



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:17 AM UTC

PDB ID : 8T2X / pdb_00008t2x
EMDB ID : EMD-40990
Title : Hypomethylated yeast 80S bound with cycloheximide, P-site tRNA, A-site tRNA, messenger RNA and eIF5A, PRE
Authors : Zhao, Y.; Li, H.
Deposited on : 2023-06-07
Resolution : 2.46 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:

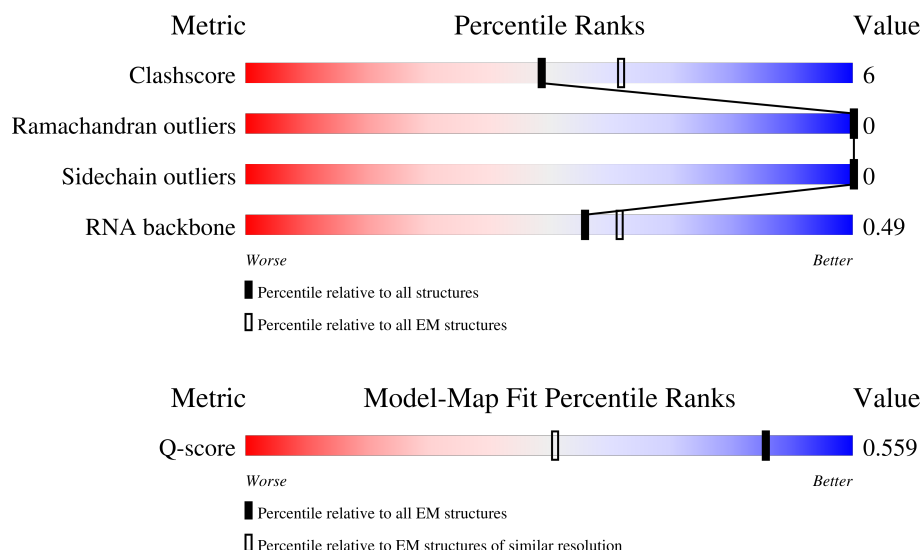
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.46 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	6014 (1.96 - 2.96)

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	E	217	
80	tP	75	
81	tA	76	
82	MR	12	
83	eI	155	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 207315 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	102	Total	C	N	O	S	0	0
			804	511	153	139	1		

- 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	1782	Total	C	N	O	P	1	0
			37987	16988	6718	12499	1782		

- 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	3216	Total	C	N	O	P	0	0
			68786	30729	12387	22454	3216		

- 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	0	0
			1543	962	315	266		

- 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	0	0
			1053	675	199	177	2		

- 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	0	0
			1720	1077	361	281	1		

- 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	197	0
			1555	1003	289	262	1		

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

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

- 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	0	0
			1441	908	290	241	2		

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

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

- 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 protein called RPL1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	E	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
80	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 81 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	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

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

- Molecule 82 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	MR	12	Total	C	N	O	P	0	0
			259	117	51	79	12		

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	eI	155	Total	C	N	O	S	0	0
			1148	712	196	231	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
eI	17	ALA	-	insertion	UNP A0A8H8ULI0

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
84	B5	39	Total	Mg	0
			39	39	
84	A1	139	Total	Mg	0
			139	139	
84	A4	1	Total	Mg	0
			1	1	
84	AP	1	Total	Mg	0
			1	1	
84	AV	1	Total	Mg	0
			1	1	

- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

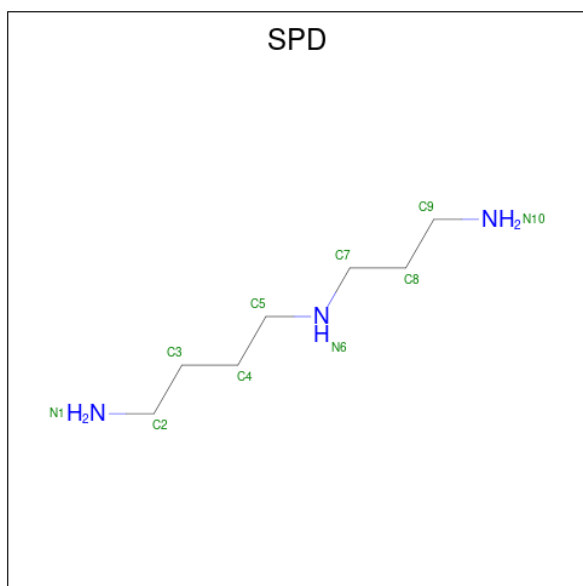
Mol	Chain	Residues	Atoms		AltConf
85	B5	10	Total	K	0
			10	10	
85	A1	12	Total	K	0
			12	12	

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Continued from previous page...

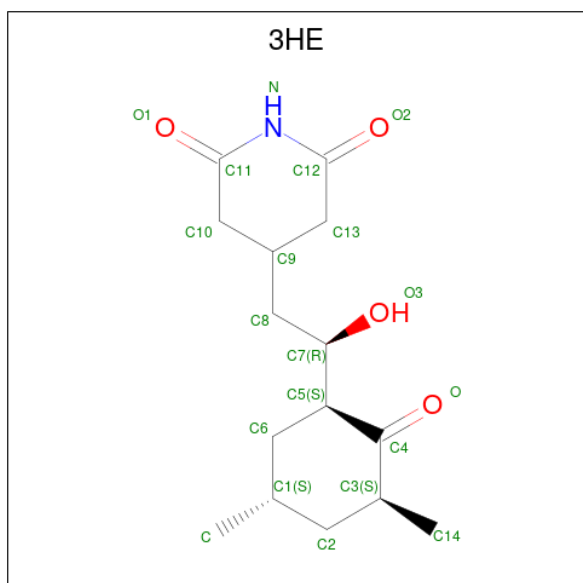
Mol	Chain	Residues	Atoms		AltConf
85	Ab	1	Total	K	0
			1	1	

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

- Molecule 87 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
87	A1	1	Total	C	N	O	0
			20	15	1	4	

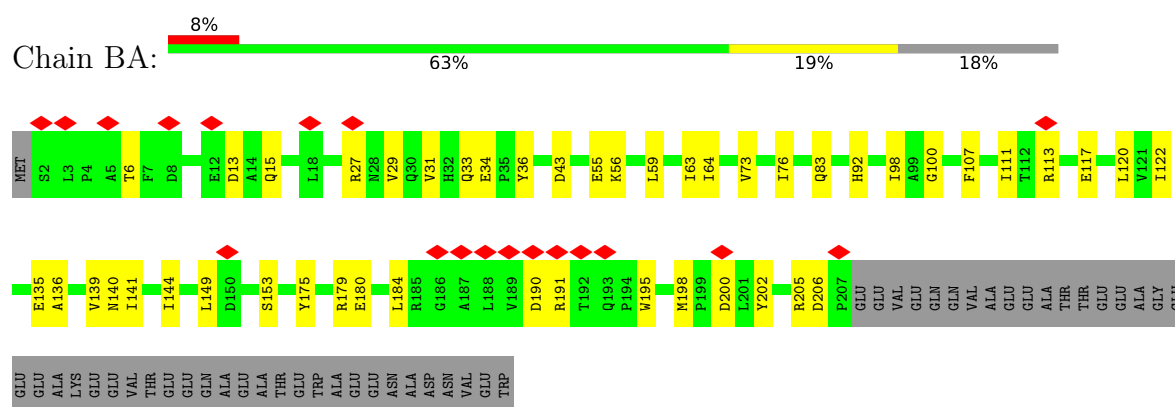
- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

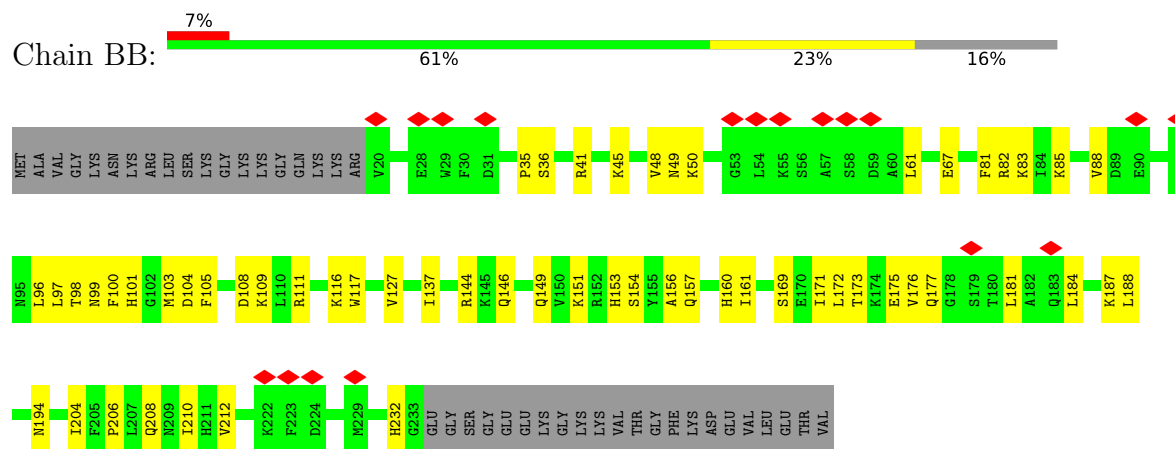
3 Residue-property plots

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.

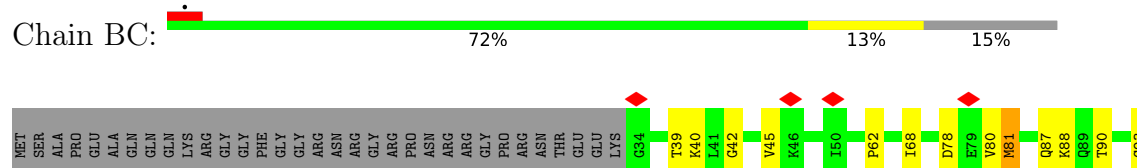
• Molecule 1: 40S ribosomal protein S0-A

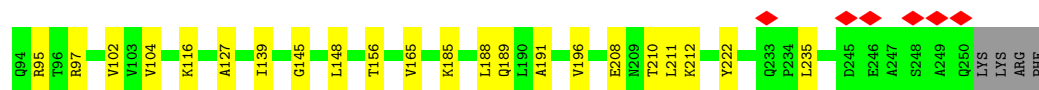


• Molecule 2: RPS1A isoform 1

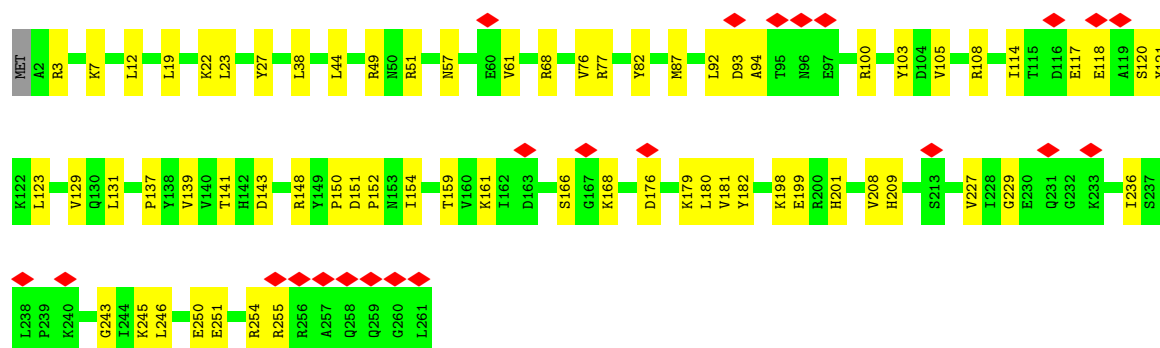
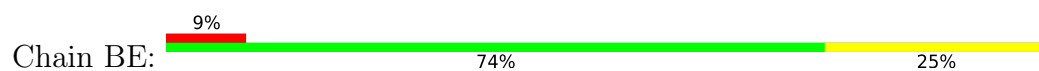


