.62	0.65
36:AB:284:ARG:NH1	36:AB:293:ASN:O	2.30	0.65
38:A1:3169:U:H2'	38:A1:3170:A:C8	2.31	0.65
45:AH:8:GLN:HB3	45:AH:72:LYS:HD2	1.78	0.65
49:AM:48:GLY:HA3	49:AM:53:VAL:HB	1.79	0.65
3:BC:116:LYS:HG2	3:BC:127:ALA:HB3	1.76	0.65
7:BI:152:ILE:HG13	7:BI:153:GLU:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BJ:87:SER:OG	8:BJ:89:ASP:OD1	2.11	0.64
1:BA:140:ASN:ND2	12:BV:31:SER:O	2.24	0.64
6:BH:104:ARG:NH1	34:B5:803:A:N3	2.44	0.64
8:BJ:126:ARG:HD3	18:Be:33:ARG:HD3	1.79	0.64
10:BN:115:LEU:O	10:BN:119:GLU:HG2	1.96	0.64
34:B5:823:G:O6	34:B5:849:C:O2'	2.15	0.64
38:A1:2679:A:HO2'	47:AJ:52:TYR:HH	1.45	0.64
45:AH:92:TYR:HB2	45:AH:142:ASP:HB3	1.79	0.64
44:AG:189:LEU:HD12	44:AG:190:VAL:HG13	1.78	0.64
69:Ag:16:ARG:HG2	69:Ag:37:LYS:HD3	1.77	0.64
33:BM:67:THR:HG22	34:B5:1228:G:H1	1.63	0.64
2:BB:48:VAL:HG13	2:BB:49:ASN:H	1.62	0.64
6:BH:8:ILE:HA	6:BH:42:GLN:HG3	1.80	0.64
13:BW:53:ILE:HD13	17:Bb:24:LEU:HD11	1.79	0.64
38:A1:2898:G:OP2	45:AH:173:ARG:NH2	2.29	0.64
41:AD:34:LYS:HA	56:AT:27:LEU:HD11	1.79	0.64
50:AN:159:ARG:HB2	50:AN:164:LEU:HB2	1.79	0.64
51:AO:61[A]:ALA:HA	51:AO:70[A]:PRO:HD2	1.80	0.64
62:AZ:103:GLN:NE2	62:AZ:106:GLN:OE1	2.31	0.64
13:BW:19:LYS:NZ	34:B5:1095:U:O2'	2.29	0.64
8:BJ:85:VAL:HG22	8:BJ:99:LEU:HD11	1.80	0.64
20:BF:189:THR:HB	20:BF:192:GLU:HG3	1.79	0.64
24:BR:70:SER:HB2	24:BR:75:GLU:OE1	1.98	0.64
38:A1:664:U:H2'	38:A1:665:A:C8	2.33	0.64
53:AQ:170:ARG:NH1	63:Aa:56:VAL:O	2.29	0.64
31:Bg:23:LEU:HD12	31:Bg:33:LEU:HD11	1.79	0.64
31:Bg:159:ASN:HD21	31:Bg:165:ASP:H	1.43	0.64
34:B5:700:C:O2'	34:B5:740:A:N6	2.31	0.64
13:BW:88:LYS:NZ	34:B5:371:G:O3'	2.30	0.63
41:AD:50:ARG:NH2	41:AD:72:ASP:OD2	2.31	0.63
57:AU:19:VAL:HG12	57:AU:105:LEU:HD13	1.79	0.63
19:BD:55:THR:HA	19:BD:58:VAL:HG12	1.79	0.63
34:B5:205:U:H2'	34:B5:206:A:H8	1.63	0.63
38:A1:1246:G:N2	38:A1:1272:C:O2	2.31	0.63
45:AH:173:ARG:HG3	75:Am:127:LEU:HD11	1.80	0.63
45:AH:173:ARG:NH1	75:Am:125:LYS:O	2.31	0.63
23:BQ:22:VAL:HG22	23:BQ:65:ILE:HG12	1.80	0.63
38:A1:269:G:H5''	50:AN:14:LYS:HE2	1.80	0.63
38:A1:786:A:H4'	38:A1:787:G:H5'	1.80	0.63
38:A1:1307:G:H4'	38:A1:1308:A:H5'	1.80	0.63
34:B5:848:C:OP1	54:AR:166:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:674:G:O6	53:AQ:56:LYS:NZ	2.32	0.63
42:AE:34:LEU:HD21	42:AE:63:LEU:HD21	1.80	0.63
34:B5:381:C:O2'	34:B5:755:A:N1	2.27	0.63
38:A1:543:C:HO2'	38:A1:548:G:H1	1.45	0.63
44:AG:245:LYS:HE3	44:AG:249:ARG:HH21	1.63	0.63
5:BG:135:PRO:HB2	5:BG:141:ILE:HG13	1.81	0.63
75:Am:106:ARG:HD3	75:Am:106:ARG:H	1.63	0.63
4:BE:92:LEU:HD21	15:BY:17:LEU:HD21	1.81	0.63
34:B5:1592:A:H2'	34:B5:1593:A:H8	1.64	0.63
5:BG:10:ASN:ND2	5:BG:127:THR:O	2.32	0.62
28:BZ:82:HIS:O	28:BZ:85:LYS:HG2	1.99	0.62
34:B5:162:A:H3'	34:B5:163:G:N2	2.11	0.62
34:B5:1017:U:H2'	34:B5:1018:U:O2	1.98	0.62
38:A1:129:U:H2'	38:A1:130:A:C8	2.34	0.62
29:Bc:8:THR:HB	29:Bc:56:LEU:HB2	1.81	0.62
37:AC:35:VAL:HG21	37:AC:244:LEU:HD21	1.80	0.62
38:A1:662:U:H2'	38:A1:663:C:C6	2.34	0.62
39:A3:101:G:N7	55:AS:52:LYS:NZ	2.44	0.62
47:AJ:20:ASN:OD1	47:AJ:126:ASP:HB3	1.98	0.62
50:AN:46:ASP:OD1	50:AN:47:LYS:N	2.32	0.62
34:B5:894:U:H2'	34:B5:895:G:C8	2.34	0.62
38:A1:1018:G:H2'	38:A1:1019:G:H4'	1.80	0.62
27:BU:97:VAL:HA	27:BU:100:VAL:HG12	1.80	0.62
34:B5:1474:G:H2'	34:B5:1475:A:C8	2.33	0.62
35:AA:195:SER:O	35:AA:198:LYS:NZ	2.32	0.62
19:BD:42:THR:OG1	19:BD:45:LYS:O	2.12	0.62
22:BP:86:VAL:HG22	22:BP:89:MET:HE2	1.80	0.62
38:A1:551:A:O2'	38:A1:552:G:O5'	2.14	0.62
38:A1:1390:A:N6	38:A1:1418:A:O2'	2.32	0.62
79:tP:23:C:H3'	79:tP:24:G:H8	1.65	0.62
11:BO:72:LYS:O	11:BO:73:GLU:HG3	1.99	0.62
34:B5:1229:G:N2	34:B5:1255:G:O2'	2.32	0.62
34:B5:1591:C:H2'	34:B5:1592:A:H8	1.63	0.62
38:A1:38:U:H4'	63:Aa:32:ARG:HD2	1.80	0.62
23:BQ:95:LYS:NZ	23:BQ:96:TYR:OH	2.33	0.62
34:B5:12:U:H2'	34:B5:13:C:C6	2.35	0.62
34:B5:590:C:H2'	34:B5:591:A:H8	1.64	0.62
35:AA:21:ARG:HD3	38:A1:824:C:H5''	1.82	0.62
38:A1:1724:U:H1'	38:A1:1725:C:C6	2.35	0.62
55:AS:77:VAL:HG11	55:AS:106:LEU:HD22	1.81	0.62
62:AZ:33:SER:OG	62:AZ:35:SER:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:116:HIS:HD2	7:BI:117:TYR:CD1	2.18	0.62
47:AJ:91:LEU:HD22	47:AJ:95:ASN:HD22	1.65	0.62
59:AW:52:THR:HG22	59:AW:54:LEU:H	1.64	0.62
73:Ak:32:ASN:OD1	73:Ak:35:GLY:N	2.30	0.62
75:Am:79:GLU:HG3	75:Am:82:LEU:HD12	1.80	0.62
28:BZ:97:LYS:NZ	34:B5:1531:G:O6	2.30	0.62
31:Bg:249:ARG:HG3	31:Bg:251:TRP:CD1	2.35	0.62
42:AE:70:LYS:HB3	42:AE:146:ILE:HD11	1.82	0.62
38:A1:538:G:N2	38:A1:553:U:O2	2.27	0.61
38:A1:2767:U:O2'	77:Ao:30:ALA:O	2.16	0.61
46:AI:102:MET:HB3	46:AI:112:GLN:HE22	1.65	0.61
18:Be:37:ARG:NH1	34:B5:478:A:OP1	2.33	0.61
26:BT:130:ARG:HG2	26:BT:134:ARG:NH1	2.15	0.61
34:B5:1735:U:OP1	58:AV:32:ARG:NH2	2.33	0.61
57:AU:43:VAL:HG12	57:AU:44:GLU:OE2	2.00	0.61
76:An:1:MET:HE1	76:An:9:ARG:HD3	1.82	0.61
7:BI:54:LYS:NZ	34:B5:333:A:OP2	2.30	0.61
23:BQ:50:GLU:OE1	23:BQ:82:ARG:NH2	2.31	0.61
29:Bc:17:GLY:HA3	29:Bc:67:ARG:HE	1.65	0.61
36:AB:124:LYS:NZ	38:A1:3297:U:O4	2.33	0.61
38:A1:2222:A:H2'	38:A1:2223:A:C8	2.36	0.61
39:A3:64:A:N7	46:AI:209:ASN:ND2	2.47	0.61
12:BV:74:GLN:HG3	12:BV:83:TRP:HB3	1.82	0.61
13:BW:107:SER:HA	34:B5:804:A:C8	2.36	0.61
45:AH:9:GLN:CG	45:AH:52:LEU:HD11	2.31	0.61
56:AT:39:ILE:HD12	56:AT:102:ARG:HD3	1.82	0.61
31:Bg:172:ALA:HB2	31:Bg:202:LEU:HD23	1.81	0.61
62:AZ:101:PHE:HA	62:AZ:107:ARG:HE	1.66	0.61
8:BJ:93:LEU:HA	8:BJ:96:VAL:HG12	1.82	0.61
19:BD:93:ASP:HB2	19:BD:96:LEU:HD13	1.83	0.61
41:AD:119:TYR:OH	41:AD:139:PRO:O	2.17	0.61
47:AJ:112:LEU:HD21	47:AJ:127:PHE:HZ	1.66	0.61
38:A1:363:G:OP2	72:Aj:56:ARG:NH2	2.26	0.61
38:A1:1203:A:H2'	38:A1:1204:A:C8	2.35	0.61
42:AE:71:VAL:HG12	42:AE:156:LYS:HG3	1.82	0.61
48:AL:124:ILE:HD11	70:Ah:119:LYS:HD3	1.82	0.61
10:BN:33:VAL:HG21	10:BN:66:ILE:HG21	1.83	0.60
15:BY:13:ILE:HG22	15:BY:22:GLN:HG3	1.83	0.60
38:A1:543:C:O2'	38:A1:548:G:N1	2.33	0.60
42:AE:30:LEU:HD22	42:AE:34:LEU:HD23	1.82	0.60
48:AL:119:TYR:HA	48:AL:122:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:79:ARG:O	1:BA:83:GLN:HG3	2.00	0.60
38:A1:1019:G:H2'	38:A1:1020:G:H2'	1.82	0.60
38:A1:1831:U:O2'	40:A4:114:G:OP1	2.18	0.60
38:A1:2545:C:H2'	38:A1:2546:C:C6	2.36	0.60
8:BJ:57:ARG:O	8:BJ:61:THR:HG23	2.01	0.60
34:B5:58:U:O2'	34:B5:451:A:N3	2.34	0.60
34:B5:486:G:H1	34:B5:501:U:H3	1.48	0.60
34:B5:1071:U:H2'	34:B5:1072:C:C6	2.36	0.60
34:B5:1081:A:O2'	34:B5:1083:G:N7	2.24	0.60
16:Ba:8:ASN:HB3	34:B5:1791:A:H3'	1.84	0.60
25:BS:8:GLN:HG3	25:BS:9:GLY:H	1.67	0.60
34:B5:1297:G:N2	34:B5:1300:A:OP2	2.28	0.60
38:A1:3100:U:O2'	38:A1:3101:G:O5'	2.19	0.60
57:AU:12:ALA:HB2	57:AU:68:THR:HG22	1.83	0.60
66:Ad:7:VAL:HG22	66:Ad:78:LYS:HA	1.83	0.60
28:BZ:56:THR:O	28:BZ:103:ARG:NH2	2.34	0.60
36:AB:128:LYS:NZ	38:A1:3294:A:OP1	2.33	0.60
38:A1:1694:U:H5	38:A1:1752:A:N1	2.00	0.60
38:A1:2228:A:H2'	38:A1:2229:A:C8	2.36	0.60
49:AM:92:GLU:N	49:AM:92:GLU:OE2	2.32	0.60
19:BD:75:LYS:HB3	21:BK:22:VAL:HG21	1.84	0.60
31:Bg:22:SER:HB2	31:Bg:36:ALA:HB3	1.82	0.60
38:A1:2699:G:H5''	56:AT:16:GLN:NE2	2.16	0.60
70:Ah:31:LEU:HD11	70:Ah:43:LYS:HD3	1.83	0.60
75:Am:99:CYS:HB2	75:Am:114:LYS:HE3	1.82	0.60
1:BA:112:THR:HG22	1:BA:114:SER:H	1.66	0.60
24:BR:14:LYS:HG2	24:BR:69:ILE:HD11	1.84	0.60
55:AS:22:PRO:O	56:AT:146:ASN:ND2	2.29	0.60
62:AZ:97:SER:O	62:AZ:100:THR:HG22	2.01	0.60
2:BB:145:LYS:NZ	2:BB:151:LYS:O	2.34	0.60
9:BL:101:GLU:OE1	14:BX:16:ARG:NH1	2.34	0.60
10:BN:16:ILE:O	13:BW:57:ARG:NH2	2.35	0.60
18:Be:33:ARG:NH2	34:B5:477:A:O2'	2.35	0.60
27:BU:99:ILE:HA	27:BU:102:ARG:HG2	1.84	0.60
34:B5:1591:C:H2'	34:B5:1592:A:C8	2.37	0.60
37:AC:318:LEU:H	37:AC:324:LEU:HD12	1.66	0.60
38:A1:1635:G:N2	38:A1:1638:A:OP2	2.30	0.60
40:A4:88:A:O2'	40:A4:89:A:OP1	2.17	0.60
38:A1:1156:C:OP2	43:AF:94:LYS:NZ	2.34	0.60
5:BG:119:GLN:HG3	5:BG:120:GLU:H	1.67	0.60
5:BG:160:ARG:NH1	34:B5:66:U:O2	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ba:18:VAL:O	16:Ba:19:LYS:HG2	2.01	0.60
38:A1:1139:G:OP2	64:Ab:14:ARG:NH2	2.34	0.60
38:A1:1267:U:O4	38:A1:1274:A:O2'	2.20	0.60
49:AM:44:VAL:HG13	49:AM:60:LEU:HD21	1.82	0.60
38:A1:728:G:H5''	53:AQ:43:PRO:HB2	1.83	0.59
38:A1:1281:G:O6	38:A1:1282:G:O6	2.20	0.59
15:BY:10:ARG:HB2	15:BY:24:VAL:HG13	1.84	0.59
38:A1:2282:U:OP1	38:A1:2973:G:O2'	2.18	0.59
38:A1:2369:G:H2'	38:A1:2370:G:C8	2.37	0.59
38:A1:3295:A:H2'	38:A1:3296:A:C8	2.37	0.59
43:AF:138:TYR:CD2	43:AF:233:GLU:HB2	2.37	0.59
47:AJ:60:ARG:N	47:AJ:63:GLU:OE1	2.31	0.59
53:AQ:79:LYS:HG2	53:AQ:136:ASN:OD1	2.02	0.59
47:AJ:48:SER:HB2	47:AJ:66:ALA:HB3	1.84	0.59
7:BI:48:THR:OG1	7:BI:52:ASN:O	2.18	0.59
13:BW:15:ASN:ND2	13:BW:72:CYS:O	2.23	0.59
24:BR:31:ASN:HD22	24:BR:55:THR:HB	1.66	0.59
34:B5:1358:G:H2'	34:B5:1359:C:C6	2.37	0.59
34:B5:1449:U:H2'	34:B5:1450:U:O2	2.02	0.59
38:A1:370:U:H4'	38:A1:404:G:H5'	1.85	0.59
38:A1:1717:U:H2'	38:A1:1718:G:C8	2.36	0.59
40:A4:150:G:OP1	60:AX:27:ARG:NH2	2.36	0.59
5:BG:219:ARG:HA	5:BG:222:GLU:HG2	1.84	0.59
11:BO:121:VAL:O	34:B5:886:U:O2'	2.19	0.59
19:BD:105:MET:HB2	19:BD:122:VAL:HG21	1.83	0.59
25:BS:23:ASP:OD1	25:BS:24:GLY:N	2.34	0.59
38:A1:3288:G:O2'	38:A1:3289:G:O5'	2.19	0.59
68:Af:14:LEU:HD11	68:Af:31:LYS:HB2	1.83	0.59
17:Bb:67:THR:OG1	17:Bb:70:LYS:O	2.18	0.59
22:BP:111:MET:HG3	25:BS:119:ILE:HD11	1.85	0.59
38:A1:1281:G:C6	38:A1:1282:G:O6	2.54	0.59
11:BO:80:HIS:HA	11:BO:113:GLY:O	2.03	0.59
33:BM:59:LEU:O	33:BM:122:VAL:HA	2.02	0.59
38:A1:238:A:H3'	38:A1:239:G:C8	2.37	0.59
38:A1:1786:G:H2'	38:A1:1787:A:C8	2.37	0.59
39:A3:23:A:H2'	39:A3:24:A:C8	2.38	0.59
6:BH:81:LEU:HD22	6:BH:90:VAL:HB	1.84	0.59
34:B5:406:U:H2'	34:B5:407:A:H8	1.68	0.59
58:AV:135:VAL:HG11	59:AW:26:SER:HB3	1.84	0.59
65:Ac:97:ASP:OD1	65:Ac:97:ASP:N	2.36	0.59
1:BA:30:GLN:HE22	1:BA:32:HIS:HB2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:125:LYS:HB2	4:BE:226:PHE:CD1	2.38	0.59
36:AB:220:VAL:O	36:AB:334:ARG:NH1	2.36	0.59
65:Ac:32:LYS:O	65:Ac:36:GLN:HG3	2.02	0.59
4:BE:3:ARG:HB3	34:B5:93:A:H1'	1.85	0.59
6:BH:30:SER:O	6:BH:34:LEU:N	2.36	0.59
10:BN:64:ARG:NH2	34:B5:861:U:OP1	2.26	0.59
19:BD:31:GLU:HG3	19:BD:107:PHE:HE2	1.67	0.58
34:B5:119:A:H1'	34:B5:397:A:C4	2.38	0.58
34:B5:939:A:H2'	34:B5:940:A:C8	2.38	0.58
35:AA:215:ASN:ND2	38:A1:2969:A:N7	2.51	0.58
38:A1:176:G:H2'	38:A1:177:U:O4'	2.03	0.58
38:A1:241:G:H5'	38:A1:241:G:H8	1.67	0.58
38:A1:1280:C:H2'	38:A1:1281:G:C8	2.38	0.58
38:A1:2768:U:H2'	38:A1:2769:A:H8	1.68	0.58
78:Ap:6:LYS:HE3	78:Ap:7:LYS:HE3	1.85	0.58
2:BB:137:ILE:HD13	2:BB:215:VAL:HG22	1.84	0.58
4:BE:104:ASP:HB3	4:BE:110:ALA:HB2	1.85	0.58
4:BE:238:LEU:HD22	4:BE:242:LYS:HG3	1.85	0.58
6:BH:50:ASP:HA	6:BH:56:LYS:HG2	1.85	0.58
34:B5:473:A:H5'	34:B5:769:A:H1'	1.86	0.58
55:AS:152:LEU:HB2	55:AS:172:TYR:CE2	2.38	0.58
70:Ah:83:LYS:O	72:Aj:73:ARG:NH2	2.36	0.58
21:BK:70:GLU:HA	21:BK:73:VAL:HG23	1.85	0.58
38:A1:1110:PSU:H2'	38:A1:1111:U:C6	2.38	0.58
38:A1:1798:A:H2'	38:A1:1799:A:C8	2.39	0.58
42:AE:51:ARG:O	42:AE:72:ASN:ND2	2.37	0.58
47:AJ:61:ARG:NH2	79:tP:56:C:O4'	2.36	0.58
27:BU:63:LEU:O	27:BU:83:GLU:HA	2.02	0.58
31:Bg:93:ASP:HB2	31:Bg:100:TYR:HE1	1.69	0.58
34:B5:590:C:H2'	34:B5:591:A:C8	2.38	0.58
37:AC:227:THR:HG23	38:A1:689:U:H3	1.69	0.58
49:AM:24:LYS:HE2	49:AM:25:LYS:HE2	1.85	0.58
19:BD:32:GLU:OE2	19:BD:65:ARG:NH1	2.36	0.58
63:Aa:24:LYS:O	63:Aa:26:ARG:HG2	2.03	0.58
2:BB:108:ASP:OD1	2:BB:109:LYS:N	2.37	0.58
38:A1:2376:G:H2'	38:A1:2377:G:C8	2.39	0.58
1:BA:69:ASN:ND2	1:BA:71:GLU:OE2	2.29	0.58
2:BB:117:TRP:CZ3	34:B5:1799:U:H5'	2.39	0.58
11:BO:47:LYS:NZ	11:BO:66:ASP:OD2	2.27	0.58
46:AI:30:LYS:HG3	46:AI:63:GLU:HG3	1.84	0.58
46:AI:52:LEU:HB3	46:AI:136:PHE:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ae:96:ILE:HG21	67:Ae:105:ARG:HG2	1.85	0.58
8:BJ:107:ARG:NH1	8:BJ:153:GLU:OE2	2.34	0.58
22:BP:75:PRO:HA	22:BP:93:VAL:HG13	1.86	0.58
47:AJ:92:ARG:HG2	47:AJ:94:ARG:H	1.69	0.58
52:AP:67:ILE:HD11	52:AP:80:LYS:HB3	1.86	0.58
1:BA:15:GLN:HG3	24:BR:117:LEU:HD22	1.84	0.58
4:BE:49:ARG:NH1	34:B5:447:U:OP1	2.37	0.58
12:BV:36:VAL:HB	12:BV:51:VAL:HG23	1.84	0.58
30:Bd:16:LYS:NZ	34:B5:1596:C:OP1	2.36	0.58
34:B5:319:U:H4'	34:B5:323:A:C8	2.39	0.58
45:AH:9:GLN:HG3	45:AH:52:LEU:HD11	1.86	0.58
7:BI:178:ARG:NH1	34:B5:207:U:O2	2.35	0.58
19:BD:23:GLU:OE1	21:BK:61:TRP:NE1	2.32	0.58
19:BD:127:MET:HE3	19:BD:154:ASP:HB3	1.86	0.58
44:AG:78:PHE:O	44:AG:79:GLN:HG3	2.03	0.58
45:AH:80:THR:HG23	45:AH:84:LYS:HE3	1.85	0.58
68:Af:31:LYS:NZ	68:Af:78:SER:O	2.37	0.58
16:Ba:3:LYS:NZ	16:Ba:8:ASN:OD1	2.37	0.57
19:BD:46:THR:HG23	19:BD:84:ILE:HD12	1.86	0.57
26:BT:122:ARG:NH1	34:B5:1499:G:OP1	2.36	0.57
4:BE:89:VAL:HG22	4:BE:100:ARG:HG2	1.84	0.57
24:BR:107:SER:O	24:BR:111:LYS:HG2	2.05	0.57
31:Bg:221:MET:CB	31:Bg:223:TRP:HE1	2.17	0.57
34:B5:814:A:H2'	54:AR:167:ARG:HD3	1.86	0.57
38:A1:1553:U:H4'	38:A1:1554:U:H5'	1.86	0.57
4:BE:105:VAL:HG22	4:BE:243:GLY:HA2	1.86	0.57
10:BN:3:ARG:HB3	10:BN:6:SER:HB3	1.87	0.57
44:AG:115:ALA:O	44:AG:120:LYS:N	2.36	0.57
61:AY:74:TYR:CE2	61:AY:77:LYS:HD2	2.39	0.57
8:BJ:139:GLN:NE2	15:BY:64:PHE:O	2.34	0.57
25:BS:2:SER:HB2	28:BZ:78:ILE:HG23	1.86	0.57
34:B5:509:G:H2'	34:B5:510:G:C8	2.40	0.57
44:AG:52:TRP:O	44:AG:57:ARG:NH1	2.37	0.57
63:Aa:36:GLY:HA3	63:Aa:40:HIS:CE1	2.39	0.57
79:tP:19:G:N2	79:tP:56:C:O2'	2.37	0.57
31:Bg:102:ARG:NH1	34:B5:1342:C:OP1	2.33	0.57
34:B5:182:A:H2'	34:B5:183:U:C6	2.39	0.57
40:A4:9:A:H2'	40:A4:10:A:C8	2.40	0.57
47:AJ:109:HIS:CD2	47:AJ:123:PHE:H	2.21	0.57
73:Ak:71:PRO:HD2	73:Ak:72:THR:H	1.69	0.57
79:tP:53:G:H2'	79:tP:54:A:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:104:ILE:HG13	7:BI:105:ASP:H	1.70	0.57
8:BJ:63:ASP:O	8:BJ:69:ARG:HD3	2.03	0.57
34:B5:108:A:H2'	34:B5:109:G:C8	2.40	0.57
34:B5:1477:G:H2'	34:B5:1478:G:C8	2.39	0.57
38:A1:1248:C:H4'	38:A1:1266:G:H5'	1.86	0.57
44:AG:104:GLU:HA	44:AG:107:GLU:HG2	1.84	0.57
45:AH:20:ILE:HG12	45:AH:25:VAL:HG22	1.87	0.57
62:AZ:22:LYS:NZ	62:AZ:129:TRP:O	2.34	0.57
67:Ae:3:SER:HB3	67:Ae:71:HIS:CE1	2.39	0.57
80:tA:14:A:H2'	80:tA:15:G:H4'	1.86	0.57
2:BB:35:PRO:HB2	2:BB:37:THR:HG22	1.86	0.57
5:BG:121:LEU:H	5:BG:125:THR:HG1	1.50	0.57
11:BO:102:LEU:HG	16:Ba:53:LEU:HD21	1.87	0.57
31:Bg:221:MET:HB3	31:Bg:223:TRP:HE1	1.70	0.57
34:B5:800:U:H2'	34:B5:801:G:C8	2.40	0.57
56:AT:14:MET:HE1	56:AT:55:LYS:HB2	1.86	0.57
4:BE:187:ARG:HH22	34:B5:753:A:H8	1.52	0.57
6:BH:64:VAL:HB	6:BH:94:ALA:HB1	1.86	0.57
7:BI:178:ARG:NH1	34:B5:258:C:O2	2.37	0.57
15:BY:13:ILE:HG22	15:BY:22:GLN:HE21	1.68	0.57
38:A1:1255:C:N4	38:A1:1262:G:OP2	2.38	0.57
38:A1:2816:G:N2	38:A1:2819:A:OP2	2.37	0.57
60:AX:47:ALA:HB3	60:AX:50:ALA:HB2	1.87	0.57
69:Ag:91:ARG:O	69:Ag:95:ILE:HG12	2.04	0.57
34:B5:1483:A:H2'	34:B5:1484:G:C8	2.40	0.57
38:A1:1193:A:OP1	51:AO:49[A]:ARG:NH2	2.37	0.57
38:A1:1268:G:H21	38:A1:1273:A:H61	1.52	0.57
41:AD:60:ILE:HD11	41:AD:93:THR:HA	1.86	0.57
33:BM:23:THR:H	33:BM:135:MET:HE1	1.69	0.57
38:A1:655:C:H2'	38:A1:656:A:H8	1.69	0.57
38:A1:2697:A:H2'	38:A1:2698:G:C8	2.40	0.57
45:AH:128:VAL:HA	45:AH:157:ASN:HD21	1.69	0.57
5:BG:202:ARG:NH1	34:B5:127:G:N7	2.49	0.56
5:BG:65:GLN:HE21	34:B5:1682:U:H4'	1.70	0.56
7:BI:168:CYS:HB2	7:BI:184:LEU:HD21	1.87	0.56
19:BD:70:THR:HG22	19:BD:86:LEU:HB2	1.87	0.56
39:A3:28:C:OP1	47:AJ:137:ARG:NH1	2.38	0.56
46:AI:28:ASP:HB3	46:AI:32:ARG:HH21	1.70	0.56
49:AM:35:ILE:HD13	49:AM:46:ILE:HG22	1.87	0.56
70:Ah:77:PRO:HD2	70:Ah:80:LEU:HD12	1.87	0.56
77:Ao:75:VAL:HG23	77:Ao:76:LYS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:141:THR:OG1	4:BE:143:ASP:OD1	2.20	0.56
20:BF:25:LEU:HD22	23:BQ:57:LEU:HD23	1.87	0.56
25:BS:14:ILE:HG22	25:BS:23:ASP:HA	1.86	0.56
33:BM:113:ARG:NH1	34:B5:1223:A:H3'	2.20	0.56
34:B5:1382:A:HO2'	34:B5:1383:G:H8	1.53	0.56
37:AC:161:LYS:HB2	37:AC:164:GLU:HG2	1.87	0.56
38:A1:627:U:H2'	38:A1:628:A:C8	2.41	0.56
38:A1:2767:U:OP1	77:Ao:34:SER:HB3	2.05	0.56
38:A1:3047:U:H2'	38:A1:3048:A:H5''	1.87	0.56
47:AJ:25:GLU:HG3	47:AJ:26:SER:H	1.70	0.56
59:AW:45:ASN:HB3	59:AW:48:ARG:HG3	1.87	0.56
66:Ad:7:VAL:HG23	66:Ad:79:ARG:NH1	2.20	0.56
80:tA:7:G:O2'	80:tA:49:C:O5'	2.23	0.56
2:BB:176:VAL:O	2:BB:177:GLN:HG2	2.05	0.56
4:BE:256:ARG:O	4:BE:261:LEU:N	2.38	0.56
13:BW:37:PHE:O	13:BW:41:MET:HG3	2.04	0.56
36:AB:92:TYR:HB2	36:AB:157:VAL:HG13	1.87	0.56
38:A1:315:C:OP2	71:Ai:28:TYR:OH	2.20	0.56
38:A1:597:G:H5'	43:AF:41:ARG:HD2	1.85	0.56
43:AF:156:ILE:HG23	43:AF:172:ASN:HD21	1.70	0.56
5:BG:57:ASP:HA	5:BG:106:LEU:HA	1.88	0.56
13:BW:71:LYS:NZ	34:B5:1099:U:OP1	2.37	0.56
38:A1:1667:A:H2'	38:A1:1668:G:C8	2.40	0.56
38:A1:1873:U:OP1	54:AR:21:LYS:NZ	2.39	0.56
38:A1:2209:U:H3	38:A1:2236:G:H22	1.54	0.56
60:AX:135:ILE:HD12	60:AX:138:ARG:HH21	1.71	0.56
4:BE:199:GLU:OE2	4:BE:209:HIS:NE2	2.39	0.56
11:BO:45:GLY:HA2	11:BO:54:GLU:HG2	1.86	0.56
19:BD:223:LYS:HD2	19:BD:225:TYR:HE1	1.71	0.56
27:BU:28:SER:HB3	27:BU:34:LEU:HD22	1.88	0.56
29:Bc:41:VAL:HG12	29:Bc:63:ALA:HB3	1.86	0.56
48:AL:118:GLU:HG2	48:AL:145:PHE:CZ	2.41	0.56
66:Ad:9:THR:HG23	66:Ad:76:SER:HB3	1.88	0.56
77:Ao:35:LEU:HA	77:Ao:40:LYS:HG2	1.88	0.56
8:BJ:49:LEU:HA	8:BJ:52:ILE:HG22	1.88	0.56
38:A1:266:A:OP1	50:AN:5:LYS:NZ	2.39	0.56
38:A1:3291:G:H2'	38:A1:3292:A:H8	1.70	0.56
41:AD:41:LYS:HD2	56:AT:93:VAL:HG11	1.87	0.56
2:BB:33:LYS:HB3	2:BB:41:ARG:HE	1.71	0.56
5:BG:177:ARG:NH1	34:B5:143:G:N7	2.45	0.56
31:Bg:255:ALA:HB2	31:Bg:292:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:199:GLU:CD	4:BE:209:HIS:HE2	2.13	0.56
47:AJ:32:ARG:NH1	47:AJ:120:ILE:O	2.37	0.56
65:Ac:50:VAL:HA	65:Ac:53:LYS:HG2	1.88	0.56
4:BE:88:ASP:OD1	4:BE:122:LYS:NZ	2.32	0.56
34:B5:442:C:O2'	34:B5:525:A:N1	2.36	0.56
34:B5:1222:C:H2'	34:B5:1223:A:H8	1.70	0.56
34:B5:1592:A:H2'	34:B5:1593:A:C8	2.40	0.56
38:A1:2357:A:H2'	38:A1:2358:A:C8	2.41	0.56
38:A1:2795:U:OP1	77:Ao:61:LYS:NZ	2.37	0.56
47:AJ:109:HIS:HD2	47:AJ:123:PHE:H	1.54	0.56
4:BE:45:ILE:HG13	4:BE:61:VAL:HG21	1.87	0.55
33:BM:103:LEU:HB3	33:BM:115:VAL:HG11	1.86	0.55
40:A4:8:C:H2'	40:A4:9:A:C8	2.40	0.55
48:AL:141:ALA:HA	48:AL:144:THR:HG22	1.87	0.55
3:BC:238:SER:O	3:BC:242:ILE:HD12	2.06	0.55
15:BY:27:VAL:HG21	15:BY:35:VAL:HG21	1.88	0.55
28:BZ:95:HIS:ND1	28:BZ:96:SER:O	2.38	0.55
35:AA:57:PRO:HB3	78:Ap:54:ILE:HD11	1.89	0.55
38:A1:2768:U:H2'	38:A1:2769:A:C8	2.42	0.55
2:BB:39:GLU:HB3	2:BB:74:GLN:HA	1.89	0.55
2:BB:167:VAL:HA	2:BB:170:GLU:HG2	1.89	0.55
5:BG:159:ARG:HH21	5:BG:170:THR:HG23	1.71	0.55
8:BJ:81:VAL:HG21	8:BJ:91:LYS:HD2	1.87	0.55
8:BJ:112:GLN:HG3	8:BJ:148:VAL:HG21	1.88	0.55
38:A1:353:G:O6	72:Aj:55:ARG:NH2	2.40	0.55
38:A1:531:G:H2'	38:A1:532:A:C8	2.41	0.55
38:A1:3169:U:H4'	38:A1:3170:A:OP1	2.05	0.55
41:AD:196:ARG:HA	41:AD:199:ILE:HD12	1.88	0.55
45:AH:5:GLN:HE22	45:AH:7:GLU:HB3	1.70	0.55
7:BI:73:SER:OG	34:B5:257:A:H1'	2.06	0.55
9:BL:2:SER:HA	9:BL:53:TYR:HD1	1.72	0.55
26:BT:130:ARG:HG2	26:BT:134:ARG:HH12	1.70	0.55
34:B5:130:C:O2'	34:B5:131:C:OP1	2.24	0.55
38:A1:1696:A:H2'	38:A1:1697:A:C8	2.41	0.55
38:A1:3291:G:H2'	38:A1:3292:A:C8	2.42	0.55
1:BA:92:HIS:ND1	1:BA:202:TYR:OH	2.33	0.55
5:BG:71:THR:HG22	5:BG:72:ARG:H	1.70	0.55
34:B5:647:G:H21	34:B5:687:G:H1	1.53	0.55
34:B5:698:U:O2'	34:B5:699:U:O4'	2.24	0.55
38:A1:1498:A:H2'	38:A1:1499:C:C6	2.42	0.55
51:AO:143[A]:THR:OG1	51:AO:150[A]:GLU:OE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AR:165:LYS:HD2	54:AR:166:ASN:N	2.21	0.55
78:Ap:59:CYS:C	78:Ap:61:LYS:H	2.15	0.55
4:BE:180:LEU:HD11	4:BE:192:ILE:HG13	1.89	0.55
24:BR:34:LEU:O	24:BR:38:ILE:HG12	2.06	0.55
38:A1:307:A:H2'	38:A1:308:A:C8	2.42	0.55
38:A1:1176:C:H2'	38:A1:1177:G:N2	2.21	0.55
38:A1:1596:C:H2'	38:A1:1597:C:C6	2.42	0.55
38:A1:2883:U:H2'	38:A1:2884:C:C6	2.42	0.55
41:AD:95:TRP:HD1	41:AD:158:ARG:HA	1.71	0.55
45:AH:94:TYR:HA	45:AH:177:ASP:OD1	2.05	0.55
52:AP:122:ALA:HB3	52:AP:143:PRO:HB2	1.88	0.55
73:Ak:40:GLN:HE21	73:Ak:55:VAL:HG13	1.72	0.55
13:BW:31:SER:H	13:BW:34:ILE:HD12	1.70	0.55
13:BW:56:HIS:O	34:B5:861:U:O2'	2.23	0.55
34:B5:233:C:O2'	34:B5:237:C:N4	2.38	0.55
2:BB:116:LYS:HG3	34:B5:931:C:H5''	1.87	0.55
18:Be:42:ARG:NH1	34:B5:589:C:OP1	2.40	0.55
19:BD:58:VAL:HG13	19:BD:59:LEU:HD12	1.89	0.55
20:BF:49:GLU:O	20:BF:50:GLU:HG2	2.07	0.55
38:A1:656:A:H2'	38:A1:657:A:C8	2.42	0.55
38:A1:2426:U:H2'	38:A1:2427:U:C6	2.42	0.55
38:A1:2901:G:O2'	38:A1:3024:A:N1	2.39	0.55
45:AH:171:ASP:OD2	45:AH:173:ARG:HG2	2.06	0.55
46:AI:206:LEU:O	46:AI:210:ILE:HG12	2.07	0.55
80:tA:27:C:H2'	80:tA:28:A:H8	1.71	0.55
15:BY:116:LYS:NZ	34:B5:57:G:OP2	2.26	0.55
25:BS:66:LEU:O	25:BS:70:VAL:HG23	2.07	0.55
29:Bc:64:ARG:HG3	29:Bc:65:ARG:H	1.72	0.55
38:A1:2960:C:H2'	38:A1:2961:G:H8	1.72	0.55
70:Ah:9:LEU:HD21	70:Ah:54:VAL:HA	1.89	0.55
13:BW:110:ILE:HD12	13:BW:126:LEU:HD11	1.89	0.55
21:BK:59:PHE:CZ	21:BK:62:GLN:HA	2.41	0.55
22:BP:48:GLY:O	22:BP:49:MET:HE2	2.06	0.55
31:Bg:133:VAL:O	31:Bg:141:LEU:N	2.40	0.55
38:A1:943:U:H3'	63:Aa:13:GLY:HA2	1.89	0.55
38:A1:1353:U:H3'	42:AE:9:TRP:HZ3	1.72	0.55
39:A3:91:G:H2'	39:A3:92:A:C8	2.42	0.55
50:AN:9:GLU:OE2	50:AN:13:LYS:NZ	2.30	0.55
1:BA:74:VAL:HG23	1:BA:118:PRO:HB3	1.88	0.54
21:BK:53:GLY:O	21:BK:55:VAL:N	2.35	0.54
23:BQ:125:GLU:OE2	23:BQ:128:LYS:NZ	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:215:ILE:HD12	36:AB:338:LEU:HD12	1.88	0.54
38:A1:149:U:OP2	50:AN:49:ARG:NH2	2.36	0.54
38:A1:776:PSU:OP2	64:Ab:41:ARG:NH1	2.40	0.54
38:A1:2185:G:O2'	38:A1:2314:PSU:OP2	2.23	0.54
44:AG:183:LYS:HB2	44:AG:194:THR:HG23	1.89	0.54
5:BG:202:ARG:NH2	34:B5:127:G:O6	2.27	0.54
22:BP:90:ILE:HD11	22:BP:112:LEU:HD21	1.88	0.54
33:BM:62:LEU:HD13	33:BM:120:VAL:HB	1.89	0.54
36:AB:361:THR:H	36:AB:371:GLN:NE2	2.06	0.54
38:A1:240:U:O2'	38:A1:241:G:OP2	2.24	0.54
38:A1:309:U:H1'	38:A1:310:U:H5	1.73	0.54
38:A1:1799:A:H2'	38:A1:1800:A:C8	2.42	0.54
38:A1:2960:C:H2'	38:A1:2961:G:C8	2.42	0.54
20:BF:72:HIS:NE2	34:B5:1610:G:OP1	2.35	0.54
22:BP:98:ASN:ND2	22:BP:121:ILE:O	2.40	0.54
31:Bg:11:GLY:HA3	31:Bg:54:PHE:HB2	1.89	0.54
38:A1:1727:G:OP1	78:Ap:44:LYS:NZ	2.40	0.54
38:A1:3198:U:C4	45:AH:26:LYS:HD2	2.42	0.54
40:A4:57:C:H4'	40:A4:63:G:N7	2.22	0.54
41:AD:95:TRP:CD1	41:AD:158:ARG:HA	2.42	0.54
47:AJ:117:ASP:OD1	47:AJ:120:ILE:HD12	2.07	0.54
14:BX:3:LYS:HD2	14:BX:7:ARG:HH21	1.72	0.54
27:BU:70:THR:OG1	27:BU:72:ASN:OD1	2.25	0.54
34:B5:406:U:H2'	34:B5:407:A:C8	2.42	0.54
34:B5:1524:A:H2'	34:B5:1525:A:C8	2.42	0.54
34:B5:1650:U:H2'	34:B5:1651:A:C8	2.41	0.54
38:A1:2367:A:H2'	38:A1:2368:A:C8	2.42	0.54
39:A3:62:U:H4'	41:AD:285:ARG:HH12	1.73	0.54
34:B5:1114:G:O2'	34:B5:1130:G:O6	2.24	0.54
34:B5:1469:A:H4'	34:B5:1541:G:H4'	1.90	0.54
37:AC:317:PRO:C	37:AC:319:LYS:H	2.14	0.54
38:A1:1863:G:N1	38:A1:1866:C:OP2	2.32	0.54
46:AI:54:SER:HB2	46:AI:135:ILE:HD11	1.89	0.54
8:BJ:62:ARG:O	8:BJ:69:ARG:NH1	2.39	0.54
14:BX:107:PHE:CD1	14:BX:123:LYS:HB3	2.43	0.54
19:BD:40:ARG:HE	27:BU:110:PRO:HD3	1.72	0.54
24:BR:37:GLU:CD	31:Bg:150:TRP:HE1	2.15	0.54
33:BM:30:VAL:HG11	33:BM:133:LEU:HD11	1.90	0.54
34:B5:520:A:H2'	34:B5:521:A:C8	2.42	0.54
34:B5:1727:G:H2'	34:B5:1728:A:C8	2.43	0.54
38:A1:55:G:OP1	72:Aj:43:LYS:NZ	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2406:C:H2'	38:A1:2407:C:C6	2.43	0.54
38:A1:2883:U:H2'	38:A1:2884:C:H6	1.72	0.54
43:AF:58:ALA:O	43:AF:62:ILE:HD12	2.08	0.54
57:AU:38:ILE:HD11	57:AU:56:VAL:HG12	1.88	0.54
37:AC:283:THR:HG21	37:AC:288:ARG:HH21	1.73	0.54
80:tA:16:U:O4	80:tA:59:A:N7	2.41	0.54
2:BB:23:PRO:O	2:BB:27:LYS:NZ	2.41	0.54
15:BY:60:PHE:CD2	34:B5:522:U:H4'	2.43	0.54
29:Bc:5:THR:HG22	29:Bc:7:VAL:HG12	1.90	0.54
36:AB:277:SER:OG	36:AB:280:HIS:NE2	2.26	0.54
38:A1:2796:G:N7	77:Ao:63:LYS:NZ	2.51	0.54
53:AQ:93:ILE:HD13	53:AQ:96:PHE:HE1	1.73	0.54
9:BL:14:GLN:HB3	9:BL:54:ILE:HG13	1.88	0.54
10:BN:142:GLU:OE2	10:BN:145:THR:OG1	2.26	0.54
34:B5:52:U:H2'	34:B5:53:G:H8	1.73	0.54
34:B5:182:A:H2'	34:B5:183:U:H6	1.73	0.54
34:B5:210:A:N6	34:B5:255:U:H3	2.03	0.54
38:A1:655:C:H2'	38:A1:656:A:C8	2.42	0.54
38:A1:2838:A:N6	38:A1:2850:G:O2'	2.39	0.54
42:AE:149:ILE:HA	42:AE:155:LEU:HD23	1.89	0.54
4:BE:181:VAL:HG12	4:BE:227:VAL:HG22	1.89	0.54
33:BM:81:ASP:HB3	33:BM:84:ASN:OD1	2.08	0.54
34:B5:1041:G:H2'	34:B5:1042:G:C8	2.42	0.54
34:B5:1087:A:H2'	34:B5:1088:A:C8	2.42	0.54
38:A1:585:A:H5''	68:Af:70:LYS:HE3	1.90	0.54
38:A1:2282:U:O2	38:A1:2310:U:H4'	2.08	0.54
50:AN:140:LYS:HB3	50:AN:144:ARG:HH11	1.72	0.54
54:AR:23:TRP:HB3	54:AR:51:VAL:HG22	1.89	0.54
55:AS:48:LEU:HD12	55:AS:49:HIS:CD2	2.43	0.54
7:BI:81:VAL:HG22	7:BI:94:ASN:HA	1.90	0.53
34:B5:228:G:N1	34:B5:834:G:O2'	2.41	0.53
34:B5:895:G:H2'	34:B5:896:U:C6	2.43	0.53
38:A1:1234:G:O3'	38:A1:1236:G:N2	2.41	0.53
38:A1:3164:C:H2'	38:A1:3165:A:C8	2.42	0.53
39:A3:65:G:OP1	46:AI:203:LYS:HD2	2.07	0.53
19:BD:29:LEU:HD21	19:BD:69:LEU:HD11	1.90	0.53
34:B5:17:C:O2'	34:B5:1137:A:N1	2.34	0.53
65:Ac:17:VAL:HG11	65:Ac:92:ILE:HD12	1.89	0.53
68:Af:49:ILE:HD11	68:Af:71:VAL:HG22	1.90	0.53
73:Ak:24:THR:HG22	73:Ak:44:LYS:HB2	1.88	0.53
77:Ao:3:ASN:ND2	77:Ao:95:GLY:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:49:ARG:NH2	34:B5:448:C:OP1	2.39	0.53
8:BJ:60:LEU:HD11	8:BJ:93:LEU:HB3	1.90	0.53
18:Be:27:PRO:HD3	34:B5:506:A:C6	2.43	0.53
19:BD:135:GLU:OE2	19:BD:151:LYS:HG3	2.08	0.53
34:B5:1502:G:N2	34:B5:1505:A:OP2	2.39	0.53
38:A1:1534:A:H2'	38:A1:1535:A:C8	2.44	0.53
38:A1:3094:A:OP1	58:AV:14:SER:OG	2.26	0.53
38:A1:3153:U:H4'	38:A1:3154:C:C2	2.43	0.53
42:AE:154:LEU:HD12	49:AM:119:GLN:HG3	1.90	0.53
43:AF:138:TYR:CE2	43:AF:233:GLU:HB2	2.44	0.53
4:BE:23:LEU:HD22	8:BJ:3:ARG:HH21	1.73	0.53
12:BV:32:VAL:HG22	12:BV:60:ARG:HD2	1.89	0.53
15:BY:9:THR:HG23	15:BY:23:PHE:CD2	2.43	0.53
34:B5:488:G:OP1	34:B5:492:A:O2'	2.25	0.53
34:B5:1236:A:H2'	34:B5:1237:G:H8	1.73	0.53
38:A1:567:G:H2'	38:A1:568:G:C8	2.43	0.53
48:AL:118:GLU:HG2	48:AL:145:PHE:HZ	1.72	0.53
63:Aa:96:LYS:NZ	63:Aa:142:GLY:O	2.36	0.53
80:tA:27:C:H2'	80:tA:28:A:C8	2.44	0.53
2:BB:62:LYS:HD3	2:BB:90:GLU:HA	1.90	0.53
8:BJ:17:ARG:O	8:BJ:23:ARG:NH2	2.32	0.53
15:BY:7:ILE:HG13	15:BY:43:LYS:HG2	1.90	0.53
22:BP:60:LEU:HD13	22:BP:89:MET:HG2	1.91	0.53
29:Bc:19:THR:HG23	29:Bc:25:VAL:HB	1.90	0.53
38:A1:178:U:H2'	38:A1:179:C:H6	1.74	0.53
38:A1:2232:A:H2'	38:A1:2233:A:C8	2.43	0.53
38:A1:2357:A:H2'	38:A1:2358:A:H8	1.74	0.53
79:tP:60:A:H3'	79:tP:61:C:H5''	1.91	0.53
38:A1:2544:U:OP2	38:A1:2544:U:H6	1.91	0.53
38:A1:2767:U:H2'	38:A1:2768:U:C6	2.43	0.53
61:AY:48:LEU:HD13	61:AY:115:ARG:HH21	1.73	0.53
63:Aa:90:TYR:CG	63:Aa:100:PRO:HG3	2.44	0.53
79:tP:7:G:O2'	79:tP:49:C:OP2	2.21	0.53
1:BA:30:GLN:HE21	1:BA:33:GLN:HG2	1.74	0.53
5:BG:199:GLN:NE2	34:B5:127:G:O6	2.42	0.53
6:BH:14:THR:HG22	6:BH:16:LEU:H	1.74	0.53
6:BH:166:LEU:HD13	6:BH:183:PHE:HB2	1.90	0.53
12:BV:41:GLU:OE1	12:BV:41:GLU:N	2.34	0.53
15:BY:37:LYS:HG3	34:B5:522:U:H5''	1.91	0.53
23:BQ:90:VAL:HG21	23:BQ:117:LEU:HD11	1.90	0.53
24:BR:44:LYS:NZ	34:B5:1387:G:N7	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BU:95:ALA:HB1	27:BU:99:ILE:HD11	1.90	0.53
34:B5:538:A:H5'	34:B5:543:C:H41	1.74	0.53
38:A1:75:G:H5''	48:AL:58:VAL:CG1	2.39	0.53
38:A1:242:C:N4	38:A1:243:G:O6	2.42	0.53
38:A1:1108:U:H2'	38:A1:1109:U:C6	2.44	0.53
38:A1:1290:A:H2'	38:A1:1291:A:C8	2.44	0.53
38:A1:3050:U:O2'	59:AW:16:GLY:O	2.26	0.53
46:AI:145:LYS:HE3	46:AI:167:LEU:HD11	1.91	0.53
79:tP:57:G:H2'	79:tP:58:A:H5''	1.89	0.53
11:BO:20:TYR:HB3	11:BO:27:PHE:HB2	1.90	0.53
18:Be:35:TYR:HA	18:Be:38:LEU:HD23	1.91	0.53
19:BD:31:GLU:O	19:BD:54:ARG:NH2	2.39	0.53
34:B5:248:U:C4	34:B5:250:C:H1'	2.43	0.53
34:B5:412:A:H2'	34:B5:413:U:O2	2.09	0.53
34:B5:885:G:H2'	34:B5:886:U:C6	2.44	0.53
34:B5:901:G:H2'	34:B5:902:G:C8	2.44	0.53
35:AA:69:TYR:OH	38:A1:2557:A:OP1	2.25	0.53
37:AC:138:ARG:NH1	38:A1:1384:U:H5'	2.24	0.53
38:A1:1671:C:OP1	54:AR:60:LYS:NZ	2.40	0.53
40:A4:142:C:H2'	40:A4:143:U:C6	2.44	0.53
51:AO:80[A]:PHE:CE2	51:AO:84[A]:LEU:HD11	2.44	0.53
8:BJ:113:VAL:HG21	8:BJ:129:ILE:HD11	1.89	0.53
10:BN:124:ARG:NH2	34:B5:967:A:OP2	2.34	0.53
21:BK:10:LYS:NZ	21:BK:36:ASP:O	2.37	0.53
21:BK:79:TYR:HD1	21:BK:80:LEU:HD12	1.72	0.53
29:Bc:22:ARG:HD3	34:B5:1162:C:H4'	1.91	0.53
34:B5:1236:A:H2'	34:B5:1237:G:C8	2.44	0.53
34:B5:1477:G:H2'	34:B5:1478:G:H8	1.74	0.53
34:B5:1776:A:H2'	34:B5:1777:G:C8	2.44	0.53
36:AB:57:VAL:HG22	36:AB:73:VAL:HG22	1.91	0.53
37:AC:181:VAL:O	37:AC:182:LEU:HG	2.09	0.53
38:A1:1940:G:N2	38:A1:3362:A:H8	2.03	0.53
40:A4:81:U:H4'	40:A4:82:U:H5'	1.91	0.53
41:AD:80:SER:OG	41:AD:92:LEU:O	2.19	0.53
80:tA:21:A:N6	80:tA:46:G:H2'	2.24	0.53
2:BB:158:SER:HA	2:BB:161:ILE:HD12	1.91	0.53
37:AC:343:LYS:HD3	38:A1:515:C:H5''	1.91	0.53
38:A1:2961:G:H2'	38:A1:2962:U:C6	2.44	0.53
41:AD:260:PHE:HA	41:AD:264:GLN:NE2	2.25	0.53
4:BE:47:PHE:CE2	4:BE:90:ILE:HD11	2.44	0.52
5:BG:183:ARG:NH1	34:B5:141:U:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:46:ILE:HD11	6:BH:58:LEU:HB2	1.90	0.52
8:BJ:62:ARG:HB2	8:BJ:69:ARG:HD2	1.91	0.52
13:BW:31:SER:HB3	34:B5:636:A:H5''	1.90	0.52
14:BX:62:LYS:HE2	14:BX:118:PRO:HB3	1.89	0.52
22:BP:21:ASP:O	22:BP:25:LEU:HG	2.09	0.52
25:BS:42:TYR:HA	25:BS:85:PHE:HE2	1.74	0.52
25:BS:140:THR:HA	25:BS:143:ARG:HH21	1.75	0.52
27:BU:37:VAL:HG21	27:BU:112:VAL:HG11	1.90	0.52
36:AB:95:THR:HG22	38:A1:3243:A:H4'	1.90	0.52
38:A1:428:A:H2'	38:A1:429:U:C6	2.44	0.52
41:AD:116:ASP:OD1	41:AD:117:GLU:N	2.41	0.52
58:AV:11:PHE:HB3	58:AV:88:ARG:NH1	2.24	0.52
73:Ak:27:ILE:HD13	73:Ak:41:THR:HG22	1.91	0.52
1:BA:59:LEU:O	1:BA:63:ILE:HG12	2.09	0.52
18:Be:25:GLU:O	34:B5:506:A:N6	2.43	0.52
38:A1:2419:A:H2'	38:A1:2420:C:C6	2.44	0.52
38:A1:2427:U:H2'	38:A1:2428:U:C6	2.44	0.52
51:AO:125[A]:ARG:HG3	51:AO:129[A]:LEU:HD12	1.92	0.52
79:tP:10:A:H61	79:tP:25:C:H42	1.57	0.52
3:BC:148:LEU:O	3:BC:174:ARG:NH1	2.40	0.52
5:BG:14:LYS:HG3	5:BG:123:GLY:HA3	1.91	0.52
31:Bg:179:LYS:NZ	31:Bg:191:ASP:OD2	2.38	0.52
38:A1:175:C:N4	38:A1:176:G:O6	2.42	0.52
38:A1:443:G:N2	38:A1:492:C:O5'	2.41	0.52
38:A1:3121:U:H1'	38:A1:3122:A:H5''	1.92	0.52
47:AJ:54:VAL:HG21	47:AJ:57:PHE:CD2	2.44	0.52
62:AZ:90:GLU:HG3	62:AZ:93:LYS:NZ	2.25	0.52
9:BL:7:VAL:HG23	9:BL:8:GLN:HG2	1.90	0.52
34:B5:1321:A:H4'	34:B5:1322:A:O5'	2.10	0.52
38:A1:498:A:O2'	38:A1:3273:A:N1	2.38	0.52
38:A1:847:A:H2'	38:A1:848:A:C8	2.44	0.52
39:A3:84:A:H2'	39:A3:85:G:C8	2.43	0.52
45:AH:103:ILE:HD11	45:AH:134:ILE:HG21	1.91	0.52
61:AY:115:ARG:O	61:AY:119:ILE:HG12	2.10	0.52
8:BJ:72:GLU:OE2	34:B5:761:G:O2'	2.28	0.52
10:BN:54:LEU:HB3	10:BN:60:VAL:HB	1.90	0.52
13:BW:23:ARG:HH21	13:BW:66:ASN:HA	1.74	0.52
19:BD:60:GLY:HA3	19:BD:64:ARG:HB2	1.91	0.52
21:BK:52:LYS:HE3	34:B5:1220:C:H5''	1.92	0.52
34:B5:982:U:H2'	34:B5:983:A:C8	2.45	0.52
34:B5:1198:G:OP1	34:B5:1199:G:O2'	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1606:C:H2'	34:B5:1607:G:C8	2.44	0.52
38:A1:417:A:H2'	38:A1:418:A:C8	2.45	0.52
38:A1:1203:A:H2'	38:A1:1204:A:H8	1.75	0.52
7:BI:77:ARG:HH22	38:A1:3354:U:H4'	1.73	0.52
20:BF:122:ASN:HB2	20:BF:129:PRO:HG3	1.92	0.52
23:BQ:98:ASP:O	23:BQ:101:SER:OG	2.25	0.52
37:AC:325:LEU:HD23	38:A1:598:A:H4'	1.91	0.52
38:A1:2407:C:H2'	38:A1:2408:U:C6	2.45	0.52
42:AE:71:VAL:HG21	42:AE:159:LEU:HD23	1.92	0.52
48:AL:174:ARG:HG3	71:AI:9:ILE:HD13	1.92	0.52
5:BG:133:LEU:O	34:B5:166:C:O2'	2.28	0.52
7:BI:44:HIS:ND1	34:B5:1676:U:OP1	2.41	0.52
23:BQ:79:TYR:O	23:BQ:82:ARG:HG2	2.09	0.52
34:B5:184:C:H2'	34:B5:185:U:C6	2.45	0.52
35:AA:47:GLN:HG2	35:AA:49:VAL:HG13	1.91	0.52
37:AC:7:THR:HG22	37:AC:147:GLU:OE2	2.10	0.52
37:AC:181:VAL:HG11	37:AC:224:GLY:HA3	1.92	0.52
3:BC:78:ASP:HB3	3:BC:104:VAL:HG12	1.91	0.52
5:BG:137:ARG:O	5:BG:141:ILE:HD12	2.09	0.52
7:BI:72:ILE:HD13	7:BI:112:TRP:CD2	2.45	0.52
11:BO:61:MET:HG3	11:BO:104:ALA:HB2	1.91	0.52
23:BQ:46:PHE:O	23:BQ:50:GLU:HG3	2.10	0.52
31:Bg:216:LYS:HA	31:Bg:239:GLU:HG3	1.90	0.52
38:A1:240:U:H1'	38:A1:241:G:O5'	2.10	0.52
38:A1:1422:G:H21	42:AE:5:LYS:HZ3	1.56	0.52
38:A1:3113:A:OP1	45:AH:73:SER:OG	2.28	0.52
24:BR:100:LEU:N	24:BR:118:PRO:O	2.43	0.52
34:B5:226:A:H1'	34:B5:837:G:H1	1.75	0.52
34:B5:1296:A:N1	34:B5:1301:U:H5	2.08	0.52
38:A1:1915:A:H2'	38:A1:1916:U:C6	2.45	0.52
38:A1:2407:C:H2'	38:A1:2408:U:H6	1.75	0.52
38:A1:3233:C:H2'	38:A1:3234:A:C8	2.45	0.52
45:AH:18:VAL:HG12	45:AH:27:VAL:HG22	1.91	0.52
3:BC:122:ALA:O	3:BC:126:ARG:HG3	2.10	0.51
5:BG:187:LYS:O	5:BG:191:ARG:HG2	2.10	0.51
13:BW:53:ILE:HD11	13:BW:62:VAL:HG23	1.91	0.51
27:BU:106:ILE:HG13	27:BU:107:THR:HG23	1.92	0.51
35:AA:9:ARG:NH2	38:A1:912:G:N7	2.58	0.51
38:A1:874:U:OP2	38:A1:1907:C:O2'	2.24	0.51
41:AD:268:GLU:HA	41:AD:271:LYS:HE2	1.92	0.51
43:AF:156:ILE:HG12	43:AF:172:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:17:HIS:HB2	4:BE:108:ARG:HA	1.91	0.51
19:BD:105:MET:HE2	19:BD:184:ILE:HD12	1.91	0.51
20:BF:165:LEU:HD23	29:Bc:47:PRO:HG2	1.92	0.51
31:Bg:131:ILE:HB	31:Bg:144:LEU:HB2	1.93	0.51
34:B5:32:U:O2'	34:B5:594:A:N1	2.43	0.51
34:B5:221:A:H61	34:B5:839:U:H3	1.57	0.51
38:A1:2676:A:H5'	38:A1:2677:G:C8	2.46	0.51
38:A1:3243:A:C5	51:AO:156[A]:LEU:HG	2.46	0.51
11:BO:16:VAL:O	11:BO:30:VAL:HA	2.10	0.51
31:Bg:302:PHE:HD1	31:Bg:312:VAL:HG12	1.74	0.51
34:B5:62:A:H1'	34:B5:269:G:H1'	1.93	0.51
34:B5:983:A:N1	34:B5:1018:U:H5	2.07	0.51
34:B5:1175:U:H2'	34:B5:1176:G:C8	2.45	0.51
34:B5:1352:G:H2'	34:B5:1354:G:H8	1.75	0.51
38:A1:945:C:H2'	38:A1:946:U:C6	2.45	0.51
38:A1:1017:C:H3'	38:A1:1019:G:OP2	2.09	0.51
43:AF:166:ASN:O	43:AF:170:GLU:HG3	2.10	0.51
46:AI:108:ALA:O	46:AI:112:GLN:HB2	2.11	0.51
2:BB:132:ASP:HB2	2:BB:221:PRO:HB3	1.93	0.51
8:BJ:119:ALA:O	8:BJ:120:LYS:HG2	2.11	0.51
20:BF:51:VAL:O	20:BF:65:ARG:NH2	2.42	0.51
26:BT:109:GLU:OE2	26:BT:122:ARG:NE	2.42	0.51
34:B5:215:A:H2'	34:B5:216:U:H5'	1.93	0.51
34:B5:487:G:H2'	34:B5:488:G:H4'	1.92	0.51
34:B5:1359:C:H2'	34:B5:1360:A:H8	1.76	0.51
36:AB:361:THR:H	36:AB:371:GLN:HE22	1.59	0.51
38:A1:501:A:H2'	38:A1:502:U:C6	2.46	0.51
55:AS:1:MET:HE1	55:AS:36:ILE:HG21	1.92	0.51
55:AS:96:ASP:OD1	55:AS:97:VAL:N	2.37	0.51
62:AZ:52:LYS:O	62:AZ:65:ARG:HD3	2.10	0.51
4:BE:230:GLU:HG3	4:BE:231:GLN:H	1.75	0.51
8:BJ:67:PRO:HA	8:BJ:70:LEU:HG	1.93	0.51
19:BD:31:GLU:HG3	19:BD:107:PHE:CE2	2.45	0.51
31:Bg:210:LEU:HG	31:Bg:231:MET:HE1	1.91	0.51
35:AA:190:ARG:HG3	35:AA:191:LEU:HD22	1.91	0.51
38:A1:585:A:H2'	38:A1:586:C:C6	2.45	0.51
38:A1:1555:U:H5'	38:A1:1556:C:OP2	2.11	0.51
38:A1:2611:U:H2'	38:A1:2612:U:C6	2.45	0.51
40:A4:29:U:H5''	48:AL:27:ASP:HB3	1.92	0.51
40:A4:63:G:H22	40:A4:97:A:H2	1.59	0.51
55:AS:2:ALA:HB1	55:AS:104:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Ak:61:LYS:HA	73:Ak:64:LYS:HG2	1.91	0.51
3:BC:44:LEU:HD21	3:BC:247:ALA:HB2	1.93	0.51
4:BE:64:ILE:HD12	15:BY:17:LEU:HB3	1.92	0.51
4:BE:101:LEU:HG	4:BE:109:PHE:CD1	2.46	0.51
8:BJ:10:LYS:NZ	34:B5:471:A:OP1	2.36	0.51
8:BJ:73:GLY:O	8:BJ:77:ILE:HG12	2.10	0.51
20:BF:63:GLN:NE2	20:BF:66:GLN:H	2.09	0.51
26:BT:33:TYR:O	26:BT:36:ILE:HG12	2.10	0.51
38:A1:166:C:H2'	38:A1:167:U:H6	1.75	0.51
38:A1:1012:G:H2'	38:A1:1013:G:O4'	2.11	0.51
38:A1:1083:G:H2'	38:A1:1084:A:C8	2.46	0.51
5:BG:133:LEU:HD23	5:BG:134:GLY:O	2.11	0.51
34:B5:844:A:H5'	34:B5:845:G:H5''	1.91	0.51
34:B5:1466:G:O2'	34:B5:1602:C:OP1	2.25	0.51
38:A1:40:A:H5''	63:Aa:35:ALA:HB1	1.93	0.51
56:AT:100:LYS:HG2	56:AT:104:GLU:OE2	2.11	0.51
57:AU:77:LYS:HD2	57:AU:95:PHE:HD1	1.76	0.51
7:BI:110:ARG:NH2	7:BI:122:GLY:HA3	2.26	0.51
19:BD:135:GLU:HB2	19:BD:157:LEU:HD11	1.93	0.51
28:BZ:43:ASP:CG	28:BZ:44:GLN:H	2.18	0.51
32:Bf:119:ARG:NH2	32:Bf:139:LEU:HD21	2.26	0.51
34:B5:625:C:H2'	34:B5:626:U:C6	2.46	0.51
38:A1:3277:U:H5'	38:A1:3278:C:C5	2.45	0.51
45:AH:27:VAL:HG12	45:AH:82:VAL:HG21	1.93	0.51
46:AI:50:VAL:HG22	46:AI:167:LEU:HD13	1.93	0.51
55:AS:90:MET:SD	55:AS:92:LYS:HE2	2.50	0.51
57:AU:89:LEU:HB3	57:AU:93:ILE:HD12	1.93	0.51
58:AV:15:LEU:HD23	58:AV:53:SER:HB3	1.92	0.51
58:AV:30:GLY:HA3	58:AV:66:LYS:HD2	1.91	0.51
7:BI:76:THR:HG21	7:BI:104:ILE:HD12	1.92	0.51
26:BT:97:SER:OG	34:B5:1504:G:OP1	2.25	0.51
27:BU:50:LEU:HD11	27:BU:94:GLU:O	2.11	0.51
31:Bg:98:GLU:HG3	31:Bg:98:GLU:O	2.10	0.51
34:B5:16:G:H2'	34:B5:17:C:C6	2.46	0.51
34:B5:651:G:H2'	34:B5:652:G:H3'	1.92	0.51
34:B5:1641:C:H2'	34:B5:1642:G:C8	2.45	0.51
38:A1:1389:G:OP1	67:Ae:104:ASN:ND2	2.39	0.51
45:AH:129:ARG:H	45:AH:157:ASN:ND2	2.09	0.51
21:BK:77:ARG:HH21	21:BK:88:PRO:HA	1.75	0.51
33:BM:28:LEU:HA	33:BM:31:VAL:HG22	1.93	0.51
34:B5:983:A:C2	34:B5:1018:U:H5	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:26:A:H2'	38:A1:27:C:H6	1.75	0.51
38:A1:3013:U:H2'	38:A1:3014:U:C6	2.46	0.51
38:A1:3275:U:O2'	68:Af:99:ARG:NH1	2.44	0.51
46:AI:69:ARG:NH2	80:tA:54:A:O2'	2.44	0.51
63:Aa:2:PRO:HG2	63:Aa:5:PHE:CD2	2.46	0.51
26:BT:102:ARG:NH2	34:B5:1502:G:N7	2.53	0.50
34:B5:181:A:H2'	34:B5:182:A:C8	2.46	0.50
37:AC:322:GLN:NE2	38:A1:597:G:H21	2.08	0.50
38:A1:309:U:O2'	38:A1:310:U:OP2	2.28	0.50
38:A1:2801:A:O2'	38:A1:2802:A:H2'	2.10	0.50
44:AG:90:THR:HG23	44:AG:214:LEU:HD21	1.93	0.50
44:AG:104:GLU:O	44:AG:108:ARG:HG3	2.11	0.50
45:AH:19:SER:HB2	45:AH:26:LYS:HG2	1.93	0.50
50:AN:140:LYS:HB3	50:AN:144:ARG:NH1	2.26	0.50
73:Ak:65:LEU:HA	73:Ak:68:SER:HB3	1.93	0.50
77:Ao:104:LEU:HD11	79:tP:56:C:H42	1.76	0.50
8:BJ:89:ASP:O	8:BJ:90:LYS:HG2	2.12	0.50
31:Bg:50:ASP:OD1	31:Bg:51:ASP:N	2.42	0.50
34:B5:1689:A:N6	34:B5:1714:A:O2'	2.45	0.50
38:A1:216:G:OP1	61:AY:16:ARG:NH1	2.42	0.50
38:A1:1899:G:O2'	38:A1:2334:U:O4	2.22	0.50
38:A1:2203:U:H2'	38:A1:2204:C:C6	2.47	0.50
38:A1:2568:C:O2'	38:A1:2569:A:O4'	2.28	0.50
38:A1:3222:U:O2	38:A1:3263:G:O6	2.29	0.50
40:A4:26:U:H2'	40:A4:27:U:C6	2.47	0.50
51:AO:16[A]:VAL:HG23	51:AO:80[A]:PHE:HD1	1.75	0.50
53:AQ:176:ARG:HA	53:AQ:182:LYS:O	2.11	0.50
4:BE:191:ARG:HD3	4:BE:245:LYS:HE3	1.92	0.50
6:BH:82:GLU:OE2	6:BH:90:VAL:HG12	2.11	0.50
19:BD:76:ARG:HA	21:BK:63:TYR:CZ	2.45	0.50
31:Bg:87:LYS:HG2	31:Bg:108:SER:C	2.37	0.50
33:BM:66:VAL:HG21	33:BM:71:ILE:HD11	1.91	0.50
34:B5:153:G:H2'	34:B5:154:G:H8	1.77	0.50
38:A1:121:A:C2	44:AG:129:PRO:HB3	2.46	0.50
38:A1:577:C:O2'	38:A1:579:G:OP1	2.26	0.50
39:A3:23:A:HO2'	39:A3:24:A:P	2.34	0.50
41:AD:85:ARG:NH1	41:AD:254:LYS:HG2	2.25	0.50
42:AE:137:ASP:HA	42:AE:140:VAL:HG12	1.93	0.50
46:AI:66:GLU:O	46:AI:70:ILE:HD12	2.11	0.50
54:AR:109:TYR:HB3	54:AR:115:ILE:HG12	1.94	0.50
70:Ah:31:LEU:HD22	70:Ah:41:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Ap:38:ASP:OD1	78:Ap:45:LYS:HD3	2.11	0.50
9:BL:57:LYS:HD3	9:BL:131:ILE:HG23	1.93	0.50
28:BZ:43:ASP:OD2	28:BZ:44:GLN:N	2.44	0.50
34:B5:895:G:H1	34:B5:917:U:H3	1.59	0.50
38:A1:872:U:H2'	38:A1:873:C:C6	2.46	0.50
43:AF:49:ALA:HB1	43:AF:53:LYS:NZ	2.27	0.50
46:AI:181:TYR:CE2	46:AI:185:ARG:HD2	2.47	0.50
61:AY:83:ASP:O	61:AY:84:LYS:HG2	2.11	0.50
69:Ag:51:LEU:HB3	69:Ag:54:ILE:HD13	1.93	0.50
69:Ag:74:ARG:NH2	69:Ag:82:ALA:HB2	2.26	0.50
80:tA:18:G:O2'	80:tA:57:G:N2	2.25	0.50
15:BY:16:PRO:HA	15:BY:19:ALA:HA	1.93	0.50
17:Bb:74:SER:O	17:Bb:77:THR:HG22	2.11	0.50
26:BT:131:ASP:OD1	26:BT:132:LEU:HD12	2.11	0.50
28:BZ:68:ARG:C	28:BZ:69:LEU:HD12	2.37	0.50
34:B5:304:U:H2'	34:B5:305:C:C6	2.46	0.50
38:A1:12:A:H2'	38:A1:13:A:C8	2.46	0.50
38:A1:129:U:H2'	38:A1:130:A:H8	1.76	0.50
38:A1:1659:U:H2'	38:A1:1660:C:C6	2.47	0.50
38:A1:1740:U:H1'	38:A1:1741:A:H2	1.77	0.50
38:A1:3089:C:H2'	38:A1:3090:U:O4'	2.11	0.50
74:Al:5:LYS:HD3	74:Al:13:MET:HE1	1.94	0.50
7:BI:137:LYS:O	34:B5:190:C:N4	2.44	0.50
30:Bd:41:GLN:O	30:Bd:45:GLU:HG3	2.12	0.50
34:B5:286:C:H2'	34:B5:287:G:O4'	2.11	0.50
34:B5:514:G:O2'	34:B5:515:A:H8	1.94	0.50
38:A1:1495:U:H5	38:A1:1835:A:N1	2.09	0.50
61:AY:55:GLU:HG2	61:AY:108:LYS:HB3	1.93	0.50
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.94	0.50
21:BK:11:ILE:HD11	21:BK:42:VAL:HG22	1.93	0.50
33:BM:29:LYS:HE2	33:BM:100:TRP:CD1	2.46	0.50
34:B5:103:A:H4'	34:B5:105:A:C8	2.47	0.50
34:B5:1360:A:N1	34:B5:1363:U:H5	2.09	0.50
36:AB:29:VAL:HG22	36:AB:218:ILE:HD13	1.92	0.50
38:A1:993:G:N3	38:A1:2637:A:H2'	2.26	0.50
38:A1:2594:C:H2'	38:A1:2595:A:O4'	2.12	0.50
41:AD:177:GLU:HB2	41:AD:190:ILE:HD12	1.93	0.50
4:BE:182:TYR:N	4:BE:226:PHE:O	2.45	0.50
27:BU:22:ILE:HD11	27:BU:116:VAL:HG12	1.94	0.50
34:B5:1564:U:H2'	34:B5:1565:C:C6	2.47	0.50
38:A1:2344:U:H2'	38:A1:2345:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3322:A:H2'	38:A1:3323:A:C8	2.46	0.50
44:AG:28:HIS:CE1	62:AZ:128:GLN:HE22	2.29	0.50
51:AO:84[A]:LEU:HD13	51:AO:102[A]:LEU:HD21	1.94	0.50
71:Ai:66:GLU:OE1	71:Ai:91:ASN:ND2	2.44	0.50
2:BB:137:ILE:HG21	2:BB:172:LEU:HD22	1.93	0.50
20:BF:80:LYS:HB2	20:BF:83:ARG:HB2	1.94	0.50
30:Bd:34:TYR:OH	34:B5:1487:A:OP1	2.18	0.50
31:Bg:214:ALA:HB2	31:Bg:220:ILE:HG12	1.92	0.50
33:BM:22:VAL:HA	33:BM:135:MET:HE1	1.94	0.50
34:B5:199:G:H2'	34:B5:200:A:C8	2.46	0.50
34:B5:1350:U:H2'	34:B5:1351:G:H8	1.76	0.50
37:AC:60:THR:HG23	38:A1:364:G:OP1	2.12	0.50
38:A1:990:PSU:H1'	56:AT:101:CYS:HB2	1.93	0.50
38:A1:1084:A:H2'	38:A1:1085:A:C8	2.47	0.50
50:AN:70:ASN:ND2	50:AN:93:LYS:HE3	2.27	0.50
6:BH:104:ARG:HD2	34:B5:803:A:C4	2.47	0.49
18:Be:35:TYR:HA	18:Be:38:LEU:CD2	2.42	0.49
34:B5:1144:U:H2'	34:B5:1145:U:C6	2.46	0.49
37:AC:317:PRO:O	37:AC:318:LEU:HB2	2.11	0.49
38:A1:976:U:OP1	53:AQ:144:ARG:NH2	2.43	0.49
38:A1:1259:A:H1'	38:A1:1280:C:H1'	1.94	0.49
38:A1:2555:G:O6	69:Ag:99:LYS:NZ	2.44	0.49
38:A1:3225:C:H2'	38:A1:3226:A:H8	1.76	0.49
41:AD:286:VAL:HG23	46:AI:206:LEU:HD22	1.94	0.49
44:AG:97:TYR:OH	44:AG:207:ASP:OD2	2.23	0.49
48:AL:51:LEU:HD22	48:AL:139:LEU:HD11	1.93	0.49
75:Am:80:PRO:HA	75:Am:83:LYS:HB3	1.92	0.49
77:Ao:14:GLY:C	77:Ao:16:THR:H	2.19	0.49
5:BG:160:ARG:HD3	34:B5:66:U:O2	2.11	0.49
5:BG:176:GLN:NE2	34:B5:65:A:OP1	2.29	0.49
9:BL:133:LYS:HB2	34:B5:337:G:H3'	1.95	0.49
15:BY:32:ARG:NH2	15:BY:39:GLU:OE1	2.44	0.49
21:BK:3:MET:SD	21:BK:41:TYR:HB3	2.52	0.49
31:Bg:46:LYS:HE3	31:Bg:56:VAL:HG22	1.93	0.49
34:B5:15:U:H2'	34:B5:16:G:O4'	2.12	0.49
34:B5:120:PSU:H2'	34:B5:121:U:H6	1.76	0.49