• Molecule 3: RPS2 isoform 1

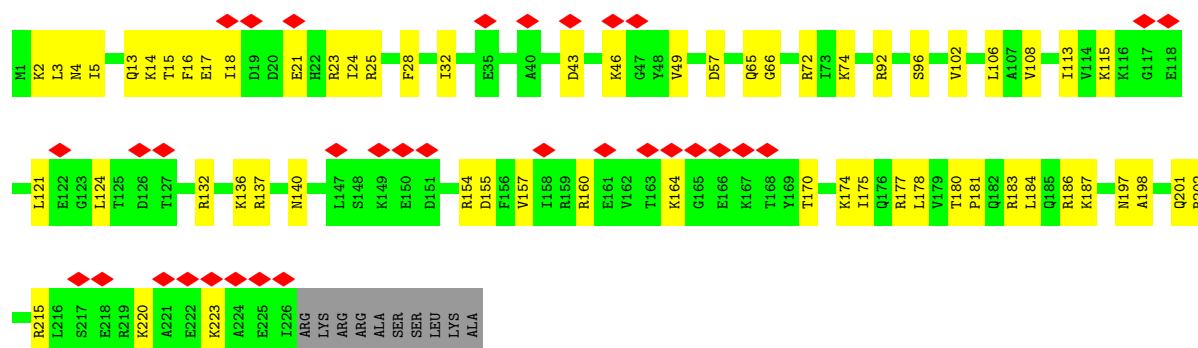
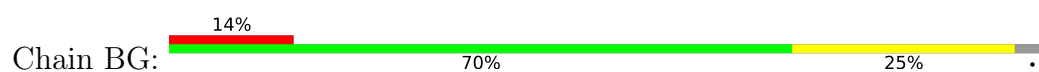




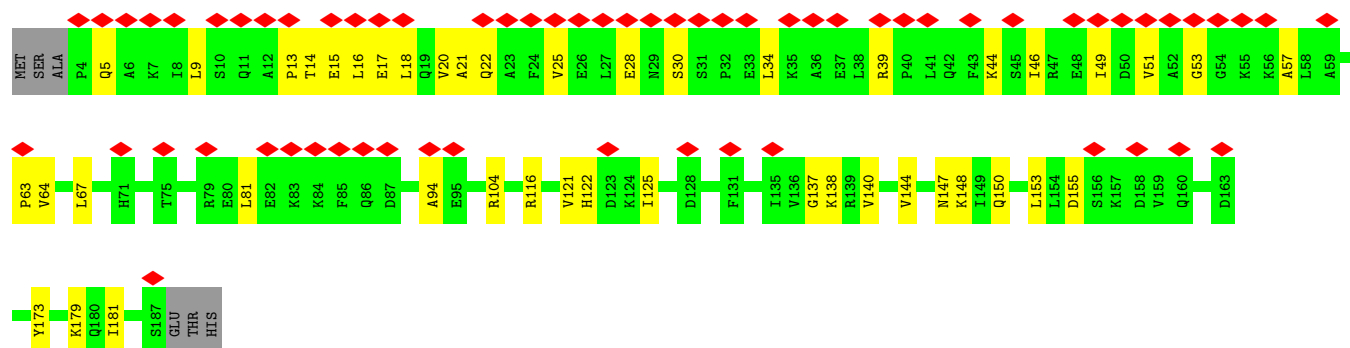
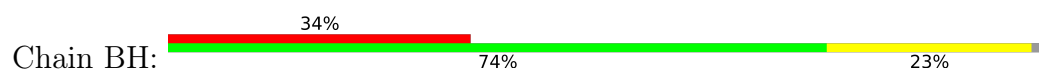
• Molecule 4: 40S ribosomal protein S4-A



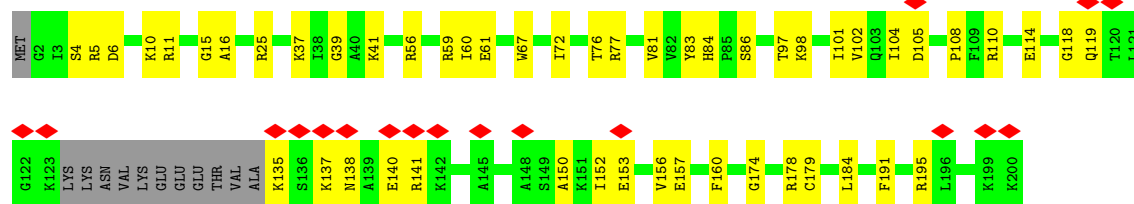
• Molecule 5: 40S ribosomal protein S6-A



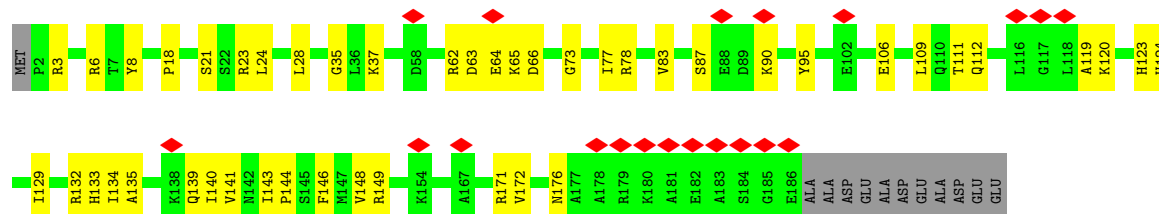
• Molecule 6: 40S ribosomal protein S7-A



• Molecule 7: 40S ribosomal protein S8-A



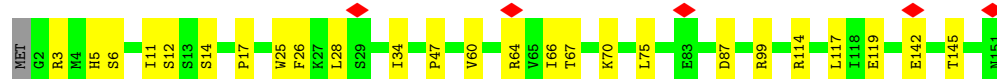
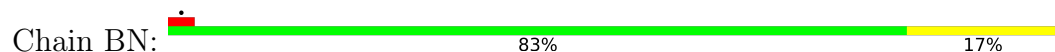
• Molecule 8: 40S ribosomal protein S9-A



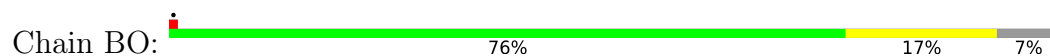
• Molecule 9: 40S ribosomal protein S11-A



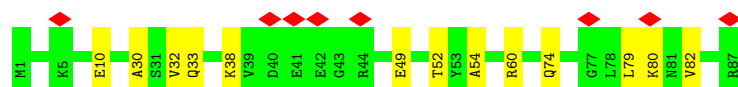
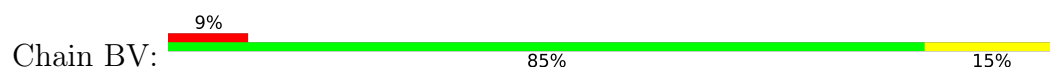
• Molecule 10: 40S ribosomal protein S13



• Molecule 11: 40S ribosomal protein S14-A

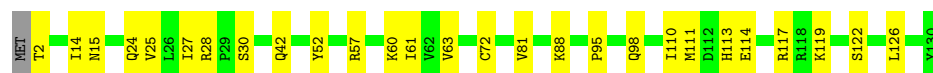


• Molecule 12: 40S ribosomal protein S21-A



- Molecule 13: RPS22A isoform 1

Chain BW:  78% 21%



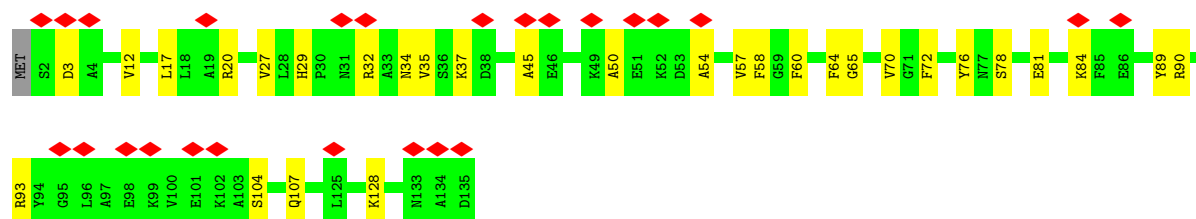
- Molecule 14: 40S ribosomal protein S23-A

Chain BX:  83% 16%



- Molecule 15: 40S ribosomal protein S24-A

Chain BY:  19% 77% 22%



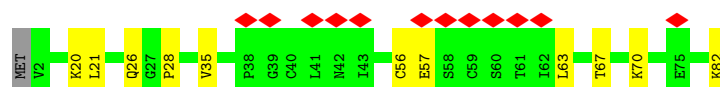
- Molecule 16: RPS26B isoform 1

Chain Ba:  71% 10% 18%



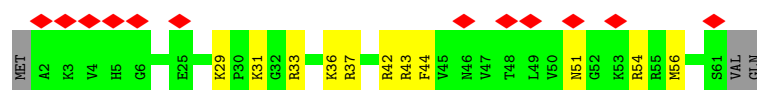
- Molecule 17: 40S ribosomal protein S27-A