34:B5:1175:U:H2'	34:B5:1176:G:H8	1.78	0.49
38:A1:651:G:O2'	38:A1:1435:A:OP1	2.30	0.49
38:A1:716:A:C5	63:Aa:117:ARG:HG3	2.46	0.49
38:A1:3016:A:H2'	38:A1:3017:A:H8	1.77	0.49
40:A4:151:C:C5	60:AX:24:LEU:HD11	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AJ:82:ARG:NH2	47:AJ:113:GLY:O	2.45	0.49
8:BJ:108:ARG:HH12	8:BJ:145:SER:HB3	1.76	0.49
15:BY:128:LYS:HE3	34:B5:153:G:N7	2.27	0.49
22:BP:110:GLU:HB2	25:BS:119:ILE:HD13	1.94	0.49
34:B5:31:C:O2'	34:B5:547:U:OP1	2.31	0.49
35:AA:65:ASP:HB3	35:AA:68:LYS:O	2.12	0.49
38:A1:1422:G:H21	42:AE:5:LYS:NZ	2.09	0.49
75:Am:105:PRO:HD2	75:Am:106:ARG:HH11	1.78	0.49
80:tA:1:A:H2'	80:tA:2:G:H8	1.77	0.49
2:BB:117:TRP:CH2	34:B5:1799:U:H5'	2.47	0.49
6:BH:22:GLN:HA	6:BH:25:VAL:HG22	1.94	0.49
7:BI:57:ALA:HB2	7:BI:177:GLY:HA2	1.94	0.49
8:BJ:75:ALA:O	8:BJ:79:ARG:HG3	2.13	0.49
11:BO:42:VAL:HA	11:BO:46:MET:HE2	1.93	0.49
14:BX:56:LYS:HD2	14:BX:93:LEU:HD11	1.93	0.49
33:BM:41:LEU:HD21	33:BM:101:ALA:HB1	1.94	0.49
34:B5:199:G:H2'	34:B5:200:A:H8	1.77	0.49
34:B5:413:U:H5	34:B5:420:A:N1	2.10	0.49
38:A1:966:PSU:OP1	63:Aa:44:ASN:ND2	2.43	0.49
38:A1:1615:C:H2'	38:A1:1616:U:C6	2.48	0.49
38:A1:2836:C:H5	38:A1:2852:C:H42	1.60	0.49
38:A1:3268:A:H5''	42:AE:46:ARG:NH1	2.27	0.49
43:AF:237:ASN:O	43:AF:241:LYS:HG2	2.13	0.49
2:BB:48:VAL:HG13	2:BB:49:ASN:N	2.27	0.49
5:BG:71:THR:HG22	5:BG:72:ARG:N	2.26	0.49
5:BG:220:LYS:HG3	5:BG:223:LYS:HE3	1.95	0.49
20:BF:208:SER:O	20:BF:212:LYS:HG2	2.12	0.49
27:BU:89:ARG:HH22	34:B5:1383:G:P	2.35	0.49
34:B5:615:A:O2'	34:B5:621:A:N1	2.42	0.49
34:B5:1171:A:O2'	34:B5:1570:A:N3	2.41	0.49
34:B5:1203:A:C2	34:B5:1556:A:C4	3.01	0.49
38:A1:166:C:H2'	38:A1:167:U:C6	2.48	0.49
38:A1:2213:A:H2'	38:A1:2214:A:H8	1.75	0.49
40:A4:8:C:H2'	40:A4:9:A:H8	1.77	0.49
50:AN:9:GLU:HG3	71:Ai:44:VAL:HG11	1.94	0.49
76:An:1:MET:CE	76:An:6:ARG:HD2	2.32	0.49
1:BA:70:PRO:HB2	1:BA:94:GLY:HA3	1.95	0.49
2:BB:135:LEU:HB3	2:BB:217:LEU:HD23	1.94	0.49
2:BB:153:HIS:CD2	2:BB:155:TYR:CD2	3.00	0.49
6:BH:44:LYS:HD2	6:BH:63:PRO:HB3	1.95	0.49
10:BN:42:ARG:HH11	10:BN:80:LEU:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BK:91:TYR:CD2	21:BK:92:ILE:HD12	2.47	0.49
30:Bd:13:ARG:NH2	34:B5:1554:U:OP1	2.41	0.49
34:B5:1044:U:H2'	34:B5:1045:C:C6	2.48	0.49
34:B5:1222:C:H2'	34:B5:1223:A:C8	2.47	0.49
35:AA:44:ILE:HD13	35:AA:87:PHE:CE1	2.47	0.49
38:A1:2520:A:H2'	38:A1:2521:U:C6	2.47	0.49
38:A1:2909:U:H2'	38:A1:2910:A:O4'	2.12	0.49
42:AE:52:VAL:HG11	42:AE:65:ILE:HD12	1.95	0.49
48:AL:58:VAL:HG21	48:AL:72:GLY:HA3	1.94	0.49
5:BG:142:ARG:HG3	5:BG:147:LEU:HB2	1.95	0.49
20:BF:144:GLU:HG2	20:BF:221:ALA:HB1	1.95	0.49
22:BP:109:PRO:O	22:BP:112:LEU:HD23	2.12	0.49
25:BS:144:ARG:HD2	34:B5:1172:G:OP1	2.13	0.49
31:Bg:9:LEU:HB3	31:Bg:313:TRP:NE1	2.28	0.49
31:Bg:151:VAL:HA	31:Bg:173:GLY:HA2	1.95	0.49
33:BM:63:VAL:HG11	33:BM:94:ALA:HB2	1.95	0.49
38:A1:19:U:H2'	38:A1:20:A:C8	2.47	0.49
38:A1:955:U:H2'	38:A1:956:U:C6	2.47	0.49
38:A1:3294:A:H2'	38:A1:3295:A:O4'	2.13	0.49
79:tP:60:A:OP2	79:tP:60:A:H8	1.95	0.49
6:BH:108:GLN:OE1	34:B5:810:G:N2	2.46	0.49
29:Bc:16:LEU:HD12	29:Bc:27:GLN:HB3	1.95	0.49
31:Bg:221:MET:HB3	31:Bg:223:TRP:NE1	2.27	0.49
38:A1:792:G:H2'	38:A1:793:C:C6	2.48	0.49
38:A1:2413:A:H2'	38:A1:2414:G:H8	1.78	0.49
40:A4:58:G:O6	72:Aj:63:ARG:NH1	2.40	0.49
53:AQ:170:ARG:O	53:AQ:171:LYS:HB2	2.12	0.49
68:Af:58:GLU:HB2	68:Af:63:LYS:HZ2	1.77	0.49
80:tA:26:G:O6	80:tA:44:A:N1	2.46	0.49
7:BI:83:TYR:HB3	7:BI:101:ILE:HB	1.95	0.49
11:BO:124:ASP:OD2	34:B5:928:U:H4'	2.13	0.49
22:BP:22:LEU:HA	22:BP:25:LEU:HD12	1.95	0.49
26:BT:61:VAL:O	26:BT:65:ILE:HG12	2.13	0.49
34:B5:1146:G:H2'	34:B5:1147:A:C8	2.47	0.49
36:AB:173:GLN:HG3	38:A1:3313:U:H4'	1.94	0.49
36:AB:283:TYR:N	36:AB:323:MET:O	2.43	0.49
38:A1:277:G:H2'	38:A1:278:U:C6	2.48	0.49
38:A1:770:G:OP1	48:AL:171:ARG:HG2	2.13	0.49
39:A3:98:C:O2'	43:AF:131:GLU:OE1	2.29	0.49
40:A4:149:A:H2'	40:A4:150:G:C8	2.47	0.49
42:AE:45:GLY:O	42:AE:48:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AP:40:GLU:HA	52:AP:113:TYR:HA	1.94	0.49
74:Al:10:LYS:HA	74:Al:13:MET:HE3	1.95	0.49
6:BH:108:GLN:HE22	34:B5:809:A:H2	1.61	0.49
10:BN:62:GLN:HB2	10:BN:65:VAL:HB	1.95	0.49
32:Bf:114:VAL:HG21	33:BM:78:LEU:HD22	1.95	0.49
34:B5:1755:A:H4'	34:B5:1756[A]:A:OP1	2.13	0.49
38:A1:3006:A:H2'	38:A1:3007:U:O4'	2.13	0.49
38:A1:3169:U:O2'	38:A1:3170:A:H5'	2.12	0.49
57:AU:93:ILE:HG21	57:AU:105:LEU:HD23	1.94	0.49
58:AV:66:LYS:HE2	58:AV:68:GLU:OE2	2.13	0.49
59:AW:45:ASN:O	59:AW:49:ILE:HG12	2.12	0.49
3:BC:178:ILE:O	3:BC:185:LYS:NZ	2.32	0.48
5:BG:63:MET:HE2	5:BG:106:LEU:HD21	1.94	0.48
5:BG:197:ASN:O	5:BG:201:GLN:HG2	2.13	0.48
15:BY:13:ILE:CG2	15:BY:22:GLN:HE21	2.25	0.48
34:B5:845:G:H1'	34:B5:846:G:C5	2.48	0.48
34:B5:1359:C:H2'	34:B5:1360:A:C8	2.47	0.48
35:AA:97:ASN:ND2	78:Ap:87:ARG:HH11	2.11	0.48
38:A1:874:U:H5''	38:A1:2950:G:OP1	2.13	0.48
38:A1:1049:C:OP1	46:AI:21:ARG:NH2	2.46	0.48
39:A3:3:U:H2'	39:A3:4:U:C6	2.48	0.48
47:AJ:27:GLY:O	47:AJ:31:THR:HG23	2.13	0.48
49:AM:19:ARG:HG2	49:AM:65:LEU:HD22	1.95	0.48
49:AM:39:ILE:HB	49:AM:43:LYS:HB2	1.95	0.48
51:AO:186[A]:ALA:O	51:AO:187[A]:GLU:HG2	2.13	0.48
52:AP:60:PHE:HB3	52:AP:64:ASN:HB3	1.95	0.48
4:BE:27:TYR:O	34:B5:447:U:O2'	2.30	0.48
14:BX:114:LYS:HD2	34:B5:571:G:H4'	1.95	0.48
20:BF:73:THR:HG22	20:BF:91:GLU:OE1	2.13	0.48
21:BK:53:GLY:C	21:BK:55:VAL:H	2.21	0.48
34:B5:610:G:H2'	34:B5:610:G:N3	2.27	0.48
34:B5:843:U:C2	34:B5:844:A:H1'	2.48	0.48
34:B5:891:A:O2'	34:B5:892:A:H5'	2.13	0.48
34:B5:1164:G:O2'	34:B5:1612:U:O2	2.31	0.48
38:A1:938:C:OP1	38:A1:963:G:H5'	2.13	0.48
38:A1:1264:G:H22	38:A1:1276:U:H3	1.61	0.48
38:A1:2700:G:H5''	56:AT:17:ARG:HG2	1.95	0.48
49:AM:23:ILE:O	49:AM:30:GLY:N	2.46	0.48
73:Ak:7:ASP:HB3	73:Ak:10:GLN:HB2	1.95	0.48
12:BV:73:ALA:HB1	12:BV:78:LEU:HB2	1.93	0.48
18:Be:35:TYR:CE2	18:Be:39:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1391:A:H2'	34:B5:1392:U:C6	2.48	0.48
36:AB:123:TYR:CZ	36:AB:124:LYS:HG3	2.49	0.48
38:A1:371:G:H4'	38:A1:396:A:N1	2.28	0.48
38:A1:963:G:O2'	63:Aa:29:PRO:O	2.28	0.48
38:A1:2148:U:H2'	38:A1:2149:A:C5	2.49	0.48
38:A1:2406:C:H2'	38:A1:2407:C:H6	1.77	0.48
47:AJ:83:GLY:HA2	47:AJ:112:LEU:HG	1.96	0.48
79:tP:11:C:H2'	79:tP:12:G:C8	2.48	0.48
7:BI:34:ALA:HB2	7:BI:56:ARG:HD2	1.95	0.48
7:BI:184:LEU:HD22	7:BI:188:GLU:HG2	1.94	0.48
22:BP:44:ARG:HE	22:BP:49:MET:HE1	1.77	0.48
23:BQ:5:PRO:HG2	23:BQ:24:ALA:HB2	1.96	0.48
28:BZ:96:SER:OG	34:B5:1530:C:OP2	2.25	0.48
31:Bg:170:ILE:HD12	31:Bg:202:LEU:HD13	1.95	0.48
32:Bf:133:ALA:HB2	34:B5:1252:C:O4'	2.14	0.48
34:B5:814:A:H3'	54:AR:167:ARG:HG2	1.94	0.48
39:A3:112:G:H2'	39:A3:113:C:C6	2.48	0.48
40:A4:143:U:OP1	50:AN:38:ARG:NH2	2.44	0.48
41:AD:108:ARG:CZ	41:AD:253:PHE:HB2	2.44	0.48
44:AG:148:ALA:HA	44:AG:201:THR:HG22	1.95	0.48
45:AH:89:LYS:HB2	45:AH:183:HIS:HB3	1.95	0.48
56:AT:132:PRO:O	56:AT:134:GLN:NE2	2.44	0.48
59:AW:18:GLY:HA3	59:AW:31:PHE:O	2.13	0.48
32:Bf:135:HIS:CD2	34:B5:1250:U:H3	2.31	0.48
34:B5:876:G:H1'	34:B5:944:A:O4'	2.14	0.48
35:AA:10:LYS:HA	35:AA:16:PHE:CD2	2.48	0.48
38:A1:1129:A:OP1	46:AI:13:LYS:NZ	2.39	0.48
45:AH:28:VAL:HG22	45:AH:33:THR:HG23	1.95	0.48
51:AO:108[A]:ILE:HD12	51:AO:160[A]:ARG:CZ	2.44	0.48
54:AR:90:PRO:O	54:AR:93:VAL:HG22	2.13	0.48
70:Ah:86:ARG:O	70:Ah:90:ARG:HG2	2.12	0.48
1:BA:36:TYR:CD1	1:BA:161:PRO:HG3	2.49	0.48
1:BA:76:ILE:HD13	1:BA:98:ILE:HB	1.94	0.48
1:BA:107:PHE:N	1:BA:135:GLU:OE2	2.45	0.48
4:BE:187:ARG:NH1	34:B5:753:A:H5''	2.28	0.48
6:BH:63:PRO:C	6:BH:65:PRO:HD3	2.39	0.48
20:BF:36:ALA:HB2	20:BF:44:ASN:HD21	1.79	0.48
21:BK:21:VAL:HG23	21:BK:66:TYR:HB2	1.94	0.48
32:Bf:145:HIS:ND1	34:B5:1234:A:O2'	2.37	0.48
34:B5:980:G:H4'	34:B5:1776:A:H4'	1.95	0.48
38:A1:225:C:OP1	61:AY:46:LYS:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:422:A:C2	38:A1:2363:A:H4'	2.48	0.48
42:AE:170:LYS:HB3	42:AE:172:HIS:CE1	2.49	0.48
43:AF:85:PHE:CZ	43:AF:147:LEU:HD21	2.48	0.48
46:AI:99:ILE:HG22	46:AI:123:HIS:HB2	1.96	0.48
52:AP:175:ARG:O	52:AP:179:GLN:HG2	2.14	0.48
77:Ao:28:TYR:HB3	77:Ao:69:VAL:HB	1.96	0.48
6:BH:37:GLU:HG2	6:BH:38:LEU:HD12	1.96	0.48
7:BI:42:ARG:O	7:BI:58:LEU:HB2	2.13	0.48
34:B5:17:C:H2'	34:B5:18:C:C6	2.49	0.48
34:B5:209:U:H2'	34:B5:210:A:H5''	1.96	0.48
34:B5:1091:A:H4'	34:B5:1092:A:O4'	2.12	0.48
34:B5:1344:A:H2'	34:B5:1345:A:C8	2.48	0.48
39:A3:47:C:OP2	41:AD:158:ARG:HD3	2.14	0.48
80:tA:21:A:H61	80:tA:46:G:H2'	1.77	0.48
1:BA:144:ILE:HG12	1:BA:158:VAL:HB	1.95	0.48
2:BB:70:LEU:HD13	2:BB:84:ILE:HG13	1.96	0.48
5:BG:119:GLN:HG3	5:BG:120:GLU:N	2.29	0.48
22:BP:33:PHE:CZ	22:BP:112:LEU:HD12	2.48	0.48
27:BU:102:ARG:O	27:BU:106:ILE:HG12	2.14	0.48
29:Bc:16:LEU:O	29:Bc:67:ARG:NH2	2.46	0.48
31:Bg:112:SER:OG	31:Bg:154:VAL:HG22	2.14	0.48
32:Bf:100:LEU:HB3	32:Bf:103:LEU:HD23	1.95	0.48
33:BM:112:ALA:HB3	33:BM:115:VAL:HG22	1.96	0.48
34:B5:950:C:H2'	34:B5:951:A:C8	2.48	0.48
34:B5:1684:U:H2'	34:B5:1685:G:C8	2.49	0.48
38:A1:238:A:H3'	38:A1:239:G:H8	1.77	0.48
38:A1:3204:C:H2'	38:A1:3205:G:C8	2.48	0.48
39:A3:3:U:H2'	39:A3:4:U:H6	1.79	0.48
39:A3:71:G:H2'	39:A3:72:A:H8	1.79	0.48
42:AE:66:SER:HB2	42:AE:76:LEU:HD12	1.94	0.48
54:AR:182:ASP:HA	54:AR:186:LYS:HB2	1.95	0.48
4:BE:125:LYS:HB2	4:BE:226:PHE:CE1	2.49	0.48
5:BG:85:ARG:O	5:BG:87:ARG:NH1	2.47	0.48
19:BD:223:LYS:HD2	19:BD:223:LYS:O	2.14	0.48
19:BD:223:LYS:HE3	31:Bg:191:ASP:HB2	1.96	0.48
20:BF:82:PHE:HB3	29:Bc:49:ARG:NH2	2.28	0.48
27:BU:33:GLN:HB3	27:BU:109:GLU:OE2	2.12	0.48
32:Bf:99:LYS:HG2	32:Bf:100:LEU:HD23	1.96	0.48
34:B5:207:U:H2'	34:B5:208:U:C6	2.49	0.48
34:B5:407:A:H2'	34:B5:408:C:C6	2.49	0.48
38:A1:787:G:H2'	38:A1:788:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AD:164:LYS:HE2	41:AD:195:LEU:HD21	1.96	0.48
73:Ak:14:LEU:HD21	73:Ak:52:TYR:CG	2.49	0.48
77:Ao:71:ARG:CZ	77:Ao:80:ARG:HD3	2.44	0.48
11:BO:16:VAL:HG12	11:BO:18:ARG:HG3	1.95	0.48
12:BV:1:MET:HG2	12:BV:10:GLU:CD	2.39	0.48
29:Bc:64:ARG:HG3	29:Bc:65:ARG:N	2.29	0.48
34:B5:52:U:H2'	34:B5:53:G:C8	2.49	0.48
34:B5:73:U:H5	34:B5:74:U:C2	2.31	0.48
34:B5:1352:G:H2'	34:B5:1354:G:C8	2.49	0.48
38:A1:507:U:H2'	38:A1:508:U:C6	2.49	0.48
38:A1:640:U:H2'	38:A1:641:C:C6	2.49	0.48
38:A1:736:A:H5''	38:A1:737:G:C8	2.49	0.48
38:A1:952:A:H4'	38:A1:968:G:N2	2.28	0.48
38:A1:987:U:H2'	38:A1:988:U:C6	2.49	0.48
38:A1:1016:C:H2'	38:A1:1017:C:C4'	2.44	0.48
38:A1:2510:U:H2'	38:A1:2511:A:H8	1.79	0.48
38:A1:2683:U:H2'	38:A1:2684:C:C6	2.49	0.48
38:A1:3252:G:H2'	38:A1:3253:G:C8	2.48	0.48
52:AP:127:ARG:HB2	52:AP:139:TYR:O	2.13	0.48
5:BG:187:LYS:NZ	34:B5:139:C:O2'	2.32	0.47
22:BP:77:ARG:HG2	34:B5:1241:G:H5'	1.94	0.47
25:BS:144:ARG:NH1	34:B5:1570:A:O2'	2.47	0.47
34:B5:855:A:C2	34:B5:857:U:H1'	2.49	0.47
36:AB:360:ASP:OD2	36:AB:364:LYS:NZ	2.41	0.47
38:A1:1687:U:O4	57:AU:45:GLY:N	2.43	0.47
38:A1:1765:U:H5''	54:AR:43:LYS:NZ	2.28	0.47
56:AT:119:ALA:HA	56:AT:122:GLN:O	2.14	0.47
4:BE:94:ALA:C	4:BE:96:ASN:H	2.22	0.47
5:BG:98:ARG:HD3	5:BG:99:GLY:O	2.13	0.47
7:BI:84:HIS:NE2	7:BI:97:THR:OG1	2.28	0.47
19:BD:80:ALA:O	19:BD:83:THR:HG22	2.14	0.47
34:B5:1039:A:O2'	34:B5:1040:G:H8	1.97	0.47
38:A1:1477:A:OP1	38:A1:3075:G:O2'	2.30	0.47
38:A1:3343:G:H21	38:A1:3362:A:H2	1.62	0.47
45:AH:57:VAL:HG23	45:AH:68:LEU:HD13	1.95	0.47
52:AP:45:GLN:O	52:AP:49:GLU:HG3	2.13	0.47
54:AR:166:ASN:O	54:AR:170:ARG:HD3	2.14	0.47
4:BE:139:VAL:HG13	4:BE:150:PRO:HG3	1.95	0.47
15:BY:49:LYS:NZ	34:B5:782:U:O4	2.47	0.47
26:BT:31:PRO:HD3	26:BT:54:PHE:CZ	2.50	0.47
34:B5:972:G:O2'	38:A1:847:A:N1	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1158:C:H5	34:B5:1163:A:H61	1.62	0.47
38:A1:551:A:O2'	38:A1:552:G:H8	1.97	0.47
38:A1:2160:G:H2'	38:A1:2161:G:H8	1.78	0.47
38:A1:2927:C:H2'	38:A1:2928:C:C6	2.48	0.47
38:A1:3296:A:H2'	38:A1:3297:U:H6	1.79	0.47
50:AN:60:VAL:HG21	50:AN:113:LEU:HD13	1.95	0.47
7:BI:152:ILE:HG13	7:BI:153:GLU:N	2.28	0.47
10:BN:5:HIS:HB3	10:BN:117:LEU:HD23	1.96	0.47
14:BX:92:CYS:HA	14:BX:95:PHE:HD2	1.79	0.47
34:B5:184:C:H2'	34:B5:185:U:H6	1.79	0.47
34:B5:1338:C:H1'	34:B5:1410:A:C4	2.50	0.47
34:B5:1776:A:H2'	34:B5:1777:G:H8	1.79	0.47
35:AA:52:SER:HB3	35:AA:191:LEU:HD12	1.94	0.47
36:AB:222:LYS:HE2	36:AB:331:ASN:HB3	1.96	0.47
38:A1:1034:U:H1'	38:A1:1035:G:C8	2.49	0.47
38:A1:1247:U:H3	38:A1:1267:U:H5	1.62	0.47
38:A1:2882:U:H2'	38:A1:2883:U:C6	2.49	0.47
38:A1:3072:C:H2'	38:A1:3073:A:O4'	2.14	0.47
41:AD:211:LEU:HD11	41:AD:218:ARG:HD2	1.95	0.47
47:AJ:18:VAL:HG22	47:AJ:70:THR:HG22	1.95	0.47
61:AY:109:LEU:HD22	61:AY:115:ARG:NH2	2.30	0.47
80:tA:25:C:C2	80:tA:26:G:C8	3.03	0.47
1:BA:31:VAL:HA	1:BA:34:GLU:HG3	1.96	0.47
2:BB:179:SER:HB3	2:BB:183:GLN:HB2	1.96	0.47
4:BE:151:ASP:OD1	5:BG:215:ARG:NH1	2.25	0.47
5:BG:180:THR:HG23	5:BG:183:ARG:H	1.79	0.47
6:BH:46:ILE:HD13	6:BH:60:ILE:HG13	1.97	0.47
8:BJ:90:LYS:HB2	8:BJ:95:TYR:CD2	2.49	0.47
31:Bg:83:ALA:HB2	31:Bg:113:VAL:HB	1.96	0.47
31:Bg:295:SER:OG	31:Bg:297:ASP:OD1	2.28	0.47
34:B5:1170:G:C2	34:B5:1171:A:C8	3.02	0.47
34:B5:1227:A:H61	34:B5:1256:A:H2'	1.79	0.47
34:B5:1231:U:O2'	34:B5:1258:U:O2'	2.29	0.47
38:A1:8:C:H2'	38:A1:9:U:C6	2.50	0.47
38:A1:2777:G:C2	63:Aa:60:TYR:CE1	3.02	0.47
38:A1:2813:A:H2'	38:A1:2814:G:O4'	2.15	0.47
1:BA:175:TYR:CD2	1:BA:199:PRO:HB3	2.49	0.47
3:BC:205:ARG:NH1	34:B5:7:G:N7	2.56	0.47
23:BQ:97:VAL:HG12	23:BQ:98:ASP:N	2.30	0.47
25:BS:8:GLN:HG3	25:BS:9:GLY:N	2.29	0.47
31:Bg:46:LYS:HE3	31:Bg:56:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:327:U:H2'	34:B5:328:A:C8	2.50	0.47
35:AA:178:PRO:HG2	78:Ap:26:VAL:HG23	1.96	0.47
37:AC:138:ARG:HH21	37:AC:240:PRO:HG2	1.79	0.47
38:A1:94:G:H2'	38:A1:95:A:C8	2.50	0.47
38:A1:314:U:H2'	38:A1:315:C:C6	2.49	0.47
38:A1:999:G:N3	38:A1:1002:A:N6	2.62	0.47
38:A1:1157:G:H2'	38:A1:1158:A:O4'	2.15	0.47
38:A1:1927:G:C8	78:Ap:16:VAL:HG12	2.49	0.47
38:A1:3106:A:H2'	38:A1:3107:U:O4'	2.15	0.47
43:AF:131:GLU:HG3	43:AF:230:GLY:HA2	1.97	0.47
49:AM:113:THR:OG1	49:AM:116:GLU:HG3	2.14	0.47
58:AV:38:ALA:HB3	58:AV:59:MET:HB2	1.97	0.47
4:BE:47:PHE:O	4:BE:51:ARG:HB2	2.14	0.47
4:BE:148:ARG:HH11	34:B5:125:U:H5''	1.80	0.47
5:BG:174:LYS:HG2	34:B5:78:A:H2	1.79	0.47
6:BH:163:ASP:OD1	6:BH:164:TYR:N	2.47	0.47
7:BI:76:THR:OG1	7:BI:105:ASP:HB3	2.15	0.47
8:BJ:129:ILE:HG12	8:BJ:134:ILE:HG13	1.95	0.47
9:BL:109:VAL:HG22	9:BL:137:PHE:HB2	1.95	0.47
11:BO:40:ALA:HB2	11:BO:70:LYS:HB3	1.96	0.47
22:BP:57:MET:HE1	22:BP:89:MET:HG3	1.95	0.47
25:BS:4:VAL:HG21	28:BZ:82:HIS:CG	2.50	0.47
27:BU:61:LYS:HB2	27:BU:86:ILE:HB	1.97	0.47
33:BM:76:GLU:OE2	33:BM:88:LEU:HD21	2.14	0.47
34:B5:196:G:O2'	34:B5:197:A:OP1	2.29	0.47
34:B5:585:A:H2'	34:B5:586:G:H8	1.79	0.47
36:AB:161:LEU:HD22	36:AB:178:LEU:HD21	1.96	0.47
38:A1:39:A:H5''	63:Aa:35:ALA:HB2	1.96	0.47
38:A1:292:U:OP2	50:AN:68:ARG:NH2	2.46	0.47
38:A1:506:U:H2'	38:A1:507:U:O4'	2.15	0.47
38:A1:616:G:H2'	38:A1:617:G:C8	2.49	0.47
38:A1:2807:U:O2'	38:A1:2809:C:OP1	2.30	0.47
38:A1:2812:C:H2'	38:A1:2813:A:C8	2.50	0.47
38:A1:2930:A:H2'	38:A1:2931:C:C6	2.50	0.47
39:A3:71:G:H2'	39:A3:72:A:C8	2.50	0.47
40:A4:106:C:H5''	40:A4:108:C:OP2	2.15	0.47
44:AG:228:GLU:HA	44:AG:231:LYS:HZ3	1.78	0.47
49:AM:23:ILE:HG13	49:AM:63:VAL:HG12	1.97	0.47
59:AW:52:THR:HG22	59:AW:54:LEU:N	2.28	0.47
60:AX:72:ALA:O	60:AX:76:VAL:HG23	2.15	0.47
61:AY:85:VAL:HG12	61:AY:97:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:47:LEU:O	11:BO:37:GLU:HG3	2.15	0.47
4:BE:222:LEU:O	4:BE:225:VAL:HG12	2.14	0.47
15:BY:56:SER:OG	15:BY:74:LEU:HB2	2.14	0.47
20:BF:175:LEU:HD22	20:BF:198:LEU:HD23	1.97	0.47
21:BK:38:LYS:HE2	21:BK:41:TYR:CZ	2.50	0.47
21:BK:50:THR:HG21	21:BK:57:THR:OG1	2.15	0.47
26:BT:63:ARG:O	26:BT:67:MET:HG2	2.15	0.47
31:Bg:42:LEU:HB2	31:Bg:61:PHE:HB2	1.97	0.47
31:Bg:50:ASP:CG	31:Bg:51:ASP:H	2.21	0.47
31:Bg:93:ASP:HB2	31:Bg:100:TYR:CE1	2.48	0.47
31:Bg:106:HIS:CE1	31:Bg:132:LYS:HD2	2.49	0.47
34:B5:235:G:O6	34:B5:237:C:N4	2.47	0.47
34:B5:1345:A:N1	34:B5:1380:U:H5	2.12	0.47
38:A1:264:G:OP1	71:Ai:34:SER:HB2	2.15	0.47
38:A1:528:U:H2'	38:A1:529:A:C8	2.50	0.47
38:A1:863:C:H2'	38:A1:864:G:O4'	2.15	0.47
38:A1:1329:U:OP1	68:Af:17:GLN:NE2	2.42	0.47
38:A1:1621:A:H2'	38:A1:1622:U:H6	1.80	0.47
38:A1:3192:U:H2'	38:A1:3193:C:C6	2.50	0.47
53:AQ:96:PHE:CE2	53:AQ:113:LYS:HG2	2.50	0.47
62:AZ:25:ILE:HA	62:AZ:43:VAL:HG12	1.97	0.47
2:BB:127:VAL:HG11	2:BB:173:THR:HG22	1.96	0.47
7:BI:116:HIS:HD2	7:BI:117:TYR:CE1	2.32	0.47
8:BJ:8:TYR:H	34:B5:25:C:H41	1.61	0.47
8:BJ:123:HIS:CE1	18:Be:37:ARG:HB2	2.50	0.47
18:Be:17:GLN:NE2	34:B5:563:U:H4'	2.30	0.47
18:Be:27:PRO:HG3	34:B5:506:A:C4	2.50	0.47
19:BD:64:ARG:NE	19:BD:64:ARG:HA	2.29	0.47
19:BD:191:ASP:HB3	19:BD:194:LYS:HE2	1.96	0.47
34:B5:1451:C:H2'	34:B5:1452:U:H6	1.80	0.47
37:AC:285:ASP:OD2	37:AC:288:ARG:HB2	2.14	0.47
38:A1:830:A:H2'	38:A1:831:G:O4'	2.15	0.47
38:A1:2218:G:H2'	38:A1:2219:A:H8	1.80	0.47
38:A1:2398:A:OP1	38:A1:2873:U:H4'	2.15	0.47
38:A1:2881:C:H2'	38:A1:2882:U:C6	2.50	0.47
39:A3:39:C:H4'	47:AJ:44:THR:HG23	1.97	0.47
2:BB:28:GLU:OE2	2:BB:50:LYS:HD3	2.15	0.47
4:BE:23:LEU:HD22	8:BJ:3:ARG:NH2	2.30	0.47
6:BH:150:GLN:HB3	6:BH:181:ILE:HG22	1.98	0.47
20:BF:205:SER:O	20:BF:206:SER:OG	2.30	0.47
21:BK:17:GLN:HE21	21:BK:90:THR:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:89:LEU:HD21	31:Bg:124:SER:HB2	1.97	0.47
34:B5:1414:U:H3'	34:B5:1415:PSU:H5'	1.95	0.47
38:A1:407:A:C2	40:A4:17:A:H1'	2.49	0.47
38:A1:444:U:P	38:A1:445:G:H21	2.38	0.47
38:A1:673:U:H2'	38:A1:674:G:C8	2.50	0.47
38:A1:708:G:N2	38:A1:711:A:OP2	2.41	0.47
38:A1:817:A:O2'	72:Aj:11:ARG:HG2	2.15	0.47
38:A1:1119:C:H2'	38:A1:1120:A:H8	1.80	0.47
47:AJ:82:ARG:NH2	47:AJ:112:LEU:O	2.48	0.47
50:AN:35:VAL:O	50:AN:64:VAL:HA	2.15	0.47
61:AY:42:GLN:O	61:AY:125:LYS:NZ	2.41	0.47
63:Aa:84:GLU:OE2	63:Aa:87:ARG:NH1	2.48	0.47
3:BC:88:LYS:HD2	3:BC:95:ARG:CZ	2.46	0.46
9:BL:19:ILE:HG13	9:BL:19:ILE:O	2.15	0.46
34:B5:30:G:H2'	34:B5:31:C:C6	2.51	0.46
34:B5:208:U:H2'	34:B5:209:U:C6	2.50	0.46
36:AB:250:ALA:HB3	38:A1:2880:PSU:H1'	1.97	0.46
36:AB:266:ARG:HD3	38:A1:2988:C:O2'	2.15	0.46
38:A1:604:G:H2'	38:A1:605:U:C6	2.50	0.46
38:A1:1765:U:H3'	54:AR:43:LYS:NZ	2.30	0.46
38:A1:2876:C:H2'	38:A1:2877:G:O4'	2.16	0.46
50:AN:80:THR:OG1	50:AN:87:GLN:HA	2.15	0.46
55:AS:80:ARG:HG2	55:AS:122:HIS:HB2	1.95	0.46
63:Aa:116:GLY:HA3	63:Aa:137:LYS:NZ	2.29	0.46
65:Ac:14:LEU:O	65:Ac:18:ILE:HG12	2.15	0.46
80:tA:39:C:H2'	80:tA:40:C:O2	2.15	0.46
1:BA:89:PHE:O	1:BA:93:THR:OG1	2.29	0.46
4:BE:201:HIS:ND1	4:BE:207:LEU:HD13	2.30	0.46
9:BL:19:ILE:HG21	9:BL:34:TRP:HB2	1.96	0.46
15:BY:83:LYS:NZ	15:BY:97:ALA:HB2	2.30	0.46
19:BD:145:ALA:O	34:B5:1275:A:O2'	2.26	0.46
34:B5:82:U:H2'	34:B5:83:G:O4'	2.15	0.46
34:B5:205:U:C2	34:B5:206:A:C8	3.03	0.46
34:B5:886:U:H2'	34:B5:887:A:H8	1.79	0.46
34:B5:968:U:H2'	34:B5:969:C:O4'	2.15	0.46
34:B5:1160:A:H2'	34:B5:1161:C:C6	2.50	0.46
34:B5:1451:C:H2'	34:B5:1452:U:C6	2.50	0.46
38:A1:20:A:H2'	38:A1:21:G:C8	2.49	0.46
38:A1:29:C:H4'	38:A1:62:A:H4'	1.96	0.46
38:A1:240:U:HO2'	38:A1:241:G:P	2.37	0.46
38:A1:718:G:OP1	63:Aa:117:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1447:G:OP1	52:AP:65:SER:OG	2.33	0.46
38:A1:2152:A:H2'	38:A1:2153:U:H6	1.80	0.46
38:A1:2444:C:H6	38:A1:2503:G:H5''	1.81	0.46
72:Aj:52:LYS:HG2	72:Aj:55:ARG:NH2	2.29	0.46
7:BI:39:GLY:HA2	7:BI:61:GLU:CG	2.41	0.46
10:BN:35:GLU:HA	10:BN:38:VAL:HG22	1.97	0.46
19:BD:40:ARG:HH12	19:BD:49:ILE:HD11	1.80	0.46
25:BS:39:GLY:H	34:B5:1566:U:H5''	1.80	0.46
25:BS:88:ARG:NH2	25:BS:112:ASP:OD1	2.49	0.46
34:B5:196:G:HO2'	34:B5:197:A:P	2.37	0.46
34:B5:329:G:H2'	34:B5:330:G:H8	1.79	0.46
34:B5:887:A:H2'	34:B5:888:U:H6	1.80	0.46
34:B5:1107:G:O2'	34:B5:1108:G:H5'	2.15	0.46
38:A1:1203:A:N3	38:A1:2855:U:O2'	2.45	0.46
38:A1:1950:U:H2'	38:A1:1951:C:C6	2.50	0.46
38:A1:2222:A:O2'	38:A1:2223:A:OP1	2.30	0.46
38:A1:2662:G:H2'	38:A1:2663:G:C8	2.50	0.46
40:A4:6:U:H2'	40:A4:7:U:C6	2.50	0.46
46:AI:49:CYS:HB3	46:AI:168:SER:HB3	1.98	0.46
53:AQ:90:ASP:OD1	53:AQ:92:ARG:NE	2.34	0.46
55:AS:93:GLU:OE1	55:AS:135:VAL:HG13	2.16	0.46
56:AT:8:ARG:O	56:AT:11:THR:OG1	2.31	0.46
62:AZ:4:PHE:HA	62:AZ:6:LYS:NZ	2.31	0.46
6:BH:76:LYS:O	6:BH:79:ARG:HG2	2.15	0.46
23:BQ:99:GLU:OE2	31:Bg:57:PRO:HB2	2.15	0.46
34:B5:800:U:H2'	34:B5:801:G:H8	1.78	0.46
34:B5:1457:C:O2'	34:B5:1458:G:H5'	2.15	0.46
34:B5:1525:A:H2'	34:B5:1526:A:C8	2.51	0.46
34:B5:1556:A:H1'	34:B5:1560:U:OP2	2.16	0.46
38:A1:45:A:P	50:AN:85:THR:HG21	2.55	0.46
38:A1:945:C:H2'	38:A1:946:U:H6	1.81	0.46
38:A1:1081:U:H5''	38:A1:1082:U:H5	1.80	0.46
40:A4:67:U:H5''	72:Aj:85:LYS:O	2.15	0.46
46:AI:102:MET:SD	46:AI:112:GLN:NE2	2.88	0.46
73:Ak:43:PHE:HE1	73:Ak:66:ILE:HD13	1.80	0.46
5:BG:25:ARG:HA	5:BG:28:PHE:CD2	2.50	0.46
8:BJ:108:ARG:NH1	8:BJ:145:SER:HB3	2.30	0.46
8:BJ:171:ARG:NH2	34:B5:538:A:OP2	2.48	0.46
23:BQ:46:PHE:HA	23:BQ:49:TYR:HB2	1.97	0.46
33:BM:87:PRO:HB3	33:BM:137:MET:HE2	1.98	0.46
34:B5:408:C:O2'	34:B5:1732:A:O2'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:118:U:O2	38:A1:121:A:H5''	2.15	0.46
38:A1:792:G:H5''	63:Aa:2:PRO:HD3	1.96	0.46
38:A1:966:PSU:H2'	38:A1:967:A:C8	2.50	0.46
38:A1:1033:U:H5'	38:A1:1034:U:H5	1.81	0.46
40:A4:69:U:H2'	40:A4:70:G:O4'	2.16	0.46
40:A4:88:A:HO2'	40:A4:89:A:P	2.38	0.46
41:AD:85:ARG:HH12	41:AD:254:LYS:H	1.63	0.46
42:AE:7:PRO:HG2	42:AE:10:TYR:CE2	2.50	0.46
42:AE:43:LEU:HD11	42:AE:85:ILE:HG13	1.97	0.46
44:AG:74:THR:HG22	44:AG:164:VAL:HG22	1.98	0.46
55:AS:16:THR:HG22	55:AS:17:GLU:N	2.31	0.46
62:AZ:90:GLU:OE1	62:AZ:90:GLU:N	2.48	0.46
76:An:1:MET:HE1	76:An:9:ARG:HH11	1.80	0.46
79:tP:22:G:N7	79:tP:46:G:O6	2.48	0.46
2:BB:129:THR:OG1	2:BB:131:ASP:O	2.29	0.46
4:BE:42:LEU:HD23	4:BE:101:LEU:HD11	1.96	0.46
6:BH:70:PHE:O	6:BH:74:GLN:HB2	2.15	0.46
20:BF:134:VAL:O	20:BF:138:THR:HG23	2.16	0.46
25:BS:38:VAL:HG23	25:BS:42:TYR:HB3	1.97	0.46
34:B5:183:U:H2'	34:B5:184:C:C6	2.50	0.46
34:B5:183:U:H2'	34:B5:184:C:H6	1.79	0.46
34:B5:524:U:H1'	34:B5:527:A:N7	2.30	0.46
34:B5:752:A:O2'	34:B5:753:A:OP1	2.32	0.46
38:A1:70:A:H5'	63:Aa:64:GLN:HE22	1.80	0.46
38:A1:734:C:H3'	38:A1:735:A:C8	2.50	0.46
38:A1:3283:U:O2'	38:A1:3284:G:OP1	2.32	0.46
40:A4:74:U:C4	61:AY:74:TYR:HD1	2.34	0.46
57:AU:98:THR:HG22	57:AU:99:LYS:HD2	1.97	0.46
62:AZ:90:GLU:HG3	62:AZ:93:LYS:HZ2	1.81	0.46
63:Aa:90:TYR:CD1	63:Aa:100:PRO:HG3	2.51	0.46
5:BG:102:VAL:HG13	5:BG:106:LEU:HD12	1.97	0.46
15:BY:41:ARG:HH21	15:BY:53:ASP:HA	1.81	0.46
16:Ba:44:ILE:HG23	16:Ba:45:VAL:HG23	1.97	0.46
16:Ba:88:SER:OG	16:Ba:90:GLU:OE2	2.25	0.46
17:Bb:33:LEU:HD23	17:Bb:81:ARG:HA	1.96	0.46
18:Be:14:VAL:HA	18:Be:17:GLN:HG2	1.98	0.46
20:BF:182:ALA:O	20:BF:186:ASN:ND2	2.49	0.46
21:BK:29:GLN:HG3	21:BK:31:LYS:H	1.80	0.46
32:Bf:139:LEU:O	32:Bf:147:VAL:HA	2.16	0.46
34:B5:116:U:H2'	34:B5:117:U:C6	2.50	0.46
34:B5:121:U:H2'	34:B5:122:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AA:2:GLY:HA2	35:AA:207:VAL:HG23	1.96	0.46
38:A1:275:U:H2'	38:A1:276:U:C6	2.51	0.46
38:A1:599:C:H2'	38:A1:600:G:O4'	2.15	0.46
38:A1:774:G:O2'	38:A1:775:A:H5'	2.15	0.46
38:A1:2510:U:H2'	38:A1:2511:A:C8	2.50	0.46
38:A1:3096:C:H2'	38:A1:3097:C:C6	2.51	0.46
38:A1:3255:U:H2'	38:A1:3256:G:H8	1.80	0.46
38:A1:3298:C:C2	38:A1:3299:A:C8	3.04	0.46
38:A1:3332:U:H2'	38:A1:3333:G:O4'	2.16	0.46
42:AE:64:LEU:HD11	42:AE:76:LEU:HG	1.97	0.46
49:AM:32:LEU:HD11	49:AM:94:TRP:CD1	2.51	0.46
73:Ak:62:ALA:O	73:Ak:66:ILE:HG12	2.16	0.46
78:Ap:8:VAL:O	78:Ap:11:THR:OG1	2.34	0.46
80:tA:3:C:H2'	80:tA:4:G:C8	2.51	0.46
80:tA:43:G:H2'	80:tA:44:A:C8	2.51	0.46
4:BE:125:LYS:HB2	4:BE:226:PHE:HD1	1.80	0.46
4:BE:131:LEU:HD12	34:B5:251:A:C2	2.51	0.46
4:BE:166:SER:O	4:BE:168:LYS:N	2.45	0.46
29:Bc:17:GLY:HA3	29:Bc:67:ARG:NE	2.31	0.46
34:B5:1759:C:H2'	34:B5:1760:G:O4'	2.16	0.46
36:AB:208:VAL:O	36:AB:340:LYS:NZ	2.48	0.46
37:AC:125:ALA:O	37:AC:129:THR:HG23	2.15	0.46
38:A1:1456:A:N1	38:A1:1476:G:O2'	2.43	0.46
38:A1:2206:G:H21	38:A1:2208:A:N6	2.14	0.46
38:A1:3085:G:H5''	38:A1:3086:A:OP1	2.16	0.46
38:A1:3154:C:O2'	38:A1:3157:U:H1'	2.16	0.46
45:AH:31:ARG:HD2	45:AH:81:GLY:O	2.16	0.46
58:AV:18:PRO:HA	58:AV:51:ALA:HA	1.98	0.46
2:BB:131:ASP:OD1	2:BB:180:THR:HG23	2.16	0.46
26:BT:105:LEU:HD13	26:BT:122:ARG:HD3	1.97	0.46
34:B5:237:C:O2'	34:B5:835:U:OP1	2.34	0.46
34:B5:1001:A:OP1	79:tP:38:A:O2'	2.31	0.46
34:B5:1350:U:H2'	34:B5:1351:G:C8	2.51	0.46
35:AA:183:GLY:HA2	38:A1:896:A:H5''	1.98	0.46
37:AC:344:ALA:HB2	38:A1:516:A:H5''	1.97	0.46
38:A1:209:A:H4'	38:A1:211:A:N7	2.31	0.46
38:A1:1194:G:H2'	38:A1:1195:A:C8	2.51	0.46
38:A1:1951:C:H2'	38:A1:1952:G:C8	2.51	0.46
38:A1:2609:A:H2'	38:A1:2610:G:C8	2.51	0.46
38:A1:2840:C:H2'	38:A1:2841:G:O4'	2.16	0.46
50:AN:153:ASP:OD2	50:AN:154:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AT:18:ASP:HB2	56:AT:21:LYS:HB2	1.97	0.46
60:AX:97:LYS:O	60:AX:101:GLU:OE1	2.34	0.46
71:AI:96:ALA:HA	71:AI:99:ARG:HG2	1.98	0.46
4:BE:148:ARG:NH1	34:B5:125:U:H5'	2.31	0.46
4:BE:230:GLU:HG3	4:BE:231:GLN:N	2.31	0.46
5:BG:26:VAL:HG11	5:BG:40:ALA:HB3	1.97	0.46
17:Bb:46:VAL:HG12	17:Bb:54:VAL:HG11	1.98	0.46
20:BF:77:TYR:HD1	20:BF:83:ARG:HG3	1.81	0.46
21:BK:25:LYS:NZ	34:B5:1435:G:N7	2.52	0.46
25:BS:126:ARG:HB2	25:BS:133:VAL:HG12	1.98	0.46
26:BT:12:GLN:OE1	34:B5:1529:C:O2'	2.30	0.46
31:Bg:150:TRP:HB2	31:Bg:174:ASN:ND2	2.26	0.46
34:B5:751:G:H2'	34:B5:752:A:H8	1.81	0.46
34:B5:1391:A:H2'	34:B5:1392:U:H6	1.81	0.46
35:AA:152:SER:OG	38:A1:2157:G:N7	2.40	0.46
38:A1:11:A:H2'	38:A1:12:A:C8	2.51	0.46
38:A1:394:G:N1	38:A1:397:A:OP2	2.49	0.46
38:A1:412:G:H2'	38:A1:413:U:C6	2.51	0.46
38:A1:2588:U:OP1	44:AG:241:LYS:NZ	2.48	0.46
40:A4:74:U:C4	61:AY:74:TYR:CD1	3.03	0.46
44:AG:68:ARG:HD3	44:AG:237:ILE:O	2.16	0.46
44:AG:172:LYS:HG3	44:AG:173:MET:HE2	1.98	0.46
58:AV:84:SER:HA	58:AV:94:TYR:HB3	1.97	0.46
79:tP:51:C:C2	79:tP:52:G:C8	3.04	0.46
5:BG:137:ARG:HH12	34:B5:144:U:H5	1.65	0.45
5:BG:142:ARG:CZ	5:BG:149:LYS:HA	2.46	0.45
10:BN:92:ILE:HG23	10:BN:141:TYR:HE2	1.81	0.45
14:BX:92:CYS:HG	14:BX:136:TRP:CD1	2.34	0.45
34:B5:1358:G:H2'	34:B5:1359:C:H6	1.79	0.45
38:A1:1666:G:H2'	38:A1:1667:A:H8	1.82	0.45
38:A1:2430:A:H2'	38:A1:2431:C:C6	2.51	0.45
38:A1:3166:C:H2'	38:A1:3167:A:C8	2.51	0.45
40:A4:103:G:OP2	40:A4:105:A:O2'	2.28	0.45
48:AL:42:ARG:O	48:AL:46:ILE:HG12	2.15	0.45
52:AP:40:GLU:HG2	52:AP:43:LYS:HG2	1.96	0.45
4:BE:90:ILE:HG12	4:BE:99:PHE:HB2	1.98	0.45
11:BO:40:ALA:HB2	11:BO:70:LYS:HG2	1.98	0.45
19:BD:76:ARG:HA	21:BK:63:TYR:OH	2.16	0.45
20:BF:133:VAL:HG22	20:BF:198:LEU:HD13	1.97	0.45
23:BQ:28:LEU:HD11	23:BQ:30:LYS:HE3	1.98	0.45
24:BR:28:PHE:CZ	24:BR:32:LYS:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BT:106:GLN:O	26:BT:110:LYS:HG2	2.16	0.45
27:BU:69:LYS:HG2	27:BU:80:GLU:HG3	1.97	0.45
28:BZ:60:VAL:HG12	28:BZ:80:LEU:HD11	1.97	0.45
28:BZ:76:ALA:O	28:BZ:80:LEU:HD23	2.16	0.45
34:B5:156:A:H2'	34:B5:157:A:O4'	2.16	0.45
34:B5:1782:MA6:H5''	76:An:1:MET:SD	2.57	0.45
38:A1:929:A:H2'	38:A1:930:U:C6	2.51	0.45
38:A1:1018:G:H21	38:A1:1019:G:HO2'	1.42	0.45
38:A1:1805:C:H2'	38:A1:1806:A:H8	1.81	0.45
40:A4:141:C:OP1	50:AN:109:ARG:NH2	2.45	0.45
46:AI:36:LEU:HD13	46:AI:73:ASN:HB2	1.98	0.45
53:AQ:62:VAL:HG13	53:AQ:66:ARG:HD2	1.98	0.45
55:AS:79:VAL:HG21	55:AS:106:LEU:HD21	1.98	0.45
58:AV:104:ASN:HB2	58:AV:105:PRO:HD2	1.99	0.45
4:BE:250:GLU:O	4:BE:254:ARG:HD3	2.16	0.45
20:BF:81:ARG:HA	34:B5:1615:C:C5	2.52	0.45
21:BK:64:TYR:OH	34:B5:1435:G:O6	2.30	0.45
27:BU:83:GLU:OE2	27:BU:85:ARG:NH2	2.49	0.45
34:B5:1138:A:H2'	34:B5:1139:A:H8	1.82	0.45
34:B5:1171:A:H2'	34:B5:1172:G:H8	1.76	0.45
34:B5:1688:U:H5''	34:B5:1714:A:N1	2.31	0.45
38:A1:2679:A:O2'	47:AJ:52:TYR:OH	2.23	0.45
38:A1:3335:A:H2'	38:A1:3336:A:C8	2.51	0.45
62:AZ:70:PRO:HG3	62:AZ:115:LYS:HB2	1.97	0.45
64:Ab:40:ARG:HH11	64:Ab:40:ARG:HG3	1.80	0.45
5:BG:45:PHE:HE1	5:BG:121:LEU:HD21	1.81	0.45
10:BN:108:ASP:OD1	34:B5:878:G:O2'	2.30	0.45
14:BX:144:ARG:HA	14:BX:144:ARG:HD3	1.77	0.45
16:Ba:46:GLU:O	16:Ba:50:VAL:HG23	2.16	0.45
21:BK:84:GLU:O	21:BK:86:ILE:HD12	2.16	0.45
34:B5:120:PSU:H2'	34:B5:121:U:C6	2.51	0.45
34:B5:1575:G7M:O2'	34:B5:1576:A:O5'	2.34	0.45
38:A1:1219:C:O2'	38:A1:1286:A:N1	2.41	0.45
38:A1:3288:G:O2'	38:A1:3289:G:H8	2.00	0.45
38:A1:3295:A:H2'	38:A1:3296:A:H8	1.79	0.45
39:A3:4:U:H2'	39:A3:5:G:C8	2.52	0.45
45:AH:85:GLY:HA3	45:AH:187:ILE:HD12	1.99	0.45
49:AM:42:LYS:C	49:AM:60:LEU:HD23	2.41	0.45
55:AS:109:ASP:OD1	55:AS:113:ARG:NE	2.44	0.45
79:tP:18:G:N2	79:tP:58:A:O4'	2.50	0.45
80:tA:30:G:H22	80:tA:40:C:H5	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:103:TYR:HA	4:BE:109:PHE:HA	1.98	0.45
6:BH:86:GLN:O	6:BH:87:ASP:OD1	2.35	0.45
9:BL:27:THR:OG1	9:BL:28:SER:N	2.48	0.45
17:Bb:32:PHE:O	17:Bb:82:LYS:HG2	2.16	0.45
19:BD:29:LEU:HB2	19:BD:34:TYR:HB2	1.97	0.45
20:BF:41:LYS:HB3	20:BF:44:ASN:HA	1.99	0.45
26:BT:91:TYR:HB2	34:B5:1590:G:OP1	2.17	0.45
37:AC:329:PRO:HB3	43:AF:41:ARG:NH2	2.31	0.45
38:A1:649:A:H2'	38:A1:650:C:C6	2.52	0.45
38:A1:727:G:O6	38:A1:742:G:O2'	2.33	0.45
38:A1:1120:A:H2'	38:A1:1121:U:C6	2.51	0.45
38:A1:1265:U:C5	38:A1:1277:C:H1'	2.51	0.45
38:A1:2504:U:H4'	71:Ai:63:ASN:HD21	1.82	0.45
40:A4:63:G:OP1	40:A4:90:U:H5''	2.17	0.45
42:AE:66:SER:HB2	42:AE:76:LEU:CD1	2.47	0.45
44:AG:162:LEU:HA	50:AN:7:LEU:HD11	1.99	0.45
50:AN:183:THR:O	50:AN:183:THR:OG1	2.34	0.45
63:Aa:83:PRO:HG2	63:Aa:86:LYS:HG2	1.98	0.45
65:Ac:73:GLY:N	65:Ac:76:GLU:OE2	2.39	0.45
80:tA:63:G:H2'	80:tA:64:A:H8	1.81	0.45
7:BI:41:LYS:HA	7:BI:59:ARG:O	2.15	0.45
8:BJ:149:ARG:O	8:BJ:151:ASP:N	2.49	0.45
12:BV:7:GLN:HG2	12:BV:7:GLN:O	2.17	0.45
15:BY:10:ARG:NH2	34:B5:778:G:N7	2.64	0.45
17:Bb:69:GLY:HA3	34:B5:1048:G:O3'	2.16	0.45
34:B5:1628:U:H2'	34:B5:1629:G:C8	2.51	0.45
38:A1:1480:G:O2'	38:A1:1871:U:O4	2.28	0.45
24:BR:72:LYS:HE2	24:BR:76:GLU:OE2	2.16	0.45
26:BT:86:ARG:NH1	26:BT:90:PRO:O	2.47	0.45
34:B5:1003:A:H1'	34:B5:1005:A:N7	2.32	0.45
34:B5:1511:U:H2'	34:B5:1512:G:C8	2.51	0.45
38:A1:718:G:C2	38:A1:721:G:H1'	2.52	0.45
38:A1:1073:U:H2'	38:A1:1074:U:C6	2.52	0.45
38:A1:3349:C:H2'	38:A1:3350:C:O4'	2.17	0.45
54:AR:162:ARG:HD2	54:AR:162:ARG:C	2.42	0.45
73:Ak:14:LEU:HD12	73:Ak:17:ARG:HD3	1.98	0.45
1:BA:63:ILE:CD1	12:BV:36:VAL:HG22	2.47	0.45
4:BE:180:LEU:HD12	4:BE:193:GLY:O	2.16	0.45
9:BL:109:VAL:HG21	9:BL:125:VAL:HG11	1.98	0.45
15:BY:135:ASP:OD1	15:BY:135:ASP:N	2.48	0.45
19:BD:118:ALA:O	19:BD:122:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BF:146:THR:HB	20:BF:157:ARG:HB3	1.99	0.45
24:BR:13:SER:O	24:BR:17:ILE:HG13	2.17	0.45
34:B5:29:U:H2'	34:B5:30:G:H8	1.81	0.45
34:B5:181:A:H2'	34:B5:182:A:H8	1.81	0.45
34:B5:1138:A:H2'	34:B5:1139:A:C8	2.52	0.45
38:A1:310:U:C2	38:A1:2779:A:N6	2.81	0.45
38:A1:2144:A:H1'	38:A1:2281:A:N6	2.31	0.45
38:A1:2683:U:H2'	38:A1:2684:C:H6	1.82	0.45
39:A3:92:A:C5	39:A3:93:C:H1'	2.52	0.45
40:A4:6:U:H2'	40:A4:7:U:H6	1.82	0.45
41:AD:79:TYR:O	41:AD:82:GLU:HG2	2.17	0.45
46:AI:192:ASP:HA	46:AI:197:VAL:HG12	1.98	0.45
47:AJ:112:LEU:HD21	47:AJ:127:PHE:CZ	2.50	0.45
53:AQ:83:VAL:O	53:AQ:103:ALA:HA	2.16	0.45
55:AS:77:VAL:HG13	55:AS:126:VAL:HG22	1.99	0.45
58:AV:6:ALA:HB1	58:AV:125:LEU:HD11	1.99	0.45
1:BA:126:PRO:HG2	1:BA:151:SER:HB3	1.98	0.45
10:BN:55:ARG:HD3	34:B5:960:U:H5'	1.98	0.45
19:BD:169:ASP:OD1	19:BD:188:ILE:HB	2.17	0.45
25:BS:41:ARG:NH1	26:BT:46:PRO:HG3	2.32	0.45
37:AC:179:LEU:O	37:AC:183:LYS:HG2	2.17	0.45
38:A1:38:U:H2'	38:A1:39:A:O4'	2.17	0.45
38:A1:178:U:H2'	38:A1:179:C:C6	2.50	0.45
48:AL:185:LYS:O	48:AL:189:GLU:OE1	2.35	0.45
59:AW:45:ASN:HD22	59:AW:48:ARG:HG3	1.82	0.45
1:BA:40:ALA:HA	1:BA:46:HIS:HA	1.99	0.45
25:BS:18:LEU:HD21	25:BS:101:LEU:HD13	1.99	0.45
32:Bf:145:HIS:CE1	34:B5:1234:A:HO2'	2.31	0.45
33:BM:72:ILE:H	33:BM:72:ILE:HD12	1.82	0.45
34:B5:604:A:H2'	34:B5:605:A:O4'	2.17	0.45
36:AB:256:HIS:HA	36:AB:257:PRO:C	2.42	0.45
38:A1:952:A:OP1	64:Ab:18:ARG:NH2	2.49	0.45
38:A1:1128:U:H2'	38:A1:1129:A:O4'	2.16	0.45
38:A1:2203:U:H2'	38:A1:2204:C:H6	1.80	0.45
38:A1:2585:G:H2'	38:A1:2585:G:N3	2.32	0.45
39:A3:14:U:H5	39:A3:66:A:N1	2.15	0.45
43:AF:163:LEU:O	43:AF:165:ASP:N	2.50	0.45
59:AW:47:ARG:HG2	59:AW:54:LEU:HG	1.99	0.45
75:Am:79:GLU:HG2	75:Am:82:LEU:HB2	1.99	0.45
20:BF:40:ILE:HB	20:BF:67:PRO:HB2	1.98	0.44
34:B5:193:U:O2'	34:B5:195:G:H8	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:297:U:H2'	34:B5:298:C:C6	2.51	0.44
34:B5:340:U:H2'	34:B5:341:A:C8	2.52	0.44
34:B5:556:A:H1'	34:B5:590:C:C1'	2.47	0.44
34:B5:886:U:C2	34:B5:887:A:C8	3.05	0.44
36:AB:212:ASN:OD1	36:AB:354:VAL:HG22	2.17	0.44
36:AB:219:ALA:HB2	36:AB:336:VAL:HG23	1.99	0.44
38:A1:87:U:OP1	53:AQ:167:SER:OG	2.32	0.44
38:A1:675:C:O2'	38:A1:679:U:OP1	2.32	0.44
38:A1:712:G:H5'	48:AL:174:ARG:NH1	2.32	0.44
38:A1:733:G:H21	38:A1:736:A:H2	1.65	0.44
38:A1:1658:G:H2'	38:A1:1659:U:C6	2.52	0.44
38:A1:1925:U:O2'	38:A1:1927:G:N7	2.49	0.44
38:A1:2094:C:H2'	38:A1:2095:G:C8	2.52	0.44
38:A1:3278:C:OP1	68:Af:54:ARG:NH2	2.41	0.44
38:A1:3334:U:H4'	38:A1:3335:A:H5'	1.99	0.44
46:AI:179:PRO:HA	46:AI:182:LEU:HG	1.99	0.44
49:AM:14:LEU:H	49:AM:19:ARG:NH2	2.15	0.44
54:AR:14:VAL:HG21	54:AR:42:ARG:HG3	2.00	0.44
60:AX:46:TYR:CD1	70:Ah:75:TYR:HB3	2.52	0.44
65:Ac:24:THR:HG23	65:Ac:93:LEU:HD11	1.99	0.44
69:Ag:22:VAL:HG11	69:Ag:30:LEU:HD23	1.98	0.44
2:BB:124:ASN:HD21	2:BB:136:ARG:CG	2.31	0.44
4:BE:72:VAL:HG22	4:BE:90:ILE:HG22	1.99	0.44
5:BG:7:TYR:HD1	5:BG:113:ILE:HB	1.82	0.44
11:BO:53:ASP:CG	20:BF:156:ARG:HH22	2.24	0.44
15:BY:5:VAL:HG13	15:BY:35:VAL:HG11	2.00	0.44
18:Be:20:LYS:NZ	18:Be:22:GLU:OE2	2.48	0.44
19:BD:66:ILE:O	19:BD:70:THR:HG23	2.16	0.44
31:Bg:70:ASP:HB3	31:Bg:113:VAL:HG12	1.99	0.44
34:B5:891:A:H2'	34:B5:892:A:C8	2.52	0.44
34:B5:1120:U:H2'	34:B5:1121:C:C6	2.51	0.44
37:AC:159:ILE:HG23	37:AC:164:GLU:HG3	1.99	0.44
38:A1:293:C:H2'	38:A1:294:U:O4'	2.17	0.44
38:A1:589:A:H8	38:A1:590:G:C8	2.35	0.44
38:A1:1818:U:O2'	38:A1:1819:U:OP1	2.34	0.44
38:A1:2674:A:H2'	38:A1:2675:C:C6	2.52	0.44
38:A1:2793:G:H4'	77:Ao:66:LYS:HE3	2.00	0.44
38:A1:3302:U:H3	38:A1:3312:U:H3	1.64	0.44
42:AE:154:LEU:HD23	42:AE:157:GLN:HE21	1.83	0.44
44:AG:103:ALA:O	44:AG:106:LYS:HG2	2.17	0.44
52:AP:85:ALA:HB1	52:AP:89:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AY:99:LEU:HD13	61:AY:104:LEU:HD21	1.98	0.44
62:AZ:4:PHE:HA	62:AZ:6:LYS:HZ1	1.82	0.44
9:BL:8:GLN:NE2	9:BL:14:GLN:O	2.43	0.44
22:BP:18:ARG:NH1	25:BS:90:ASN:O	2.50	0.44
23:BQ:97:VAL:HG12	23:BQ:98:ASP:H	1.83	0.44
27:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.98	0.44
33:BM:66:VAL:HG23	33:BM:72:ILE:HD11	1.98	0.44
34:B5:1080:U:H2'	34:B5:1081:A:O4'	2.18	0.44
38:A1:976:U:H2'	38:A1:977:C:O4'	2.17	0.44
38:A1:1120:A:H2'	38:A1:1121:U:H6	1.82	0.44
38:A1:1332:A:H2'	38:A1:1333:C:C6	2.53	0.44
38:A1:1809:A:H2'	38:A1:1810:A:O4'	2.17	0.44
38:A1:2723:U:H2'	38:A1:2724:U:C6	2.52	0.44
44:AG:112:GLU:OE2	44:AG:123:GLN:HG2	2.17	0.44
49:AM:17:VAL:HG11	49:AM:74:ARG:HA	1.99	0.44
60:AX:131:ASP:O	60:AX:135:ILE:HG12	2.18	0.44
62:AZ:17:ARG:HG2	69:Ag:73:SER:O	2.17	0.44
66:Ad:7:VAL:HG23	66:Ad:79:ARG:HH12	1.83	0.44
66:Ad:41:LYS:NZ	66:Ad:47:ASP:OD1	2.44	0.44
72:Aj:2:GLY:O	72:Aj:7:SER:OG	2.25	0.44
2:BB:150:VAL:HG23	34:B5:1067:C:H5''	1.99	0.44
4:BE:127:LYS:HA	4:BE:127:LYS:HD2	1.78	0.44
4:BE:205:PHE:O	4:BE:207:LEU:HD12	2.17	0.44
15:BY:112:LYS:NZ	34:B5:55:A:OP1	2.50	0.44
19:BD:223:LYS:NZ	19:BD:225:TYR:OH	2.42	0.44
34:B5:292:U:H2'	34:B5:293:U:O2	2.17	0.44
34:B5:1158:C:O2	34:B5:1158:C:H2'	2.17	0.44
34:B5:1186:U:OP2	34:B5:1456:C:O2'	2.22	0.44
36:AB:347:SER:C	36:AB:349:LYS:H	2.26	0.44
38:A1:291:C:H2'	38:A1:292:U:C6	2.52	0.44
38:A1:2160:G:H2'	38:A1:2161:G:C8	2.52	0.44
38:A1:2502:A:H5''	38:A1:2504:U:O2	2.18	0.44
38:A1:2696:A:H2'	38:A1:2697:A:C8	2.52	0.44
38:A1:3337:G:H2'	38:A1:3338:C:C6	2.53	0.44
46:AI:72:ALA:O	46:AI:76:MET:HG2	2.17	0.44
56:AT:102:ARG:O	56:AT:106:LEU:HG	2.17	0.44
4:BE:68:ARG:HG2	4:BE:76:VAL:HG11	2.00	0.44
31:Bg:214:ALA:HB2	31:Bg:220:ILE:HG23	1.99	0.44
34:B5:282:C:H2'	34:B5:283:U:O4'	2.16	0.44
34:B5:1429:G:H2'	34:B5:1430:U:C6	2.53	0.44
38:A1:44:U:H5''	50:AN:85:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1621:A:H2'	38:A1:1622:U:C6	2.53	0.44
38:A1:2129:PSU:H2'	38:A1:2130:G:C8	2.52	0.44
38:A1:3119:U:H4'	75:Am:104:PRO:HG3	1.99	0.44
38:A1:3276:G:O2'	52:AP:175:ARG:HD2	2.18	0.44
42:AE:71:VAL:HG23	42:AE:72:ASN:OD1	2.18	0.44
44:AG:74:THR:O	44:AG:77:GLN:HG2	2.17	0.44
44:AG:78:PHE:C	44:AG:80:TYR:H	2.25	0.44
62:AZ:23:VAL:HG12	62:AZ:45:GLY:HA3	1.98	0.44
65:Ac:24:THR:HG1	65:Ac:91:SER:HG	1.50	0.44
66:Ad:25:PHE:HA	66:Ad:28:ARG:HG3	1.99	0.44
2:BB:67:GLU:OE1	2:BB:85:LYS:HG2	2.17	0.44
20:BF:92:ARG:NH2	34:B5:1613:U:OP1	2.51	0.44
22:BP:33:PHE:O	22:BP:36:LEU:HD23	2.18	0.44
34:B5:556:A:H1'	34:B5:590:C:H1'	1.99	0.44
34:B5:1220:C:H2'	34:B5:1221:A:H8	1.82	0.44
37:AC:318:LEU:HD11	43:AF:146:GLN:HA	2.00	0.44
38:A1:1708:C:H2'	38:A1:1709:C:H6	1.83	0.44
38:A1:2537:U:O2'	38:A1:2539:C:OP2	2.31	0.44
38:A1:3066:U:H2'	38:A1:3067:C:C6	2.52	0.44
47:AJ:32:ARG:O	47:AJ:36:VAL:HG23	2.17	0.44
68:Af:13:HIS:HA	68:Af:30:ILE:HD13	1.99	0.44
2:BB:176:VAL:C	2:BB:178:GLY:H	2.26	0.44
4:BE:87:MET:HG3	4:BE:100:ARG:HH21	1.81	0.44
8:BJ:70:LEU:HD12	8:BJ:71:PHE:N	2.33	0.44
8:BJ:80:LEU:HA	8:BJ:83:VAL:HG12	2.00	0.44
15:BY:76:TYR:HB2	15:BY:82:ALA:HB2	1.99	0.44
16:Ba:45:VAL:HB	16:Ba:64:LEU:HD11	2.00	0.44
24:BR:52:GLY:HA2	24:BR:55:THR:HG22	1.99	0.44
34:B5:86:A:H2'	34:B5:87:C:H6	1.82	0.44
34:B5:107:C:H2'	34:B5:108:A:H8	1.82	0.44
34:B5:343:C:H2'	34:B5:344:A:H8	1.83	0.44
36:AB:47:LEU:HD11	36:AB:179:ALA:HB3	1.99	0.44
36:AB:222:LYS:NZ	38:A1:3089:C:OP1	2.37	0.44
36:AB:297:SER:O	36:AB:300:ARG:NH1	2.51	0.44
38:A1:524:U:OP1	49:AM:77:ARG:NH2	2.46	0.44
38:A1:630:A:H2'	38:A1:631:U:C6	2.53	0.44
38:A1:818:C:H2'	38:A1:819:U:O4'	2.18	0.44
38:A1:1037:C:H2'	38:A1:1038:C:H6	1.82	0.44
38:A1:1504:A:N1	38:A1:1515:A:O2'	2.45	0.44
38:A1:3268:A:OP1	42:AE:46:ARG:NH2	2.44	0.44
39:A3:23:A:O2'	39:A3:24:A:OP1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AD:125:VAL:HG11	41:AD:199:ILE:HG21	1.99	0.44
47:AJ:116:TYR:HE2	47:AJ:122:ILE:HG13	1.83	0.44
63:Aa:87:ARG:O	63:Aa:91:LEU:HG	2.18	0.44
5:BG:4:ASN:ND2	34:B5:152:U:O2	2.27	0.44
5:BG:58:LYS:O	5:BG:59:GLN:HB2	2.17	0.44
7:BI:110:ARG:O	7:BI:114:GLU:OE1	2.36	0.44
18:Be:14:VAL:HA	18:Be:17:GLN:HE21	1.82	0.44
20:BF:94:THR:OG1	20:BF:114:ILE:HG13	2.18	0.44
22:BP:60:LEU:HD21	22:BP:64:LYS:HE3	2.00	0.44
34:B5:163:G:C8	34:B5:164:A:C8	3.06	0.44
34:B5:872:G:H2'	34:B5:873:U:O4'	2.18	0.44
34:B5:1393:C:H2'	34:B5:1394:G:H8	1.83	0.44
38:A1:716:A:C6	63:Aa:117:ARG:HG3	2.53	0.44
38:A1:833:G:OP1	54:AR:86:GLU:HB3	2.17	0.44
38:A1:969:C:O2'	64:Ab:18:ARG:NH2	2.51	0.44
38:A1:975:C:H2'	38:A1:976:U:C6	2.53	0.44
38:A1:1641:U:O2'	38:A1:1642:A:H3'	2.18	0.44
38:A1:1688:U:H2'	38:A1:1689:U:C6	2.52	0.44
38:A1:1765:U:H3'	54:AR:43:LYS:HZ1	1.83	0.44
38:A1:1799:A:H2'	38:A1:1800:A:H8	1.83	0.44
38:A1:2283:G:H1'	38:A1:2285:C:N4	2.33	0.44
38:A1:2714:G:H4'	38:A1:2715:A:H5''	2.00	0.44
38:A1:2986:U:H2'	38:A1:2987:A:H8	1.83	0.44
38:A1:3274:A:H5''	38:A1:3276:G:OP2	2.18	0.44
38:A1:3296:A:H2'	38:A1:3297:U:C6	2.53	0.44
48:AL:76:THR:HG22	48:AL:101:ARG:HB3	1.99	0.44
61:AY:51:ARG:HG2	61:AY:52:ARG:H	1.82	0.44
75:Am:105:PRO:HD2	75:Am:106:ARG:NH1	2.32	0.44
2:BB:110:LEU:O	2:BB:114:VAL:HG23	2.18	0.44
4:BE:253:ASP:OD1	4:BE:254:ARG:HD2	2.17	0.44
8:BJ:66:ASP:HB3	8:BJ:69:ARG:HB2	2.00	0.44
20:BF:48:PHE:HE2	20:BF:68:ILE:H	1.66	0.44
34:B5:1466:G:H2'	34:B5:1467:C:C6	2.53	0.44
35:AA:117:GLU:HG2	35:AA:124:GLY:H	1.82	0.44
37:AC:11:LEU:HD22	37:AC:168:ALA:HB1	2.00	0.44
37:AC:193:LYS:HB2	37:AC:198:ARG:HA	1.98	0.44
38:A1:594:U:H2'	38:A1:609:G:O6	2.18	0.44
38:A1:2542:U:H4'	38:A1:2544:U:OP1	2.18	0.44
39:A3:89:G:N2	39:A3:92:A:OP2	2.37	0.44
40:A4:5:U:H2'	40:A4:6:U:C6	2.53	0.44
44:AG:203:VAL:HG22	44:AG:207:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ad:7:VAL:HA	66:Ad:77:ARG:O	2.17	0.44
4:BE:87:MET:SD	4:BE:123:LEU:HB2	2.58	0.43
14:BX:90:ASP:HA	34:B5:568:G:H4'	1.99	0.43
19:BD:23:GLU:CD	21:BK:61:TRP:HE1	2.22	0.43
24:BR:71:PHE:O	24:BR:75:GLU:HG2	2.18	0.43
34:B5:413:U:H2'	34:B5:414:C:C6	2.53	0.43
34:B5:448:C:H2'	34:B5:449:C:H6	1.83	0.43
35:AA:117:GLU:HB2	35:AA:162:ALA:HB1	2.00	0.43
37:AC:120:TYR:CE2	37:AC:277:PRO:HB3	2.53	0.43
38:A1:637:C:C2	38:A1:638:C:C5	3.05	0.43
38:A1:1230:G:N2	38:A1:1259:A:H2'	2.33	0.43
38:A1:1801:U:H2'	38:A1:1802:C:C6	2.53	0.43
38:A1:3322:A:H2'	38:A1:3323:A:H8	1.83	0.43
46:AI:171:TRP:HB2	46:AI:178:ARG:HA	2.00	0.43
47:AJ:25:GLU:HG3	47:AJ:26:SER:N	2.32	0.43
48:AL:109:PHE:CB	71:AI:20:MET:HE1	2.48	0.43
66:Ad:26:LYS:HD3	66:Ad:26:LYS:HA	1.84	0.43
74:Al:9:ILE:HG22	74:Al:13:MET:CE	2.46	0.43
8:BJ:133:HIS:NE2	34:B5:512:A:O2'	2.30	0.43
18:Be:29:LYS:HD2	18:Be:38:LEU:HD11	2.00	0.43
23:BQ:42:GLU:HG3	23:BQ:45:ARG:CZ	2.48	0.43
38:A1:156:G:OP2	71:AI:25:LYS:HB3	2.19	0.43
38:A1:887:G:H2'	38:A1:888:A:C8	2.52	0.43
38:A1:3056:U:O2	66:Ad:28:ARG:NH2	2.49	0.43
38:A1:3258:U:O2'	38:A1:3260:G:OP1	2.25	0.43
40:A4:5:U:H2'	40:A4:6:U:H6	1.83	0.43
40:A4:37:A:H5''	40:A4:39:G:O4'	2.17	0.43
52:AP:179:GLN:HA	52:AP:182:ILE:HG22	1.99	0.43
79:tP:60:A:H3'	79:tP:61:C:C5'	2.48	0.43
1:BA:121:VAL:HG23	1:BA:141:ILE:HG21	2.00	0.43
2:BB:30:PHE:N	2:BB:46:THR:O	2.51	0.43
4:BE:53:LYS:HG3	4:BE:53:LYS:O	2.18	0.43
5:BG:154:ARG:NE	34:B5:78:A:OP2	2.52	0.43
5:BG:175:ILE:HG12	34:B5:78:A:C4	2.53	0.43
10:BN:130:ARG:NH1	10:BN:139:TRP:O	2.50	0.43
23:BQ:132:LYS:NZ	34:B5:1603:U:OP2	2.49	0.43
25:BS:27:LYS:HG3	25:BS:57:ARG:CZ	2.48	0.43
26:BT:6:VAL:O	26:BT:6:VAL:HG13	2.19	0.43
34:B5:158:U:C4	34:B5:420:A:H4'	2.54	0.43
34:B5:830:U:H1'	34:B5:831:U:H5	1.83	0.43
34:B5:838:G:H3'	34:B5:838:G:N3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:948:G:H2'	34:B5:949:C:C6	2.53	0.43