Chain Bb:  15% 85% 13%

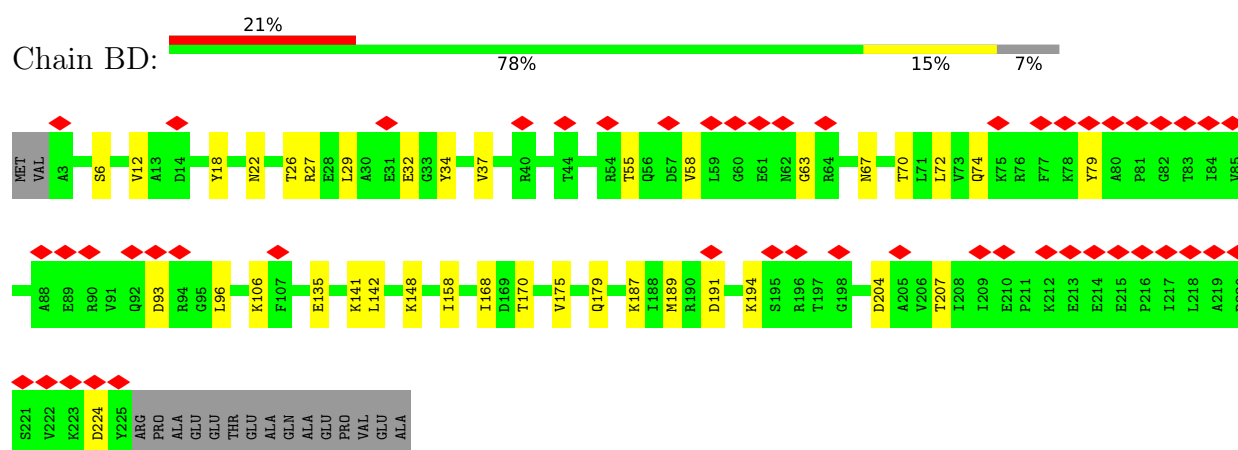


- Molecule 18: 40S ribosomal protein S30-A

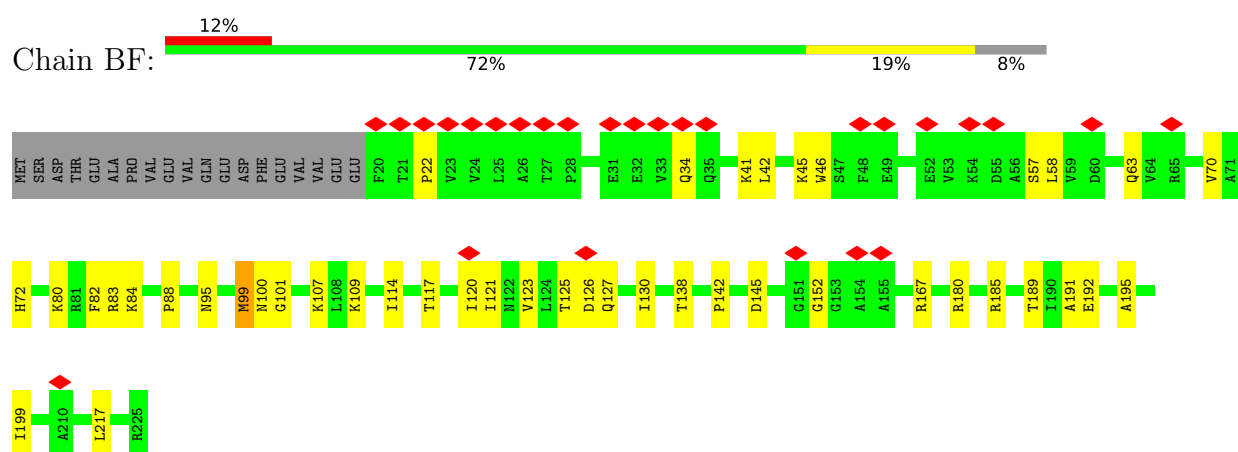
Chain Be:  19% 78% 17% 5%



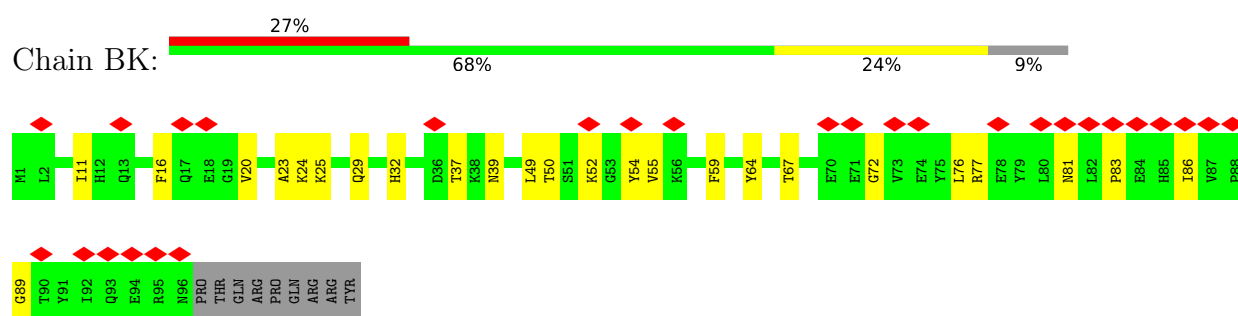
- Molecule 19: RPS3 isoform 1



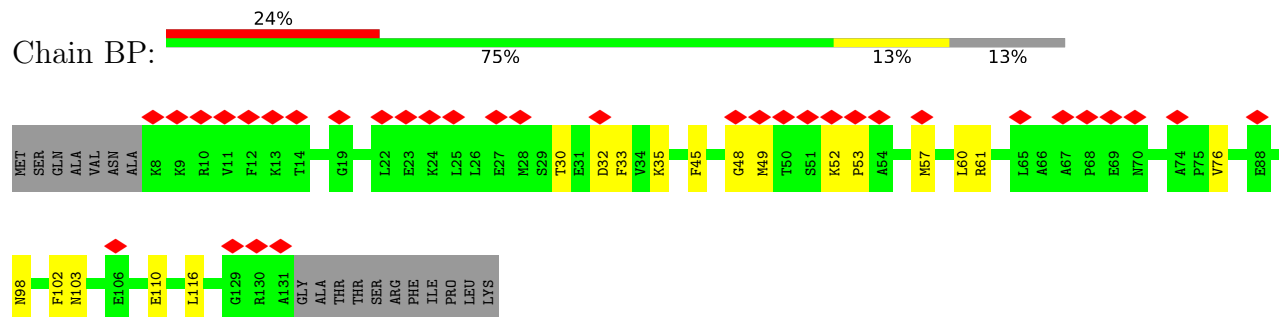
- Molecule 20: Rps5p



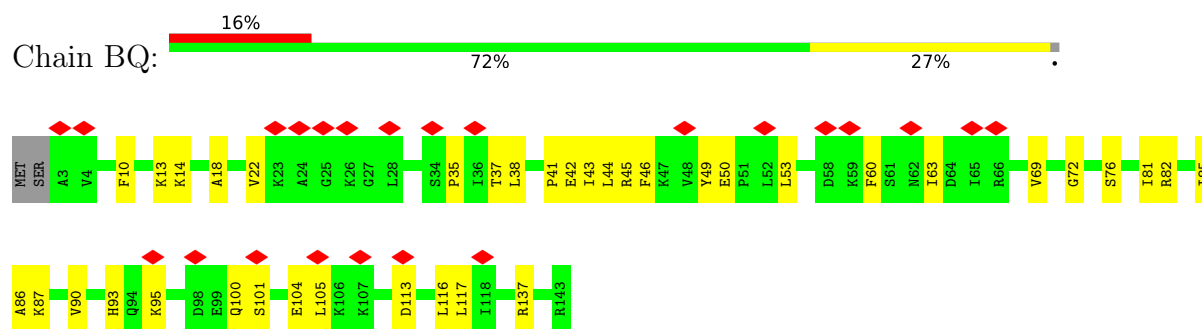
- Molecule 21: 40S ribosomal protein S10-A



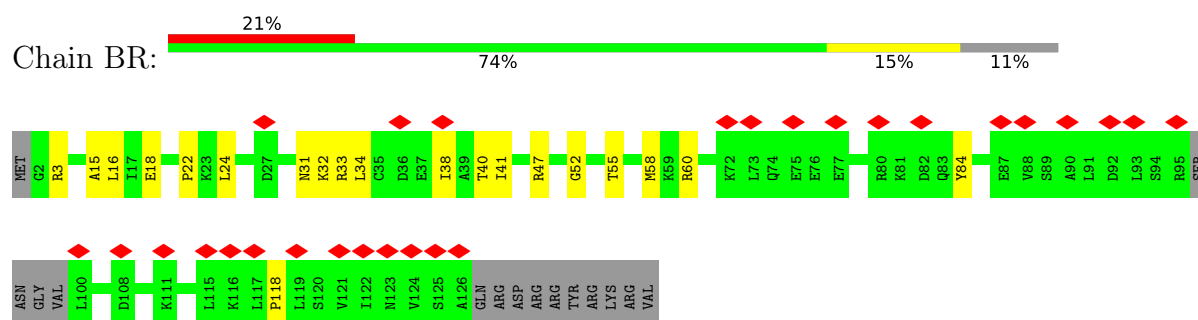
- Molecule 22: RPS15 isoform 1



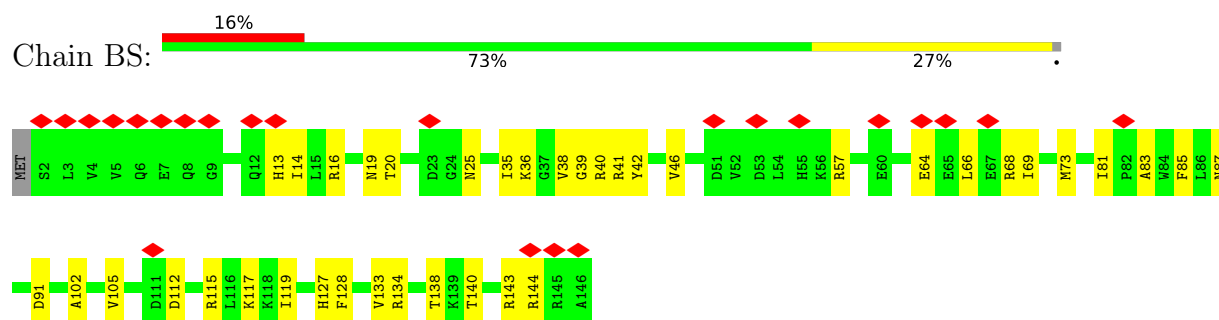
- Molecule 23: 40S ribosomal protein S16-A



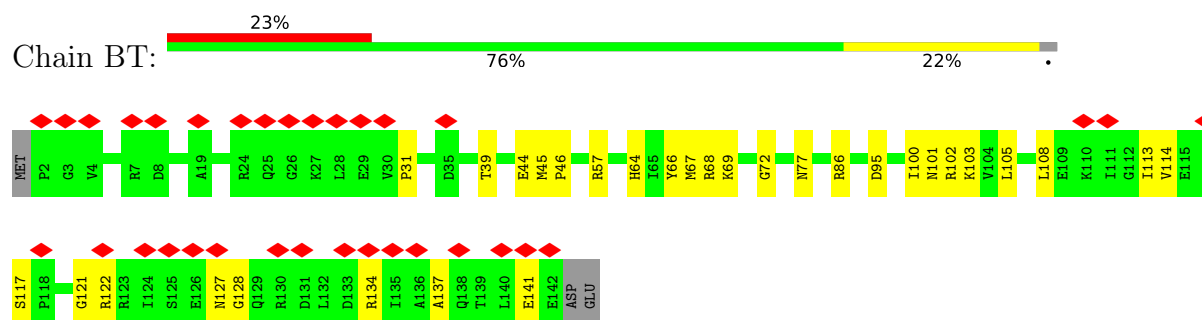
- Molecule 24: 40S ribosomal protein S17-A



- Molecule 25: 40S ribosomal protein S18-A

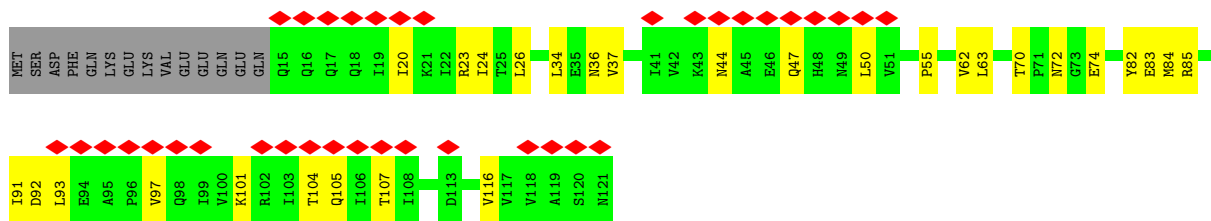


- Molecule 26: 40S ribosomal protein S19-A

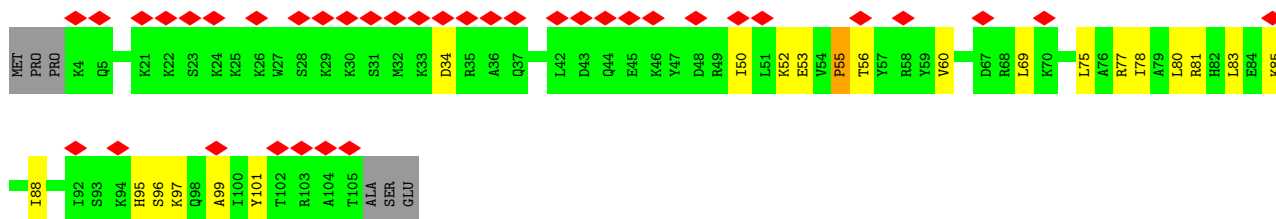
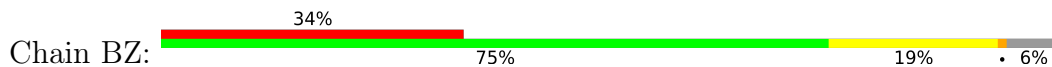


- Molecule 27: RPS20 isoform 1

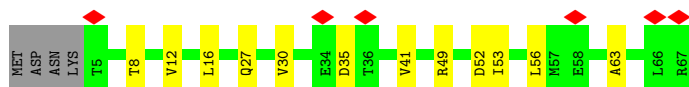
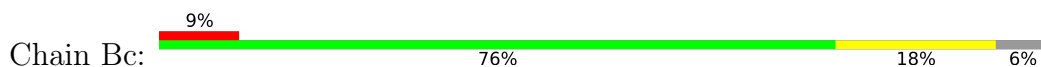




• Molecule 28: RPS25A isoform 1



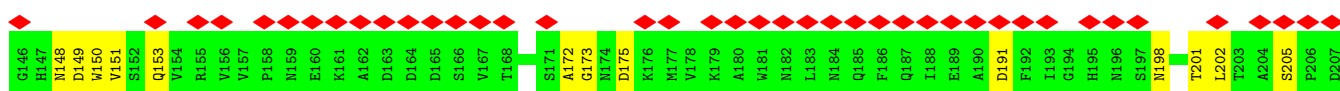
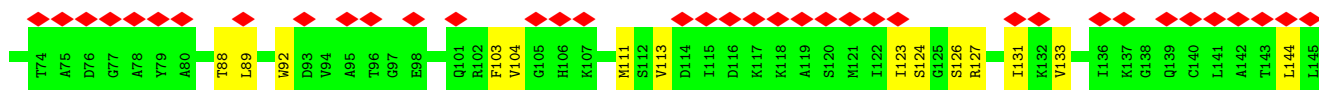
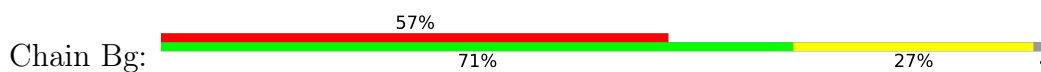
• Molecule 29: RPS28A isoform 1



• Molecule 30: RPS29A isoform 1



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

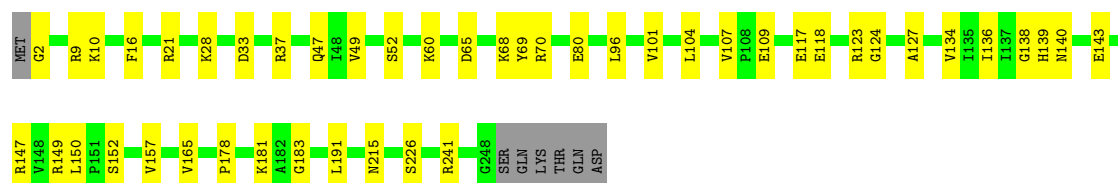






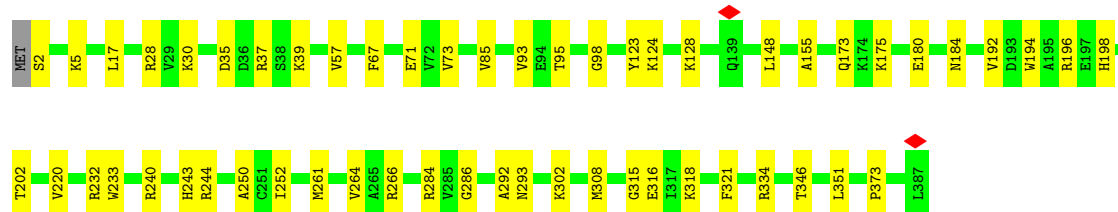
• Molecule 35: 60S ribosomal protein L2-A