34:B5:1488:G:H3'	34:B5:1515:A:H61	1.82	0.43
37:AC:282:SER:OG	53:AQ:125:ASP:OD1	2.24	0.43
38:A1:95:A:H5''	63:Aa:34:MET:HB2	2.00	0.43
38:A1:543:C:H2'	38:A1:544:C:H5'	1.99	0.43
38:A1:748:U:H2'	38:A1:749:C:C6	2.52	0.43
38:A1:1715:A:N7	65:Ac:84:LEU:HD12	2.33	0.43
38:A1:3122:A:O2'	45:AH:63:LYS:HD3	2.17	0.43
38:A1:3154:C:N4	38:A1:3293:U:H3	2.16	0.43
38:A1:3174:A:OP1	68:Af:97:SER:OG	2.14	0.43
39:A3:90:U:H2'	39:A3:91:G:O4'	2.17	0.43
44:AG:81:THR:HG21	44:AG:181:LYS:HG3	1.99	0.43
44:AG:88:ALA:O	44:AG:92:LYS:HG3	2.18	0.43
1:BA:154:GLU:OE1	1:BA:154:GLU:N	2.51	0.43
4:BE:192:ILE:HG22	4:BE:243:GLY:O	2.19	0.43
6:BH:5:GLN:HB2	6:BH:18:LEU:HD11	2.00	0.43
7:BI:72:ILE:HG21	7:BI:112:TRP:CE2	2.54	0.43
15:BY:12:VAL:HG22	34:B5:783:G:H8	1.83	0.43
20:BF:48:PHE:CD1	20:BF:130:ILE:HD13	2.54	0.43
20:BF:95:ASN:O	34:B5:1611:A:O2'	2.36	0.43
33:BM:23:THR:H	33:BM:135:MET:CE	2.32	0.43
33:BM:62:LEU:HD22	33:BM:120:VAL:HG23	1.99	0.43
34:B5:453:U:O2	34:B5:453:U:H2'	2.17	0.43
34:B5:751:G:H2'	34:B5:752:A:C8	2.54	0.43
38:A1:656:A:H2'	38:A1:657:A:H8	1.84	0.43
38:A1:2986:U:H2'	38:A1:2987:A:C8	2.54	0.43
47:AJ:86:VAL:HG11	47:AJ:111:ASP:HB3	2.00	0.43
54:AR:68:GLN:NE2	54:AR:71:ARG:HH21	2.16	0.43
58:AV:39:VAL:HG13	58:AV:42:SER:HB3	2.01	0.43
62:AZ:41:ALA:HB2	62:AZ:77:TYR:HE1	1.83	0.43
73:Ak:40:GLN:HE21	73:Ak:55:VAL:CG1	2.31	0.43
74:Al:44:TRP:CE2	74:Al:45:ARG:HG3	2.54	0.43
77:Ao:73:GLU:OE2	77:Ao:78:LYS:HD3	2.18	0.43
78:Ap:84:ARG:O	78:Ap:88:GLU:HG2	2.18	0.43
2:BB:157:GLN:C	2:BB:159:SER:H	2.25	0.43
4:BE:112:HIS:NE2	4:BE:237:SER:O	2.52	0.43
7:BI:81:VAL:CG2	7:BI:94:ASN:HA	2.48	0.43
7:BI:107:THR:HB	7:BI:108:PRO:HD3	2.00	0.43
15:BY:37:LYS:NZ	34:B5:522:U:OP1	2.38	0.43
20:BF:42:LEU:HB2	20:BF:48:PHE:CZ	2.54	0.43
22:BP:125:PRO:HB3	25:BS:129:TRP:CH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BQ:42:GLU:HG3	23:BQ:45:ARG:NH1	2.32	0.43
34:B5:36:C:H2'	34:B5:37:U:H6	1.83	0.43
34:B5:340:U:H2'	34:B5:341:A:H8	1.82	0.43
38:A1:664:U:H2'	38:A1:665:A:H8	1.83	0.43
38:A1:1448:U:H2'	38:A1:1449:A:H8	1.83	0.43
38:A1:1618:G:O2'	40:A4:126:A:N1	2.51	0.43
38:A1:1914:G:O2'	54:AR:82:LYS:O	2.32	0.43
38:A1:2652:U:OP1	77:Ao:65:THR:OG1	2.23	0.43
45:AH:38:LEU:O	45:AH:41:ILE:HG22	2.18	0.43
54:AR:68:GLN:HE21	54:AR:71:ARG:HH21	1.65	0.43
57:AU:25:ASN:HB2	57:AU:27:VAL:HG22	2.01	0.43
73:Ak:60:GLY:O	73:Ak:63:LYS:HG2	2.19	0.43
1:BA:28:ASN:O	1:BA:150:ASP:HB3	2.18	0.43
2:BB:41:ARG:HH21	2:BB:97:LEU:HD22	1.83	0.43
3:BC:91:ARG:NE	34:B5:1147:A:OP1	2.52	0.43
4:BE:85:GLY:O	4:BE:101:LEU:HD23	2.19	0.43
7:BI:137:LYS:NZ	34:B5:196:G:O6	2.52	0.43
9:BL:146:ALA:O	9:BL:150:ASN:ND2	2.46	0.43
19:BD:132:LYS:HD3	19:BD:132:LYS:HA	1.78	0.43
24:BR:61:ILE:HD11	24:BR:69:ILE:HG21	2.01	0.43
31:Bg:11:GLY:HA2	31:Bg:52:GLN:HA	2.00	0.43
33:BM:50:LYS:HA	33:BM:53:THR:HG22	2.01	0.43
33:BM:96:GLN:HE21	33:BM:100:TRP:HE1	1.63	0.43
34:B5:404:G:H2'	34:B5:405:C:C6	2.53	0.43
34:B5:1235:C:C2	34:B5:1236:A:C8	3.07	0.43
34:B5:1483:A:N3	34:B5:1607:G:O2'	2.37	0.43
34:B5:1487:A:H2'	34:B5:1488:G:C8	2.53	0.43
36:AB:308:MET:HE2	38:A1:3329:U:H5''	1.99	0.43
36:AB:315:GLY:HA2	38:A1:3379:C:H4'	2.00	0.43
37:AC:135:VAL:HG12	37:AC:140:HIS:HB2	1.99	0.43
38:A1:69:C:OP1	50:AN:178:HIS:ND1	2.23	0.43
38:A1:649:A:OP2	38:A1:2868:U:O2'	2.37	0.43
38:A1:796:U:H2'	38:A1:797:U:C6	2.54	0.43
38:A1:2438:A:O2'	38:A1:2439:A:OP1	2.30	0.43
38:A1:2552:C:N4	65:Ac:54:SER:OG	2.52	0.43
38:A1:2763:U:O2	82:A1:3401:SPD:N1	2.50	0.43
38:A1:2943:G:H2'	38:A1:2944:PSU:O4'	2.18	0.43
41:AD:40:HIS:CE1	56:AT:69:LYS:HA	2.53	0.43
47:AJ:28:ASP:O	47:AJ:32:ARG:HG3	2.19	0.43
48:AL:83:ALA:HA	48:AL:117:LYS:HE3	1.99	0.43
48:AL:180:ARG:HD3	71:Ai:11:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:20:ALA:HB2	24:BR:91:LEU:HD22	2.00	0.43
2:BB:133:TYR:HE1	2:BB:220:GLN:HG2	1.84	0.43
4:BE:11:ARG:NH1	4:BE:24:SER:HB2	2.33	0.43
6:BH:5:GLN:H	6:BH:5:GLN:CD	2.27	0.43
7:BI:4:SER:OG	7:BI:24:LYS:HD3	2.18	0.43
14:BX:2:GLY:N	34:B5:1102:G:N7	2.66	0.43
18:Be:31:LYS:HE2	34:B5:545:A:H2'	2.00	0.43
25:BS:39:GLY:N	34:B5:1566:U:H5''	2.34	0.43
34:B5:640:U:H2'	34:B5:641:G:O4'	2.17	0.43
34:B5:1438:G:H2'	34:B5:1439:C:C6	2.54	0.43
37:AC:22:LEU:HA	37:AC:23:PRO:HD3	1.77	0.43
38:A1:289:A:H2'	38:A1:290:G:H8	1.83	0.43
38:A1:1332:A:H2'	38:A1:1333:C:H6	1.82	0.43
38:A1:1915:A:H2'	38:A1:1916:U:H6	1.83	0.43
38:A1:2812:C:H2'	38:A1:2813:A:H8	1.84	0.43
40:A4:27:U:H2'	40:A4:28:C:C6	2.54	0.43
46:AI:156:ARG:NH1	46:AI:163:GLN:O	2.47	0.43
48:AL:179:PHE:HB2	48:AL:183:ARG:NH2	2.34	0.43
61:AY:116:LYS:O	61:AY:120:GLN:HG3	2.18	0.43
62:AZ:104:PRO:O	62:AZ:108:GLU:OE1	2.37	0.43
4:BE:183:VAL:HG11	4:BE:188:ASN:HB2	2.00	0.43
16:Ba:37:LYS:HE3	34:B5:933:A:OP2	2.19	0.43
19:BD:99:VAL:HG13	19:BD:173:ARG:NH2	2.34	0.43
26:BT:129:GLN:NE2	34:B5:1358:G:H21	2.17	0.43
33:BM:113:ARG:HG3	33:BM:114:LYS:N	2.34	0.43
34:B5:534:A:C4	34:B5:535:A:C8	3.06	0.43
34:B5:948:G:H2'	34:B5:949:C:H6	1.82	0.43
34:B5:1458:G:HO2'	34:B5:1459:C:P	2.39	0.43
34:B5:1462:G:O2'	79:tP:30:G:OP1	2.32	0.43
34:B5:1665:U:H2'	34:B5:1666:U:O2	2.18	0.43
38:A1:167:U:H2'	38:A1:168:U:H6	1.84	0.43
38:A1:616:G:H2'	38:A1:617:G:H8	1.83	0.43
38:A1:631:U:H2'	38:A1:632:G:C8	2.54	0.43
38:A1:710:A:H2'	38:A1:711:A:C8	2.52	0.43
38:A1:1666:G:H2'	38:A1:1667:A:C8	2.54	0.43
38:A1:1941:C:H2'	38:A1:1942:U:C6	2.54	0.43
38:A1:2561:A:O2'	38:A1:2562:A:H8	2.01	0.43
38:A1:3016:A:H2'	38:A1:3017:A:C8	2.54	0.43
40:A4:40:A:H2'	40:A4:41:A:C8	2.54	0.43
43:AF:98:LYS:HB3	43:AF:99:PRO:HD3	2.00	0.43
47:AJ:35:LYS:HD3	47:AJ:120:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AJ:106:ILE:HD11	47:AJ:125:MET:HB2	2.01	0.43
70:Ah:73:LYS:HG3	70:Ah:74:LYS:O	2.19	0.43
3:BC:102:VAL:HG11	3:BC:129:ILE:HG13	2.00	0.43
9:BL:105:LYS:NZ	34:B5:307:G:OP2	2.44	0.43
10:BN:128:TYR:O	10:BN:132:VAL:HG22	2.19	0.43
15:BY:117:LYS:HG2	34:B5:159:U:H5'	2.01	0.43
18:Be:13:LYS:NZ	18:Be:17:GLN:HE22	2.17	0.43
20:BF:187:ILE:HG12	28:BZ:66:VAL:HG11	2.01	0.43
24:BR:45:ARG:NH1	34:B5:1331:A:OP1	2.34	0.43
34:B5:393:C:H2'	34:B5:394:C:C6	2.54	0.43
34:B5:1405:G:H2'	34:B5:1406:A:C8	2.53	0.43
34:B5:1471:A:H2	34:B5:1474:G:N3	2.17	0.43
36:AB:35:ASP:OD2	36:AB:191:LYS:NZ	2.46	0.43
36:AB:92:TYR:HB3	36:AB:99:LEU:HG	2.01	0.43
37:AC:59:GLN:NE2	72:Aj:55:ARG:HH12	2.16	0.43
38:A1:551:A:HO2'	38:A1:552:G:P	2.39	0.43
38:A1:1251:A:H5'	38:A1:1252:A:H4'	2.00	0.43
38:A1:1737:U:O2	69:Ag:52:GLN:NE2	2.52	0.43
38:A1:2292:U:H2'	38:A1:2293:C:C6	2.54	0.43
38:A1:3127:A:H2'	38:A1:3128:G:O4'	2.19	0.43
38:A1:3181:C:H2'	38:A1:3182:G:C8	2.53	0.43
38:A1:3359:A:H2'	38:A1:3360:C:H6	1.83	0.43
42:AE:131:LYS:O	42:AE:135:VAL:HG23	2.19	0.43
58:AV:86:ARG:HB2	58:AV:92:PHE:CE2	2.53	0.43
12:BV:62:ARG:HH22	34:B5:1039:A:H4'	1.84	0.43
19:BD:51:ARG:HB3	19:BD:91:VAL:HG12	2.00	0.43
22:BP:44:ARG:NE	22:BP:49:MET:HE1	2.34	0.43
28:BZ:80:LEU:HD12	28:BZ:101:TYR:CD1	2.54	0.43
33:BM:61:VAL:CG1	33:BM:121:VAL:HB	2.48	0.43
34:B5:445:A:H1'	34:B5:525:A:OP1	2.18	0.43
34:B5:887:A:H2'	34:B5:888:U:C6	2.54	0.43
34:B5:1147:A:H2'	34:B5:1148:C:C6	2.54	0.43
36:AB:28:ARG:CZ	36:AB:30:LYS:HE2	2.48	0.43
38:A1:2278:5MC:OP1	76:An:23:ARG:NH2	2.51	0.43
38:A1:2989:U:H2'	38:A1:2990:G:O4'	2.19	0.43
38:A1:3318:G:O2'	38:A1:3319:U:H5''	2.19	0.43
47:AJ:47:GLN:HB3	47:AJ:64:LYS:HG2	2.00	0.43
49:AM:21:VAL:HG12	49:AM:65:LEU:HD23	2.00	0.43
5:BG:5:ILE:HG23	5:BG:124:LEU:HD11	2.01	0.42
5:BG:219:ARG:O	5:BG:222:GLU:HG2	2.18	0.42
8:BJ:123:HIS:HB3	18:Be:33:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BW:24:GLN:HA	13:BW:63:VAL:O	2.18	0.42
15:BY:23:PHE:HE2	15:BY:25:VAL:HB	1.84	0.42
15:BY:55:VAL:HG22	15:BY:75:VAL:HG22	2.00	0.42
15:BY:83:LYS:HZ1	15:BY:97:ALA:HB2	1.84	0.42
23:BQ:116:LEU:HD23	23:BQ:116:LEU:HA	1.90	0.42
26:BT:38:LYS:HA	26:BT:46:PRO:HA	2.01	0.42
34:B5:162:A:C6	34:B5:163:G:C6	3.07	0.42
34:B5:285:G:H2'	34:B5:286:C:O4'	2.19	0.42
34:B5:334:G:H2'	34:B5:335:U:C6	2.54	0.42
34:B5:1164:G:H2'	34:B5:1165:G:C8	2.53	0.42
34:B5:1308:G:H2'	34:B5:1309:C:C6	2.54	0.42
34:B5:1579:U:H2'	34:B5:1580:C:C6	2.54	0.42
34:B5:1719:A:H2'	34:B5:1720:G:O4'	2.19	0.42
35:AA:96:LEU:HD23	78:Ap:83:ILE:HG23	2.01	0.42
38:A1:1497:C:H2'	38:A1:1498:A:H8	1.84	0.42
38:A1:1643:A:H2'	38:A1:1644:C:C2	2.54	0.42
38:A1:2309:A:N3	38:A1:2961:G:O2'	2.47	0.42
38:A1:2762:A:H2'	38:A1:2763:U:H6	1.84	0.42
38:A1:2947:G:OP2	38:A1:2947:G:H4'	2.18	0.42
39:A3:50:PSU:O2'	41:AD:221:GLU:O	2.25	0.42
39:A3:77:G:H5''	55:AS:46:GLN:O	2.18	0.42
42:AE:68:PRO:HB3	42:AE:142:ASP:HB2	2.01	0.42
53:AQ:116:LYS:NZ	63:Aa:88:ASP:OD2	2.35	0.42
54:AR:105:LEU:HD23	54:AR:138:LEU:HD23	2.01	0.42
64:Ab:33:LYS:HE2	64:Ab:33:LYS:HB2	1.89	0.42
1:BA:31:VAL:HG13	34:B5:1041:G:OP1	2.19	0.42
2:BB:39:GLU:HG3	2:BB:40:ASN:N	2.25	0.42
8:BJ:8:TYR:H	34:B5:25:C:N4	2.17	0.42
15:BY:124:ARG:HG2	15:BY:128:LYS:HD2	2.01	0.42
23:BQ:13:LYS:HG2	23:BQ:76:SER:HA	2.01	0.42
28:BZ:99:ALA:HB1	28:BZ:101:TYR:HE1	1.84	0.42
34:B5:407:A:H2'	34:B5:408:C:H6	1.84	0.42
34:B5:522:U:H2'	34:B5:523:G:O4'	2.19	0.42
34:B5:585:A:H2'	34:B5:586:G:C8	2.53	0.42
34:B5:888:U:H2'	34:B5:889:U:C6	2.54	0.42
35:AA:28:LYS:HB2	35:AA:123:ARG:HB3	2.01	0.42
38:A1:629:U:H2'	38:A1:630:A:C8	2.54	0.42
38:A1:671:U:H2'	38:A1:672:A:H8	1.84	0.42
38:A1:1011:A:H2'	38:A1:1012:G:C8	2.54	0.42
39:A3:66:A:OP2	46:AI:203:LYS:NZ	2.51	0.42
43:AF:233:GLU:HG2	43:AF:234:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AM:43:LYS:HD2	49:AM:59:ASN:HA	2.01	0.42
71:AI:61:ILE:HD11	71:AI:87:VAL:HG13	2.01	0.42
1:BA:50:VAL:HG22	24:BR:109:LEU:HD21	2.00	0.42
3:BC:226:THR:OG1	3:BC:228:ASN:OD1	2.27	0.42
4:BE:51:ARG:HD3	4:BE:51:ARG:HA	1.90	0.42
4:BE:187:ARG:HH12	34:B5:753:A:H3'	1.84	0.42
5:BG:65:GLN:HE21	34:B5:1682:U:H5'	1.84	0.42
8:BJ:74:ASN:HA	8:BJ:77:ILE:HG12	2.02	0.42
15:BY:19:ALA:HB3	15:BY:81:GLU:OE2	2.19	0.42
23:BQ:69:VAL:HG11	23:BQ:81:ILE:HD11	2.02	0.42
23:BQ:143:ARG:NH1	79:tP:33:U:OP2	2.43	0.42
25:BS:57:ARG:N	25:BS:60:GLU:OE2	2.50	0.42
28:BZ:81:ARG:NH2	34:B5:1532:U:OP2	2.51	0.42
34:B5:989:U:H2'	34:B5:990:C:C6	2.54	0.42
34:B5:1174:C:O2'	34:B5:1196:A:N6	2.51	0.42
34:B5:1783:C:OP2	76:An:1:MET:HG3	2.20	0.42
34:B5:1783:C:P	76:An:1:MET:HG3	2.60	0.42
38:A1:947:G:H2'	38:A1:948:C:C6	2.53	0.42
38:A1:1062:A:O2'	56:AT:108:ARG:NH2	2.51	0.42
38:A1:1771:C:H2'	38:A1:1772:U:O4'	2.19	0.42
38:A1:1836:C:H41	74:Al:3:ALA:HB2	1.84	0.42
38:A1:2344:U:H2'	38:A1:2345:A:H8	1.84	0.42
38:A1:2426:U:H2'	38:A1:2427:U:H6	1.83	0.42
38:A1:2651:G:H5''	38:A1:2652:U:O4'	2.19	0.42
38:A1:3251:U:H2'	38:A1:3252:G:C8	2.54	0.42
39:A3:113:C:H2'	39:A3:114:U:O4'	2.19	0.42
41:AD:41:LYS:HB2	56:AT:68:THR:O	2.19	0.42
41:AD:85:ARG:NH2	41:AD:86:TYR:OH	2.52	0.42
44:AG:54:GLU:O	44:AG:58:VAL:HG23	2.19	0.42
47:AJ:92:ARG:NH2	47:AJ:174:LYS:HB3	2.33	0.42
3:BC:81:MET:HE1	3:BC:186:LYS:HB3	2.01	0.42
4:BE:186:GLY:HA3	34:B5:753:A:OP2	2.19	0.42
8:BJ:83:VAL:HG21	8:BJ:147:MET:HG3	2.01	0.42
16:Ba:71:LEU:HD13	16:Ba:73:TYR:OH	2.18	0.42
19:BD:159:HIS:N	34:B5:1328:G:OP1	2.42	0.42
26:BT:117:SER:HB3	26:BT:121:GLY:O	2.19	0.42
27:BU:19:ILE:HD11	27:BU:94:GLU:HG3	2.01	0.42
27:BU:71:PRO:HB3	30:Bd:41:GLN:HG2	2.02	0.42
34:B5:1323:C:H2'	34:B5:1324:G:O4'	2.19	0.42
34:B5:1428:G:OP2	34:B5:1428:G:H8	2.02	0.42
35:AA:181:LYS:HB2	38:A1:860:G:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:68:C:OP2	38:A1:301:G:N2	2.51	0.42
38:A1:1054:A:H5''	38:A1:2637:A:H61	1.85	0.42
38:A1:1596:C:O2'	38:A1:1696:A:N3	2.51	0.42
38:A1:2697:A:H2'	38:A1:2698:G:H8	1.84	0.42
38:A1:3267:A:N6	42:AE:69:PHE:O	2.53	0.42
40:A4:10:A:H2'	40:A4:11:C:C6	2.55	0.42
42:AE:154:LEU:HA	42:AE:157:GLN:HE21	1.84	0.42
47:AJ:19:LEU:HD23	47:AJ:125:MET:SD	2.58	0.42
48:AL:46:ILE:HD11	48:AL:51:LEU:HA	2.00	0.42
51:AO:27[A]:LEU:HD11	51:AO:102[A]:LEU:HD13	2.01	0.42
62:AZ:9:LYS:HD2	62:AZ:83:THR:O	2.20	0.42
62:AZ:101:PHE:HB3	62:AZ:107:ARG:HH21	1.84	0.42
79:tP:25:C:H2'	79:tP:26:G:O4'	2.18	0.42
80:tA:29:G:H2'	80:tA:30:G:C8	2.54	0.42
1:BA:56:LYS:HA	1:BA:56:LYS:HD2	1.84	0.42
5:BG:3:LEU:O	5:BG:15:THR:HA	2.19	0.42
9:BL:36:LYS:HE2	34:B5:248:U:OP1	2.19	0.42
9:BL:57:LYS:O	9:BL:138:ASN:ND2	2.50	0.42
9:BL:149:ALA:HB1	9:BL:153:PHE:CD2	2.54	0.42
15:BY:12:VAL:HG22	34:B5:783:G:C8	2.55	0.42
30:Bd:33:LYS:O	30:Bd:36:LEU:HD23	2.19	0.42
34:B5:1254:U:H2'	34:B5:1255:G:C8	2.55	0.42
34:B5:1600:A:H4'	34:B5:1601:G:OP1	2.20	0.42
36:AB:159:ARG:HG2	36:AB:182:GLN:HA	2.00	0.42
37:AC:74:ILE:HG12	37:AC:94:CYS:SG	2.59	0.42
38:A1:324:A:H2'	38:A1:325:A:C8	2.55	0.42
38:A1:568:G:H2'	38:A1:569:A:O4'	2.19	0.42
38:A1:968:G:H2'	38:A1:969:C:C6	2.54	0.42
38:A1:2615:G:H2'	38:A1:2616:C:H6	1.85	0.42
38:A1:3225:C:C2	38:A1:3226:A:N7	2.88	0.42
43:AF:77:VAL:HB	56:AT:139:ARG:HG2	2.01	0.42
49:AM:28:SER:HB3	49:AM:31:LYS:HD2	2.02	0.42
51:AO:83[A]:ALA:O	51:AO:87[A]:MET:HG3	2.20	0.42
69:Ag:74:ARG:CZ	69:Ag:82:ALA:HB2	2.49	0.42
72:Aj:39:TYR:CD1	72:Aj:40:PRO:HA	2.53	0.42
77:Ao:15:LYS:HA	77:Ao:18:ARG:NE	2.34	0.42
80:tA:14:A:C2'	80:tA:15:G:H4'	2.49	0.42
5:BG:23:ARG:NH1	5:BG:41:VAL:O	2.52	0.42
5:BG:27:PHE:CE1	5:BG:36:VAL:HG21	2.54	0.42
6:BH:104:ARG:NH2	34:B5:805:U:O4	2.51	0.42
8:BJ:168:ARG:HD2	8:BJ:168:ARG:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BL:16:GLN:HB2	9:BL:19:ILE:CD1	2.49	0.42
14:BX:107:PHE:CE2	14:BX:114:LYS:HB3	2.55	0.42
26:BT:129:GLN:HE22	34:B5:1358:G:H21	1.67	0.42
27:BU:109:GLU:HB2	27:BU:110:PRO:HD2	2.01	0.42
31:Bg:294:TRP:CE2	31:Bg:301:LEU:HD13	2.55	0.42
34:B5:446:A:C6	34:B5:447:U:C4	3.07	0.42
37:AC:130:ALA:HA	37:AC:148:ILE:HG22	2.02	0.42
38:A1:1016:C:H2'	38:A1:1017:C:H4'	2.01	0.42
38:A1:1448:U:H2'	38:A1:1449:A:C8	2.54	0.42
38:A1:2139:A:C4	72:Aj:3:LYS:HE2	2.55	0.42
38:A1:3166:C:H2'	38:A1:3167:A:H8	1.84	0.42
40:A4:91:C:H2'	40:A4:92:A:C8	2.54	0.42
42:AE:41:ILE:HB	42:AE:85:ILE:HB	2.02	0.42
46:AI:110:ARG:NH2	79:tP:74:C:H3'	2.35	0.42
54:AR:70:LYS:HE2	54:AR:70:LYS:HB3	1.81	0.42
66:Ad:87:ASN:HA	66:Ad:88:PRO:HD3	1.88	0.42
70:Ah:69:LEU:HD23	70:Ah:69:LEU:HA	1.85	0.42
80:tA:75:C:H2'	80:tA:76:A:C8	2.54	0.42
4:BE:133:LYS:HD3	4:BE:133:LYS:HA	1.87	0.42
5:BG:175:ILE:HG12	34:B5:78:A:N3	2.35	0.42
22:BP:76:VAL:O	22:BP:94:VAL:HA	2.20	0.42
22:BP:78:THR:HA	34:B5:1241:G:H4'	2.01	0.42
25:BS:36:LYS:HE2	25:BS:36:LYS:HB3	1.88	0.42
31:Bg:161:LYS:HA	31:Bg:161:LYS:HD2	1.80	0.42
34:B5:55:A:N6	34:B5:403:G:H1'	2.34	0.42
34:B5:830:U:H1'	34:B5:831:U:C5	2.54	0.42
34:B5:892:A:H2'	34:B5:893:U:C6	2.55	0.42
34:B5:1061:A:N3	34:B5:1061:A:H2'	2.35	0.42
36:AB:106:TRP:HB2	36:AB:133:TYR:CE1	2.54	0.42
38:A1:1497:C:H2'	38:A1:1498:A:C8	2.55	0.42
38:A1:2218:G:H2'	38:A1:2219:A:C8	2.54	0.42
43:AF:239:LEU:O	43:AF:243:MET:HG3	2.19	0.42
47:Aj:91:LEU:HD12	47:Aj:163:PHE:CZ	2.55	0.42
54:AR:19:LYS:HB2	54:AR:19:LYS:HE3	1.93	0.42
62:AZ:61:LYS:O	62:AZ:65:ARG:HB3	2.20	0.42
1:BA:84:ARG:HE	1:BA:88:LYS:NZ	2.18	0.42
2:BB:124:ASN:HD21	2:BB:136:ARG:HG2	1.85	0.42
4:BE:200:ARG:HG3	4:BE:201:HIS:H	1.84	0.42
7:BI:22:ARG:HB3	34:B5:385:A:H5''	2.02	0.42
8:BJ:32:GLY:HA3	18:Be:40:TYR:CG	2.55	0.42
8:BJ:52:ILE:CD1	8:BJ:76:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BJ:124:HIS:HA	8:BJ:127:VAL:HG12	2.02	0.42
9:BL:36:LYS:HE2	34:B5:248:U:P	2.59	0.42
20:BF:117:THR:HG21	20:BF:194:LEU:HD23	2.02	0.42
24:BR:33:ARG:HD3	24:BR:33:ARG:HA	1.81	0.42
34:B5:315:A:H4'	34:B5:316:A:H4'	2.01	0.42
37:AC:343:LYS:HD2	38:A1:516:A:OP1	2.19	0.42
38:A1:810:A:H2'	38:A1:811:U:C6	2.55	0.42
38:A1:954:U:H5	38:A1:967:A:N1	2.18	0.42
38:A1:1048:A:H2'	46:AI:22:TYR:CZ	2.55	0.42
38:A1:1245:A:O2'	38:A1:1246:G:H5''	2.19	0.42
40:A4:9:A:H2'	40:A4:10:A:H8	1.84	0.42
40:A4:143:U:H2'	40:A4:144:G:O4'	2.20	0.42
44:AG:166:LEU:HD23	44:AG:166:LEU:HA	1.83	0.42
46:AI:102:MET:HB3	46:AI:112:GLN:NE2	2.32	0.42
50:AN:66:VAL:HG21	50:AN:98:LEU:HB3	2.02	0.42
69:Ag:3:GLN:NE2	69:Ag:30:LEU:H	2.17	0.42
69:Ag:44:CYS:HB2	69:Ag:81:CYS:HB3	2.01	0.42
70:Ah:15:GLU:CD	70:Ah:15:GLU:H	2.28	0.42
79:tP:53:G:H2'	79:tP:54:A:H8	1.82	0.42
3:BC:219:GLY:O	12:BV:25:LYS:NZ	2.53	0.42
11:BO:114:ARG:HG2	16:Ba:59:TYR:HE2	1.85	0.42
30:Bd:10:HIS:ND1	34:B5:1452:U:OP1	2.44	0.42
34:B5:174:U:H2'	34:B5:175:G:C8	2.54	0.42
34:B5:300:A:H2'	34:B5:301:A:C8	2.54	0.42
34:B5:368:U:H2'	34:B5:369:A:O4'	2.20	0.42
34:B5:390:G:O2'	34:B5:1731:A:H5''	2.20	0.42
34:B5:848:C:H5''	54:AR:165:LYS:NZ	2.35	0.42
34:B5:1382:A:O2'	34:B5:1383:G:H8	2.02	0.42
35:AA:206:PRO:HG3	35:AA:213:GLY:HA3	2.02	0.42
36:AB:295:ALA:HB2	36:AB:301:THR:O	2.20	0.42
38:A1:956:U:H2'	38:A1:957:C:C6	2.55	0.42
38:A1:1129:A:H2'	38:A1:1130:A:C8	2.55	0.42
38:A1:1597:C:H2'	38:A1:1598:G:C8	2.54	0.42
38:A1:2254:U:H2'	38:A1:2261:G:N2	2.33	0.42
38:A1:3291:G:C2	38:A1:3292:A:C5	3.08	0.42
38:A1:3310:A:OP1	52:AP:74:LYS:NZ	2.38	0.42
42:AE:51:ARG:HB3	42:AE:159:LEU:HD12	2.01	0.42
44:AG:50:VAL:HG21	60:AX:27:ARG:HD2	2.00	0.42
53:AQ:96:PHE:CD2	53:AQ:113:LYS:HG2	2.55	0.42
58:AV:108:GLU:HG3	58:AV:128:ARG:HG3	2.02	0.42
74:Al:6:SER:OG	74:Al:9:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:tA:22:G:N7	80:tA:46:G:O6	2.53	0.42
80:tA:63:G:H2'	80:tA:64:A:C8	2.54	0.42
4:BE:64:ILE:HD13	4:BE:64:ILE:HA	1.76	0.42
4:BE:100:ARG:HB2	4:BE:112:HIS:HD2	1.85	0.42
5:BG:186:ARG:NH2	34:B5:269:G:OP2	2.47	0.42
15:BY:61:ARG:NH2	34:B5:530:C:O2	2.29	0.42
17:Bb:51:GLN:NE2	34:B5:870:C:H1'	2.35	0.42
21:BK:22:VAL:HB	21:BK:63:TYR:CZ	2.55	0.42
22:BP:37:ALA:O	22:BP:42:ARG:NH1	2.53	0.42
25:BS:73:MET:HG2	25:BS:101:LEU:HD11	2.01	0.42
31:Bg:206:PRO:HG3	31:Bg:247:PRO:HA	2.02	0.42
33:BM:70:ASN:O	33:BM:73:LYS:HG3	2.20	0.42
34:B5:29:U:H2'	34:B5:30:G:C8	2.55	0.42
34:B5:145:A:O2'	34:B5:146:U:H5''	2.20	0.42
34:B5:162:A:H2'	34:B5:163:G:N3	2.34	0.42
34:B5:1292:G:H2'	34:B5:1293:U:C6	2.55	0.42
34:B5:1560:U:H2'	34:B5:1561:U:O4'	2.20	0.42
38:A1:1188:U:OP1	38:A1:1210:U:O2'	2.23	0.42
38:A1:1463:U:H2'	38:A1:1464:G:O4'	2.20	0.42
38:A1:2180:G:H2'	38:A1:2181:C:C6	2.55	0.42
38:A1:2413:A:H2'	38:A1:2414:G:C8	2.54	0.42
38:A1:2689:A:N3	38:A1:2689:A:H2'	2.35	0.42
38:A1:2799:A:H5''	38:A1:2800:G:O5'	2.20	0.42
46:AI:76:MET:HE2	46:AI:151:GLY:HA3	2.01	0.42
50:AN:36:ILE:HG12	50:AN:64:VAL:HG23	2.02	0.42
53:AQ:175:ALA:C	63:Aa:51:GLY:HA2	2.44	0.42
80:tA:37:A:H2'	80:tA:38:A:O4'	2.20	0.42
8:BJ:76:LEU:HD23	8:BJ:79:ARG:NH2	2.35	0.41
10:BN:32:SER:O	10:BN:35:GLU:HG3	2.20	0.41
12:BV:7:GLN:O	12:BV:9:VAL:HG13	2.20	0.41
19:BD:163:PRO:HA	19:BD:166:ASP:HB2	2.02	0.41
19:BD:176:LEU:HD11	34:B5:1437:U:H4'	2.02	0.41
33:BM:115:VAL:HG12	33:BM:116:VAL:O	2.20	0.41
34:B5:291:G:H2'	34:B5:292:U:O2	2.20	0.41
34:B5:301:A:H2'	34:B5:302:PSU:C6	2.54	0.41
34:B5:736:C:H2'	34:B5:737:A:C8	2.55	0.41
34:B5:1061:A:O2'	34:B5:1062:A:OP1	2.34	0.41
34:B5:1564:U:H2'	34:B5:1565:C:H6	1.84	0.41
38:A1:144:A:H2'	38:A1:145:G:O4'	2.20	0.41
38:A1:591:G:C2	42:AE:18:LEU:HD12	2.55	0.41
38:A1:761:A:C2	38:A1:771:A:H1'	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:967:A:OP1	63:Aa:47:LYS:NZ	2.53	0.41
38:A1:1341:U:H2'	38:A1:1342:C:C6	2.54	0.41
38:A1:1729:A:O4'	65:Ac:52:ARG:NH1	2.50	0.41
38:A1:2674:A:H1'	47:AJ:107:ASP:OD1	2.19	0.41
40:A4:146:U:H2'	40:A4:147:U:C6	2.55	0.41
49:AM:55:ARG:NH1	49:AM:76:ALA:O	2.48	0.41
62:AZ:95:VAL:HG21	62:AZ:113:VAL:HG11	2.02	0.41
65:Ac:17:VAL:HG21	65:Ac:100:ILE:HG21	2.02	0.41
66:Ad:75:ILE:HG12	66:Ad:93:VAL:HG22	2.02	0.41
70:Ah:9:LEU:HG	70:Ah:17:LEU:HD21	2.02	0.41
75:Am:93:LYS:HB2	75:Am:124:LYS:CD	2.50	0.41
79:tP:66:C:H2'	79:tP:67:G:C8	2.55	0.41
3:BC:188:LEU:HD13	3:BC:196:VAL:HG11	2.02	0.41
6:BH:51:VAL:HG22	6:BH:55:LYS:O	2.21	0.41
8:BJ:93:LEU:O	8:BJ:96:VAL:HG12	2.20	0.41
15:BY:92:VAL:HG21	15:BY:99:LYS:HE2	2.02	0.41
24:BR:58:MET:HE3	24:BR:58:MET:HB3	1.82	0.41
34:B5:326:G:H2'	34:B5:327:U:C6	2.55	0.41
34:B5:384:G:H2'	34:B5:385:A:C8	2.55	0.41
34:B5:821:U:H1'	34:B5:852:C:H1'	2.01	0.41
35:AA:40:TYR:O	38:A1:2550:U:H5	2.03	0.41
38:A1:393:U:H2'	38:A1:394:G:O4'	2.20	0.41
38:A1:698:U:H2'	38:A1:699:A:O4'	2.20	0.41
38:A1:820:A:H2'	38:A1:821:U:C6	2.55	0.41
38:A1:2115:G:H22	38:A1:2120:A:H1'	1.85	0.41
38:A1:3000:A:H2'	38:A1:3001:C:C6	2.55	0.41
38:A1:3042:U:OP2	38:A1:3092:C:N4	2.43	0.41
39:A3:4:U:H2'	39:A3:5:G:H8	1.85	0.41
47:AJ:29:ARG:NH1	47:AJ:123:PHE:HE1	2.18	0.41
49:AM:103:ILE:O	49:AM:106:ARG:HG2	2.20	0.41
62:AZ:95:VAL:HG11	62:AZ:113:VAL:CG1	2.50	0.41
62:AZ:121:ARG:HG3	62:AZ:131:PHE:CZ	2.55	0.41
77:Ao:15:LYS:O	77:Ao:15:LYS:HD3	2.21	0.41
2:BB:157:GLN:O	2:BB:159:SER:N	2.51	0.41
4:BE:130:GLN:OE1	34:B5:251:A:O2'	2.24	0.41
7:BI:10:LYS:HE3	7:BI:10:LYS:HB3	1.94	0.41
7:BI:184:LEU:C	7:BI:189:LEU:HB2	2.45	0.41
13:BW:40:VAL:HG11	13:BW:103:ILE:HD12	2.01	0.41
17:Bb:40:CYS:SG	17:Bb:41:LEU:N	2.94	0.41
18:Be:40:TYR:CD1	18:Be:44:PHE:HD2	2.38	0.41
19:BD:92:GLN:O	19:BD:93:ASP:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BS:32:LEU:HD23	25:BS:32:LEU:HA	1.89	0.41
26:BT:23:GLN:NE2	26:BT:51:GLU:O	2.54	0.41
27:BU:33:GLN:O	27:BU:37:VAL:HG22	2.21	0.41
29:Bc:31:GLU:HB3	29:Bc:39:THR:HG22	2.02	0.41
31:Bg:266:ASP:HB3	31:Bg:267:PRO:HD3	2.02	0.41
34:B5:36:C:H2'	34:B5:37:U:C6	2.55	0.41
34:B5:196:G:H2'	34:B5:197:A:O4'	2.20	0.41
34:B5:1077:C:H2'	34:B5:1078:C:H6	1.85	0.41
35:AA:150:LEU:HD11	35:AA:156:LYS:HD2	2.02	0.41
36:AB:19:ARG:HB2	36:AB:232:ARG:NH2	2.35	0.41
36:AB:36:ASP:O	36:AB:185:GLY:HA2	2.20	0.41
38:A1:2533:G:H2'	38:A1:2534:G:H8	1.85	0.41
38:A1:2779:A:C6	38:A1:2780:A:C5	3.08	0.41
38:A1:3193:C:H2'	38:A1:3194:C:C6	2.56	0.41
41:AD:40:HIS:CE1	41:AD:42:ALA:HB3	2.55	0.41
46:AI:191:LYS:HE2	46:AI:212:GLU:OE1	2.20	0.41
47:AJ:9:MET:HE2	47:AJ:9:MET:HB3	1.87	0.41
65:Ac:15:ALA:O	65:Ac:19:LYS:HG3	2.20	0.41
4:BE:49:ARG:HH22	34:B5:448:C:P	2.43	0.41
8:BJ:115:LYS:HA	8:BJ:115:LYS:HD3	1.60	0.41
11:BO:70:LYS:O	11:BO:70:LYS:HG3	2.20	0.41
25:BS:64:GLU:OE1	25:BS:64:GLU:N	2.37	0.41
33:BM:71:ILE:O	33:BM:75:VAL:HG22	2.20	0.41
34:B5:5:U:H2'	34:B5:6:G:H8	1.86	0.41
34:B5:889:U:H2'	34:B5:890:C:C6	2.56	0.41
34:B5:1471:A:C8	34:B5:1540:G:H1'	2.55	0.41
34:B5:1490:C:N3	34:B5:1492:A:N6	2.69	0.41
38:A1:159:A:H2'	38:A1:160:G:H8	1.86	0.41
38:A1:875:G:O2'	38:A1:1891:A:OP1	2.35	0.41
38:A1:1438:U:H2'	38:A1:1439:U:C6	2.55	0.41
38:A1:1444:G:H2'	38:A1:1445:U:O4'	2.21	0.41
38:A1:1470:U:H2'	38:A1:1471:U:C6	2.55	0.41
38:A1:1784:G:H2'	38:A1:1785:U:O4'	2.20	0.41
38:A1:1809:A:OP2	62:AZ:65:ARG:NH2	2.48	0.41
38:A1:2103:U:H2'	38:A1:2104:A:C8	2.55	0.41
38:A1:2223:A:H2'	38:A1:2224:A:C8	2.54	0.41
38:A1:3065:G:H2'	38:A1:3066:U:C6	2.55	0.41
42:AE:135:VAL:HG12	42:AE:139:LYS:NZ	2.35	0.41
44:AG:137:ASN:HD22	50:AN:3:ALA:H	1.66	0.41
54:AR:80:LYS:HA	54:AR:80:LYS:HD2	1.92	0.41
61:AY:43:TYR:CE2	61:AY:109:LEU:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ae:94:ALA:O	67:Ae:119:VAL:HA	2.20	0.41
73:Ak:71:PRO:HD2	73:Ak:72:THR:N	2.34	0.41
78:Ap:17:ARG:H	78:Ap:17:ARG:HG2	1.72	0.41
3:BC:36:VAL:O	3:BC:36:VAL:HG13	2.21	0.41
8:BJ:146:PHE:HD2	8:BJ:148:VAL:HG12	1.86	0.41
9:BL:16:GLN:HB2	9:BL:19:ILE:HD11	2.03	0.41
14:BX:109:ARG:O	14:BX:112:LYS:HB2	2.20	0.41
15:BY:113:ASN:HD22	15:BY:113:ASN:HA	1.68	0.41
19:BD:177:MET:HE3	19:BD:177:MET:HB3	1.90	0.41
21:BK:11:ILE:CD1	21:BK:42:VAL:HG22	2.51	0.41
22:BP:34:VAL:HG21	22:BP:45:PHE:CG	2.56	0.41
22:BP:111:MET:HG2	22:BP:119:PHE:CZ	2.56	0.41
24:BR:72:LYS:O	24:BR:76:GLU:OE1	2.38	0.41
24:BR:91:LEU:HD12	24:BR:91:LEU:O	2.20	0.41
25:BS:48:LYS:HE2	25:BS:54:LEU:HD11	2.02	0.41
27:BU:94:GLU:O	27:BU:94:GLU:HG2	2.20	0.41
34:B5:329:G:H2'	34:B5:330:G:C8	2.56	0.41
34:B5:592:A:H2'	34:B5:593:U:O4'	2.20	0.41
34:B5:752:A:O2'	34:B5:753:A:P	2.78	0.41
34:B5:1539:G:H5'	34:B5:1539:G:N3	2.34	0.41
34:B5:1544:U:H3	34:B5:1567:U:H3	1.69	0.41
37:AC:23:PRO:HD2	37:AC:26:PHE:CE2	2.56	0.41
38:A1:1744:G:H2'	38:A1:1745:C:C6	2.55	0.41
38:A1:1805:C:H2'	38:A1:1806:A:C8	2.56	0.41
38:A1:2711:C:O2'	38:A1:2744:U:OP1	2.31	0.41
39:A3:11:A:N1	39:A3:67:G:O2'	2.50	0.41
43:AF:130:ILE:HD12	43:AF:134:VAL:HG11	2.03	0.41
45:AH:41:ILE:HG12	45:AH:71:VAL:CG2	2.51	0.41
57:AU:77:LYS:HD2	57:AU:95:PHE:CD1	2.54	0.41
63:Aa:28:HIS:CD2	63:Aa:32:ARG:HG2	2.55	0.41
77:Ao:98:LYS:HB2	77:Ao:98:LYS:HE3	1.83	0.41
5:BG:160:ARG:O	5:BG:170:THR:HA	2.21	0.41
7:BI:135:LYS:HD2	7:BI:135:LYS:HA	1.85	0.41
8:BJ:149:ARG:C	8:BJ:151:ASP:H	2.26	0.41
9:BL:2:SER:HA	9:BL:53:TYR:CD1	2.53	0.41
17:Bb:20:LYS:NZ	34:B5:959:U:OP2	2.52	0.41
19:BD:135:GLU:HB3	19:BD:187:LYS:HB3	2.02	0.41
20:BF:84:LYS:NZ	34:B5:1614:A:OP2	2.50	0.41
21:BK:6:GLU:O	21:BK:10:LYS:HE2	2.21	0.41
22:BP:57:MET:O	22:BP:61:ARG:HG2	2.21	0.41
23:BQ:58:ASP:OD1	23:BQ:58:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:523:G:N1	34:B5:528:U:OP2	2.38	0.41
34:B5:919:A:H2'	34:B5:920:U:C6	2.55	0.41
34:B5:1221:A:H2'	34:B5:1222:C:C6	2.55	0.41
34:B5:1344:A:H4'	34:B5:1345:A:OP1	2.20	0.41
38:A1:1803:C:H2'	38:A1:1804:A:C8	2.56	0.41
38:A1:2673:A:H4'	47:AJ:103:GLY:C	2.44	0.41
38:A1:3107:U:H2'	38:A1:3108:G:C8	2.55	0.41
38:A1:3271:G:C2	42:AE:108:LYS:HG3	2.55	0.41
38:A1:3277:U:H3'	38:A1:3278:C:H5'	2.02	0.41
38:A1:3359:A:H2'	38:A1:3360:C:C6	2.55	0.41
40:A4:141:C:H2'	40:A4:142:C:H6	1.85	0.41
43:AF:124:LEU:HD23	43:AF:124:LEU:HA	1.89	0.41
44:AG:75:ILE:O	44:AG:76:ALA:HB3	2.20	0.41
44:AG:173:MET:HE3	71:AI:39:PHE:CE1	2.56	0.41
47:AJ:94:ARG:C	47:AJ:96:PHE:H	2.29	0.41
53:AQ:92:ARG:HG3	63:Aa:76:ASP:HB2	2.01	0.41
61:AY:63:LYS:HA	61:AY:63:LYS:HD3	1.87	0.41
67:Ae:74:PHE:HB3	67:Ae:85:LEU:HD11	2.02	0.41
3:BC:49:LYS:HG3	3:BC:246:GLU:OE2	2.20	0.41
7:BI:43:ILE:HD11	7:BI:60:ILE:HD11	2.03	0.41
7:BI:56:ARG:HH22	34:B5:332:U:P	2.43	0.41
8:BJ:141:VAL:HG11	8:BJ:146:PHE:CD1	2.55	0.41
10:BN:2:GLY:HA3	34:B5:866:G:OP1	2.21	0.41
14:BX:90:ASP:HA	34:B5:568:G:O5'	2.21	0.41
16:Ba:10:ARG:HB2	16:Ba:33:ASP:OD2	2.20	0.41
28:BZ:45:GLU:HG2	28:BZ:46:LYS:N	2.36	0.41
31:Bg:111:MET:HG2	31:Bg:127:ARG:HG3	2.03	0.41
31:Bg:117:LYS:HB3	31:Bg:117:LYS:HE2	1.86	0.41
33:BM:30:VAL:HA	33:BM:33:ARG:HG2	2.03	0.41
34:B5:61:A:H2'	34:B5:62:A:O4'	2.21	0.41
34:B5:756:A:H2'	34:B5:757:A:O4'	2.21	0.41
34:B5:953:G:H2'	34:B5:954:G:C8	2.55	0.41
36:AB:212:ASN:ND2	36:AB:353:GLU:OE1	2.53	0.41
38:A1:807:A:H61	38:A1:934:G:H22	1.68	0.41
38:A1:1913:A:N3	38:A1:2120:A:H2'	2.35	0.41
38:A1:2148:U:H2'	38:A1:2149:A:C8	2.56	0.41
38:A1:2389:C:O2'	38:A1:3307:A:N1	2.51	0.41
40:A4:142:C:H2'	40:A4:143:U:H6	1.85	0.41
42:AE:133:GLU:HA	42:AE:136:GLU:HG3	2.03	0.41
44:AG:118:GLU:HG2	44:AG:119:GLY:N	2.36	0.41
3:BC:178:ILE:HB	3:BC:185:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:100:ARG:CG	4:BE:114:ILE:HD13	2.41	0.41
15:BY:11:LYS:HB2	15:BY:24:VAL:HG12	2.02	0.41
15:BY:60:PHE:H	15:BY:71:GLY:HA2	1.84	0.41
25:BS:83:ALA:C	25:BS:85:PHE:H	2.28	0.41
27:BU:21:LYS:HE2	27:BU:94:GLU:HB3	2.02	0.41
27:BU:58:LEU:HD11	34:B5:1347:U:N3	2.36	0.41
34:B5:119:A:H1'	34:B5:397:A:C5	2.55	0.41
34:B5:730:G:N2	34:B5:732:G:H21	2.19	0.41
36:AB:283:TYR:OH	36:AB:325:LYS:HD2	2.21	0.41
37:AC:140:HIS:CD2	37:AC:247:PHE:H	2.39	0.41
38:A1:230:U:H2'	38:A1:231:G:O4'	2.20	0.41
38:A1:241:G:O2'	38:A1:242:C:H6	1.99	0.41
38:A1:252:U:O2'	38:A1:253:A:P	2.79	0.41
38:A1:438:A:H3'	38:A1:439:C:H2'	2.03	0.41
38:A1:640:U:OP1	63:Aa:21:ARG:NH1	2.52	0.41
38:A1:947:G:H5''	67:Ae:55:ILE:HB	2.03	0.41
38:A1:1184:A:H2'	38:A1:1185:C:C6	2.55	0.41
38:A1:2106:A:H2'	38:A1:2107:A:C8	2.56	0.41
38:A1:2676:A:H5'	38:A1:2677:G:N7	2.36	0.41
38:A1:2709:C:H2'	38:A1:2710:C:C6	2.56	0.41
46:AI:48:LEU:HD11	46:AI:167:LEU:HD12	2.02	0.41
47:AJ:40:LEU:HD23	47:AJ:125:MET:HE1	2.03	0.41
47:AJ:90:GLN:HG3	47:AJ:172:LEU:HD23	2.02	0.41
65:Ac:55:GLU:HB2	69:Ag:94:LEU:HD11	2.02	0.41
70:Ah:31:LEU:HB3	70:Ah:44:ILE:HG12	2.03	0.41
1:BA:90:ALA:HA	1:BA:95:ALA:HB3	2.02	0.41
4:BE:105:VAL:CG2	4:BE:243:GLY:HA2	2.51	0.41
7:BI:98:LYS:HB3	34:B5:329:G:H5''	2.03	0.41
8:BJ:94:ASP:OD1	8:BJ:95:TYR:N	2.54	0.41
10:BN:81:ALA:HA	10:BN:82:PRO:HD3	1.94	0.41
11:BO:92:LYS:HE3	11:BO:92:LYS:HB3	1.77	0.41
12:BV:62:ARG:HA	12:BV:62:ARG:HD2	1.93	0.41
13:BW:30:SER:O	13:BW:30:SER:OG	2.39	0.41
16:Ba:84:VAL:HB	34:B5:1797:A:N6	2.36	0.41
18:Be:3:LYS:HD3	18:Be:3:LYS:HA	1.79	0.41
19:BD:72:LEU:HD22	21:BK:65:TYR:HD2	1.85	0.41
19:BD:211:PRO:O	19:BD:212:LYS:HG2	2.20	0.41
28:BZ:40:VAL:HG13	28:BZ:41:ILE:HG12	2.03	0.41
34:B5:34:G:O6	34:B5:474:A:H2	2.04	0.41
34:B5:153:G:H2'	34:B5:154:G:C8	2.56	0.41
34:B5:205:U:H2'	34:B5:206:A:C8	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1057:U:O2	34:B5:1062:A:N6	2.54	0.41
34:B5:1458:G:H2'	34:B5:1458:G:N3	2.36	0.41
34:B5:1738:U:H2'	34:B5:1739:C:C6	2.56	0.41
34:B5:1770:U:H2'	34:B5:1771:U:C6	2.56	0.41
35:AA:127:ALA:HB2	35:AA:134:VAL:HG23	2.03	0.41
36:AB:92:TYR:O	36:AB:155:ALA:HA	2.21	0.41
38:A1:179:C:H2'	38:A1:180:C:H6	1.86	0.41
38:A1:503:C:H2'	38:A1:504:A:H8	1.85	0.41
38:A1:717:C:OP1	38:A1:751:A:O2'	2.37	0.41
38:A1:759:U:H2'	38:A1:760:G:O4'	2.21	0.41
38:A1:1035:G:C4	38:A1:1036:A:C8	3.09	0.41
38:A1:1070:U:H2'	38:A1:1071:U:O4'	2.21	0.41
38:A1:2359:C:H2'	38:A1:2360:C:C6	2.56	0.41
38:A1:2366:C:H2'	38:A1:2367:A:H8	1.86	0.41
38:A1:2568:C:O2'	38:A1:2569:A:O5'	2.37	0.41
38:A1:3047:U:C2'	38:A1:3048:A:H5''	2.49	0.41
38:A1:3163:A:H2'	38:A1:3164:C:O4'	2.20	0.41
38:A1:3237:U:H2'	38:A1:3238:G:O4'	2.20	0.41
39:A3:1:G:C2	39:A3:2:G:C8	3.09	0.41
44:AG:45:ASN:HD22	60:AX:26:VAL:HG13	1.86	0.41
47:AJ:71:VAL:HG11	47:AJ:79:ILE:HD12	2.02	0.41
50:AN:158:HIS:HB3	50:AN:161:ALA:HB3	2.03	0.41
53:AQ:72:LYS:HB2	53:AQ:72:LYS:HE3	1.90	0.41
54:AR:181:ARG:HA	54:AR:185:LEU:HB3	2.02	0.41
55:AS:135:VAL:HG12	55:AS:141:LYS:HG3	2.02	0.41
62:AZ:104:PRO:HA	62:AZ:107:ARG:HG3	2.02	0.41
64:Ab:14:ARG:O	64:Ab:18:ARG:HG3	2.20	0.41
70:Ah:41:LEU:HD22	70:Ah:44:ILE:HG13	2.02	0.41
71:Ai:66:GLU:CD	71:Ai:91:ASN:HD21	2.27	0.41
5:BG:20:ASP:O	5:BG:23:ARG:HG2	2.21	0.41
5:BG:188:ARG:NH2	34:B5:284:G:N7	2.65	0.41
6:BH:41:LEU:O	6:BH:41:LEU:HD12	2.21	0.41
10:BN:48:SER:OG	10:BN:86:GLU:OE2	2.26	0.41
17:Bb:50:ALA:C	17:Bb:52:THR:H	2.28	0.41
19:BD:64:ARG:C	19:BD:66:ILE:H	2.29	0.41
21:BK:49:LEU:O	21:BK:52:LYS:N	2.54	0.41
31:Bg:68:VAL:HA	31:Bg:84:SER:HA	2.02	0.41
31:Bg:295:SER:HB3	31:Bg:300:THR:OG1	2.21	0.41
34:B5:71:A:H2'	34:B5:72:A:C8	2.56	0.41
34:B5:446:A:N6	34:B5:461:G:H21	2.19	0.41
36:AB:328:ILE:HD12	36:AB:336:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:3:ARG:HA	37:AC:3:ARG:HD2	1.82	0.41
38:A1:308:A:H1'	38:A1:2222:A:N3	2.36	0.41
38:A1:366:A:H2'	38:A1:367:A:O4'	2.20	0.41
38:A1:490:C:H2'	38:A1:491:A:O4'	2.21	0.41
38:A1:1015:U:H1'	38:A1:1016:C:N3	2.36	0.41
38:A1:1169:A:H2'	38:A1:1170:A:C8	2.56	0.41
38:A1:1329:U:O3'	68:Af:19:SER:HB3	2.21	0.41
38:A1:3160:U:H2'	38:A1:3161:C:C6	2.55	0.41
38:A1:3305:A:H2'	38:A1:3306:U:O4'	2.20	0.41
48:AL:138:VAL:CG2	70:Ah:118:ILE:HB	2.51	0.41
49:AM:65:LEU:HG	55:AS:172:TYR:OH	2.21	0.41
53:AQ:177:GLY:O	53:AQ:186:VAL:N	2.51	0.41
65:Ac:77:LEU:O	65:Ac:81:VAL:HG22	2.21	0.41
70:Ah:28:LEU:HG	70:Ah:32:LYS:HE2	2.02	0.41
2:BB:34:ALA:O	2:BB:41:ARG:HG3	2.20	0.40
3:BC:175:GLY:O	8:BJ:53:ARG:HD2	2.21	0.40
4:BE:61:VAL:O	4:BE:65:LEU:HD23	2.21	0.40
5:BG:65:GLN:NE2	34:B5:1682:U:H5'	2.36	0.40
6:BH:31:SER:HA	6:BH:34:LEU:HB3	2.03	0.40
29:Bc:12:VAL:HA	29:Bc:30:VAL:HG12	2.02	0.40
34:B5:646:C:H2'	34:B5:647:G:O4'	2.21	0.40
34:B5:891:A:H2'	34:B5:892:A:H8	1.86	0.40
34:B5:892:A:H2'	34:B5:893:U:H6	1.86	0.40
34:B5:1392:U:H2'	34:B5:1393:C:C6	2.56	0.40
34:B5:1516:A:O2'	34:B5:1517:U:H5'	2.21	0.40
34:B5:1652:C:H2'	34:B5:1653:C:H6	1.86	0.40
34:B5:1683:C:O2'	34:B5:1684:U:O5'	2.28	0.40
38:A1:1647:A:C2	38:A1:1809:A:H1'	2.56	0.40
38:A1:2824:G:H2'	38:A1:2825:C:H6	1.86	0.40
40:A4:27:U:H2'	40:A4:28:C:H6	1.87	0.40
44:AG:108:ARG:HE	44:AG:108:ARG:HB3	1.37	0.40
44:AG:172:LYS:HE2	44:AG:172:LYS:HB2	1.75	0.40
53:AQ:175:ALA:O	63:Aa:51:GLY:HA2	2.22	0.40
58:AV:11:PHE:HB3	58:AV:88:ARG:HH12	1.85	0.40
66:Ad:6:ASP:OD1	66:Ad:7:VAL:N	2.54	0.40
2:BB:110:LEU:HD21	2:BB:213:ARG:HG3	2.04	0.40
3:BC:157:LYS:HG2	13:BW:95:PRO:HA	2.03	0.40
4:BE:64:ILE:CD1	15:BY:17:LEU:HB3	2.50	0.40
11:BO:18:ARG:HD3	34:B5:918:U:H4'	2.04	0.40
15:BY:20:ARG:HB3	15:BY:76:TYR:CD2	2.56	0.40
15:BY:112:LYS:HE3	15:BY:112:LYS:HB3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ba:97:PRO:HG2	16:Ba:98:PRO:HD3	2.03	0.40
20:BF:30:PRO:O	20:BF:34:GLN:HG2	2.22	0.40
20:BF:146:THR:HG23	20:BF:221:ALA:HA	2.03	0.40
25:BS:41:ARG:HH11	26:BT:46:PRO:HG3	1.86	0.40
25:BS:55:HIS:ND1	25:BS:55:HIS:O	2.54	0.40
29:Bc:58:GLU:OE2	29:Bc:60:GLU:HB2	2.22	0.40
34:B5:97:C:O2	34:B5:425:A:O2'	2.37	0.40
34:B5:126:A:H62	34:B5:291:G:H21	1.70	0.40
34:B5:445:A:H1'	34:B5:525:A:H5'	2.03	0.40
34:B5:978:A:H2'	34:B5:979:A:O4'	2.20	0.40
34:B5:1451:C:C2	34:B5:1452:U:C5	3.09	0.40
34:B5:1617:U:H2'	34:B5:1618:C:C6	2.56	0.40
34:B5:1740:A:H2'	34:B5:1741:U:C6	2.56	0.40
37:AC:349:THR:HG23	43:AF:71:ALA:HB2	2.02	0.40
38:A1:1326:A:H2'	38:A1:1327:C:O4'	2.21	0.40
38:A1:2347:U:H2'	38:A1:2348:A:O4'	2.21	0.40
38:A1:3212:C:H2'	38:A1:3213:A:O4'	2.21	0.40
43:AF:151:ARG:HD2	43:AF:207:LEU:HD23	2.03	0.40
44:AG:45:ASN:ND2	60:AX:27:ARG:H	2.19	0.40
44:AG:82:LEU:HD13	44:AG:222:PHE:HE2	1.86	0.40
44:AG:156:ASP:N	44:AG:156:ASP:OD1	2.54	0.40
47:AJ:59:ILE:O	47:AJ:59:ILE:HG13	2.21	0.40
52:AP:116:HIS:HB3	52:AP:149:VAL:HB	2.03	0.40
58:AV:81:GLN:HG2	58:AV:83:LYS:H	1.86	0.40
58:AV:82:ALA:HB2	58:AV:97:ASP:O	2.21	0.40
61:AY:126:LEU:HD23	61:AY:126:LEU:O	2.21	0.40
62:AZ:95:VAL:HG11	62:AZ:113:VAL:HG11	2.02	0.40
65:Ac:34:LEU:HD13	65:Ac:59:TYR:HB3	2.02	0.40
80:tA:69:C:H2'	80:tA:70:G:C8	2.56	0.40
1:BA:206:ASP:HA	1:BA:207:PRO:HA	1.76	0.40
2:BB:32:ILE:HD13	2:BB:66:VAL:HG21	2.02	0.40
2:BB:111:ARG:HB3	16:Ba:68:TYR:HB2	2.02	0.40
8:BJ:67:PRO:O	8:BJ:70:LEU:HG	2.21	0.40
31:Bg:74:THR:HG21	31:Bg:79:TYR:HB2	2.03	0.40
31:Bg:142:ALA:HB2	31:Bg:186:PHE:CD2	2.55	0.40
34:B5:524:U:O2'	34:B5:526:A:N7	2.51	0.40
34:B5:1356:U:O2	34:B5:1367:G:N2	2.42	0.40
37:AC:112:LYS:HE2	50:AN:202:TYR:HB3	2.02	0.40
38:A1:677:A:OP2	53:AQ:107:THR:HG21	2.21	0.40
38:A1:996:A:H2'	38:A1:997:A:O4'	2.21	0.40
38:A1:1143:A:H4'	38:A1:1144:U:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1242:G:P	38:A1:1243:G:H5''	2.61	0.40
38:A1:1443:G:H2'	38:A1:1444:G:C8	2.57	0.40
38:A1:2419:A:H2'	38:A1:2420:C:H6	1.87	0.40
38:A1:2701:U:OP1	56:AT:17:ARG:NH1	2.54	0.40
38:A1:3234:A:H2	38:A1:3253:G:H22	1.69	0.40
40:A4:19:C:H2'	40:A4:20:U:C6	2.55	0.40
40:A4:44:A:H2'	40:A4:45:C:C6	2.57	0.40
43:AF:120:THR:HB	56:AT:132:PRO:HB2	2.03	0.40
61:AY:63:LYS:HG3	61:AY:97:ILE:HD11	2.02	0.40
71:Ai:70:ARG:HD3	71:Ai:84:LYS:HG2	2.04	0.40
2:BB:151:LYS:HG2	2:BB:152:ARG:N	2.36	0.40
5:BG:78:THR:OG1	5:BG:79:LYS:N	2.50	0.40
10:BN:34:ILE:O	10:BN:38:VAL:HG13	2.22	0.40
11:BO:17:ALA:HA	11:BO:30:VAL:HG22	2.04	0.40
12:BV:36:VAL:HB	12:BV:51:VAL:CG2	2.50	0.40
14:BX:6:PRO:HG3	14:BX:14:LYS:HG2	2.02	0.40
15:BY:43:LYS:O	15:BY:46:GLU:HG3	2.22	0.40
20:BF:48:PHE:CD2	20:BF:67:PRO:HA	2.56	0.40
23:BQ:113:ASP:OD1	23:BQ:115:THR:HG22	2.22	0.40
27:BU:42:VAL:HG13	27:BU:52:LYS:HE3	2.02	0.40
32:Bf:140:TYR:CE1	32:Bf:145:HIS:HA	2.56	0.40
33:BM:97:LEU:HG	33:BM:118:ALA:HB3	2.04	0.40
34:B5:1553:G:N2	34:B5:1555:A:H3'	2.37	0.40
34:B5:1695:G:N3	34:B5:1695:G:H2'	2.36	0.40
37:AC:82:THR:OG1	38:A1:355:A:N1	2.49	0.40
38:A1:130:A:H2'	38:A1:131:C:C6	2.57	0.40
38:A1:595:G:H2'	38:A1:596:C:C6	2.57	0.40
38:A1:633:C:O2'	68:Af:21:ARG:O	2.36	0.40
38:A1:989:A:H2'	38:A1:990:PSU:O4'	2.22	0.40
38:A1:1740:U:C1'	38:A1:1741:A:H2	2.34	0.40
38:A1:1751:G:H5'	73:Ak:26:LYS:HE2	2.04	0.40
38:A1:2318:U:H2'	38:A1:2319:U:O4'	2.21	0.40
38:A1:2615:G:H2'	38:A1:2616:C:C6	2.56	0.40
38:A1:2673:A:O2'	47:AJ:126:ASP:OD1	2.25	0.40
58:AV:40:LYS:HE3	58:AV:40:LYS:HB3	1.94	0.40
63:Aa:94:ALA:HB2	63:Aa:121:VAL:HG22	2.04	0.40
67:Ae:11:LYS:O	67:Ae:12:LYS:HB2	2.19	0.40
71:Ai:90:MET:HE2	71:Ai:93:ILE:HD12	2.03	0.40
17:Bb:17:ARG:O	34:B5:1071:U:H5'	2.21	0.40
24:BR:26:LEU:HD11	24:BR:62:GLN:HG3	2.02	0.40
31:Bg:292:LEU:HA	31:Bg:302:PHE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:119:A:H1'	34:B5:397:A:C8	2.55	0.40
34:B5:1244:A:C5	34:B5:1246:C:C2	3.10	0.40
37:AC:23:PRO:HD2	37:AC:26:PHE:CD2	2.56	0.40
38:A1:100:A:H3'	38:A1:101:G:H21	1.86	0.40
38:A1:571:U:H2'	38:A1:572:A:H8	1.87	0.40
38:A1:627:U:H2'	38:A1:628:A:H8	1.86	0.40
38:A1:1011:A:H2'	38:A1:1012:G:H8	1.86	0.40
38:A1:1306:G:C6	51:AO:62[A]:THR:HA	2.56	0.40
38:A1:2722:U:O2'	56:AT:88:ARG:O	2.35	0.40
38:A1:2727:A:N1	63:Aa:43:ILE:HG12	2.37	0.40
38:A1:2836:C:H5	38:A1:2852:C:N4	2.20	0.40
38:A1:2921:OMU:H6	38:A1:2921:OMU:O5'	2.21	0.40
38:A1:3268:A:C6	42:AE:69:PHE:HE2	2.40	0.40
43:AF:186:HIS:HA	43:AF:189:ILE:HG22	2.03	0.40
48:AL:113:VAL:O	48:AL:117:LYS:HG2	2.22	0.40
55:AS:48:LEU:HD12	55:AS:49:HIS:CG	2.57	0.40
61:AY:37:LYS:NZ	61:AY:40:ARG:HH11	2.20	0.40
63:Aa:75:LEU:HB3	63:Aa:118:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	185 (91%)	19 (9%)	0	100	100
2	BB	212/255 (83%)	191 (90%)	21 (10%)	0	100	100
3	BC	215/254 (85%)	210 (98%)	5 (2%)	0	100	100
4	BE	258/261 (99%)	247 (96%)	11 (4%)	0	100	100
5	BG	224/236 (95%)	219 (98%)	5 (2%)	0	100	100
6	BH	182/190 (96%)	168 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BI	184/200 (92%)	170 (92%)	14 (8%)	0	100	100
8	BJ	183/197 (93%)	171 (93%)	12 (7%)	0	100	100
9	BL	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
10	BN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
11	BO	125/137 (91%)	114 (91%)	11 (9%)	0	100	100
12	BV	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
13	BW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	BX	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
15	BY	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
16	Ba	95/119 (80%)	86 (90%)	9 (10%)	0	100	100
17	Bb	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
18	Be	58/63 (92%)	54 (93%)	4 (7%)	0	100	100
19	BD	221/240 (92%)	213 (96%)	8 (4%)	0	100	100
20	BF	204/225 (91%)	194 (95%)	10 (5%)	0	100	100
21	BK	94/105 (90%)	85 (90%)	9 (10%)	0	100	100
22	BP	122/142 (86%)	117 (96%)	5 (4%)	0	100	100
23	BQ	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
24	BR	117/136 (86%)	115 (98%)	2 (2%)	0	100	100
25	BS	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
26	BT	139/144 (96%)	128 (92%)	11 (8%)	0	100	100
27	BU	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
28	BZ	69/108 (64%)	69 (100%)	0	0	100	100
29	Bc	61/67 (91%)	59 (97%)	2 (3%)	0	100	100
30	Bd	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
31	Bg	310/319 (97%)	286 (92%)	24 (8%)	0	100	100
32	Bf	73/152 (48%)	69 (94%)	4 (6%)	0	100	100
33	BM	122/143 (85%)	116 (95%)	6 (5%)	0	100	100
35	AA	245/254 (96%)	233 (95%)	12 (5%)	0	100	100
36	AB	383/387 (99%)	368 (96%)	15 (4%)	0	100	100
37	AC	359/362 (99%)	338 (94%)	21 (6%)	0	100	100
41	AD	290/297 (98%)	279 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	AE	163/176 (93%)	155 (95%)	8 (5%)	0	100	100
43	AF	220/244 (90%)	212 (96%)	8 (4%)	0	100	100
44	AG	228/256 (89%)	219 (96%)	9 (4%)	0	100	100
45	AH	188/191 (98%)	177 (94%)	11 (6%)	0	100	100
46	AI	215/221 (97%)	204 (95%)	11 (5%)	0	100	100
47	AJ	167/174 (96%)	161 (96%)	6 (4%)	0	100	100
48	AL	191/199 (96%)	183 (96%)	8 (4%)	0	100	100
49	AM	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
50	AN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
52	AP	171/184 (93%)	165 (96%)	6 (4%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
55	AS	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
56	AT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
57	AU	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
58	AV	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	115 (97%)	4 (3%)	0	100	100
61	AY	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
62	AZ	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
63	Aa	146/149 (98%)	137 (94%)	9 (6%)	0	100	100
64	Ab	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
65	Ac	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
66	Ad	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
67	Ae	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
68	Af	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
69	Ag	110/121 (91%)	104 (94%)	6 (6%)	0	100	100
70	Ah	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
71	Ai	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
72	Aj	85/88 (97%)	82 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Ak	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
74	Al	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
75	Am	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	90 (87%)	13 (13%)	0	100	100
78	Ap	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
All	All	10921/11886 (92%)	10389 (95%)	532 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	136 (100%)	0	100	100
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	96 (100%)	0	100	100
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	182 (100%)	0	100	100
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	104 (100%)	0	100	100
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	101/124 (82%)	101 (100%)	0	100	100
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	62/89 (70%)	62 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	66/135 (49%)	66 (100%)	0	100	100
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	321/322 (100%)	321 (100%)	0	100	100
37	AC	288/289 (100%)	288 (100%)	0	100	100
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	137/153 (90%)	137 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	170 (100%)	0	100	100
46	AI	185/187 (99%)	185 (100%)	0	100	100
47	AJ	147/150 (98%)	147 (100%)	0	100	100
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	141 (100%)	0	100	100
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	136 (100%)	0	100	100
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
All	All	9293/9988 (93%)	9293 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165)

such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	30	GLN
1	BA	39	ASN
1	BA	46	HIS
1	BA	109	ASN
2	BB	124	ASN
2	BB	199	ASN
2	BB	211	HIS
3	BC	82	ASN
3	BC	89	GLN
4	BE	36	HIS
4	BE	157	ASN
4	BE	223	ASN
4	BE	224	ASN
5	BG	56	ASN
5	BG	65	GLN
5	BG	197	ASN
6	BH	22	GLN
6	BH	42	GLN
6	BH	71	HIS
6	BH	170	GLN
7	BI	116	HIS
7	BI	175	GLN
8	BJ	74	ASN
8	BJ	155	HIS
9	BL	92	HIS
12	BV	7	GLN
13	BW	56	HIS
13	BW	64	GLN
14	BX	28	ASN
15	BY	22	GLN
15	BY	107	GLN
15	BY	113	ASN
16	Ba	69	ASN
17	Bb	42	ASN
18	Be	17	GLN
18	Be	46	ASN
19	BD	111	ASN
19	BD	165	ASN
20	BF	44	ASN
20	BF	128	ASN
20	BF	131	GLN
20	BF	186	ASN

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Mol	Chain	Res	Type
20	BF	224	ASN
21	BK	13	GLN
21	BK	17	GLN
21	BK	28	ASN
22	BP	79	HIS
22	BP	103	ASN
22	BP	104	GLN
23	BQ	32	ASN
25	BS	12	GLN
25	BS	13	HIS
25	BS	63	GLN
25	BS	71	GLN
26	BT	129	GLN
27	BU	15	GLN
27	BU	36	ASN
27	BU	48	HIS
27	BU	105	GLN
30	Bd	37	ASN
31	Bg	101	GLN
31	Bg	153	GLN
31	Bg	159	ASN
31	Bg	198	ASN
31	Bg	224	ASN
31	Bg	268	GLN
31	Bg	308	ASN
31	Bg	314	GLN
33	BM	38	HIS
33	BM	96	GLN
35	AA	97	ASN
36	AB	121	ASN
36	AB	211	GLN
36	AB	224	HIS
36	AB	293	ASN
36	AB	371	GLN
37	AC	59	GLN
37	AC	140	HIS
37	AC	160	GLN
37	AC	175	HIS
37	AC	196	ASN
37	AC	237	GLN
37	AC	291	ASN
37	AC	322	GLN