Chain AA: 79% 18%



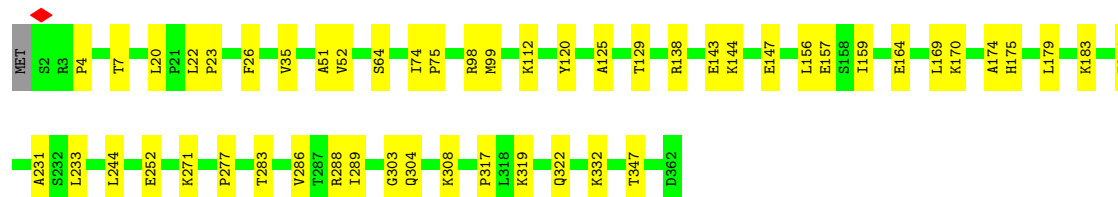
• Molecule 36: 60S ribosomal protein L3

Chain AB: 86% 14%



• Molecule 37: RPL4A isoform 1

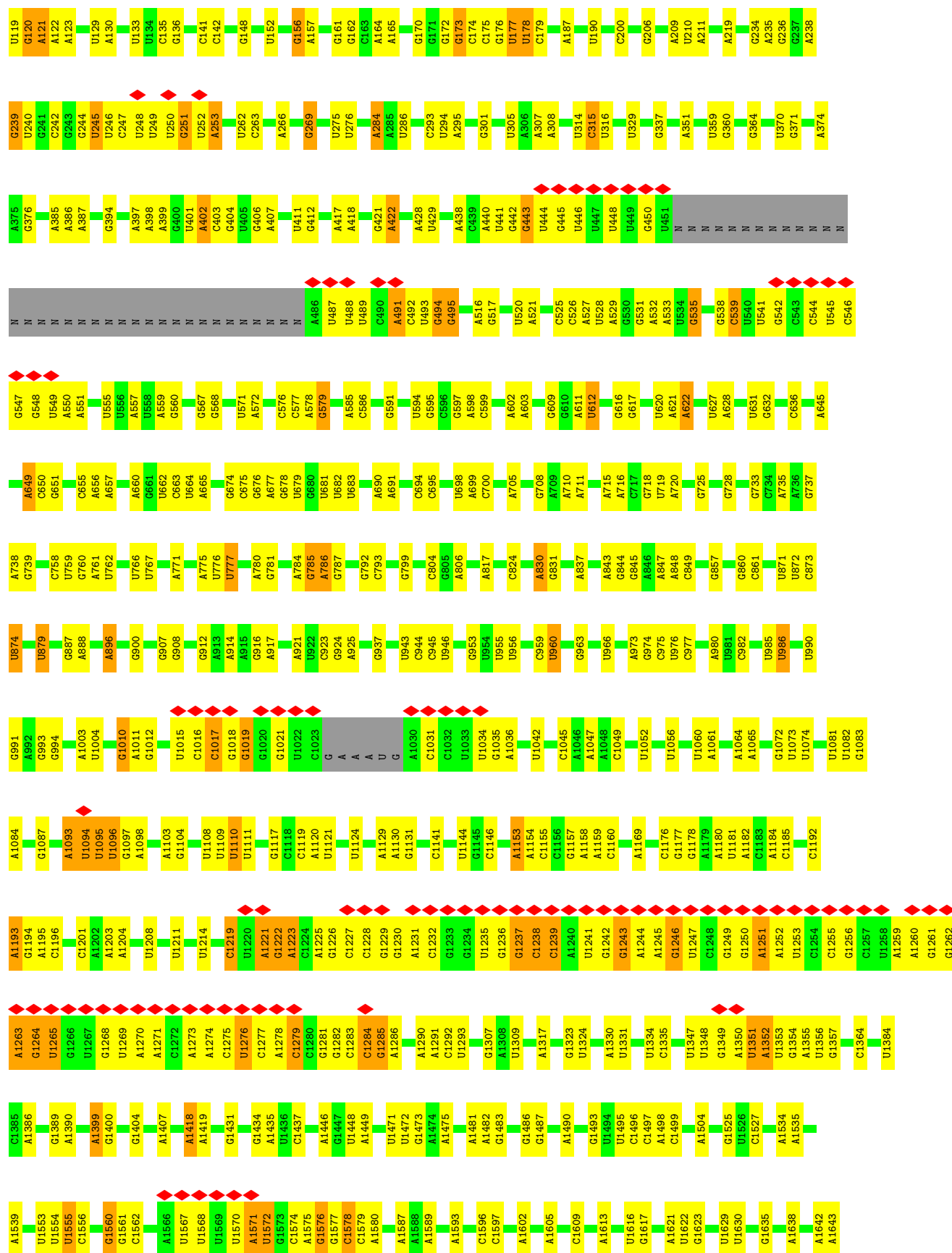
Chain AC: 86% 14%



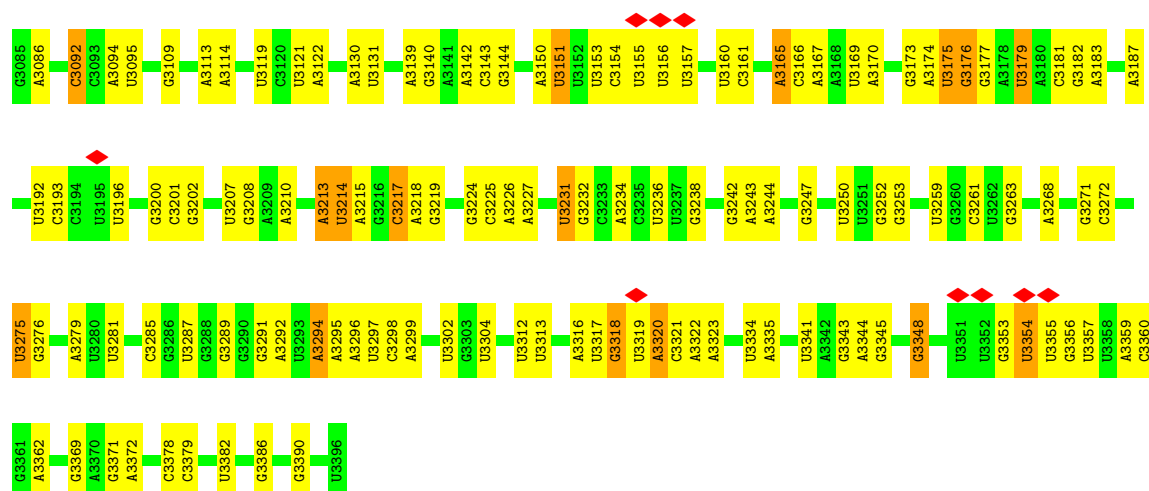
• Molecule 38: 25S rRNA

Chain A1: 60% 30% 5%

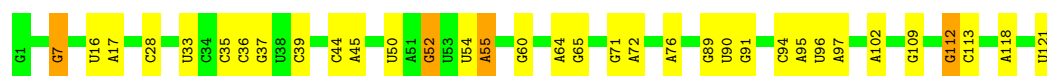




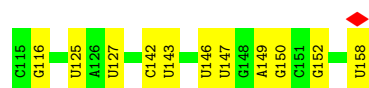
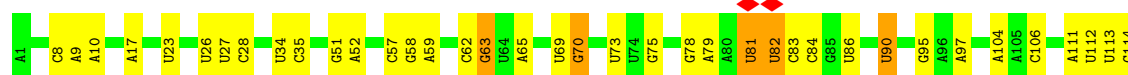




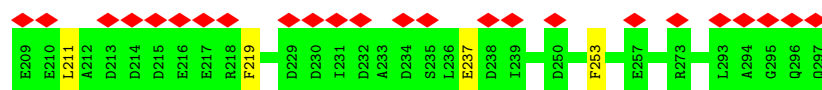
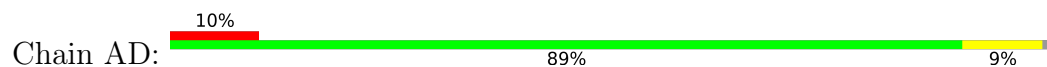
• Molecule 39: 5s rRNA



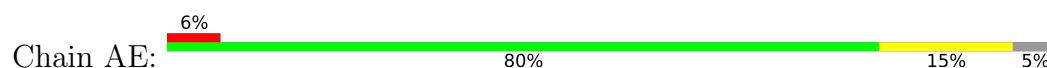
• Molecule 40: 5.8 S rRNA

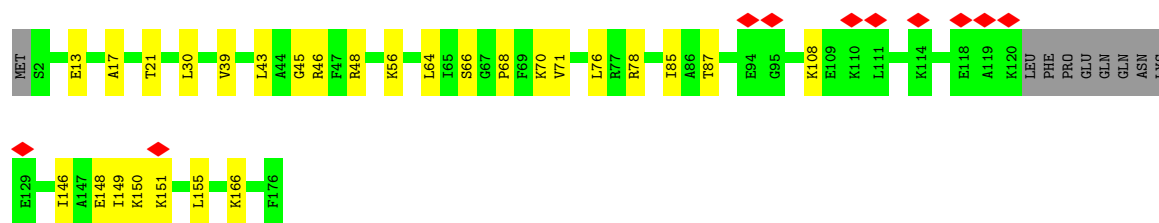


• Molecule 41: RPL5 isoform 1

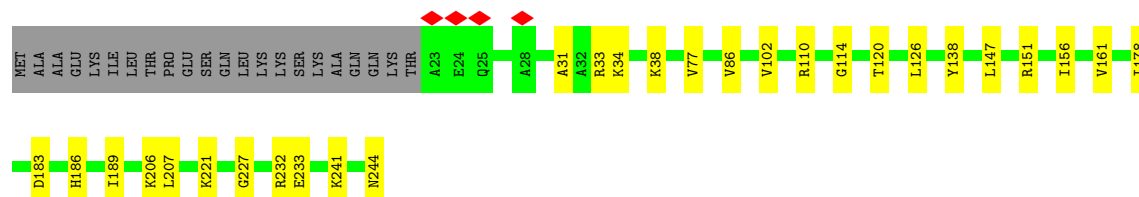
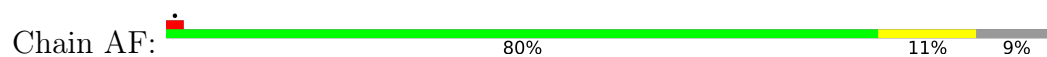


• Molecule 42: 60S ribosomal protein L6-A

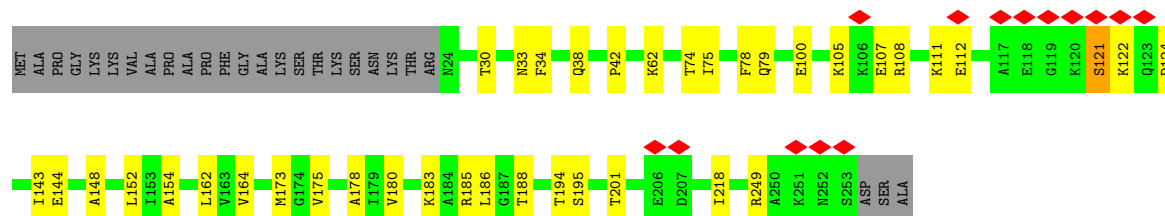
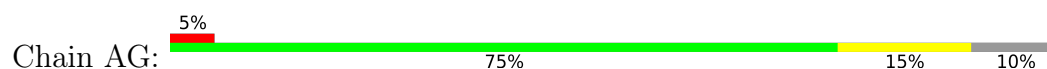