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Mol	Chain	Res	Type
37	AC	361	HIS
41	AD	57	ASN
41	AD	81	HIS
41	AD	151	GLN
41	AD	264	GLN
41	AD	274	GLN
42	AE	57	HIS
42	AE	157	GLN
43	AF	93	ASN
43	AF	104	GLN
43	AF	112	ASN
43	AF	159	GLN
43	AF	166	ASN
43	AF	172	ASN
43	AF	186	HIS
43	AF	231	ASN
44	AG	45	ASN
44	AG	137	ASN
44	AG	192	GLN
45	AH	8	GLN
45	AH	58	HIS
45	AH	100	ASN
45	AH	157	ASN
45	AH	162	GLN
46	AI	112	GLN
47	AJ	68	HIS
47	AJ	95	ASN
47	AJ	109	HIS
47	AJ	150	ASN
48	AL	37	ASN
48	AL	103	ASN
48	AL	106	GLN
48	AL	129	ASN
49	AM	27	GLN
49	AM	41	GLN
49	AM	105	GLN
49	AM	126	GLN
50	AN	15	GLN
50	AN	32	GLN
50	AN	70	ASN
50	AN	95	GLN
50	AN	182	ASN

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Mol	Chain	Res	Type
52	AP	10	ASN
52	AP	133	HIS
52	AP	137	ASN
53	AQ	9	GLN
54	AR	34	GLN
54	AR	68	GLN
55	AS	3	HIS
55	AS	49	HIS
55	AS	138	GLN
56	AT	5	HIS
56	AT	26	HIS
56	AT	98	HIS
57	AU	40	HIS
57	AU	49	ASN
57	AU	101	ASN
58	AV	98	ASN
59	AW	45	ASN
60	AX	53	HIS
60	AX	137	ASN
61	AY	110	HIS
62	AZ	122	HIS
62	AZ	128	GLN
63	Aa	64	GLN
63	Aa	65	GLN
65	Ac	75	ASN
67	Ae	20	HIS
69	Ag	3	GLN
69	Ag	61	GLN
70	Ah	16	GLN
70	Ah	34	GLN
70	Ah	62	GLN
70	Ah	76	GLN
70	Ah	108	GLN
71	Ai	63	ASN
72	Aj	69	HIS
74	Al	11	GLN
74	Al	32	ASN
75	Am	117	HIS
77	Ao	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1754/1798 (97%)	408 (23%)	10 (0%)
38	A1	3156/3395 (92%)	574 (18%)	29 (0%)
39	A3	120/121 (99%)	15 (12%)	1 (0%)
40	A4	157/158 (99%)	26 (16%)	1 (0%)
79	tP	74/75 (98%)	31 (41%)	0
80	tA	75/76 (98%)	15 (20%)	0
81	MR	11/12 (91%)	1 (9%)	0
All	All	5347/5635 (94%)	1070 (20%)	41 (0%)

All (1070) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	17	C
34	B5	25	C
34	B5	34	G
34	B5	47	A
34	B5	57	G
34	B5	59	C
34	B5	61	A
34	B5	62	A
34	B5	68	A
34	B5	73	U
34	B5	74	U
34	B5	75	U
34	B5	76	A
34	B5	77	U
34	B5	78	A
34	B5	84	A
34	B5	104	A
34	B5	114	C
34	B5	119	A
34	B5	121	U
34	B5	127	G
34	B5	130	C
34	B5	131	C
34	B5	132	U
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U

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Mol	Chain	Res	Type
34	B5	138	A
34	B5	140	A
34	B5	141	U
34	B5	144	U
34	B5	145	A
34	B5	153	G
34	B5	160	C
34	B5	161	U
34	B5	166	C
34	B5	178	U
34	B5	179	A
34	B5	180	A
34	B5	188	A
34	B5	189	C
34	B5	190	C
34	B5	191	C
34	B5	193	U
34	B5	194	U
34	B5	195	G
34	B5	197	A
34	B5	210	A
34	B5	215	A
34	B5	216	U
34	B5	217	A
34	B5	218	A
34	B5	220	A
34	B5	224	C
34	B5	225	A
34	B5	226	A
34	B5	228	G
34	B5	231	U
34	B5	233	C
34	B5	235	G
34	B5	236	A
34	B5	238	U
34	B5	239	C
34	B5	240	U
34	B5	241	U
34	B5	242	U
34	B5	249	U
34	B5	252	U
34	B5	253	A

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Mol	Chain	Res	Type
34	B5	257	A
34	B5	260	U
34	B5	261	U
34	B5	262	U
34	B5	265	A
34	B5	272	U
34	B5	273	G
34	B5	278	U
34	B5	280	U
34	B5	284	G
34	B5	286	C
34	B5	288	A
34	B5	289	U
34	B5	293	U
34	B5	299	A
34	B5	314	C
34	B5	316	A
34	B5	322	G
34	B5	337	G
34	B5	338	C
34	B5	352	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	404	G
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	428	A
34	B5	439	U
34	B5	444	C
34	B5	454	U
34	B5	460	A
34	B5	461	G
34	B5	468	A
34	B5	474	A
34	B5	475	A
34	B5	477	A

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Mol	Chain	Res	Type
34	B5	481	A
34	B5	482	U
34	B5	483	A
34	B5	484	C
34	B5	486	G
34	B5	487	G
34	B5	488	G
34	B5	489	C
34	B5	490	C
34	B5	491	C
34	B5	493	U
34	B5	494	U
34	B5	495	C
34	B5	496	G
34	B5	497	G
34	B5	499	U
34	B5	500	C
34	B5	501	U
34	B5	502	U
34	B5	505	A
34	B5	508	U
34	B5	514	G
34	B5	515	A
34	B5	519	C
34	B5	527	A
34	B5	534	A
34	B5	538	A
34	B5	540	G
34	B5	542	A
34	B5	543	C
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	561	G
34	B5	565	C
34	B5	574	G
34	B5	580	A
34	B5	594	A
34	B5	595	G
34	B5	606	A
34	B5	610	G

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Mol	Chain	Res	Type
34	B5	611	U
34	B5	619	A
34	B5	620	A
34	B5	623	A
34	B5	624	G
34	B5	649	U
34	B5	650	U
34	B5	651	G
34	B5	652	G
34	B5	656	G
34	B5	657	U
34	B5	658	C
34	B5	677	G
34	B5	679	U
34	B5	680	U
34	B5	681	U
34	B5	682	C
34	B5	684	A
34	B5	685	A
34	B5	691	C
34	B5	694	U
34	B5	696	C
34	B5	697	C
34	B5	698	U
34	B5	699	U
34	B5	700	C
34	B5	701	U
34	B5	702	G
34	B5	703	G
34	B5	704	C
34	B5	731	C
34	B5	732	G
34	B5	733	A
34	B5	734	A
34	B5	735	C
34	B5	736	C
34	B5	738	G
34	B5	739	G
34	B5	740	A
34	B5	741	C
34	B5	742	U
34	B5	743	U

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Mol	Chain	Res	Type
34	B5	753	A
34	B5	765	G
34	B5	766	PSU
34	B5	771	A
34	B5	774	A
34	B5	779	U
34	B5	780	A
34	B5	782	U
34	B5	783	G
34	B5	784	C
34	B5	789	A
34	B5	793	A
34	B5	794	U
34	B5	812	A
34	B5	814	A
34	B5	819	G
34	B5	823	G
34	B5	825	U
34	B5	826	U
34	B5	827	C
34	B5	828	U
34	B5	829	A
34	B5	830	U
34	B5	831	U
34	B5	832	U
34	B5	834	G
34	B5	835	U
34	B5	836	U
34	B5	837	G
34	B5	838	G
34	B5	843	U
34	B5	847	A
34	B5	849	C
34	B5	851	U
34	B5	852	C
34	B5	857	U
34	B5	860	U
34	B5	863	A
34	B5	873	U
34	B5	889	U
34	B5	890	C
34	B5	892	A

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Mol	Chain	Res	Type
34	B5	898	A
34	B5	914	G
34	B5	921	U
34	B5	927	C
34	B5	933	A
34	B5	935	U
34	B5	959	U
34	B5	960	U
34	B5	966	A
34	B5	969	C
34	B5	992	A
34	B5	1003	A
34	B5	1004	U
34	B5	1010	C
34	B5	1021	C
34	B5	1026	A
34	B5	1028	C
34	B5	1031	U
34	B5	1032	G
34	B5	1039	A
34	B5	1040	G
34	B5	1052	U
34	B5	1053	G
34	B5	1056	U
34	B5	1057	U
34	B5	1059	U
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1063	U
34	B5	1064	G
34	B5	1076	A
34	B5	1081	A
34	B5	1082	C
34	B5	1092	A
34	B5	1100	G
34	B5	1126	G
34	B5	1138	A
34	B5	1150	G
34	B5	1158	C
34	B5	1185	U
34	B5	1186	U

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Mol	Chain	Res	Type
34	B5	1194	A
34	B5	1196	A
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1202	A
34	B5	1203	A
34	B5	1217	A
34	B5	1218	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1250	U
34	B5	1251	U
34	B5	1255	G
34	B5	1256	A
34	B5	1265	G
34	B5	1291	G
34	B5	1314	U
34	B5	1315	U
34	B5	1318	G
34	B5	1321	A
34	B5	1340	U
34	B5	1344	A
34	B5	1345	A
34	B5	1348	A
34	B5	1353	U
34	B5	1354	G
34	B5	1362	U
34	B5	1363	U
34	B5	1366	U
34	B5	1369	U
34	B5	1370	U
34	B5	1378	U
34	B5	1388	A
34	B5	1390	U
34	B5	1398	U
34	B5	1399	C
34	B5	1400	A
34	B5	1413	U
34	B5	1415	PSU
34	B5	1422	A

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Mol	Chain	Res	Type
34	B5	1423	U
34	B5	1427	A
34	B5	1428	G
34	B5	1435	G
34	B5	1436	A
34	B5	1458	G
34	B5	1459	C
34	B5	1460	A
34	B5	1471	A
34	B5	1490	C
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1510	U
34	B5	1514	U
34	B5	1515	A
34	B5	1516	A
34	B5	1521	G
34	B5	1523	G
34	B5	1524	A
34	B5	1531	G
34	B5	1534	G
34	B5	1537	C
34	B5	1540	G
34	B5	1557	U
34	B5	1559	A
34	B5	1573	A
34	B5	1574	G
34	B5	1575	G7M
34	B5	1577	A
34	B5	1578	U
34	B5	1583	A
34	B5	1584	G
34	B5	1590	G
34	B5	1601	G
34	B5	1607	G
34	B5	1611	A
34	B5	1616	G
34	B5	1634	C
34	B5	1657	U
34	B5	1658	G
34	B5	1678	A

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Mol	Chain	Res	Type
34	B5	1680	G
34	B5	1683	C
34	B5	1684	U
34	B5	1687	U
34	B5	1688	U
34	B5	1689	A
34	B5	1690	G
34	B5	1692	G
34	B5	1693	A
34	B5	1694	A
34	B5	1698	G
34	B5	1699	G
34	B5	1700	C
34	B5	1701	A
34	B5	1702	A
34	B5	1703	C
34	B5	1704	U
34	B5	1705	C
34	B5	1707	A
34	B5	1708	U
34	B5	1709	C
34	B5	1711	C
34	B5	1712	A
34	B5	1713	G
34	B5	1714	A
34	B5	1716	C
34	B5	1728	A
34	B5	1732	A
34	B5	1755	A
34	B5	1756[A]	A
34	B5	1757	G
34	B5	1762	A
34	B5	1769	U
34	B5	1780	G
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1795	U
34	B5	1796	C
34	B5	1798	U
34	B5	1799	U
38	A1	6	A

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Mol	Chain	Res	Type
38	A1	26	A
38	A1	34	A
38	A1	40	A
38	A1	49	A
38	A1	59	G
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	92	G
38	A1	99	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	122	A
38	A1	135	C
38	A1	136	G
38	A1	150	A
38	A1	156	G
38	A1	157	A
38	A1	165	A
38	A1	166	C
38	A1	169	U
38	A1	170	G
38	A1	171	G
38	A1	172	G
38	A1	173	G
38	A1	174	C
38	A1	175	C
38	A1	187	A
38	A1	188	U
38	A1	190	U
38	A1	191	U
38	A1	200	C
38	A1	210	U
38	A1	219	A
38	A1	238	A
38	A1	239	G
38	A1	240	U
38	A1	241	G
38	A1	242	C
38	A1	243	G

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Mol	Chain	Res	Type
38	A1	244	G
38	A1	245	U
38	A1	246	U
38	A1	247	C
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	253	A
38	A1	254	A
38	A1	258	G
38	A1	261	U
38	A1	262	U
38	A1	263	C
38	A1	269	G
38	A1	284	A
38	A1	286	U
38	A1	295	A
38	A1	305	U
38	A1	309	U
38	A1	310	U
38	A1	315	C
38	A1	329	U
38	A1	349	A
38	A1	376	G
38	A1	387	A
38	A1	398	A
38	A1	403	C
38	A1	421	G
38	A1	422	A
38	A1	437	G
38	A1	439	C
38	A1	440	A
38	A1	441	U
38	A1	443	G
38	A1	444	U
38	A1	445	G
38	A1	446	U
38	A1	447	U
38	A1	448	U
38	A1	449	U

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Mol	Chain	Res	Type
38	A1	450	G
38	A1	451	U
38	A1	487	U
38	A1	488	U
38	A1	490	C
38	A1	493	U
38	A1	494	G
38	A1	495	G
38	A1	520	U
38	A1	521	A
38	A1	536	U
38	A1	540	U
38	A1	543	C
38	A1	544	C
38	A1	545	U
38	A1	547	G
38	A1	548	G
38	A1	552	G
38	A1	557	A
38	A1	559	A
38	A1	560	G
38	A1	567	G
38	A1	569	A
38	A1	579	G
38	A1	589	A
38	A1	592	A
38	A1	597	G
38	A1	600	G
38	A1	603	A
38	A1	607	A
38	A1	611	A
38	A1	612	U
38	A1	620	U
38	A1	621	A
38	A1	622	A
38	A1	649	A
38	A1	660	A
38	A1	677	A
38	A1	691	A
38	A1	705	A
38	A1	715	A
38	A1	719	U

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Mol	Chain	Res	Type
38	A1	734	C
38	A1	735	A
38	A1	738	A
38	A1	750	G
38	A1	767	U
38	A1	776	PSU
38	A1	777	U
38	A1	780	A
38	A1	781	G
38	A1	785	G
38	A1	806	A
38	A1	817	A
38	A1	830	A
38	A1	832	G
38	A1	837	A
38	A1	848	A
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	890	C
38	A1	896	A
38	A1	907	G
38	A1	908	G
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	921	A
38	A1	923	C
38	A1	925	A
38	A1	937	G
38	A1	944	C
38	A1	959	C
38	A1	960	PSU
38	A1	980	A
38	A1	982	C
38	A1	994	G
38	A1	1000	C
38	A1	1010	G
38	A1	1013	G
38	A1	1014	U
38	A1	1015	U
38	A1	1016	C

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Mol	Chain	Res	Type
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1020	G
38	A1	1021	G
38	A1	1022	U
38	A1	1023	C
38	A1	1031	C
38	A1	1032	C
38	A1	1033	U
38	A1	1034	U
38	A1	1035	G
38	A1	1036	A
38	A1	1037	C
38	A1	1041	U
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1083	G
38	A1	1087	G
38	A1	1092	C
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1131	G
38	A1	1143	A
38	A1	1153	A
38	A1	1159	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1197	A
38	A1	1201	C
38	A1	1206	G
38	A1	1208	U

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Mol	Chain	Res	Type
38	A1	1218	U
38	A1	1220	U
38	A1	1221	A
38	A1	1222	G
38	A1	1225	A
38	A1	1228	C
38	A1	1232	C
38	A1	1233	G
38	A1	1234	G
38	A1	1235	U
38	A1	1236	G
38	A1	1237	G
38	A1	1238	C
38	A1	1239	C
38	A1	1240	A
38	A1	1241	U
38	A1	1242	G
38	A1	1244	A
38	A1	1246	G
38	A1	1248	C
38	A1	1249	G
38	A1	1250	G
38	A1	1251	A
38	A1	1252	A
38	A1	1253	U
38	A1	1257	C
38	A1	1258	U
38	A1	1259	A
38	A1	1260	A
38	A1	1262	G
38	A1	1263	A
38	A1	1264	G
38	A1	1265	U
38	A1	1266	G
38	A1	1267	U
38	A1	1268	G
38	A1	1269	U
38	A1	1271	A
38	A1	1272	C
38	A1	1273	A
38	A1	1274	A
38	A1	1276	U

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Mol	Chain	Res	Type
38	A1	1280	C
38	A1	1282	G
38	A1	1283	C
38	A1	1285	G
38	A1	1286	A
38	A1	1287	A
38	A1	1309	U
38	A1	1330	A
38	A1	1331	U
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1355	A
38	A1	1366	A
38	A1	1386	A
38	A1	1399	A
38	A1	1400	G
38	A1	1418	A
38	A1	1419	A
38	A1	1425	U
38	A1	1434	G
38	A1	1437	C
38	A1	1446	A
38	A1	1475	A
38	A1	1481	A
38	A1	1482	A
38	A1	1483	G
38	A1	1488	G
38	A1	1502	C
38	A1	1527	C
38	A1	1539	A
38	A1	1555	U
38	A1	1556	C
38	A1	1557	A
38	A1	1561	G
38	A1	1562	C
38	A1	1563	C
38	A1	1564	U
38	A1	1565	G

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Mol	Chain	Res	Type
38	A1	1566	A
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1570	U
38	A1	1571	A
38	A1	1572	U
38	A1	1575	A
38	A1	1576	G
38	A1	1577	G
38	A1	1580	A
38	A1	1582	C
38	A1	1589	A
38	A1	1628	C
38	A1	1642	A
38	A1	1643	A
38	A1	1645	U
38	A1	1686	U
38	A1	1724	U
38	A1	1736	G
38	A1	1741	A
38	A1	1750	A
38	A1	1751	G
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1796	G
38	A1	1797	A
38	A1	1813	A
38	A1	1816	A
38	A1	1818	U
38	A1	1819	U
38	A1	1821	U
38	A1	1824	U
38	A1	1842	A
38	A1	1849	C
38	A1	1867	A
38	A1	1880	U
38	A1	1886	A
38	A1	1893	A

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Mol	Chain	Res	Type
38	A1	1906	G
38	A1	1952	G
38	A1	1953	G
38	A1	1954	G
38	A1	2094	C
38	A1	2095	G
38	A1	2111	G
38	A1	2112	U
38	A1	2114	C
38	A1	2122	G
38	A1	2131	A
38	A1	2140	U
38	A1	2144	A
38	A1	2158	A
38	A1	2169	G
38	A1	2170	U
38	A1	2188	A
38	A1	2206	G
38	A1	2207	A
38	A1	2208	A
38	A1	2209	U
38	A1	2222	A
38	A1	2223	A
38	A1	2226	U
38	A1	2227	C
38	A1	2249	G
38	A1	2269	U
38	A1	2272	G
38	A1	2273	G
38	A1	2280	A
38	A1	2281	A
38	A1	2282	U
38	A1	2307	G
38	A1	2310	U
38	A1	2313	A
38	A1	2315	G
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G

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Mol	Chain	Res	Type
38	A1	2383	C
38	A1	2393	G
38	A1	2394	G
38	A1	2397	A
38	A1	2398	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2435	G
38	A1	2437	G
38	A1	2439	A
38	A1	2440	G
38	A1	2441	A
38	A1	2442	G
38	A1	2443	A
38	A1	2444	C
38	A1	2501	U
38	A1	2502	A
38	A1	2503	G
38	A1	2504	U
38	A1	2506	U
38	A1	2507	C
38	A1	2508	U
38	A1	2509	U
38	A1	2514	U
38	A1	2515	A
38	A1	2522	G
38	A1	2523	A
38	A1	2530	G
38	A1	2532	U
38	A1	2536	A
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2541	U
38	A1	2542	U
38	A1	2543	U
38	A1	2544	U
38	A1	2545	C
38	A1	2546	C

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Mol	Chain	Res	Type
38	A1	2547	A
38	A1	2549	G
38	A1	2552	C
38	A1	2554	A
38	A1	2569	A
38	A1	2570	U
38	A1	2571	U
38	A1	2572	C
38	A1	2573	G
38	A1	2575	G
38	A1	2585	G
38	A1	2587	U
38	A1	2593	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2636	A
38	A1	2637	A
38	A1	2652	U
38	A1	2656	A
38	A1	2674	A
38	A1	2677	G
38	A1	2678	A
38	A1	2680	A
38	A1	2681	U
38	A1	2689	A
38	A1	2691	A
38	A1	2694	A
38	A1	2704	A
38	A1	2705	A
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G
38	A1	2729	U
38	A1	2747	A
38	A1	2749	G
38	A1	2752	U
38	A1	2753	G
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2779	A

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Mol	Chain	Res	Type
38	A1	2796	G
38	A1	2799	A
38	A1	2800	G
38	A1	2801	A
38	A1	2802	A
38	A1	2808	A
38	A1	2810	C
38	A1	2814	G
38	A1	2817	A
38	A1	2842	U
38	A1	2845	A
38	A1	2847	A
38	A1	2849	C
38	A1	2860	U
38	A1	2861	U
38	A1	2871	G
38	A1	2875	U
38	A1	2887	A
38	A1	2894	C
38	A1	2904	U
38	A1	2923	PSU
38	A1	2935	U
38	A1	2936	A
38	A1	2942	C
38	A1	2947	G
38	A1	2951	G
38	A1	2971	A
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3012	A
38	A1	3018	C
38	A1	3022	G
38	A1	3023	U
38	A1	3035	A
38	A1	3048	A
38	A1	3059	G
38	A1	3078	U
38	A1	3079	U
38	A1	3086	A
38	A1	3092	C
38	A1	3101	G

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Mol	Chain	Res	Type
38	A1	3104	U
38	A1	3113	A
38	A1	3122	A
38	A1	3129	A
38	A1	3130	A
38	A1	3131	U
38	A1	3134	A
38	A1	3142	A
38	A1	3143	C
38	A1	3153	U
38	A1	3154	C
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3163	A
38	A1	3165	A
38	A1	3166	C
38	A1	3168	A
38	A1	3170	A
38	A1	3171	U
38	A1	3173	G
38	A1	3174	A
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3196	U
38	A1	3206	C
38	A1	3207	U
38	A1	3210	A
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3228	C
38	A1	3229	G
38	A1	3232	G
38	A1	3238	G
38	A1	3243	A
38	A1	3247	G
38	A1	3259	U
38	A1	3263	G

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Mol	Chain	Res	Type
38	A1	3270	U
38	A1	3276	G
38	A1	3277	U
38	A1	3278	C
38	A1	3279	A
38	A1	3282	U
38	A1	3284	G
38	A1	3285	C
38	A1	3286	G
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U
38	A1	3313	U
38	A1	3316	A
38	A1	3320	A
38	A1	3324	C
38	A1	3341	U
38	A1	3342	A
38	A1	3345	G
38	A1	3350	C
38	A1	3352	U
38	A1	3354	U
38	A1	3369	G
38	A1	3378	C
38	A1	3382	U
38	A1	3383	G
38	A1	3396	U
39	A3	7	G
39	A3	11	A
39	A3	17	A
39	A3	22	A
39	A3	23	A
39	A3	24	A
39	A3	38	U
39	A3	54	U
39	A3	55	A
39	A3	65	G
39	A3	73	C
39	A3	76	A
39	A3	102	A
39	A3	112	G
39	A3	121	U

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Mol	Chain	Res	Type
40	A4	23	U
40	A4	34	U
40	A4	35	C
40	A4	51	G
40	A4	52	A
40	A4	59	A
40	A4	62	C
40	A4	63	G
40	A4	81	U
40	A4	82	U
40	A4	84	C
40	A4	86	U
40	A4	87	G
40	A4	89	A
40	A4	90	U
40	A4	95	G
40	A4	104	A
40	A4	105	A
40	A4	106	C
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	130	C
40	A4	152	G
40	A4	158	U
79	tP	10	A
79	tP	16	U
79	tP	18	G
79	tP	19	G
79	tP	20	A
79	tP	22	G
79	tP	23	C
79	tP	24	G
79	tP	30	G
79	tP	31	G
79	tP	33	U
79	tP	42	U
79	tP	44	A
79	tP	45	U
79	tP	46	G
79	tP	47	U

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Mol	Chain	Res	Type
79	tP	48	C
79	tP	50	U
79	tP	52	G
79	tP	54	A
79	tP	55	U
79	tP	57	G
79	tP	58	A
79	tP	60	A
79	tP	61	C
79	tP	62	C
79	tP	66	C
79	tP	69	C
79	tP	70	G
79	tP	73	A
79	tP	76	A
80	tA	9	G
80	tA	14	A
80	tA	15	G
80	tA	16	U
80	tA	17	A
80	tA	18	G
80	tA	19	G
80	tA	20	A
80	tA	31	G
80	tA	46	G
80	tA	48	C
80	tA	49	C
80	tA	54	A
80	tA	59	A
80	tA	74	C
81	MR	8	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	130	C
34	B5	196	G
34	B5	610	G
34	B5	752	A
34	B5	889	U
34	B5	1061	A
34	B5	1344	A

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Mol	Chain	Res	Type
34	B5	1458	G
34	B5	1683	C
34	B5	1755	A
38	A1	43	A
38	A1	116	A
38	A1	165	A
38	A1	240	U
38	A1	252	U
38	A1	309	U
38	A1	588	G
38	A1	734	C
38	A1	873	C
38	A1	916	G
38	A1	1020	G
38	A1	1022	U
38	A1	1034	U
38	A1	1035	G
38	A1	1560	G
38	A1	1818	U
38	A1	1953	G
38	A1	2094	C
38	A1	2222	A
38	A1	2438	A
38	A1	2586	G
38	A1	2772	C
38	A1	2801	A
38	A1	3022	G
38	A1	3121	U
38	A1	3154	C
38	A1	3169	U
38	A1	3227	A
38	A1	3283	U
39	A3	23	A
40	A4	88	A