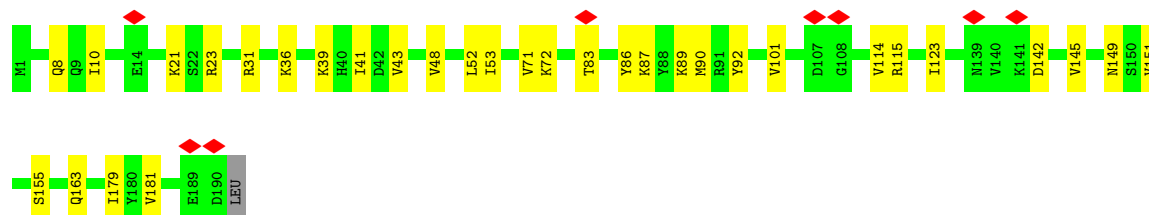
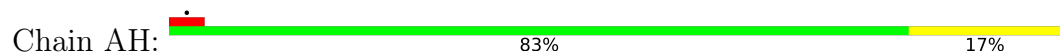
- Molecule 43: 60S ribosomal protein L7-A



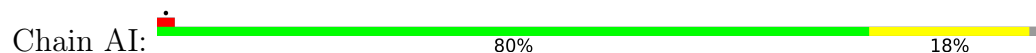
- Molecule 44: 60S ribosomal protein L8-A



- Molecule 45: 60S ribosomal protein L9-A

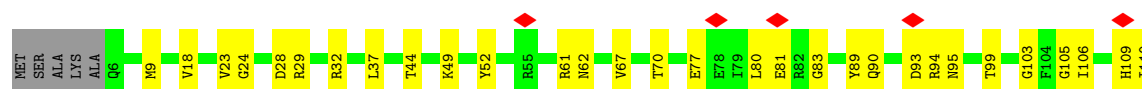
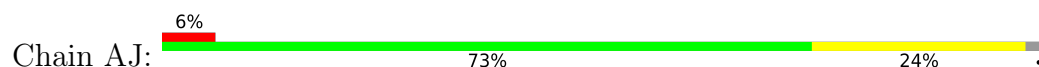


- Molecule 46: RPL10 isoform 1

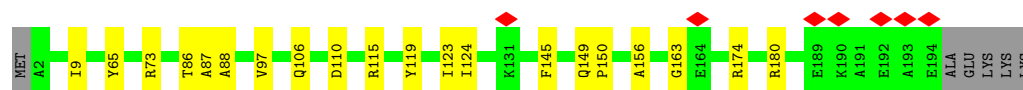




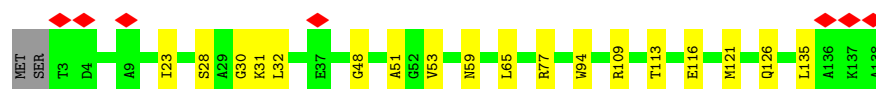
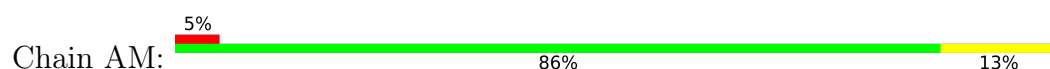
- Molecule 47: RPL11A isoform 1



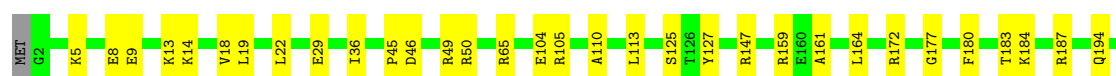
- Molecule 48: 60S ribosomal protein L13-A



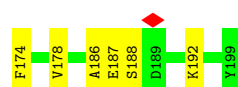
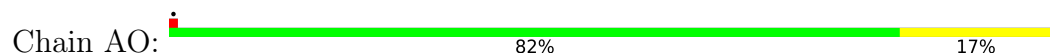
- Molecule 49: 60S ribosomal protein L14-A



- Molecule 50: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L17-A

Chain AP:  82% 13% 5%



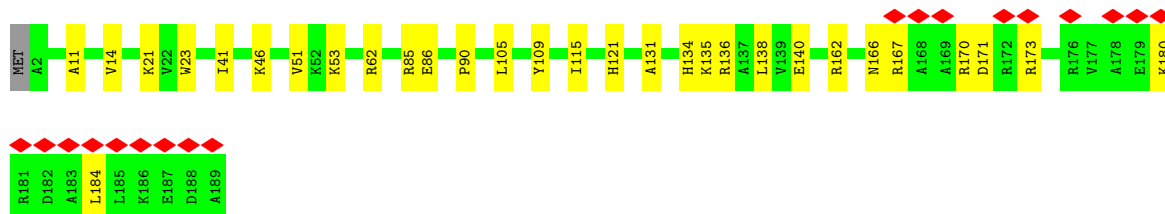
- Molecule 53: 60S ribosomal protein L18-A

Chain AQ:  88% 11%



- Molecule 54: 60S ribosomal protein L19-A

Chain AR:  10% 84% 16%



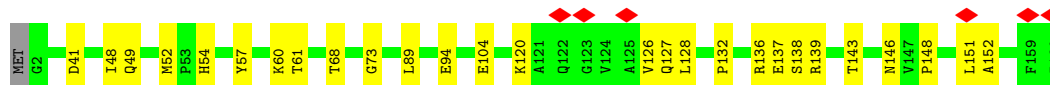
- Molecule 55: 60S ribosomal protein L20

Chain AS:  77% 20%



- Molecule 56: 60S ribosomal protein L21-A

Chain AT:  82% 17%

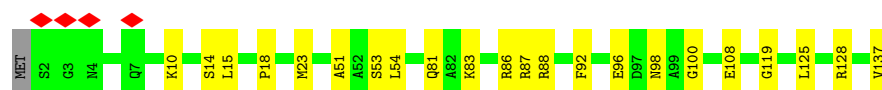
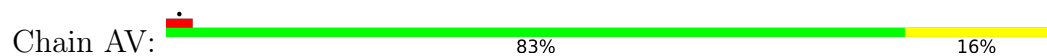


- Molecule 57: 60S ribosomal protein L22-A

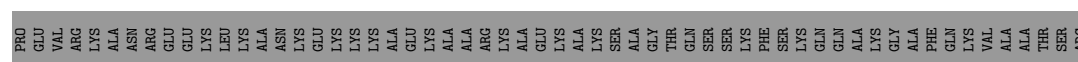
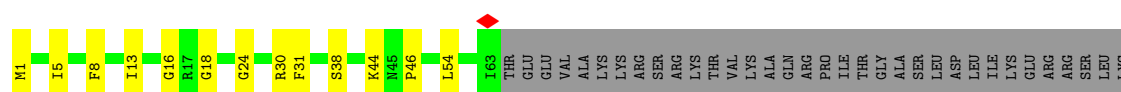
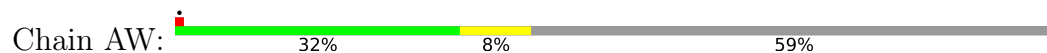
Chain AU:  74% 9% 17%



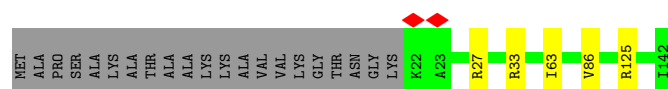
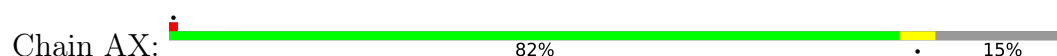
- Molecule 58: 60S ribosomal protein L23-A



- Molecule 59: RPL24A isoform 1



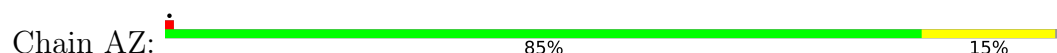
- Molecule 60: 60S ribosomal protein L25



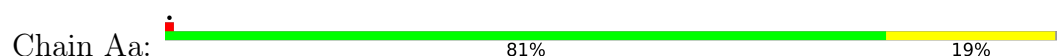
- Molecule 61: 60S ribosomal protein L26-A



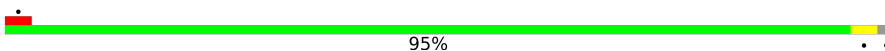
- Molecule 62: 60S ribosomal protein L27-A



- Molecule 63: 60S ribosomal protein L28



- Molecule 64: RPL29 isoform 1

Chain Ab:  95%



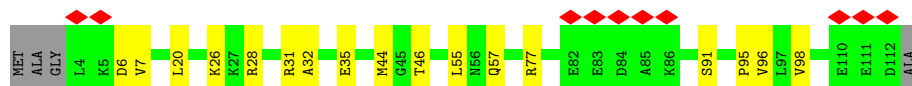
- Molecule 65: 60S ribosomal protein L30

Chain Ac:  76% 16% 8%



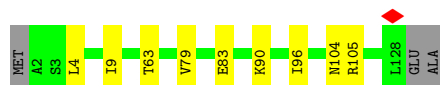
- Molecule 66: 60S ribosomal protein L31-A

Chain Ad:  9% 81% 15%



- Molecule 67: RPL32 isoform 1

Chain Ae:  91% 7%



- Molecule 68: 60S ribosomal protein L33-A

Chain Af:  91% 8%



- Molecule 69: 60S ribosomal protein L34-A

Chain Ag:  6% 81% 12% 7%



- Molecule 70: 60S ribosomal protein L35-A

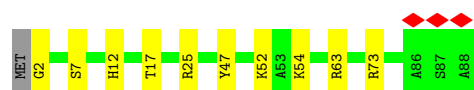
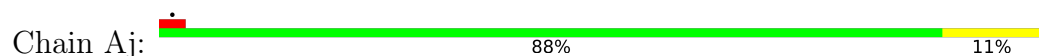
Chain Ah:  81% 18%



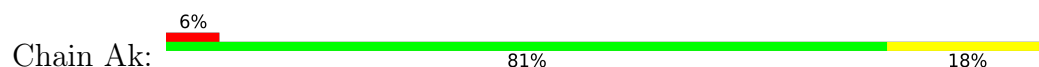
- Molecule 71: 60S ribosomal protein L36-A



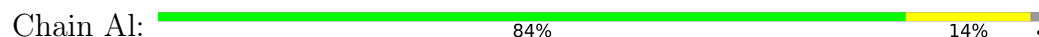
- Molecule 72: 60S ribosomal protein L37-A



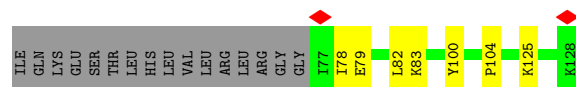
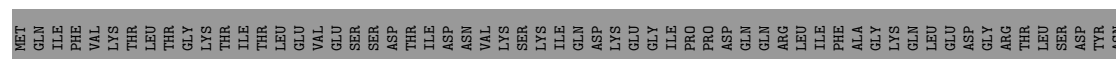
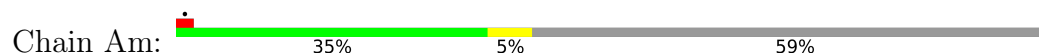
- Molecule 73: RPL38 isoform 1



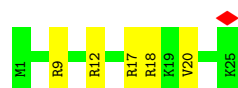
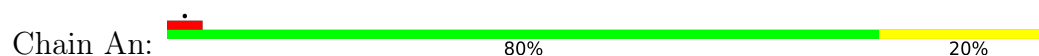
- Molecule 74: 60S ribosomal protein L39



- Molecule 75: Ubiquitin-60S ribosomal protein L40

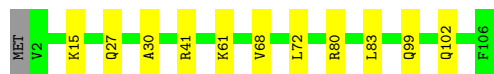


- Molecule 76: 60S ribosomal protein L41-A



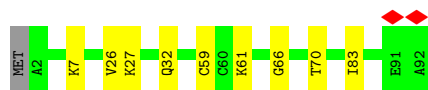
- Molecule 77: 60S ribosomal protein L42-A

Chain Ao:  89% 10%



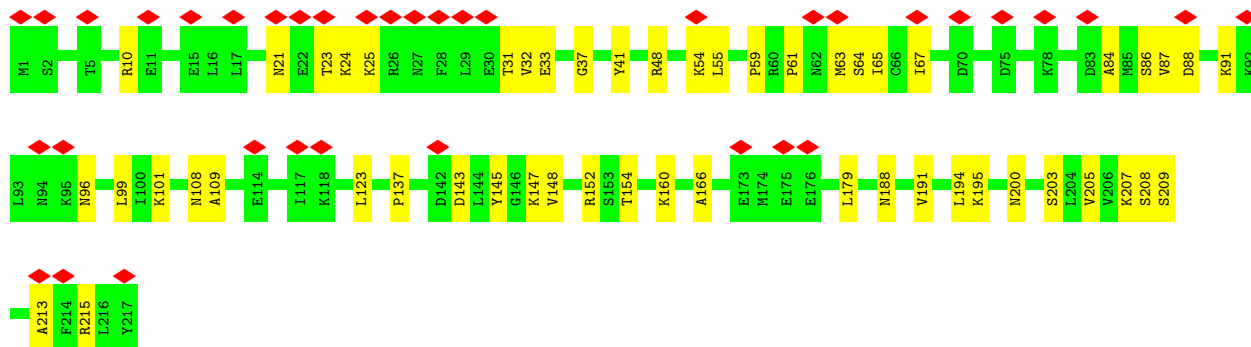
- Molecule 78: 60S ribosomal protein L43-A