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

59 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
34	PSU	B5	999	34	18,21,22	1.40	3 (16%)	21,30,33	2.05	4 (19%)
38	PSU	A1	2133	38	18,21,22	1.44	3 (16%)	21,30,33	2.09	5 (23%)
38	PSU	A1	1052	38	18,21,22	1.41	3 (16%)	21,30,33	2.00	4 (19%)
38	PSU	A1	966	38	18,21,22	1.43	4 (22%)	21,30,33	2.14	4 (19%)
36	HIC	AB	243	36	10,11,12	1.45	1 (10%)	9,14,16	1.37	2 (22%)
38	5MC	A1	2278	38	19,22,23	1.55	3 (15%)	26,32,35	1.09	3 (11%)
40	PSU	A4	73	40	18,21,22	1.40	3 (16%)	21,30,33	2.07	4 (19%)
38	PSU	A1	2923	80,38	18,21,22	1.42	2 (11%)	21,30,33	2.06	3 (14%)
38	OMG	A1	2922	80,38	23,26,27	1.18	4 (17%)	32,38,41	1.93	6 (18%)
38	1MA	A1	645	38	21,25,26	1.34	4 (19%)	30,37,40	1.64	6 (20%)
38	PSU	A1	2351	38	18,21,22	1.42	4 (22%)	21,30,33	2.08	4 (19%)
38	PSU	A1	2264	38	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
38	PSU	A1	2266	38	18,21,22	1.40	3 (16%)	21,30,33	2.06	4 (19%)
38	PSU	A1	2944	38	18,21,22	1.46	4 (22%)	21,30,33	2.20	5 (23%)
38	PSU	A1	2975	38	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
34	B8N	B5	1191	34	25,29,30	1.34	3 (12%)	28,42,45	1.64	6 (21%)
38	PSU	A1	2260	38	18,21,22	1.40	3 (16%)	21,30,33	1.99	3 (14%)
38	PSU	A1	1110	38	18,21,22	1.46	3 (16%)	21,30,33	2.05	4 (19%)
38	PSU	A1	2258	38	18,21,22	1.43	3 (16%)	21,30,33	2.04	3 (14%)
38	PSU	A1	2314	38	18,21,22	1.41	3 (16%)	21,30,33	2.10	4 (19%)
34	PSU	B5	1290	34	18,21,22	1.39	3 (16%)	21,30,33	2.10	5 (23%)
38	PSU	A1	1042	38	18,21,22	1.39	4 (22%)	21,30,33	2.03	3 (14%)
38	PSU	A1	2880	38	18,21,22	1.42	3 (16%)	21,30,33	2.22	5 (23%)
38	PSU	A1	960	38	18,21,22	1.49	4 (22%)	21,30,33	2.09	4 (19%)
34	PSU	B5	302	34	18,21,22	1.40	3 (16%)	21,30,33	2.08	4 (19%)
34	PSU	B5	120	34	18,21,22	1.35	3 (16%)	21,30,33	2.04	4 (19%)
38	PSU	A1	2191	38	18,21,22	1.41	4 (22%)	21,30,33	2.12	4 (19%)
34	PSU	B5	211	34	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
38	PSU	A1	2826	38	18,21,22	1.39	4 (22%)	21,30,33	2.05	5 (23%)
38	PSU	A1	986	38	18,21,22	1.42	3 (16%)	21,30,33	2.02	4 (19%)
38	OMU	A1	2921	38	19,22,23	1.26	3 (15%)	25,31,34	1.83	5 (20%)
34	PSU	B5	632	34	18,21,22	1.38	3 (16%)	21,30,33	2.08	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PSU	B5	1187	34	18,21,22	1.36	2 (11%)	21,30,33	2.09	4 (19%)
38	PSU	A1	1124	38	18,21,22	1.37	2 (11%)	21,30,33	2.23	4 (19%)
38	PSU	A1	2416	38	18,21,22	1.46	3 (16%)	21,30,33	2.07	4 (19%)
38	5MC	A1	2870	38	19,22,23	1.70	3 (15%)	26,32,35	1.33	3 (11%)
34	PSU	B5	1415	34	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
34	PSU	B5	766	34	18,21,22	1.44	3 (16%)	21,30,33	2.06	4 (19%)
38	PSU	A1	990	38	18,21,22	1.38	3 (16%)	21,30,33	2.08	4 (19%)
38	PSU	A1	2340	38	18,21,22	1.45	3 (16%)	21,30,33	2.12	4 (19%)
34	PSU	B5	759	34	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
34	PSU	B5	466	34	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
38	PSU	A1	2129	38	18,21,22	1.41	3 (16%)	21,30,33	2.18	4 (19%)
38	PSU	A1	2349	38	18,21,22	1.43	4 (22%)	21,30,33	2.02	4 (19%)
38	PSU	A1	2735	38	18,21,22	1.41	3 (16%)	21,30,33	2.11	4 (19%)
38	PSU	A1	1004	38	18,21,22	1.40	2 (11%)	21,30,33	2.10	4 (19%)
39	PSU	A3	50	39	18,21,22	1.37	2 (11%)	21,30,33	2.10	4 (19%)
38	PSU	A1	776	38	18,21,22	1.46	3 (16%)	21,30,33	2.00	4 (19%)
34	4AC	B5	1280	34	21,24,25	1.00	1 (4%)	28,34,37	1.12	3 (10%)
38	PSU	A1	1056	38	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
34	PSU	B5	106	34	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
38	UR3	A1	2634	38	19,22,23	0.93	0	26,32,35	1.71	2 (7%)
38	1MA	A1	2142	38	21,25,26	1.34	3 (14%)	30,37,40	1.75	5 (16%)
34	PSU	B5	1181	34	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)
34	MA6	B5	1782	34	23,26,27	1.45	5 (21%)	33,38,41	2.17	10 (30%)
34	G7M	B5	1575	79,34	23,26,27	2.54	6 (26%)	34,39,42	3.15	15 (44%)
34	MA6	B5	1781	34	23,26,27	1.45	4 (17%)	33,38,41	2.05	10 (30%)
38	PSU	A1	2865	38	18,21,22	1.42	3 (16%)	21,30,33	2.14	4 (19%)
34	4AC	B5	1773	34	21,24,25	0.98	2 (9%)	28,34,37	2.22	5 (17%)

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
34	PSU	B5	999	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2133	38	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	1052	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	966	38	-	0/7/25/26	0/2/2/2
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
38	5MC	A1	2278	38	-	0/7/25/26	0/2/2/2
40	PSU	A4	73	40	-	0/7/25/26	0/2/2/2
38	PSU	A1	2923	80,38	-	3/7/25/26	0/2/2/2
38	OMG	A1	2922	80,38	-	1/9/27/28	0/3/3/3
38	1MA	A1	645	38	-	2/7/25/26	0/3/3/3
38	PSU	A1	2351	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2264	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2266	38	-	1/7/25/26	0/2/2/2
38	PSU	A1	2944	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2975	38	-	0/7/25/26	0/2/2/2
34	B8N	B5	1191	34	-	0/16/34/35	0/2/2/2
38	PSU	A1	2260	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	1110	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2258	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	2314	38	-	1/7/25/26	0/2/2/2
34	PSU	B5	1290	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	1042	38	-	3/7/25/26	0/2/2/2
38	PSU	A1	2880	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	960	38	-	2/7/25/26	0/2/2/2
34	PSU	B5	302	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	120	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2191	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	211	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2826	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	986	38	-	0/7/25/26	0/2/2/2
38	OMU	A1	2921	38	-	0/9/27/28	0/2/2/2
34	PSU	B5	632	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	1187	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	1124	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2416	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
34	PSU	B5	1415	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	766	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	990	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2340	38	-	1/7/25/26	0/2/2/2
34	PSU	B5	759	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	466	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2129	38	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	2349	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2735	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1004	38	-	0/7/25/26	0/2/2/2
39	PSU	A3	50	39	-	0/7/25/26	0/2/2/2
38	PSU	A1	776	38	-	2/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	0/11/29/30	0/2/2/2
38	PSU	A1	1056	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	106	34	-	0/7/25/26	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	1MA	A1	2142	38	-	1/7/25/26	0/3/3/3
34	PSU	B5	1181	34	-	0/7/25/26	0/2/2/2
34	MA6	B5	1782	34	-	3/11/29/30	0/3/3/3
34	G7M	B5	1575	79,34	-	0/7/25/26	0/3/3/3
34	MA6	B5	1781	34	-	0/11/29/30	0/3/3/3
38	PSU	A1	2865	38	-	0/7/25/26	0/2/2/2
34	4AC	B5	1773	34	-	3/11/29/30	0/2/2/2

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N7	7.80	1.46	1.33
38	A1	2870	5MC	C5-C4	6.02	1.48	1.44
38	A1	2278	5MC	C5-C4	5.50	1.48	1.44
34	B5	1575	G7M	C5-N7	-4.90	1.33	1.39
34	B5	1781	MA6	C5-C4	4.39	1.46	1.39
34	B5	1782	MA6	C5-C4	4.29	1.46	1.39
34	B5	1575	G7M	C8-N9	4.09	1.46	1.35
34	B5	1191	B8N	C4-C5	-3.73	1.39	1.47
38	A1	2416	PSU	C6-C5	3.62	1.39	1.35
34	B5	1575	G7M	C5-C4	3.49	1.47	1.38
34	B5	766	PSU	C6-C5	3.42	1.39	1.35
38	A1	2340	PSU	C6-C5	3.41	1.39	1.35
34	B5	759	PSU	C6-C5	3.37	1.39	1.35
38	A1	2129	PSU	C6-C5	3.35	1.39	1.35
38	A1	2258	PSU	C6-C5	3.31	1.39	1.35
38	A1	2923	PSU	C6-C5	3.30	1.38	1.35
39	A3	50	PSU	C6-C5	3.30	1.38	1.35
38	A1	1110	PSU	C6-C5	3.29	1.38	1.35
38	A1	986	PSU	C6-C5	3.28	1.38	1.35
38	A1	2975	PSU	C6-C5	3.28	1.38	1.35
34	B5	1415	PSU	C6-C5	3.27	1.38	1.35
34	B5	211	PSU	C6-C5	3.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	1052	PSU	C6-C5	3.23	1.38	1.35
34	B5	106	PSU	C6-C5	3.20	1.38	1.35
38	A1	2314	PSU	C6-C5	3.20	1.38	1.35
38	A1	2944	PSU	C6-C5	3.20	1.38	1.35
38	A1	2133	PSU	C4-N3	-3.19	1.32	1.38
34	B5	1187	PSU	C6-C5	3.16	1.38	1.35
38	A1	2735	PSU	C6-C5	3.16	1.38	1.35
34	B5	466	PSU	C6-C5	3.13	1.38	1.35
38	A1	776	PSU	C6-C5	3.12	1.38	1.35
38	A1	2264	PSU	C6-C5	3.12	1.38	1.35
38	A1	2266	PSU	C6-C5	3.12	1.38	1.35
34	B5	120	PSU	C6-C5	3.12	1.38	1.35
38	A1	2260	PSU	C6-C5	3.11	1.38	1.35
38	A1	966	PSU	C6-C5	3.10	1.38	1.35
34	B5	302	PSU	C6-C5	3.09	1.38	1.35
38	A1	1004	PSU	C6-C5	3.09	1.38	1.35
38	A1	1056	PSU	C6-C5	3.08	1.38	1.35
38	A1	1110	PSU	C4-N3	-3.08	1.33	1.38
40	A4	73	PSU	C6-C5	3.06	1.38	1.35
34	B5	632	PSU	C6-C5	3.04	1.38	1.35
38	A1	2880	PSU	C6-C5	3.03	1.38	1.35
38	A1	2826	PSU	C4-N3	-3.03	1.33	1.38
38	A1	990	PSU	C6-C5	3.03	1.38	1.35
38	A1	2921	OMU	C4-N3	-3.03	1.33	1.38
38	A1	2142	1MA	C6-N6	3.03	1.35	1.28
34	B5	1181	PSU	C6-C5	3.02	1.38	1.35
38	A1	2349	PSU	C6-C5	3.02	1.38	1.35
34	B5	999	PSU	C6-C5	3.02	1.38	1.35
34	B5	1782	MA6	C5-C6	3.01	1.49	1.41
38	A1	1124	PSU	C6-C5	2.99	1.38	1.35
38	A1	2142	1MA	C5-C4	2.99	1.47	1.38
38	A1	1042	PSU	C6-C5	2.99	1.38	1.35
38	A1	2865	PSU	C6-C5	2.99	1.38	1.35
38	A1	2133	PSU	C6-C5	2.98	1.38	1.35
38	A1	645	1MA	C5-C4	2.98	1.46	1.38
38	A1	2944	PSU	C4-N3	-2.97	1.33	1.38
38	A1	2191	PSU	C4-N3	-2.96	1.33	1.38
38	A1	2351	PSU	C6-C5	2.95	1.38	1.35
38	A1	645	1MA	C6-N6	2.94	1.35	1.28
38	A1	2880	PSU	C4-N3	-2.93	1.33	1.38
38	A1	2191	PSU	C6-C5	2.93	1.38	1.35
38	A1	2351	PSU	C4-N3	-2.93	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2922	OMG	C5-C4	2.93	1.46	1.38
38	A1	960	PSU	C6-C5	2.93	1.38	1.35
38	A1	2735	PSU	C4-N3	-2.93	1.33	1.38
34	B5	999	PSU	C4-N3	-2.92	1.33	1.38
38	A1	2416	PSU	C4-N3	-2.92	1.33	1.38
38	A1	2129	PSU	C4-N3	-2.90	1.33	1.38
38	A1	2340	PSU	C4-N3	-2.90	1.33	1.38
38	A1	966	PSU	C4-N3	-2.90	1.33	1.38
38	A1	776	PSU	C4-N3	-2.90	1.33	1.38
38	A1	986	PSU	C4-N3	-2.89	1.33	1.38
34	B5	1290	PSU	C6-C5	2.88	1.38	1.35
34	B5	1191	B8N	C6-C5	2.87	1.39	1.35
36	AB	243	HIC	CD2-CG	2.87	1.41	1.36
38	A1	2314	PSU	C4-N3	-2.86	1.33	1.38
38	A1	2865	PSU	C4-N3	-2.86	1.33	1.38
38	A1	1052	PSU	C4-N3	-2.86	1.33	1.38
38	A1	960	PSU	O4'-C1'	-2.84	1.39	1.43
38	A1	1042	PSU	C4-N3	-2.84	1.33	1.38
38	A1	2975	PSU	C4-N3	-2.83	1.33	1.38
38	A1	2266	PSU	C4-N3	-2.83	1.33	1.38
38	A1	2923	PSU	C4-N3	-2.83	1.33	1.38
34	B5	1781	MA6	C5-C6	2.82	1.48	1.41
38	A1	2278	5MC	C6-C5	2.82	1.39	1.34
34	B5	302	PSU	C4-N3	-2.82	1.33	1.38
38	A1	2264	PSU	C4-N3	-2.81	1.33	1.38
38	A1	2870	5MC	C6-C5	2.81	1.39	1.34
34	B5	632	PSU	C4-N3	-2.80	1.33	1.38
38	A1	990	PSU	C4-N3	-2.79	1.33	1.38
38	A1	1004	PSU	C4-N3	-2.79	1.33	1.38
38	A1	1056	PSU	C4-N3	-2.79	1.33	1.38
34	B5	106	PSU	C4-N3	-2.78	1.33	1.38
34	B5	1415	PSU	C4-N3	-2.77	1.33	1.38
38	A1	2349	PSU	C4-N3	-2.77	1.33	1.38
38	A1	1124	PSU	C4-N3	-2.76	1.33	1.38
34	B5	1290	PSU	C4-N3	-2.76	1.33	1.38
38	A1	960	PSU	C4-N3	-2.75	1.33	1.38
38	A1	2260	PSU	C4-N3	-2.74	1.33	1.38
34	B5	1280	4AC	C4-N4	-2.73	1.35	1.39
40	A4	73	PSU	C4-N3	-2.73	1.33	1.38
34	B5	1181	PSU	C4-N3	-2.72	1.33	1.38
38	A1	2258	PSU	C4-N3	-2.70	1.33	1.38
34	B5	120	PSU	C4-N3	-2.69	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	766	PSU	C4-N3	-2.69	1.33	1.38
34	B5	466	PSU	C4-N3	-2.68	1.33	1.38
39	A3	50	PSU	C4-N3	-2.67	1.33	1.38
34	B5	759	PSU	C4-N3	-2.67	1.33	1.38
34	B5	1187	PSU	C4-N3	-2.64	1.33	1.38
34	B5	211	PSU	C4-N3	-2.64	1.33	1.38
38	A1	2826	PSU	C6-C5	2.62	1.38	1.35
38	A1	2922	OMG	C6-N1	-2.59	1.34	1.38
38	A1	2133	PSU	C2-N3	-2.49	1.33	1.37
34	B5	1575	G7M	C2'-C3'	-2.47	1.46	1.53
38	A1	2870	5MC	C6-N1	-2.44	1.33	1.38
34	B5	1575	G7M	C6-N1	-2.43	1.34	1.38
38	A1	2142	1MA	C5-N7	-2.40	1.34	1.39
38	A1	2921	OMU	C5-C4	-2.38	1.38	1.43
38	A1	2921	OMU	C2-N3	-2.37	1.33	1.38
38	A1	645	1MA	C5-N7	-2.36	1.34	1.39
34	B5	1782	MA6	C4-N9	-2.33	1.32	1.37
34	B5	1781	MA6	C5-N7	-2.31	1.34	1.39
34	B5	1781	MA6	C4-N9	-2.31	1.32	1.37
38	A1	776	PSU	C2-N3	-2.31	1.33	1.37
38	A1	2278	5MC	C6-N1	-2.28	1.34	1.38
38	A1	2349	PSU	C2-N3	-2.26	1.33	1.37
38	A1	2944	PSU	C2-N3	-2.26	1.33	1.37
38	A1	1042	PSU	C2-N3	-2.21	1.33	1.37
34	B5	1773	4AC	C4-N4	-2.21	1.36	1.39
38	A1	2191	PSU	C2-N3	-2.20	1.33	1.37
38	A1	966	PSU	C2-N3	-2.17	1.33	1.37
38	A1	2826	PSU	C2-N3	-2.17	1.33	1.37
38	A1	2880	PSU	C2-N3	-2.16	1.33	1.37
38	A1	1110	PSU	C2-N3	-2.16	1.33	1.37
38	A1	1052	PSU	C2-N3	-2.16	1.33	1.37
38	A1	966	PSU	C2-N1	-2.16	1.33	1.36
34	B5	999	PSU	C2-N3	-2.16	1.33	1.37
38	A1	2975	PSU	C2-N3	-2.16	1.33	1.37
34	B5	766	PSU	O4'-C1'	-2.15	1.40	1.43
38	A1	2865	PSU	C2-N3	-2.14	1.33	1.37
34	B5	1782	MA6	C5-N7	-2.14	1.35	1.39
38	A1	2416	PSU	C2-N3	-2.14	1.33	1.37
38	A1	1056	PSU	C2-N3	-2.14	1.33	1.37
38	A1	2735	PSU	C2-N3	-2.13	1.34	1.37
38	A1	960	PSU	C2-N3	-2.13	1.34	1.37
38	A1	2351	PSU	C2-N3	-2.13	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2349	PSU	C2-N1	-2.13	1.33	1.36
38	A1	645	1MA	C4-N9	-2.13	1.32	1.38
38	A1	2266	PSU	C2-N3	-2.12	1.34	1.37
38	A1	986	PSU	C2-N3	-2.12	1.34	1.37
34	B5	1782	MA6	C8-N7	2.11	1.35	1.31
38	A1	2351	PSU	C2-N1	-2.11	1.33	1.36
34	B5	1191	B8N	CN1-N1	2.10	1.50	1.46
34	B5	1290	PSU	C2-N3	-2.10	1.34	1.37
38	A1	2922	OMG	C5-N7	-2.10	1.34	1.39
38	A1	990	PSU	C2-N3	-2.10	1.34	1.37
34	B5	120	PSU	C2-N3	-2.08	1.34	1.37
38	A1	2922	OMG	C4-N9	-2.08	1.32	1.38
38	A1	2264	PSU	C2-N3	-2.07	1.34	1.37
40	A4	73	PSU	C2-N3	-2.07	1.34	1.37
38	A1	2314	PSU	C2-N3	-2.07	1.34	1.37
34	B5	1773	4AC	C6-N1	-2.06	1.33	1.38
34	B5	632	PSU	C2-N3	-2.05	1.34	1.37
38	A1	2258	PSU	C2-N3	-2.05	1.34	1.37
34	B5	302	PSU	C2-N3	-2.04	1.34	1.37
38	A1	1042	PSU	C2-N1	-2.04	1.34	1.36
38	A1	2944	PSU	O4'-C1'	-2.03	1.41	1.43
38	A1	2260	PSU	C2-N3	-2.02	1.34	1.37
38	A1	2340	PSU	C2-N3	-2.01	1.34	1.37
38	A1	2826	PSU	C2-N1	-2.01	1.34	1.36
38	A1	2191	PSU	C2-N1	-2.00	1.34	1.36
38	A1	2129	PSU	C2-N3	-2.00	1.34	1.37

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1773	4AC	N4-C4-N3	8.18	127.15	113.87
34	B5	1575	G7M	CN7-N7-C8	-7.60	113.29	124.79
38	A1	2944	PSU	N1-C2-N3	6.84	122.39	115.17
38	A1	1124	PSU	N1-C2-N3	6.83	122.38	115.17
38	A1	2129	PSU	N1-C2-N3	6.83	122.37	115.17
38	A1	2634	UR3	C4-N3-C2	-6.82	119.09	124.58
34	B5	1575	G7M	N9-C8-N7	-6.80	95.98	112.48
38	A1	2880	PSU	N1-C2-N3	6.79	122.33	115.17
38	A1	2865	PSU	N1-C2-N3	6.72	122.26	115.17
38	A1	2264	PSU	N1-C2-N3	6.70	122.24	115.17
38	A1	2340	PSU	N1-C2-N3	6.68	122.22	115.17
38	A1	2975	PSU	N1-C2-N3	6.65	122.18	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2416	PSU	N1-C2-N3	6.64	122.17	115.17
39	A3	50	PSU	N1-C2-N3	6.62	122.15	115.17
34	B5	632	PSU	N1-C2-N3	6.61	122.14	115.17
38	A1	966	PSU	N1-C2-N3	6.61	122.14	115.17
38	A1	2133	PSU	N1-C2-N3	6.60	122.14	115.17
38	A1	2314	PSU	N1-C2-N3	6.60	122.13	115.17
34	B5	106	PSU	N1-C2-N3	6.60	122.13	115.17
38	A1	2191	PSU	N1-C2-N3	6.57	122.10	115.17
34	B5	302	PSU	N1-C2-N3	6.53	122.06	115.17
38	A1	2735	PSU	N1-C2-N3	6.53	122.06	115.17
38	A1	2923	PSU	N1-C2-N3	6.52	122.05	115.17
38	A1	1004	PSU	N1-C2-N3	6.52	122.04	115.17
38	A1	960	PSU	N1-C2-N3	6.51	122.04	115.17
38	A1	990	PSU	N1-C2-N3	6.51	122.03	115.17
34	B5	999	PSU	N1-C2-N3	6.51	122.03	115.17
34	B5	1575	G7M	C8-N7-C5	6.50	115.91	107.78
38	A1	2258	PSU	N1-C2-N3	6.50	122.03	115.17
38	A1	776	PSU	N1-C2-N3	6.50	122.02	115.17
38	A1	2266	PSU	N1-C2-N3	6.49	122.02	115.17
38	A1	2351	PSU	N1-C2-N3	6.47	122.00	115.17
40	A4	73	PSU	N1-C2-N3	6.47	121.99	115.17
34	B5	1187	PSU	N1-C2-N3	6.46	121.98	115.17
38	A1	1110	PSU	N1-C2-N3	6.44	121.96	115.17
34	B5	1181	PSU	N1-C2-N3	6.42	121.94	115.17
34	B5	1290	PSU	N1-C2-N3	6.42	121.94	115.17
34	B5	759	PSU	N1-C2-N3	6.42	121.94	115.17
38	A1	1056	PSU	N1-C2-N3	6.39	121.91	115.17
34	B5	766	PSU	N1-C2-N3	6.38	121.90	115.17
38	A1	1052	PSU	N1-C2-N3	6.33	121.85	115.17
34	B5	211	PSU	N1-C2-N3	6.32	121.83	115.17
38	A1	2349	PSU	N1-C2-N3	6.31	121.82	115.17
38	A1	2826	PSU	N1-C2-N3	6.30	121.81	115.17
38	A1	1042	PSU	N1-C2-N3	6.27	121.79	115.17
38	A1	986	PSU	N1-C2-N3	6.25	121.76	115.17
34	B5	1415	PSU	N1-C2-N3	6.24	121.75	115.17
34	B5	466	PSU	N1-C2-N3	6.23	121.75	115.17
38	A1	2260	PSU	N1-C2-N3	6.19	121.70	115.17
34	B5	120	PSU	N1-C2-N3	6.12	121.62	115.17
34	B5	1575	G7M	N9-C4-N3	5.81	137.57	125.95
38	A1	2922	OMG	C5-C4-N3	-5.72	119.29	128.39
38	A1	2142	1MA	C5-C4-N3	-5.55	119.10	127.27
34	B5	1191	B8N	C4-N3-C2	-5.32	119.07	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1575	G7M	C5-C4-N3	-5.32	118.10	128.15
34	B5	1782	MA6	C5-C4-N3	-5.27	119.46	126.72
34	B5	1781	MA6	C5-C4-N3	-5.08	119.73	126.72
34	B5	1773	4AC	C5-C4-N4	-5.04	114.45	122.94
38	A1	2922	OMG	C2-N3-C4	4.95	120.83	112.30
38	A1	645	1MA	C5-C4-N3	-4.90	120.06	127.27
38	A1	2142	1MA	C2-N3-C4	4.74	121.82	112.53
38	A1	2880	PSU	C4-N3-C2	-4.74	119.85	126.37
38	A1	2921	OMU	C4-N3-C2	-4.72	120.75	126.61
34	B5	1575	G7M	C2-N3-C4	4.65	120.31	112.30
38	A1	2944	PSU	C4-N3-C2	-4.61	120.02	126.37
38	A1	1124	PSU	C4-N3-C2	-4.56	120.08	126.37
38	A1	645	1MA	C2-N3-C4	4.46	121.28	112.53
38	A1	2921	OMU	N3-C2-N1	4.43	120.66	114.89
38	A1	2129	PSU	C4-N3-C2	-4.40	120.31	126.37
38	A1	2191	PSU	C4-N3-C2	-4.39	120.32	126.37
38	A1	966	PSU	C4-N3-C2	-4.38	120.33	126.37
38	A1	2133	PSU	C4-N3-C2	-4.35	120.38	126.37
38	A1	1124	PSU	O2-C2-N1	-4.35	118.30	122.79
38	A1	2865	PSU	C4-N3-C2	-4.32	120.42	126.37
34	B5	1781	MA6	C2-N1-C6	4.31	122.35	111.83
38	A1	2340	PSU	C4-N3-C2	-4.31	120.44	126.37
34	B5	1575	G7M	O2'-C2'-C3'	4.30	125.60	111.82
38	A1	2735	PSU	C4-N3-C2	-4.29	120.46	126.37
38	A1	1056	PSU	C4-N3-C2	-4.29	120.47	126.37
39	A3	50	PSU	C4-N3-C2	-4.28	120.48	126.37
38	A1	2870	5MC	C5-C6-N1	-4.27	118.67	123.31
38	A1	2975	PSU	C4-N3-C2	-4.25	120.51	126.37
34	B5	1187	PSU	C4-N3-C2	-4.24	120.53	126.37
34	B5	120	PSU	C4-N3-C2	-4.24	120.53	126.37
38	A1	990	PSU	C4-N3-C2	-4.24	120.53	126.37
38	A1	2264	PSU	C4-N3-C2	-4.23	120.54	126.37
38	A1	2314	PSU	C4-N3-C2	-4.23	120.55	126.37
34	B5	1782	MA6	C2-N1-C6	4.22	122.14	111.83
34	B5	1181	PSU	C4-N3-C2	-4.21	120.58	126.37
38	A1	1004	PSU	C4-N3-C2	-4.20	120.58	126.37
34	B5	1290	PSU	C4-N3-C2	-4.19	120.60	126.37
38	A1	960	PSU	C4-N3-C2	-4.16	120.64	126.37
40	A4	73	PSU	C4-N3-C2	-4.15	120.65	126.37
34	B5	302	PSU	C4-N3-C2	-4.15	120.66	126.37
34	B5	759	PSU	C4-N3-C2	-4.14	120.67	126.37
34	B5	999	PSU	C4-N3-C2	-4.11	120.72	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1110	PSU	C4-N3-C2	-4.10	120.73	126.37
38	A1	2826	PSU	C4-N3-C2	-4.09	120.73	126.37
38	A1	2351	PSU	C4-N3-C2	-4.09	120.73	126.37
34	B5	106	PSU	C4-N3-C2	-4.09	120.74	126.37
34	B5	466	PSU	C4-N3-C2	-4.08	120.75	126.37
34	B5	632	PSU	C4-N3-C2	-4.08	120.75	126.37
38	A1	2266	PSU	C4-N3-C2	-4.07	120.76	126.37
38	A1	2416	PSU	C4-N3-C2	-4.07	120.77	126.37
34	B5	1415	PSU	C4-N3-C2	-4.07	120.77	126.37
38	A1	2922	OMG	N9-C4-N3	4.06	134.07	125.95
34	B5	211	PSU	C4-N3-C2	-4.06	120.78	126.37
34	B5	1782	MA6	C4-C5-N7	-4.06	105.94	110.58
34	B5	1781	MA6	C4-C5-N7	-4.05	105.95	110.58
38	A1	2349	PSU	C4-N3-C2	-4.04	120.81	126.37
38	A1	986	PSU	C4-N3-C2	-4.04	120.81	126.37
38	A1	966	PSU	O2-C2-N1	-4.03	118.63	122.79
38	A1	1042	PSU	C4-N3-C2	-4.01	120.84	126.37
38	A1	1052	PSU	C4-N3-C2	-4.01	120.85	126.37
38	A1	2264	PSU	O2-C2-N1	-4.00	118.66	122.79
34	B5	1575	G7M	C8-N9-C4	4.00	116.98	107.09
38	A1	2923	PSU	C4-N3-C2	-4.00	120.87	126.37
34	B5	1782	MA6	N3-C4-N9	3.99	133.95	127.17
34	B5	1290	PSU	O2-C2-N1	-3.96	118.70	122.79
38	A1	2351	PSU	O2-C2-N1	-3.96	118.70	122.79
38	A1	1004	PSU	O2-C2-N1	-3.96	118.71	122.79
34	B5	766	PSU	C4-N3-C2	-3.93	120.96	126.37
38	A1	2258	PSU	C4-N3-C2	-3.93	120.96	126.37
38	A1	2260	PSU	C4-N3-C2	-3.93	120.96	126.37
38	A1	2880	PSU	O2-C2-N1	-3.92	118.75	122.79
34	B5	1781	MA6	N3-C4-N9	3.90	133.79	127.17
38	A1	2865	PSU	O2-C2-N1	-3.84	118.83	122.79
34	B5	1187	PSU	O2-C2-N1	-3.84	118.83	122.79
38	A1	2921	OMU	C5-C4-N3	3.83	120.17	114.80
38	A1	2129	PSU	O2-C2-N1	-3.83	118.84	122.79
40	A4	73	PSU	O2-C2-N1	-3.83	118.84	122.79
38	A1	2260	PSU	O2-C2-N1	-3.82	118.85	122.79
34	B5	766	PSU	O2-C2-N1	-3.82	118.85	122.79
38	A1	2258	PSU	O2-C2-N1	-3.81	118.86	122.79
38	A1	2735	PSU	O2-C2-N1	-3.80	118.87	122.79
34	B5	1782	MA6	C2-N3-C4	3.77	121.04	111.83
38	A1	776	PSU	C4-N3-C2	-3.75	121.20	126.37
38	A1	2340	PSU	O2-C2-N1	-3.75	118.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2142	1MA	N9-C4-N3	3.75	135.44	126.90
38	A1	2826	PSU	O2-C2-N1	-3.73	118.94	122.79
34	B5	1181	PSU	O2-C2-N1	-3.73	118.94	122.79
39	A3	50	PSU	O2-C2-N1	-3.73	118.94	122.79
38	A1	960	PSU	O2-C2-N1	-3.72	118.95	122.79
34	B5	211	PSU	O2-C2-N1	-3.68	118.99	122.79
34	B5	302	PSU	O2-C2-N1	-3.68	118.99	122.79
38	A1	2923	PSU	O2-C2-N1	-3.66	119.01	122.79
34	B5	106	PSU	O2-C2-N1	-3.66	119.01	122.79
38	A1	2975	PSU	O2-C2-N1	-3.64	119.03	122.79
38	A1	2266	PSU	O2-C2-N1	-3.63	119.05	122.79
38	A1	2349	PSU	O2-C2-N1	-3.62	119.06	122.79
38	A1	986	PSU	O2-C2-N1	-3.60	119.08	122.79
34	B5	632	PSU	O2-C2-N1	-3.58	119.09	122.79
38	A1	2944	PSU	O2-C2-N1	-3.58	119.10	122.79
38	A1	2922	OMG	C6-C5-N7	3.56	136.77	130.29
34	B5	1781	MA6	C2-N3-C4	3.55	120.51	111.83
38	A1	990	PSU	O2-C2-N1	-3.55	119.13	122.79
38	A1	1056	PSU	O2-C2-N1	-3.55	119.13	122.79
38	A1	1042	PSU	O2-C2-N1	-3.54	119.14	122.79
38	A1	2191	PSU	O2-C2-N1	-3.51	119.17	122.79
34	B5	1782	MA6	N1-C2-N3	-3.50	123.28	128.58
34	B5	1773	4AC	CM7-C7-N4	3.47	120.86	115.27
34	B5	1773	4AC	C6-C5-C4	3.43	121.13	117.00
38	A1	2634	UR3	C5-C4-N3	3.41	119.53	115.04
38	A1	2314	PSU	O2-C2-N1	-3.41	119.27	122.79
38	A1	2278	5MC	C5-C6-N1	-3.41	119.61	123.31
34	B5	1781	MA6	N1-C2-N3	-3.36	123.50	128.58
34	B5	466	PSU	O2-C2-N1	-3.36	119.33	122.79
34	B5	999	PSU	O2-C2-N1	-3.34	119.34	122.79
38	A1	1110	PSU	O2-C2-N1	-3.31	119.38	122.79
34	B5	120	PSU	O2-C2-N1	-3.30	119.39	122.79
34	B5	1575	G7M	O2'-C2'-C1'	3.27	121.37	110.10
34	B5	1415	PSU	O2-C2-N1	-3.24	119.45	122.79
34	B5	1782	MA6	C4-N9-C8	3.22	109.12	105.74
34	B5	1575	G7M	CN7-N7-C5	3.19	130.78	126.80
38	A1	2416	PSU	O2-C2-N1	-3.17	119.52	122.79
34	B5	759	PSU	O2-C2-N1	-3.14	119.55	122.79
38	A1	645	1MA	N9-C4-N3	3.10	133.97	126.90
34	B5	1191	B8N	N3-C2-N1	3.09	120.49	116.72
38	A1	776	PSU	O2-C2-N1	-3.07	119.62	122.79
38	A1	1052	PSU	O2-C2-N1	-3.01	119.68	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2921	OMU	O4-C4-C5	-2.99	120.01	125.16
34	B5	1575	G7M	O3'-C3'-C4'	2.97	119.62	111.08
38	A1	2870	5MC	C5-C4-N3	-2.97	118.71	121.75
34	B5	1781	MA6	C4-N9-C8	2.97	108.86	105.74
34	B5	1782	MA6	C5-N7-C8	2.93	108.05	103.45
34	B5	1781	MA6	C5-N7-C8	2.87	107.95	103.45
34	B5	1280	4AC	C6-C5-C4	2.84	120.42	117.00
36	AB	243	HIC	NE2-CE1-ND1	-2.81	111.59	112.66
34	B5	1782	MA6	C6-C5-N7	2.80	137.90	133.43
38	A1	2133	PSU	O2-C2-N1	-2.76	119.94	122.79
34	B5	1191	B8N	C31-N3-C4	2.71	121.01	117.18
34	B5	1773	4AC	C5-C4-N3	-2.68	118.40	122.60
38	A1	2922	OMG	C4-C5-N7	-2.62	106.52	110.67
38	A1	2880	PSU	C5-C6-N1	-2.61	118.52	122.14
34	B5	1781	MA6	C6-C5-N7	2.61	137.59	133.43
34	B5	1782	MA6	N9-C8-N7	-2.57	110.30	113.94
38	A1	2944	PSU	C5-C6-N1	-2.51	118.65	122.14
38	A1	2921	OMU	O2-C2-N1	-2.50	119.54	122.80
38	A1	2278	5MC	C5-C4-N3	-2.49	119.20	121.75
38	A1	2133	PSU	C5-C6-N1	-2.47	118.70	122.14
34	B5	1575	G7M	C3'-C2'-C1'	2.47	106.13	101.46
34	B5	1575	G7M	O3'-C3'-C2'	2.46	119.69	111.82
38	A1	1124	PSU	C5-C6-N1	-2.42	118.78	122.14
34	B5	1191	B8N	C1'-C5-C4	2.39	121.23	117.61
34	B5	1575	G7M	O6-C6-C5	-2.38	122.69	128.01
38	A1	2314	PSU	C5-C6-N1	-2.36	118.87	122.14
38	A1	2826	PSU	C5-C6-N1	-2.34	118.90	122.14
34	B5	1280	4AC	O7-C7-N4	2.32	125.54	121.90
38	A1	2865	PSU	C5-C6-N1	-2.30	118.95	122.14
38	A1	645	1MA	C4-C5-N7	-2.29	107.04	110.67
38	A1	2870	5MC	O2-C2-N3	-2.28	118.73	122.33
38	A1	2129	PSU	C5-C6-N1	-2.28	118.98	122.14
38	A1	966	PSU	C5-C6-N1	-2.27	118.99	122.14
34	B5	1191	B8N	O4'-C1'-C2'	2.27	108.29	105.15
38	A1	645	1MA	C6-C5-N7	2.26	136.16	132.16
38	A1	990	PSU	C5-C6-N1	-2.26	119.00	122.14
34	B5	1290	PSU	C5-C6-N1	-2.25	119.02	122.14
34	B5	1781	MA6	N9-C8-N7	-2.24	110.75	113.94
34	B5	1280	4AC	C5-C4-N3	-2.23	119.10	122.60
38	A1	2264	PSU	C5-C6-N1	-2.23	119.04	122.14
34	B5	999	PSU	C5-C6-N1	-2.23	119.05	122.14
38	A1	1056	PSU	C5-C6-N1	-2.22	119.06	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1575	G7M	C1'-N9-C8	-2.22	119.24	126.74
38	A1	2133	PSU	O2-C2-N3	-2.22	117.93	121.86
38	A1	2340	PSU	C5-C6-N1	-2.19	119.10	122.14
38	A1	2191	PSU	C5-C6-N1	-2.18	119.11	122.14
38	A1	2735	PSU	C5-C6-N1	-2.18	119.12	122.14
38	A1	2278	5MC	O2-C2-N3	-2.17	118.92	122.33
38	A1	2975	PSU	C5-C6-N1	-2.16	119.14	122.14
38	A1	2142	1MA	C4-C5-N7	-2.14	107.28	110.67
36	AB	243	HIC	CB-CG-CD2	-2.12	124.83	129.96
34	B5	1290	PSU	O4'-C1'-C2'	2.12	108.08	105.15
38	A1	2826	PSU	O4'-C1'-C2'	2.12	108.08	105.15
38	A1	645	1MA	N1-C2-N3	-2.10	123.50	126.00
38	A1	960	PSU	C5-C6-N1	-2.09	119.23	122.14
34	B5	466	PSU	C5-C6-N1	-2.09	119.24	122.14
38	A1	2922	OMG	O6-C6-C5	-2.09	121.02	126.53
34	B5	1187	PSU	C5-C6-N1	-2.09	119.24	122.14
34	B5	1191	B8N	C32-C31-N3	-2.08	108.52	112.16
38	A1	1004	PSU	C5-C6-N1	-2.07	119.27	122.14
34	B5	106	PSU	C5-C6-N1	-2.06	119.28	122.14
38	A1	2351	PSU	C5-C6-N1	-2.06	119.29	122.14
39	A3	50	PSU	C5-C6-N1	-2.05	119.29	122.14
38	A1	2880	PSU	O4'-C1'-C2'	2.05	107.99	105.15
38	A1	2266	PSU	C5-C6-N1	-2.05	119.30	122.14
38	A1	2142	1MA	N1-C2-N3	-2.05	123.56	126.00
34	B5	302	PSU	C5-C6-N1	-2.03	119.32	122.14
34	B5	120	PSU	C5-C6-N1	-2.02	119.33	122.14
38	A1	2416	PSU	C5-C6-N1	-2.02	119.33	122.14
38	A1	2349	PSU	C5-C6-N1	-2.02	119.34	122.14
38	A1	2944	PSU	O4'-C1'-C2'	2.02	107.94	105.15
38	A1	1052	PSU	C5-C6-N1	-2.01	119.35	122.14
34	B5	766	PSU	O4'-C1'-C2'	2.01	107.94	105.15
34	B5	211	PSU	C5-C6-N1	-2.01	119.35	122.14
38	A1	1110	PSU	C5-C6-N1	-2.01	119.35	122.14
34	B5	1181	PSU	C5-C6-N1	-2.01	119.36	122.14
38	A1	776	PSU	O4'-C1'-C2'	2.00	107.92	105.15
34	B5	759	PSU	C5-C6-N1	-2.00	119.36	122.14
38	A1	986	PSU	C5-C6-N1	-2.00	119.36	122.14
40	A4	73	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	1773	4AC	N3-C4-N4-C7
38	A1	776	PSU	C3'-C4'-C5'-O5'
38	A1	776	PSU	O4'-C4'-C5'-O5'
38	A1	960	PSU	C2'-C1'-C5-C4
38	A1	1042	PSU	C2'-C1'-C5-C4
38	A1	1042	PSU	O4'-C1'-C5-C4
38	A1	1042	PSU	O4'-C1'-C5-C6
38	A1	2923	PSU	C3'-C4'-C5'-O5'
38	A1	2923	PSU	O4'-C4'-C5'-O5'
38	A1	2258	PSU	C3'-C4'-C5'-O5'
38	A1	2258	PSU	O4'-C4'-C5'-O5'
34	B5	1782	MA6	O4'-C4'-C5'-O5'
38	A1	2260	PSU	C3'-C4'-C5'-O5'
38	A1	2870	5MC	C2'-C1'-N1-C6
34	B5	1782	MA6	C3'-C4'-C5'-O5'
38	A1	2260	PSU	O4'-C4'-C5'-O5'
34	B5	1773	4AC	O7-C7-N4-C4
34	B5	1773	4AC	CM7-C7-N4-C4
38	A1	2870	5MC	O4'-C1'-N1-C6
38	A1	2314	PSU	C4'-C5'-O5'-P
38	A1	2923	PSU	C4'-C5'-O5'-P
38	A1	960	PSU	O4'-C1'-C5-C4
38	A1	645	1MA	C2'-C1'-N9-C8
38	A1	2922	OMG	C3'-C2'-O2'-CM2
38	A1	645	1MA	C2'-C1'-N9-C4
38	A1	2870	5MC	O4'-C1'-N1-C2
38	A1	2340	PSU	C4'-C5'-O5'-P
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	2266	PSU	C3'-C4'-C5'-O5'
38	A1	2142	1MA	C4'-C5'-O5'-P
34	B5	1782	MA6	C4'-C5'-O5'-P

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	966	PSU	2	0
38	A1	2278	5MC	1	0
38	A1	2944	PSU	1	0
38	A1	1110	PSU	1	0
38	A1	2314	PSU	1	0
38	A1	2880	PSU	1	0
34	B5	302	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B5	120	PSU	2	0
38	A1	2921	OMU	1	0
34	B5	1415	PSU	1	0
38	A1	990	PSU	2	0
38	A1	2129	PSU	1	0
39	A3	50	PSU	1	0
38	A1	776	PSU	3	0
34	B5	1782	MA6	1	0
34	B5	1575	G7M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	SPD	A1	3401	-	9,9,9	0.34	0	8,8,8	0.97	0
83	3HE	A1	3402	-	21,21,21	0.38	0	23,30,30	0.65	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
82	SPD	A1	3401	-	-	0/7/7/7	-
83	3HE	A1	3402	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

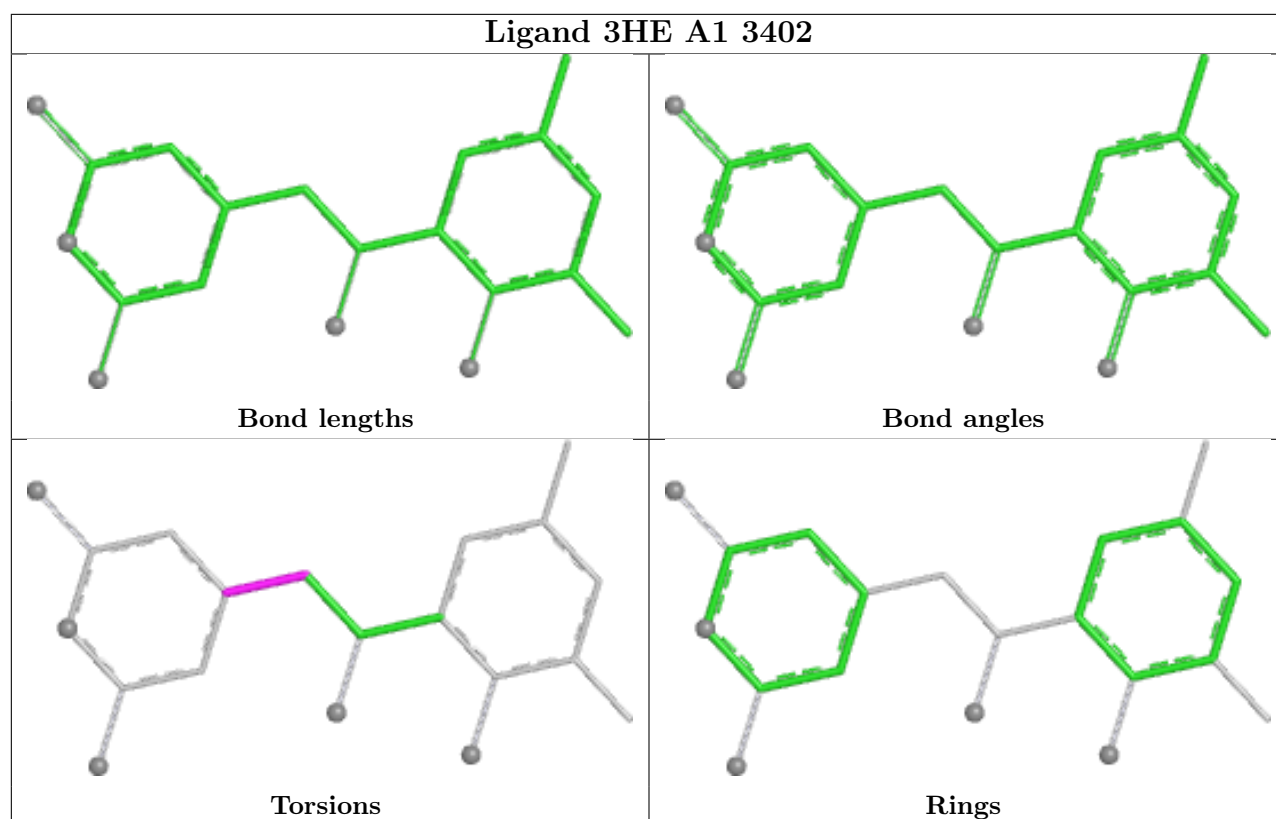
Mol	Chain	Res	Type	Atoms
83	A1	3402	3HE	C7-C8-C9-C10
83	A1	3402	3HE	C7-C8-C9-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A1	3401	SPD	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

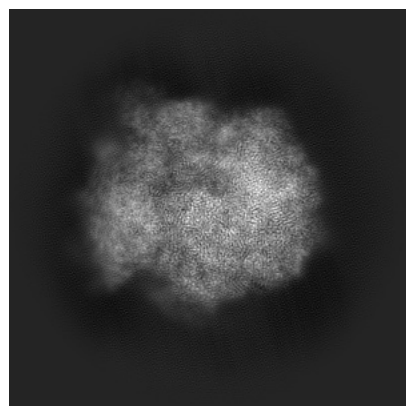
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40992. These allow visual inspection of the internal detail of the map and identification of artifacts.