Chain Ap:  89% 10%



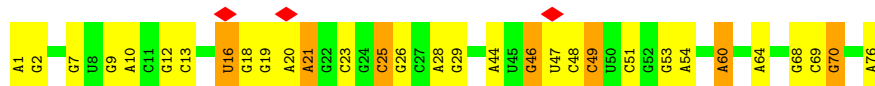
- Molecule 79: RPL1A isoform 1

Chain E:  17% 76% 24%



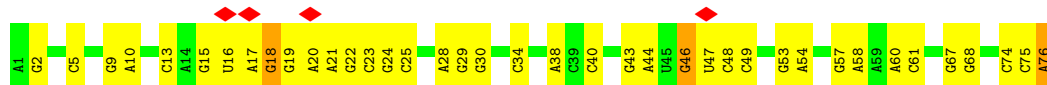
- Molecule 80: P site tRNA

Chain tP:  59% 32% 9%



- Molecule 81: A site tRNA

Chain tA:  5% 49% 47%

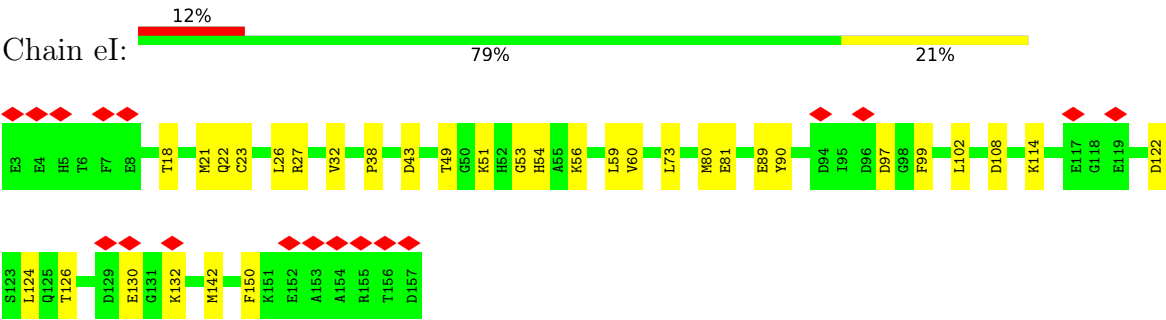


- Molecule 82: messenger RNA

Chain MR:  75% 25%



● Molecule 83: Eukaryotic translation initiation factor 5A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	295361	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	9.412	Depositor
Minimum map value	-4.108	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.255	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: SPD, G7M, 3HE, PSU, 1MA, 4AC, OMG, 5CT, 5MC, OMU, UR3, MA6, MG, B8N, K, HIC, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	BA	0.23	0/1653	0.47	0/2261
2	BB	0.26	0/1735	0.55	0/2335
3	BC	0.26	0/1665	0.48	1/2263 (0.0%)
4	BE	0.20	0/2109	0.45	0/2839
5	BG	0.21	0/1844	0.45	0/2464
6	BH	0.22	0/1506	0.53	2/2028 (0.1%)
7	BI	0.27	0/1514	0.49	0/2021
8	BJ	0.21	0/1519	0.45	0/2035
9	BL	0.26	0/1272	0.45	0/1712
10	BN	0.28	0/1215	0.51	0/1638
11	BO	0.33	0/952	0.62	0/1279
12	BV	0.23	0/693	0.54	0/935
13	BW	0.27	0/1038	0.44	0/1395
14	BX	0.31	0/1139	0.50	0/1518
15	BY	0.21	0/1087	0.47	0/1449
16	Ba	0.30	0/782	0.58	0/1047
17	Bb	0.24	0/620	0.50	0/838
18	Be	0.22	0/483	0.44	0/643
19	BD	0.23	0/1759	0.51	0/2368
20	BF	0.22	0/1629	0.49	0/2202
21	BK	0.23	0/837	0.64	2/1131 (0.2%)
22	BP	0.22	0/1012	0.53	0/1356
23	BQ	0.23	0/1125	0.50	0/1510
24	BR	0.19	0/957	0.44	0/1283
25	BS	0.23	0/1211	0.52	0/1628
26	BT	0.23	0/1113	0.57	0/1494
27	BU	0.27	0/865	0.59	0/1169
28	BZ	0.19	0/814	0.49	2/1084 (0.2%)
29	Bc	0.25	0/499	0.56	0/670
30	Bd	0.22	0/452	0.66	2/600 (0.3%)
31	Bg	0.19	0/2454	0.49	0/3340
32	Bf	0.15	0/616	0.37	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.19	0/943	0.51	0/1274
34	B5	0.28	1/42034 (0.0%)	0.37	1/65493 (0.0%)
35	AA	0.40	0/1912	0.49	0/2569
36	AB	0.31	0/3139	0.46	0/4219
37	AC	0.31	0/2800	0.49	0/3790
38	A1	0.42	0/76161	0.41	1/118749 (0.0%)
39	A3	0.29	0/2861	0.32	0/4457
40	A4	0.40	0/3724	0.37	0/5798
41	AD	0.23	0/2390	0.42	0/3225
42	AE	0.22	0/1324	0.42	0/1782
43	AF	0.32	0/1821	0.47	0/2451
44	AG	0.30	0/1830	0.51	0/2469
45	AH	0.28	0/1531	0.49	0/2062
46	AI	0.30	0/1796	0.46	0/2409
47	AJ	0.25	0/1374	0.55	0/1842
48	AL	0.29	0/1568	0.42	0/2106
49	AM	0.24	0/1068	0.42	0/1438
50	AN	0.40	0/1757	0.52	0/2354
51	AO	0.32	0/1585	0.48	1/2128 (0.0%)
52	AP	0.33	0/1410	0.44	0/1893
53	AQ	0.31	0/1465	0.43	0/1965
54	AR	0.31	0/1538	0.46	0/2050
55	AS	0.31	0/1481	0.50	0/1990
56	AT	0.33	0/1300	0.50	1/1743 (0.1%)
57	AU	0.25	0/812	0.48	0/1099
58	AV	0.35	0/1018	0.50	0/1369
59	AW	0.31	0/533	0.42	0/707
60	AX	0.32	0/983	0.44	0/1325
61	AY	0.30	0/1004	0.44	0/1341
62	AZ	0.26	0/1118	0.45	0/1497
63	Aa	0.36	0/1204	0.47	0/1612
64	Ab	0.29	0/473	0.43	0/629
65	Ac	0.27	0/751	0.42	0/1008
66	Ad	0.30	0/904	0.42	0/1213
67	Ae	0.32	0/1041	0.42	0/1394
68	Af	0.30	0/868	0.40	0/1168
69	Ag	0.34	0/890	0.46	0/1189
70	Ah	0.28	0/978	0.45	0/1301
71	Ai	0.28	0/778	0.51	0/1034
72	Aj	0.41	0/696	0.50	0/923
73	Ak	0.27	0/618	0.51	0/826
74	Al	0.36	0/443	0.46	0/588
75	Am	0.28	0/423	0.54	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.30	0/234	0.60	0/300
77	Ao	0.34	0/860	0.45	0/1136
78	Ap	0.35	0/701	0.54	0/934
79	E	0.22	0/1745	0.52	0/2342
80	tP	0.30	0/1796	0.37	0/2799
81	tA	0.28	0/1821	0.38	0/2838
82	MR	0.32	0/291	0.35	0/451
83	eI	0.31	0/1147	0.62	0/1544
All	All	0.34	1/221111 (0.0%)	0.43	13/324737 (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
11	BO	0	1
14	BX	0	1
20	BF	0	1
43	AF	0	1
44	AG	0	2
54	AR	0	1
63	Aa	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O3'-P	5.36	1.61	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Bd	4	GLU	CA-C-N	8.76	137.47	121.70
30	Bd	4	GLU	C-N-CA	8.76	137.47	121.70
21	BK	89	GLY	CA-C-N	6.63	133.63	121.70
21	BK	89	GLY	C-N-CA	6.63	133.63	121.70
6	BH	13	PRO	CA-C-N	5.93	132.38	121.70
6	BH	13	PRO	C-N-CA	5.93	132.38	121.70
38	A1	406	G	O4'-C1'-N9	5.81	116.91	108.20
34	B5	1363	U	P-O3'-C3'	5.78	128.87	120.20
3	BC	81	MET	CA-CB-CG	5.62	125.35	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BZ	55	PRO	CA-C-N	5.40	135.66	125.66
28	BZ	55	PRO	C-N-CA	5.40	135.66	125.66
51	AO	100[A]	GLU	N-CA-CB	5.25	119.23	110.41
56	AT	104	GLU	N-CA-CB	5.22	118.36	110.28

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AF	232	ARG	Peptide
44	AG	121	SER	Peptide
44	AG	30	THR	Peptide
54	AR	131	ALA	Peptide
63	Aa	115	LYS	Peptide
20	BF	99	MET	Peptide
11	BO	123	SER	Peptide
14	BX	88	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1612	0	1623	33	0
2	BB	1709	0	1784	36	0
3	BC	1635	0	1723	24	0
4	BE	2068	0	2154	46	0
5	BG	1820	0	1918	44	0
6	BH	1481	0	1572	34	0
7	BI	1489	0	1525	37	0
8	BJ	1494	0	1573	36	0
9	BL	1244	0	1314	9	0
10	BN	1192	0	1255	16	0
11	BO	941	0	979	15	0
12	BV	684	0	672	10	0
13	BW	1021	0	1060	21	0
14	BX	1121	0	1196	15	0
15	BY	1073	0	1132	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Ba	769	0	818	10	0
17	Bb	610	0	633	8	0
18	Be	475	0	525	9	0
19	BD	1734	0	1817	26	0
20	BF	1609	0	1675	34	0
21	BK	817	0	804	17	0
22	BP	991	0	1035	12	0
23	BQ	1105	0	1166	33	0
24	BR	948	0	990	18	0
25	BS	1192	0	1222	34	0
26	BT	1095	0	1114	25	0
27	BU	855	0	917	19	0
28	BZ	804	0	881	14	0
29	Bc	497	0	535	9	0
30	Bd	442	0	432	12	0
31	Bg	2401	0	2356	61	0
32	Bf	605	0	654	11	0
33	BM	935	0	975	28	0
34	B5	37987	0	19105	418	0
35	AA	1878	0	1946	35	0
36	AB	3081	0	3162	39	0
37	AC	2748	0	2859	36	0
38	A1	68786	0	34573	501	0
39	A3	2579	0	1304	19	0
40	A4	3353	0	1695	20	0
41	AD	2341	0	2290	16	0
42	AE	1303	0	1376	19	0
43	AF	1784	0	1862	18	0
44	AG	1798	0	1894	25	0
45	AH	1510	0	1576	21	0
46	AI	1759	0	1799	23	0
47	AJ	1353	0	1383	30	0
48	AL	1543	0	1608	15	0
49	AM	1053	0	1149	13	0
50	AN	1720	0	1779	25	0
51	AO	1555	0	1659	21	0
52	AP	1388	0	1423	17	0
53	AQ	1441	0	1543	16	0
54	AR	1521	0	1617	26	0
55	AS	1445	0	1487	28	0
56	AT	1276	0	1323	18	0
57	AU	796	0	812	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AV	1003	0	1048	15	0
59	AW	521	0	551	10	0
60	AX	968	0	1036	4	0
61	AY	993	0	1081	9	0
62	AZ	1092	0	1155	13	0
63	Aa	1173	0	1215	23	0
64	Ab	462	0	491	2	0
65	Ac	743	0	797	12	0
66	Ad	890	0	938	11	0
67	Ae	1020	0	1090	6	0
68	Af	850	0	880	8	0
69	Ag	880	0	945	12	0
70	Ah	969	0	1078	14	0
71	Ai	771	0	849	10	0
72	Aj	681	0	687	9	0
73	Ak	612	0	682	10	0
74	Al	436	0	475	5	0
75	Am	417	0	459	5	0
76	An	233	0	283	3	0
77	Ao	847	0	914	8	0
78	Ap	694	0	738	6	0
79	E	1718	0	1811	33	0
80	tP	1606	0	816	12	0
81	tA	1628	0	827	22	0
82	MR	259	0	130	2	0
83	eI	1148	0	1111	20	0
84	A1	139	0	0	0	0
84	A4	1	0	0	0	0
84	AP	1	0	0	0	0
84	AV	1	0	0	0	0
84	B5	39	0	0	0	0
85	A1	12	0	0	0	0
85	Ab	1	0	0	0	0
85	B5	10	0	0	0	0
86	A1	10	0	19	0	0
87	A1	20	0	23	0	0
88	Ao	1	0	0	0	0
All	All	207315	0	153382	2055	0