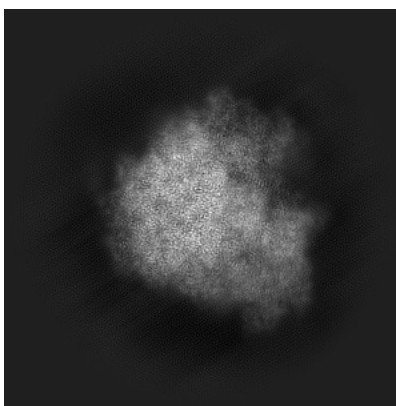
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

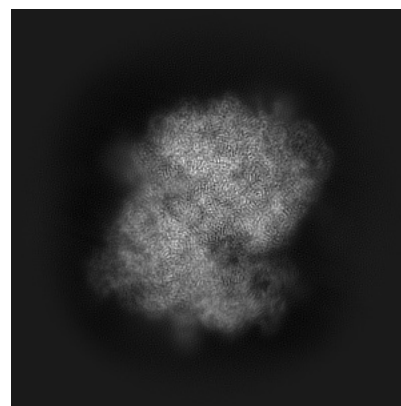
6.1.1 Primary map



X

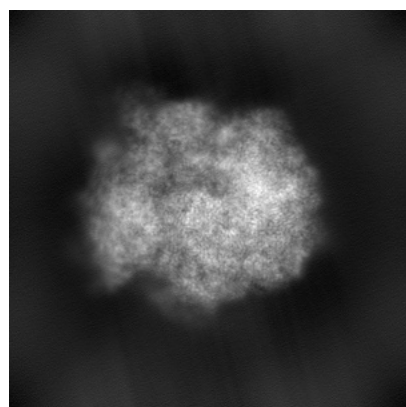


Y

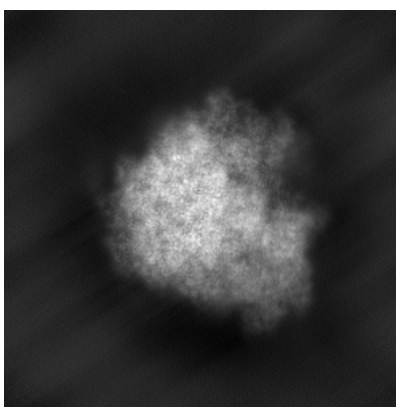


Z

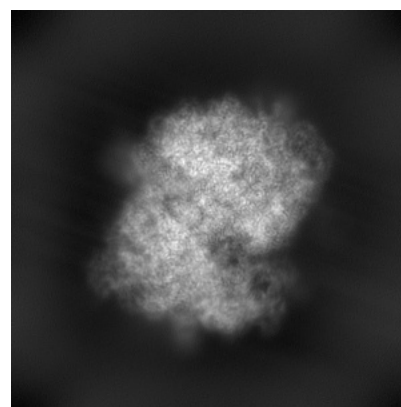
6.1.2 Raw map



X



Y

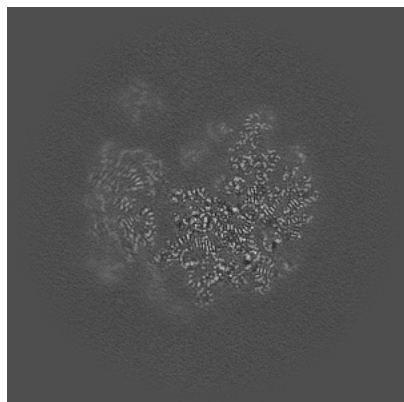


Z

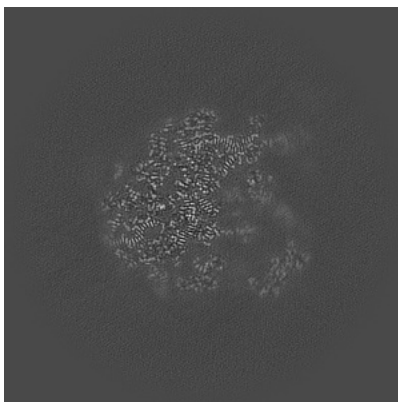
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

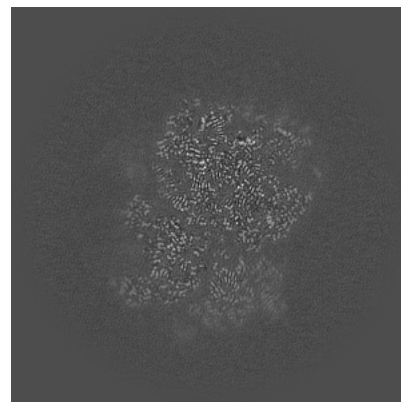
6.2.1 Primary map



X Index: 200

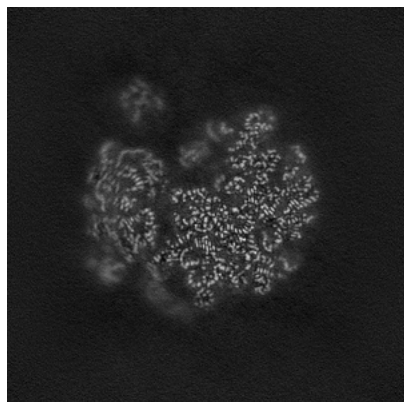


Y Index: 200

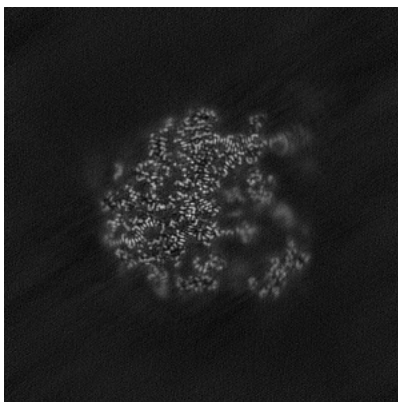


Z Index: 200

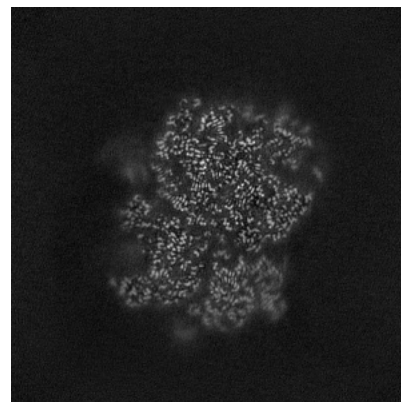
6.2.2 Raw map



X Index: 200



Y Index: 200

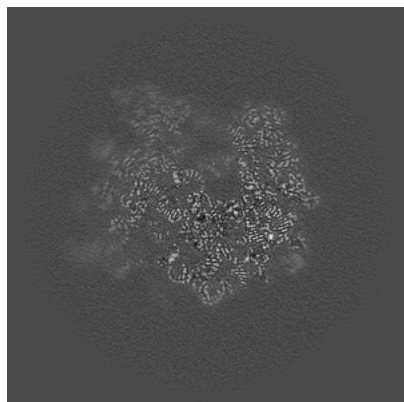


Z Index: 200

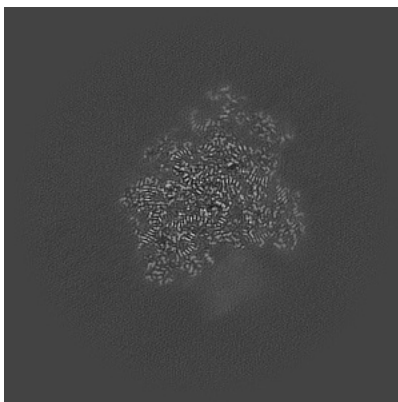
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

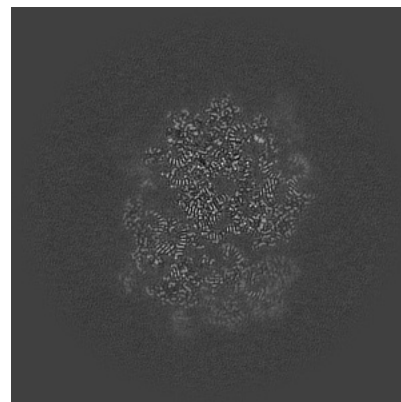
6.3.1 Primary map



X Index: 183

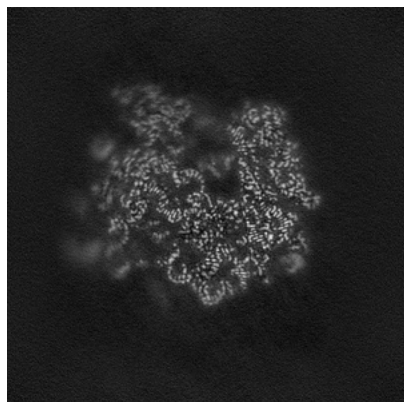


Y Index: 247

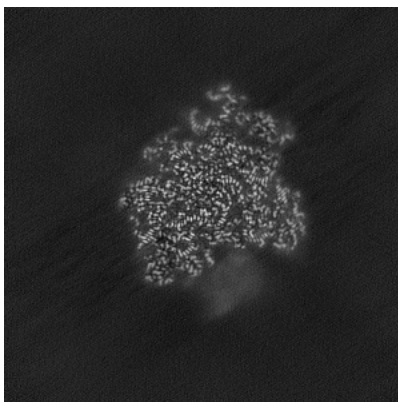


Z Index: 188

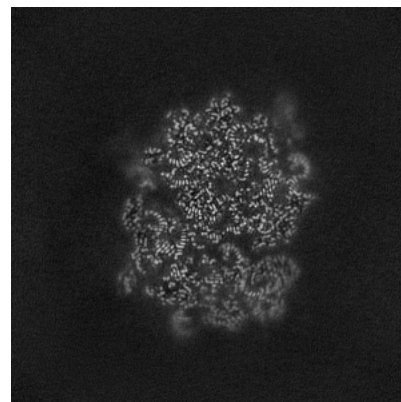
6.3.2 Raw map



X Index: 183



Y Index: 247

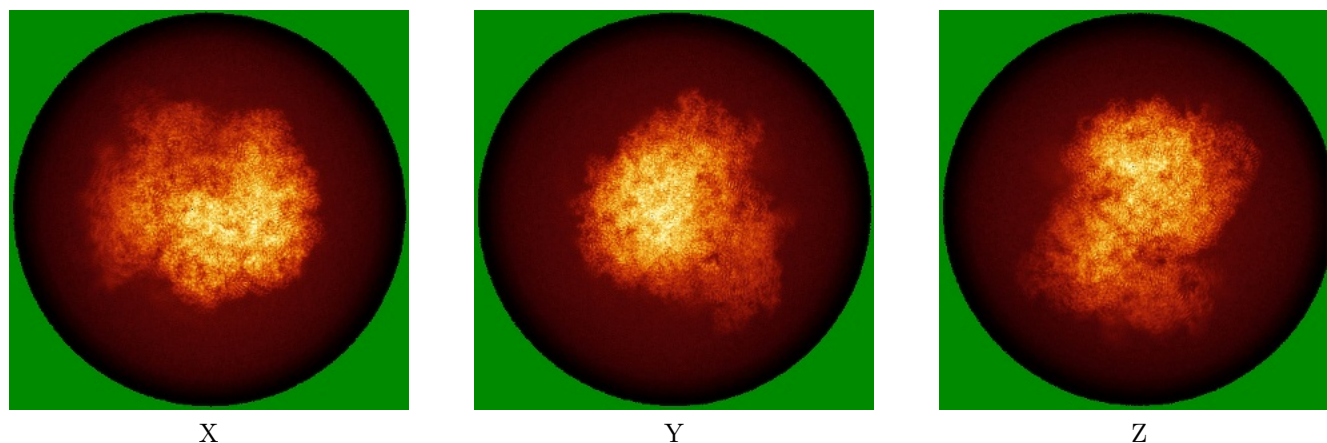


Z Index: 188

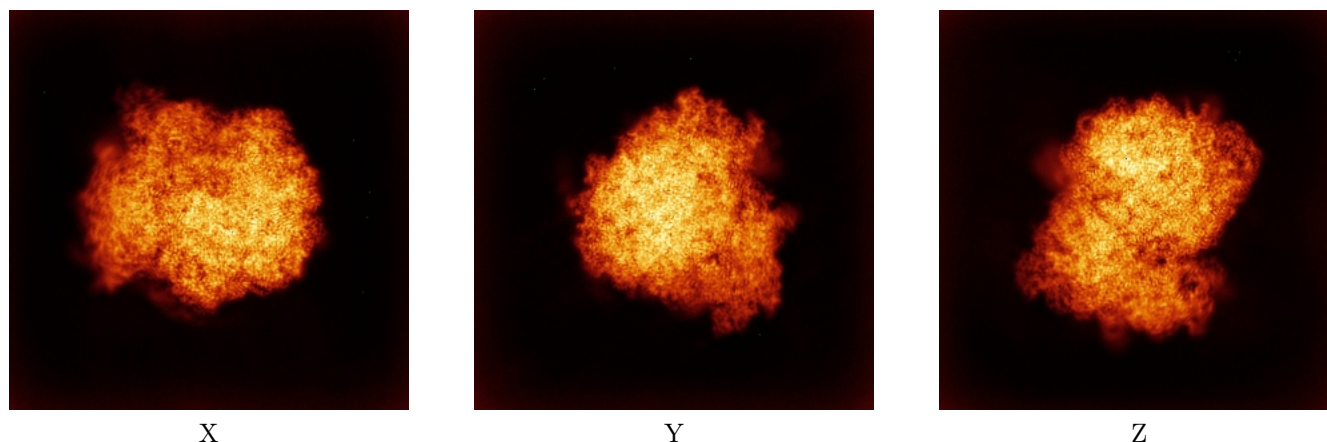
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

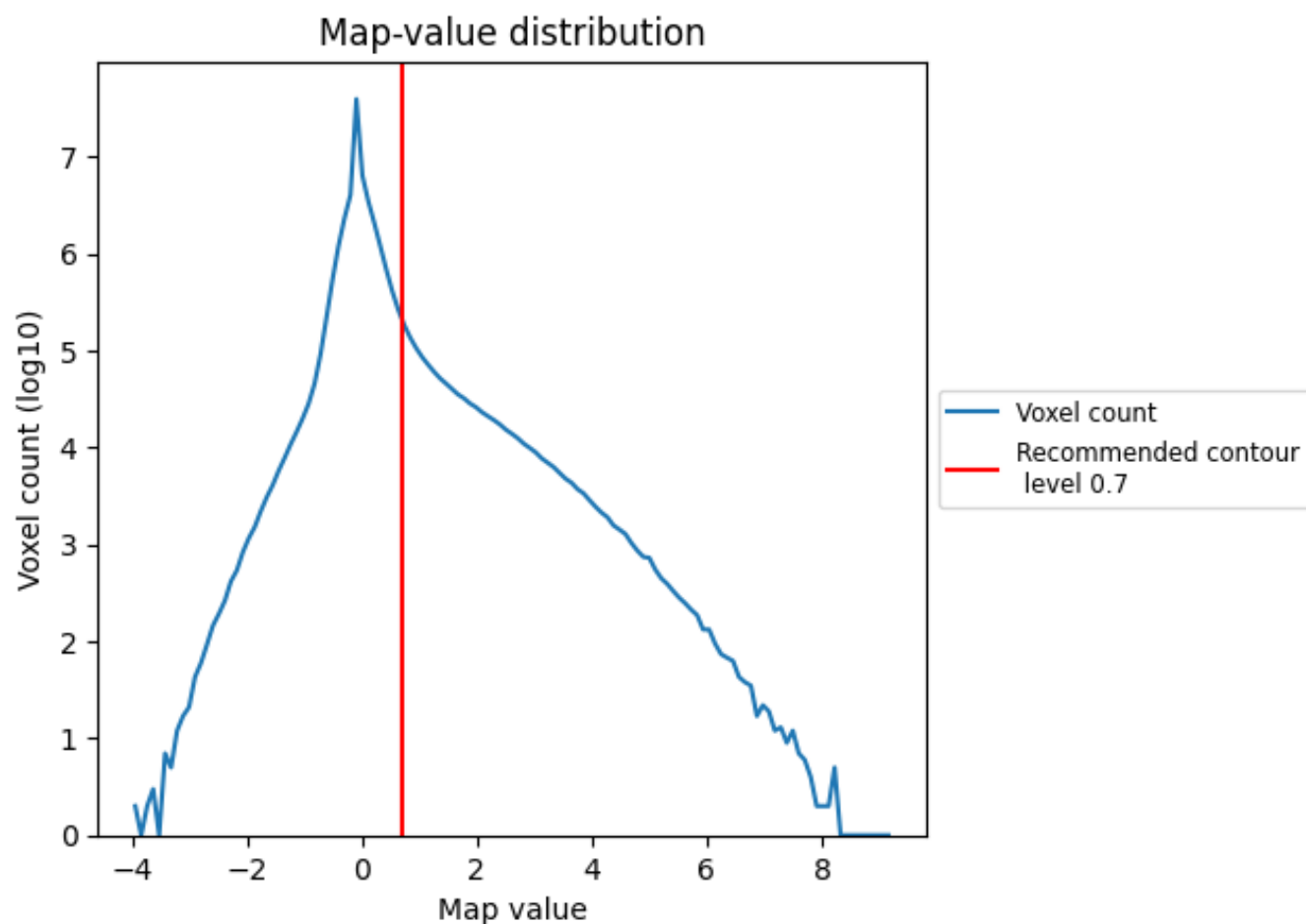
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

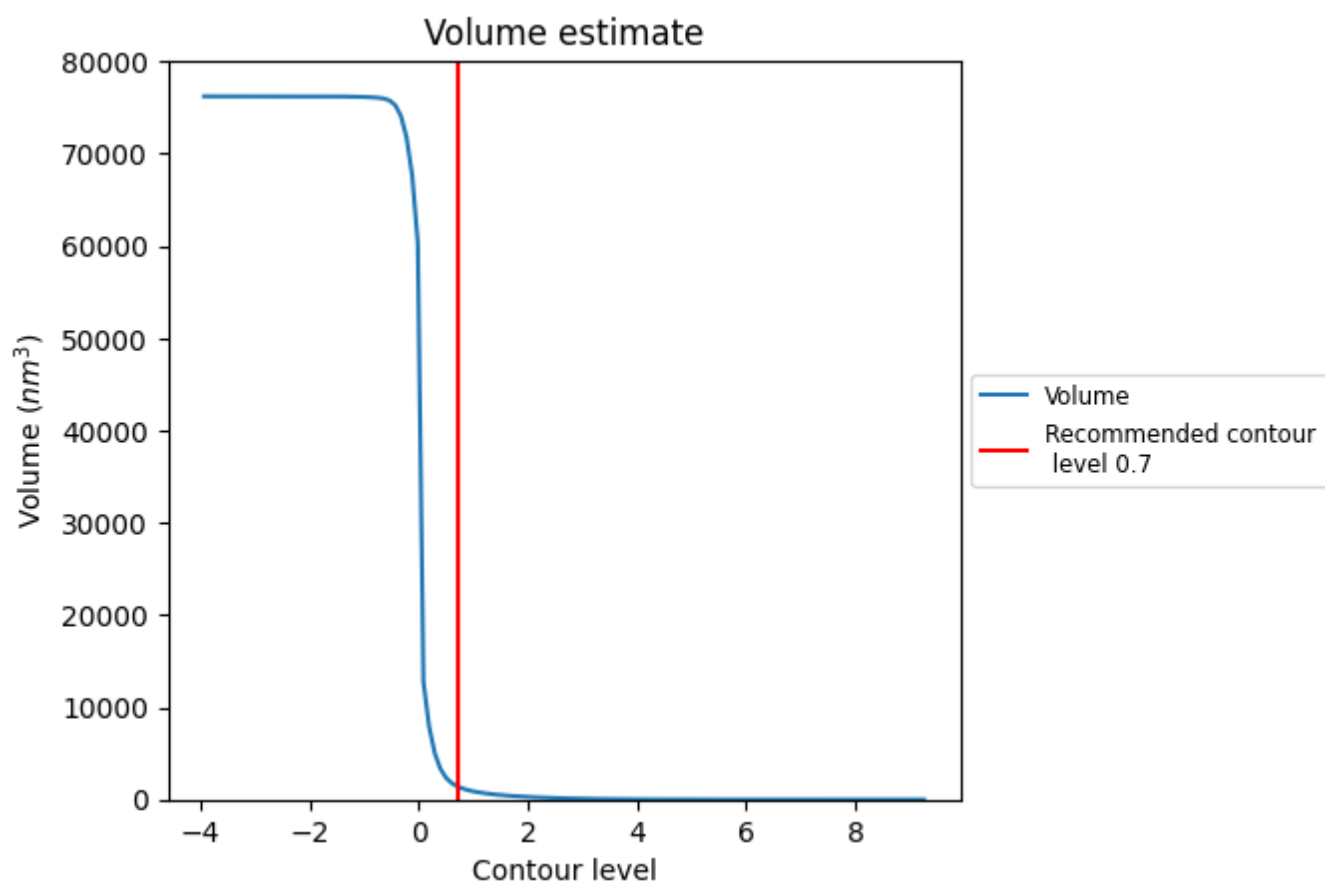
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

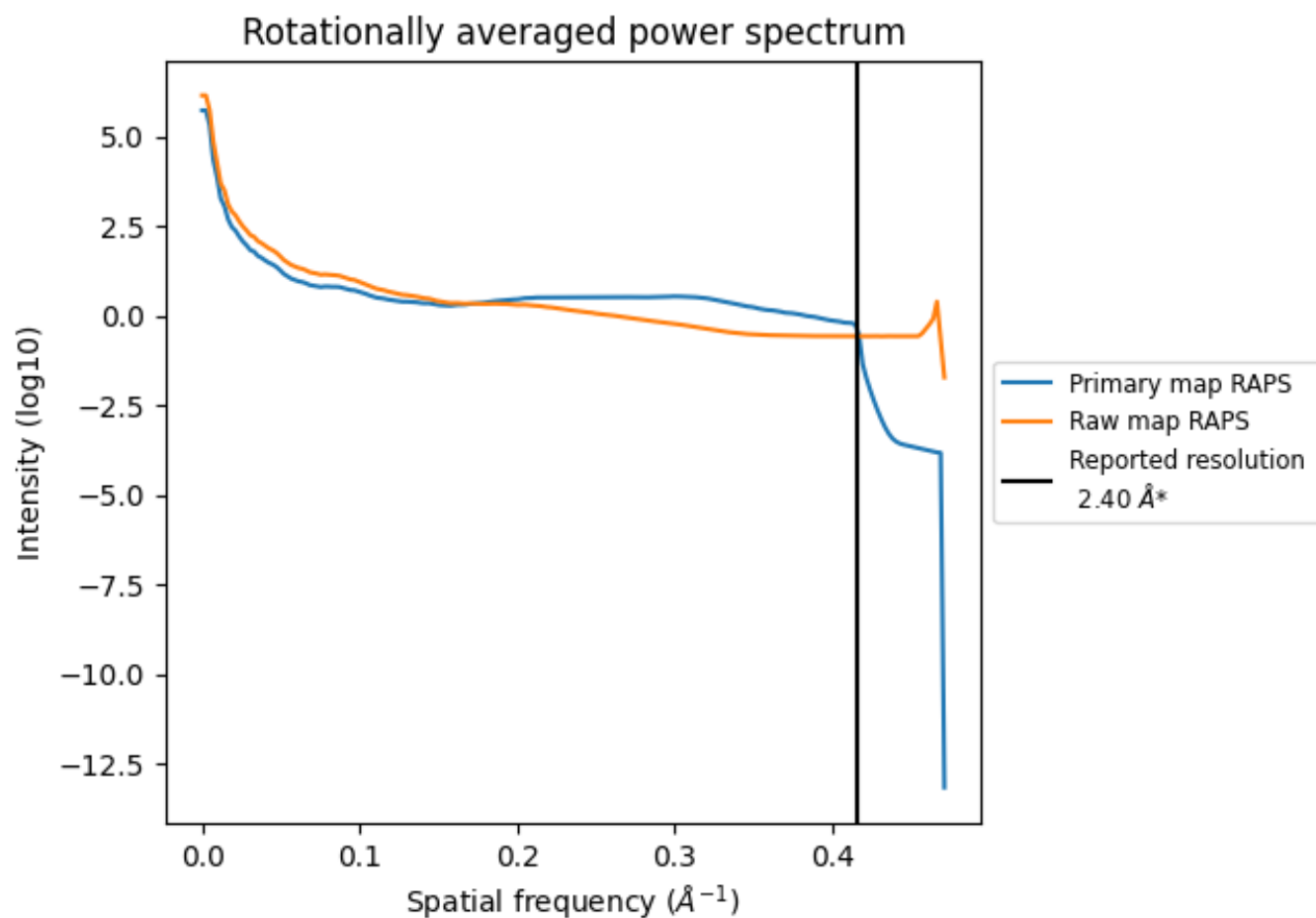
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1441 nm^3 ; this corresponds to an approximate mass of 1302 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 ⓘ

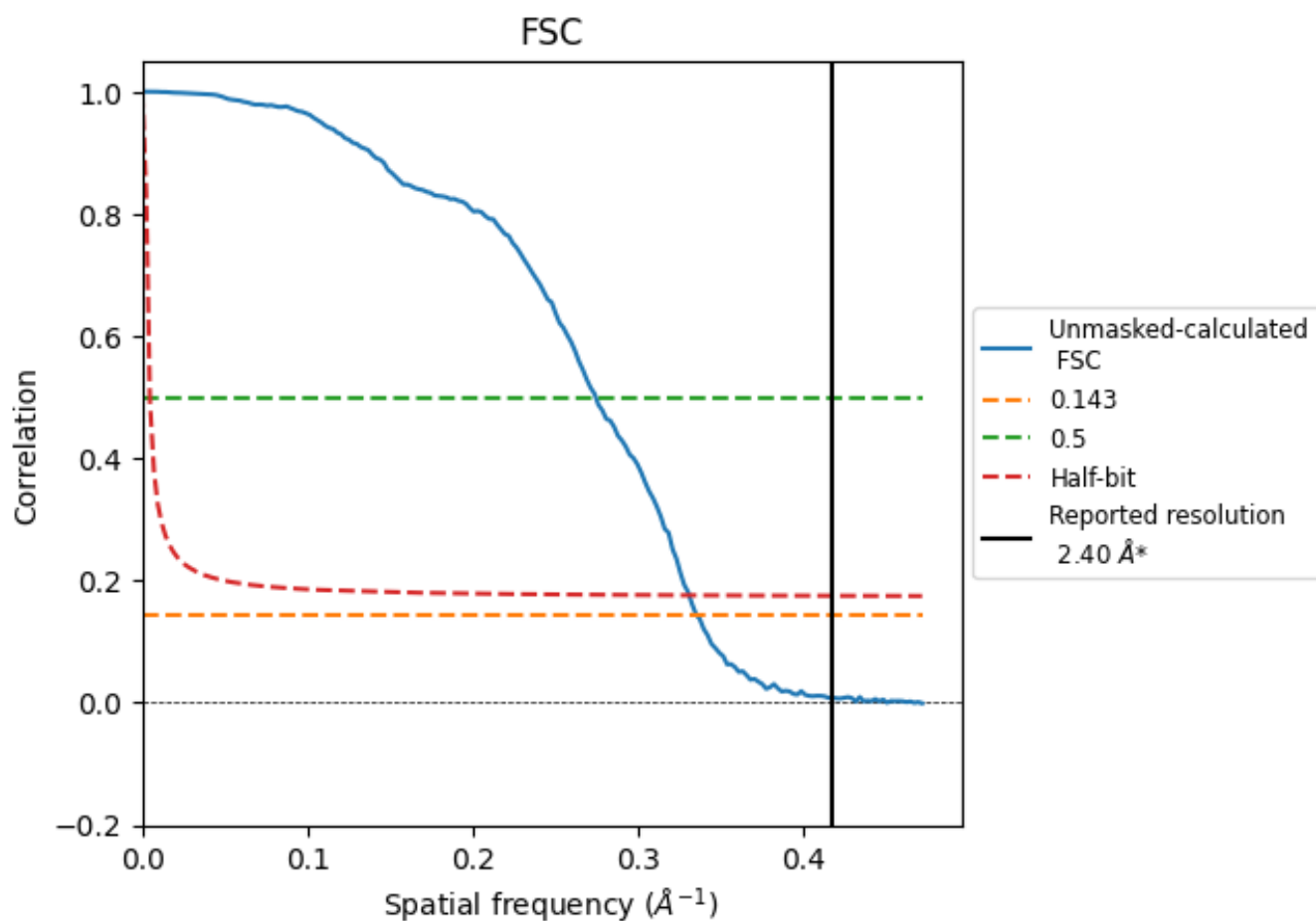


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

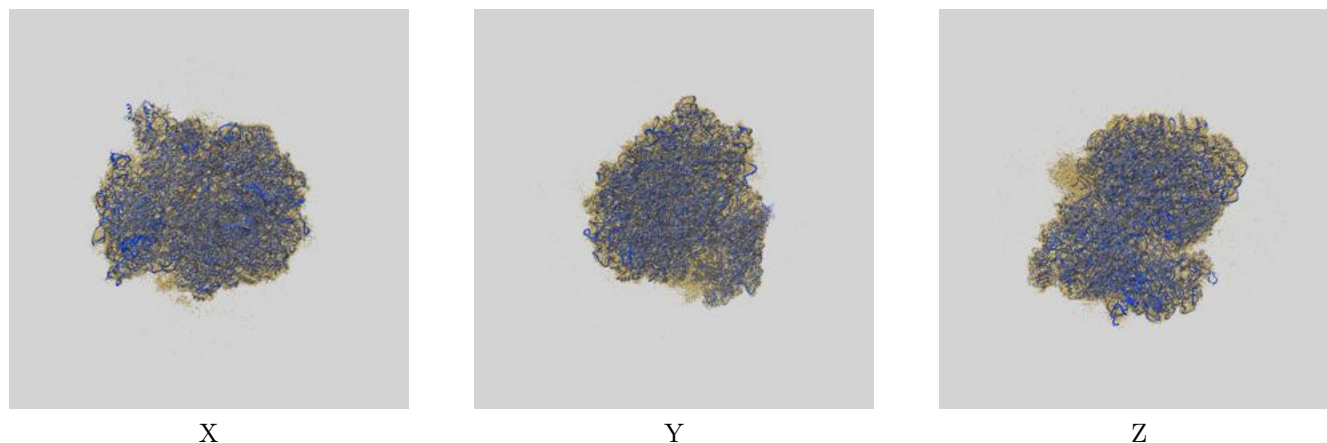
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.98	3.65	3.02

*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 2.98 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

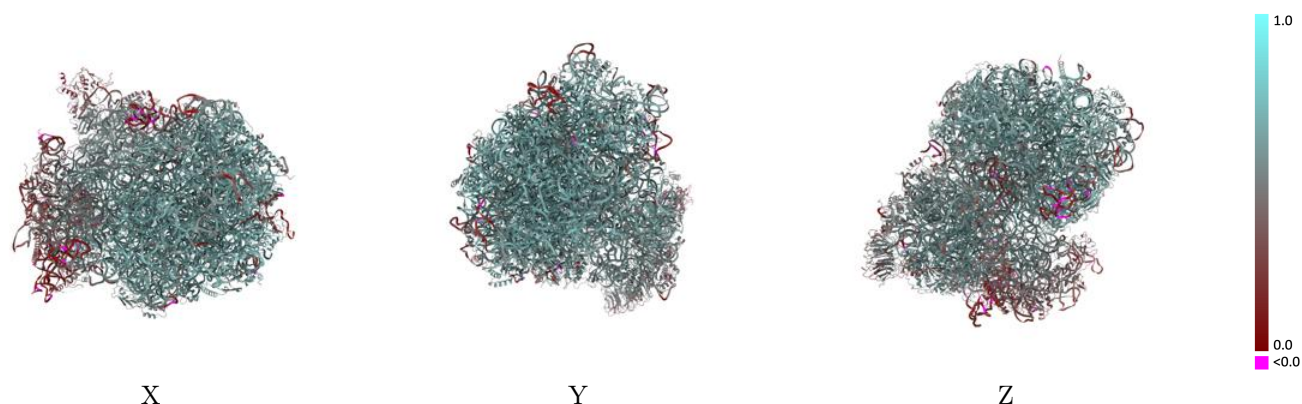
This section contains information regarding the fit between EMDB map EMD-40992 and PDB model 8T2Z. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



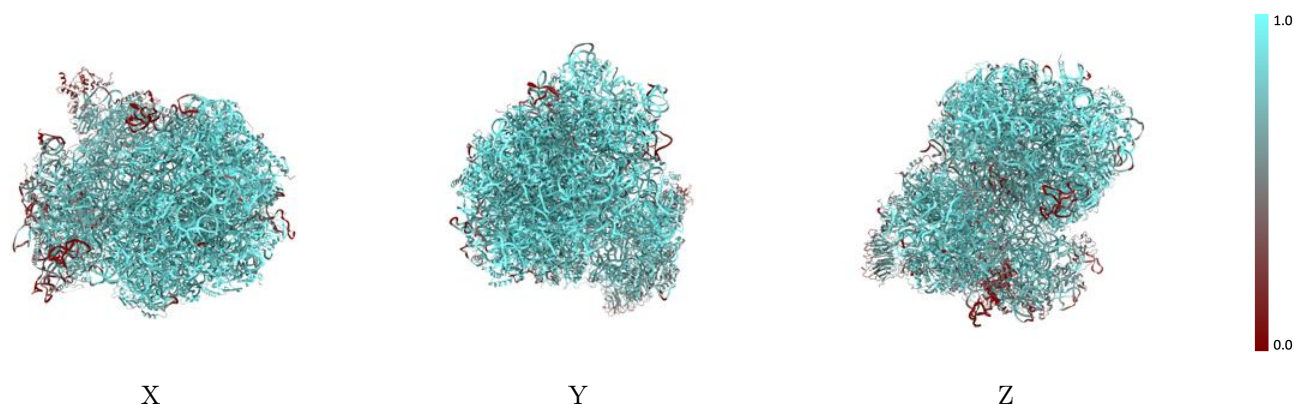
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



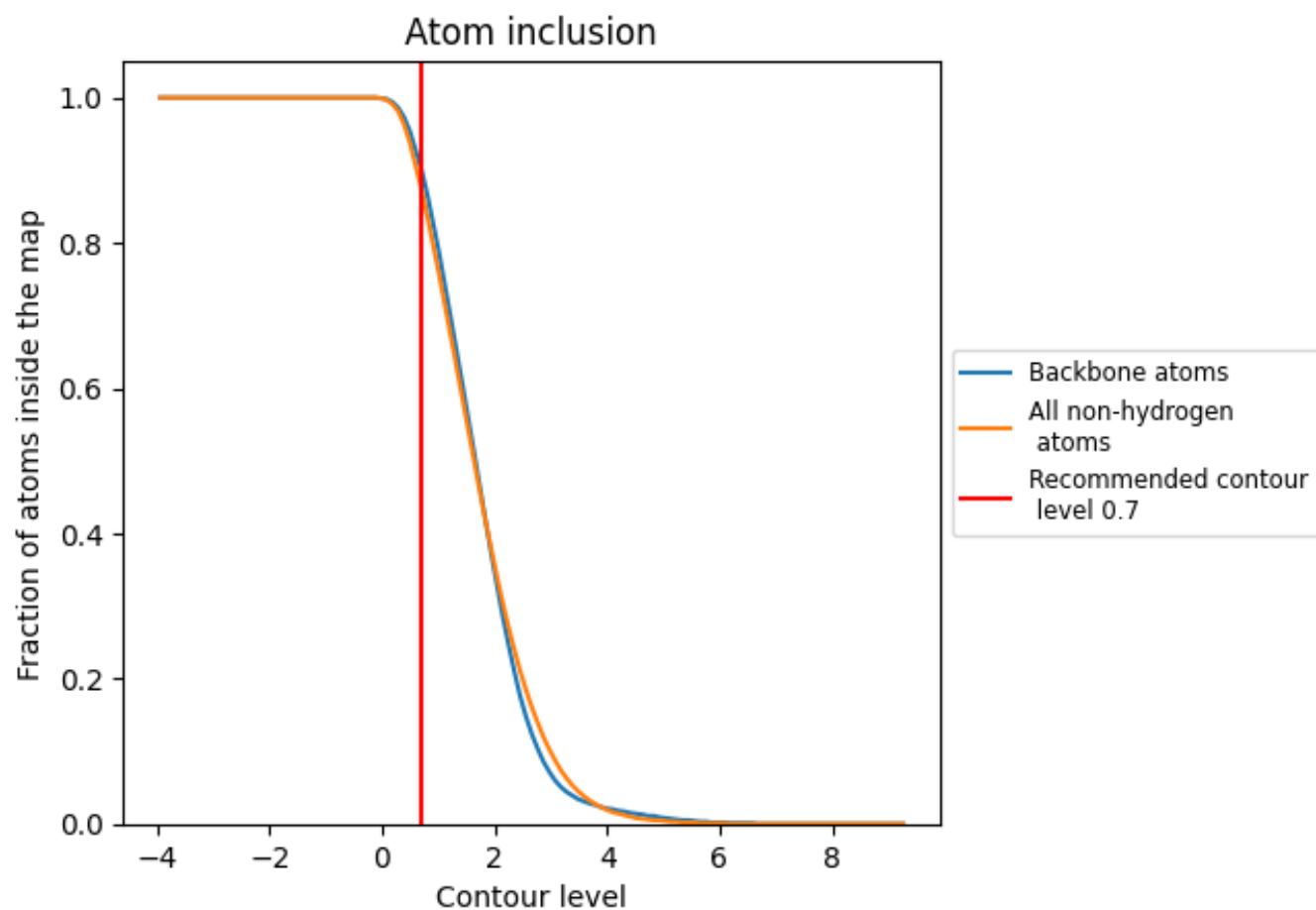
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5770
A1	 0.9350	 0.6180
A3	 0.9780	 0.6230
A4	 0.9760	 0.6520
AA	 0.9800	 0.6830
AB	 0.9520	 0.6420
AC	 0.9550	 0.6510
AD	 0.8490	 0.5680
AE	 0.8390	 0.5610
AF	 0.9410	 0.6430
AG	 0.8770	 0.5930
AH	 0.8820	 0.5950
AI	 0.8610	 0.5750
AJ	 0.8040	 0.5380
AL	 0.9240	 0.6310
AM	 0.9140	 0.6010
AN	 0.9850	 0.6800
AO	 0.9600	 0.6410
AP	 0.9490	 0.6510
AQ	 0.9690	 0.6690
AR	 0.8520	 0.5780
AS	 0.9280	 0.6220
AT	 0.9310	 0.6340
AU	 0.8410	 0.5620
AV	 0.9370	 0.6460
AW	 0.9550	 0.6530
AX	 0.9280	 0.6300
AY	 0.9320	 0.6320
AZ	 0.9040	 0.6130
Aa	 0.9630	 0.6630
Ab	 0.9340	 0.6220
Ac	 0.9270	 0.6220
Ad	 0.8820	 0.6050
Ae	 0.9530	 0.6650
Af	 0.9790	 0.6630



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Chain	Atom inclusion	Q-score
Ag	 0.9180	 0.6390
Ah	 0.9410	 0.6300
Ai	 0.9210	 0.6040
Aj	 0.9770	 0.6810
Ak	 0.8060	 0.5600
Al	 0.9780	 0.6650
Am	 0.8710	 0.6000
An	 0.9240	 0.6160
Ao	 0.9390	 0.6410
Ap	 0.9430	 0.6550
B5	 0.8470	 0.5190
BA	 0.8700	 0.5860
BB	 0.8590	 0.5820
BC	 0.9300	 0.6230
BD	 0.7410	 0.5170
BE	 0.6530	 0.3870
BF	 0.7700	 0.5390
BG	 0.5600	 0.3660
BH	 0.6710	 0.4810
BI	 0.8190	 0.5290
BJ	 0.5960	 0.3460
BK	 0.5980	 0.4390
BL	 0.7680	 0.5220
BM	 0.1380	 0.2500
BN	 0.9170	 0.6190
BO	 0.9260	 0.6120
BP	 0.5730	 0.4360
BQ	 0.8100	 0.5480
BR	 0.7920	 0.5520
BS	 0.7200	 0.4880
BT	 0.7580	 0.5020
BU	 0.6450	 0.4680
BV	 0.8790	 0.5950
BW	 0.9610	 0.6470
BX	 0.8640	 0.5870
BY	 0.5530	 0.3490
BZ	 0.6730	 0.4760
Ba	 0.9240	 0.6320
Bb	 0.8640	 0.5840
Bc	 0.7820	 0.5450
Bd	 0.9200	 0.6000
Be	 0.5750	 0.3800

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Chain	Atom inclusion	Q-score
Bf	 0.2530	 0.3260
Bg	 0.5650	 0.4450
MR	 0.9350	 0.5970
tA	 0.7200	 0.4630
tP	 0.8290	 0.4750