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

All (2055) 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)
34:B5:898:A:C2	34:B5:914:G:N2	2.11	1.19
34:B5:898:A:H2	34:B5:914:G:N2	1.53	0.99
38:A1:2437:G:H1	38:A1:2510:U:H3	1.13	0.97
38:A1:172:G:H1	38:A1:246:U:H3	1.08	0.96
34:B5:515:A:H62	34:B5:537:G:H21	1.13	0.95
13:BW:2:THR:N	34:B5:1034:C:HO2'	1.70	0.90
57:AU:58:GLU:HG2	57:AU:60:GLY:H	1.43	0.84
22:BP:57:MET:HB3	22:BP:61:ARG:HH12	1.42	0.83
34:B5:1588:G:H1	34:B5:1608:U:H3	0.88	0.83
38:A1:845:G:H21	38:A1:848:A:H2	1.27	0.79
58:AV:81:GLN:O	58:AV:98:ASN:ND2	2.14	0.78
3:BC:80:VAL:HG22	3:BC:102:VAL:HG22	1.66	0.77
26:BT:134:ARG:HH22	34:B5:1360:A:H4'	1.50	0.77
5:BG:2:LYS:HB2	5:BG:108:VAL:HG22	1.66	0.76
31:Bg:20:VAL:HG11	31:Bg:310:ILE:HD11	1.66	0.76
50:AN:183:THR:HG22	50:AN:187:ARG:HB3	1.69	0.75
39:A3:52:G:H21	47:AJ:9:MET:HE3	1.50	0.74
34:B5:1585:U:H3	34:B5:1611:A:H2	1.33	0.74
81:tA:13:C:H42	81:tA:46:G:H22	1.33	0.74
34:B5:868:G:H1	34:B5:960:U:H3	1.35	0.74
34:B5:818:C:H42	34:B5:853:G:H1	1.34	0.74
33:BM:88:LEU:HD21	33:BM:90:LYS:HZ3	1.52	0.74
38:A1:3348:G:H1	38:A1:3357:U:H3	1.36	0.73
6:BH:140:VAL:HB	13:BW:52:TYR:HB3	1.71	0.73
6:BH:150:GLN:HB3	6:BH:181:ILE:HG22	1.71	0.72
38:A1:2200:U:H4'	38:A1:2418:G:H22	1.54	0.72
38:A1:879:U:O2'	52:AP:135:ARG:NH2	2.22	0.72
32:Bf:145:HIS:HD1	34:B5:1234:A:HO2'	1.35	0.72
38:A1:1324:U:OP1	55:AS:1:MET:N	2.23	0.71
8:BJ:120:LYS:HD3	34:B5:479:C:H4'	1.72	0.71
38:A1:284:A:OP2	77:Ao:41:ARG:NH1	2.24	0.71
5:BG:13:GLN:NE2	34:B5:151:G:N3	2.39	0.71
5:BG:202:ARG:NH1	34:B5:127:G:N7	2.39	0.71
47:AJ:109:HIS:HB3	47:AJ:125:MET:HE2	1.71	0.71
12:BV:38:LYS:HD2	12:BV:49:GLU:HB3	1.71	0.71
49:AM:113:THR:HG22	49:AM:116:GLU:HG3	1.73	0.70
1:BA:33:GLN:NE2	1:BA:153:SER:OG	2.24	0.70
34:B5:1339:C:O2'	34:B5:1341:A:N7	2.24	0.70
38:A1:2467:G:H21	38:A1:2488:A:H62	1.39	0.70
34:B5:515:A:H62	34:B5:537:G:N2	1.86	0.70
31:Bg:151:VAL:HA	31:Bg:173:GLY:HA2	1.73	0.70
38:A1:676:G:HO2'	38:A1:678:G:HO2'	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AH:92:TYR:HB2	45:AH:142:ASP:HB3	1.73	0.70
23:BQ:37:THR:O	23:BQ:45:ARG:NH1	2.25	0.69
38:A1:1251:A:N7	38:A1:1263:A:N6	2.38	0.69
52:AP:132:ALA:O	52:AP:135:ARG:NH1	2.25	0.69
5:BG:72:ARG:HH21	34:B5:419:G:H5'	1.56	0.69
4:BE:129:VAL:HG22	4:BE:139:VAL:HG12	1.75	0.69
71:AI:4:LYS:O	71:AI:16:LYS:NZ	2.26	0.69
6:BH:34:LEU:HD22	6:BH:39:ARG:HH22	1.58	0.69
23:BQ:50:GLU:OE1	23:BQ:82:ARG:NH2	2.26	0.69
34:B5:139:C:N4	34:B5:175:G:O2'	2.26	0.69
34:B5:65:A:H2	34:B5:84:A:H62	1.40	0.68
8:BJ:109:LEU:HB2	8:BJ:146:PHE:HB3	1.75	0.68
38:A1:2450:G:N2	38:A1:2451:G:O6	2.24	0.68
50:AN:46:ASP:OD2	50:AN:50:ARG:NH2	2.27	0.68
19:BD:158:ILE:HG12	19:BD:189:MET:HE1	1.76	0.68
22:BP:98:ASN:ND2	22:BP:103:ASN:OD1	2.27	0.68
10:BN:3:ARG:HB3	10:BN:6:SER:HB3	1.76	0.68
26:BT:113:ILE:HG13	26:BT:114:VAL:HG13	1.75	0.68
5:BG:187:LYS:NZ	34:B5:140:A:OP2	2.28	0.67
36:AB:315:GLY:HA2	38:A1:3379:C:H4'	1.75	0.67
37:AC:308:LYS:NZ	38:A1:609:G:N7	2.42	0.67
24:BR:32:LYS:NZ	34:B5:1388:A:OP2	2.27	0.67
31:Bg:172:ALA:HB2	31:Bg:202:LEU:HD23	1.77	0.67
34:B5:992:A:O2'	34:B5:1785:U:O2	2.12	0.67
81:tA:30:G:N1	81:tA:40:C:N3	2.34	0.67
34:B5:648:G:N1	34:B5:686:C:N3	2.32	0.67
1:BA:136:ALA:HB1	1:BA:141:ILE:HB	1.75	0.67
25:BS:16:ARG:NH2	25:BS:19:ASN:OD1	2.23	0.67
34:B5:1003:A:O2'	34:B5:1005:A:N7	2.24	0.66
3:BC:39:THR:HG23	3:BC:42:GLY:H	1.60	0.66
21:BK:54:TYR:HB3	21:BK:72:GLY:HA3	1.76	0.66
38:A1:2462:A:H2	38:A1:2494:A:H61	1.44	0.66
2:BB:117:TRP:HD1	2:BB:153:HIS:HB3	1.61	0.66
52:AP:167:ARG:HB2	68:Af:60:ARG:HD2	1.77	0.66
27:BU:37:VAL:HG12	27:BU:107:THR:HG22	1.77	0.66
34:B5:898:A:N1	34:B5:914:G:N3	2.43	0.66
34:B5:1672:G:H2'	34:B5:1673:G:C8	2.30	0.66
38:A1:1093:A:H2	38:A1:1096:U:H3	1.41	0.66
81:tA:21:A:H61	81:tA:46:G:H2'	1.60	0.66
81:tA:30:G:N2	81:tA:40:C:O2	2.17	0.66
16:Ba:3:LYS:NZ	16:Ba:8:ASN:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BU:101:LYS:HA	27:BU:104:THR:HG22	1.78	0.65
3:BC:88:LYS:HD3	3:BC:95:ARG:HD3	1.77	0.65
13:BW:111:MET:HE1	13:BW:119:LYS:HD2	1.77	0.65
31:Bg:42:LEU:HB2	31:Bg:61:PHE:HB2	1.78	0.65
31:Bg:113:VAL:HG23	31:Bg:124:SER:HB2	1.78	0.65
31:Bg:248:ASN:HD21	31:Bg:249:ARG:HH11	1.42	0.65
38:A1:728:G:H5''	53:AQ:43:PRO:HB2	1.79	0.65
66:Ad:46:THR:HG1	66:Ad:91:SER:HG	1.43	0.65
5:BG:43:ASP:O	5:BG:46:LYS:NZ	2.19	0.65
15:BY:37:LYS:HG3	34:B5:522:U:H5''	1.77	0.65
44:AG:100:GLU:OE2	44:AG:108:ARG:NH1	2.29	0.65
34:B5:648:G:N2	34:B5:686:C:O2	2.17	0.64
1:BA:59:LEU:HB2	12:BV:79:LEU:HD11	1.78	0.64
34:B5:1353:U:O2	34:B5:1355:C:N4	2.31	0.64
47:AJ:49:LYS:HB3	47:AJ:62:ASN:HA	1.77	0.64
23:BQ:72:GLY:O	34:B5:1482:C:O2'	2.16	0.64
40:A4:81:U:H4'	40:A4:82:U:H5'	1.80	0.64
2:BB:111:ARG:HH12	34:B5:930:A:H1'	1.63	0.64
23:BQ:100:GLN:NE2	31:Bg:57:PRO:O	2.31	0.64
38:A1:2779:A:O2'	48:AL:180:ARG:NH2	2.31	0.64
20:BF:58:LEU:HD12	20:BF:138:THR:HG22	1.80	0.64
4:BE:199:GLU:OE2	4:BE:209:HIS:NE2	2.29	0.64
15:BY:104:SER:H	15:BY:107:GLN:HE21	1.46	0.64
33:BM:32:LEU:HB3	33:BM:100:TRP:HH2	1.63	0.64
46:AI:29:SER:OG	46:AI:32:ARG:NH2	2.29	0.64
6:BH:28:GLU:HA	6:BH:34:LEU:HD21	1.80	0.64
27:BU:101:LYS:HB3	27:BU:105:GLN:HE22	1.63	0.64
58:AV:96:GLU:OE2	59:AW:24:GLY:N	2.30	0.64
15:BY:89:TYR:OH	15:BY:90:ARG:NH2	2.31	0.64
15:BY:34:ASN:ND2	34:B5:521:A:N3	2.45	0.63
36:AB:240:ARG:NH2	38:A1:1907:C:O2	2.29	0.63
38:A1:3208:G:O2'	55:AS:161:LYS:NZ	2.31	0.63
20:BF:95:ASN:O	34:B5:1611:A:O2'	2.15	0.63
34:B5:515:A:N6	34:B5:537:G:H21	1.91	0.63
41:AD:50:ARG:NH1	41:AD:147:ASP:OD2	2.32	0.63
38:A1:1348:U:OP1	53:AQ:39:ARG:NH1	2.32	0.63
4:BE:49:ARG:NH2	34:B5:448:C:OP1	2.31	0.63
7:BI:98:LYS:HB3	34:B5:329:G:H5''	1.80	0.63
8:BJ:3:ARG:HH12	8:BJ:6:ARG:HG2	1.61	0.63
34:B5:1354:G:N1	34:B5:1369:U:N3	2.46	0.63
35:AA:215:ASN:ND2	38:A1:2969:A:N7	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1222:G:H2'	38:A1:1286:A:H61	1.64	0.63
13:BW:88:LYS:NZ	34:B5:371:G:O3'	2.32	0.63
38:A1:1010:G:N2	46:AI:193:ASP:OD2	2.32	0.63
44:AG:33:ASN:ND2	44:AG:38:GLN:OE1	2.32	0.63
45:AH:115:ARG:HG2	45:AH:123:ILE:HD12	1.80	0.63
38:A1:2213:A:H2'	38:A1:2214:A:C8	2.34	0.63
4:BE:251:GLU:OE1	4:BE:255:ARG:NH1	2.32	0.63
5:BG:65:GLN:HG3	34:B5:1681:A:H8	1.63	0.63
38:A1:1390:A:N6	38:A1:1418:A:O2'	2.31	0.63
45:AH:90:MET:HE2	45:AH:179:ILE:HG22	1.79	0.63
73:Ak:31:LEU:HA	73:Ak:37:PRO:HA	1.79	0.63
12:BV:79:LEU:HD23	12:BV:82:VAL:HG21	1.80	0.63
47:AJ:52:TYR:HA	47:AJ:61:ARG:HG2	1.80	0.63
79:E:207:LYS:HB3	79:E:213:ALA:HA	1.81	0.63
28:BZ:83:LEU:HD22	28:BZ:88:ILE:HD11	1.81	0.62
31:Bg:23:LEU:HD12	31:Bg:33:LEU:HD11	1.79	0.62
38:A1:1277:C:OP2	38:A1:1279:C:N4	2.32	0.62
31:Bg:111:MET:H	31:Bg:126:SER:HA	1.63	0.62
36:AB:244:ARG:NH1	38:A1:2948:C:OP1	2.32	0.62
38:A1:591:G:O2'	42:AE:17:ALA:O	2.16	0.62
38:A1:2673:A:H5''	47:AJ:95:ASN:HD22	1.64	0.62
51:AO:61[A]:ALA:HA	51:AO:70[A]:PRO:HD2	1.82	0.62
38:A1:2485:A:OP1	79:E:101:LYS:NZ	2.25	0.62
13:BW:81:VAL:O	13:BW:122:SER:OG	2.17	0.62
31:Bg:270:LEU:HD11	31:Bg:273:ASP:HB2	1.81	0.62
34:B5:1356:U:O4	34:B5:1367:G:O6	2.17	0.62
38:A1:1661:G:H2'	38:A1:1662:G:C8	2.34	0.62
14:BX:114:LYS:HD2	34:B5:571:G:H4'	1.80	0.62
34:B5:1171:A:H2'	34:B5:1172:G:C8	2.34	0.62
54:AR:180:LYS:HG2	54:AR:184:LEU:HD23	1.82	0.62
37:AC:35:VAL:HG21	37:AC:244:LEU:HD21	1.82	0.62
38:A1:718:G:OP1	63:Aa:117:ARG:NH2	2.32	0.62
38:A1:3275:U:O2'	68:Af:99:ARG:NH1	2.32	0.62
73:Ak:32:ASN:OD1	73:Ak:36:LYS:N	2.33	0.62
23:BQ:13:LYS:HG3	23:BQ:14:LYS:H	1.65	0.62
34:B5:898:A:N1	34:B5:914:G:C2	2.68	0.62
34:B5:1353:U:O2'	34:B5:1354:G:N7	2.33	0.62
1:BA:36:TYR:OH	1:BA:56:LYS:NZ	2.33	0.61
13:BW:15:ASN:ND2	13:BW:72:CYS:O	2.33	0.61
13:BW:57:ARG:HG2	34:B5:862:A:H4'	1.82	0.61
34:B5:236:A:H5''	34:B5:237:C:H5	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:815:G:N3	54:AR:162:ARG:NH1	2.45	0.61
38:A1:3177:G:O2'	38:A1:3179:U:OP1	2.17	0.61
79:E:61:PRO:HA	79:E:152:ARG:HD3	1.82	0.61
26:BT:69:LYS:NZ	34:B5:1367:G:OP1	2.29	0.61
26:BT:108:LEU:HD22	26:BT:113:ILE:HD11	1.82	0.61
32:Bf:129:GLY:O	33:BM:50:LYS:NZ	2.33	0.61
2:BB:149:GLN:HE21	2:BB:151:LYS:HB3	1.65	0.61
27:BU:44:ASN:HA	27:BU:47:GLN:HG2	1.82	0.61
45:AH:31:ARG:O	45:AH:149:ASN:ND2	2.31	0.61
81:tA:13:C:N4	81:tA:46:G:H22	1.98	0.61
10:BN:34:ILE:HD11	10:BN:67:THR:HG21	1.82	0.61
31:Bg:26:SER:HB2	31:Bg:29:GLN:HB2	1.81	0.61
31:Bg:213:SER:OG	31:Bg:221:MET:SD	2.59	0.61
10:BN:60:VAL:HG23	10:BN:66:ILE:HD12	1.82	0.61
16:Ba:89:ARG:HE	16:Ba:92:ARG:HH21	1.46	0.61
30:Bd:14:TYR:OH	34:B5:1555:A:N6	2.34	0.61
38:A1:2493:U:HO2'	38:A1:2494:A:H8	1.49	0.61
2:BB:175:GLU:OE1	2:BB:187:LYS:NZ	2.30	0.61
38:A1:792:G:H5''	63:Aa:2:PRO:HD3	1.83	0.61
38:A1:2631:U:OP1	38:A1:2757:U:O2'	2.19	0.61
26:BT:31:PRO:HB3	26:BT:103:LYS:HG2	1.81	0.60
18:Be:43:ARG:NH2	34:B5:590:C:OP1	2.31	0.60
34:B5:486:G:N2	34:B5:487:G:O6	2.34	0.60
11:BO:38:THR:HG21	34:B5:895:G:H21	1.64	0.60
34:B5:1356:U:H3	34:B5:1367:G:H1	0.76	0.60
5:BG:18:ILE:HD11	5:BG:23:ARG:HD3	1.82	0.60
26:BT:102:ARG:NH2	34:B5:1502:G:N7	2.50	0.60
38:A1:1389:G:OP1	67:Ae:104:ASN:ND2	2.34	0.60
38:A1:1560:G:H1	38:A1:1579:C:H42	1.48	0.60
1:BA:122:ILE:HA	1:BA:144:ILE:O	2.01	0.60
34:B5:871:G:H2'	34:B5:872:G:C8	2.36	0.60
38:A1:1193:A:OP1	51:AO:49[A]:ARG:NH2	2.33	0.60
38:A1:1364:C:OP1	43:AF:110:ARG:NH2	2.29	0.60
79:E:63:MET:O	79:E:152:ARG:NH1	2.34	0.60
1:BA:113:ARG:HH12	34:B5:1324:G:H4'	1.66	0.60
38:A1:1917:C:OP1	54:AR:85:ARG:NH2	2.34	0.60
61:AY:74:TYR:HE2	61:AY:77:LYS:HE3	1.66	0.60
79:E:205:VAL:HG22	79:E:215:ARG:HD2	1.84	0.60
2:BB:194:ASN:ND2	2:BB:210:ILE:O	2.29	0.60
21:BK:29:GLN:OE1	21:BK:39:ASN:ND2	2.33	0.60
23:BQ:35:PRO:HG2	23:BQ:38:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BU:70:THR:OG1	27:BU:72:ASN:OD1	2.20	0.60
19:BD:74:GLN:NE2	19:BD:79:TYR:O	2.34	0.60
38:A1:3050:U:O2'	59:AW:16:GLY:O	2.18	0.60
37:AC:283:THR:HG21	37:AC:288:ARG:HH21	1.66	0.60
70:Ah:83:LYS:O	72:Aj:73:ARG:NH2	2.33	0.60
34:B5:1291:G:H1	34:B5:1324:G:H22	1.49	0.59
37:AC:20:LEU:HD11	37:AC:252:GLU:HG3	1.84	0.59
45:AH:89:LYS:HG2	45:AH:145:VAL:HG22	1.82	0.59
7:BI:4:SER:OG	7:BI:6:ASP:OD2	2.20	0.59
17:Bb:35:VAL:HG11	17:Bb:63:LEU:HD21	1.83	0.59
38:A1:2138:A:HO2'	72:Aj:2:GLY:N	2.00	0.59
8:BJ:176:ASN:ND2	34:B5:511:A:OP2	2.35	0.59
11:BO:135:ARG:NH1	34:B5:1007:C:O3'	2.36	0.59
38:A1:2960:C:H2'	38:A1:2961:G:C8	2.37	0.59
25:BS:35:ILE:HG23	25:BS:102:ALA:HB2	1.83	0.59
34:B5:898:A:C2	34:B5:914:G:C2	2.89	0.59
18:Be:54:ARG:HH12	18:Be:56:MET:HE3	1.67	0.59
34:B5:773:C:O2'	34:B5:787:G:N2	2.35	0.59
38:A1:577:C:O2'	38:A1:579:G:OP1	2.20	0.59
4:BE:105:VAL:HB	4:BE:243:GLY:HA2	1.85	0.59
34:B5:1225:U:H3'	34:B5:1226:A:H8	1.67	0.59
35:AA:96:LEU:HD23	78:Ap:83:ILE:HG23	1.84	0.59
35:AA:101:VAL:HG22	35:AA:165:VAL:HG22	1.84	0.59
81:tA:13:C:N4	81:tA:46:G:N2	2.50	0.59
7:BI:178:ARG:NH1	34:B5:258:C:O2	2.36	0.59
19:BD:63:GLY:O	19:BD:67:ASN:ND2	2.36	0.59
34:B5:1213:G:H1	34:B5:1450:U:H5	1.51	0.59
35:AA:241:ARG:NH1	38:A1:2155:G:OP1	2.34	0.59
38:A1:1094:U:H4'	38:A1:1095:U:H5'	1.84	0.59
43:AF:151:ARG:HE	43:AF:244:ASN:HB2	1.66	0.59
38:A1:266:A:OP1	50:AN:5:LYS:NZ	2.35	0.59
55:AS:110:MET:HG3	55:AS:116:ALA:HB3	1.83	0.59
15:BY:54:ALA:HB1	15:BY:76:TYR:HB2	1.85	0.58
34:B5:815:G:H5''	54:AR:166:ASN:HD22	1.68	0.58
38:A1:1724:U:H1'	38:A1:1725:C:C6	2.38	0.58
38:A1:1813:A:H4'	38:A1:1817:G:H1'	1.85	0.58
37:AC:156:LEU:HD12	37:AC:159:ILE:HD12	1.85	0.58
6:BH:22:GLN:HA	6:BH:25:VAL:HG12	1.85	0.58
25:BS:38:VAL:HG23	25:BS:42:TYR:HD2	1.68	0.58
34:B5:1686:C:N4	34:B5:1715:G:O6	2.37	0.58
68:Af:14:LEU:HD11	68:Af:31:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:148:ARG:NH1	5:BG:201:GLN:OE1	2.36	0.58
7:BI:16:ALA:HB2	34:B5:354:C:H5''	1.86	0.58
79:E:88:ASP:HA	79:E:91:LYS:HG2	1.85	0.58
5:BG:160:ARG:NH2	34:B5:68:A:OP1	2.37	0.58
38:A1:1799:A:H2'	38:A1:1800:A:C8	2.38	0.58
38:A1:2679:A:O2'	47:AJ:52:TYR:OH	2.19	0.58
38:A1:3016:A:H2'	38:A1:3017:A:C8	2.38	0.58
40:A4:75:G:OP2	61:AY:74:TYR:OH	2.22	0.58
38:A1:2457:G:O2'	38:A1:2482:U:O2	2.20	0.58
38:A1:3192:U:H3	38:A1:3200:G:H1	1.52	0.58
44:AG:162:LEU:HD21	50:AN:45:PRO:HG2	1.86	0.58
51:AO:55[A]:HIS:HD1	51:AO:58[A]:LEU:HD12	1.68	0.58
65:Ac:73:GLY:N	65:Ac:76:GLU:OE1	2.33	0.58
81:tA:34:C:H42	82:MR:6:U:H3	1.50	0.58
14:BX:140:LYS:NZ	34:B5:31:C:OP1	2.37	0.58
38:A1:571:U:H2'	38:A1:572:A:H8	1.69	0.58
38:A1:2437:G:O6	38:A1:2510:U:O4	2.21	0.58
56:AT:49:GLN:HA	56:AT:52:MET:HE3	1.85	0.58
19:BD:93:ASP:HB2	19:BD:96:LEU:HD13	1.84	0.58
33:BM:34:THR:O	33:BM:38:HIS:ND1	2.34	0.58
34:B5:1575:G7M:O2'	34:B5:1576:A:O4'	2.13	0.58
38:A1:315:C:OP2	71:AI:28:TYR:OH	2.22	0.58
44:AG:62:LYS:HD2	50:AN:29:GLU:HG3	1.85	0.58
5:BG:180:THR:HG23	5:BG:183:ARG:H	1.69	0.58
22:BP:110:GLU:HB2	25:BS:119:ILE:HD13	1.86	0.58
32:Bf:138:ARG:NH2	34:B5:1235:C:N3	2.47	0.58
38:A1:1717:U:H2'	38:A1:1718:G:C8	2.39	0.58
79:E:48:ARG:NH1	79:E:160:LYS:O	2.37	0.58
33:BM:42:ALA:HB3	33:BM:122:VAL:HB	1.85	0.58
38:A1:40:A:H5''	63:Aa:35:ALA:HB1	1.85	0.58
38:A1:123:A:OP1	44:AG:105:LYS:NZ	2.37	0.58
54:AR:167:ARG:NH2	54:AR:171:ASP:OD1	2.33	0.58
56:AT:136:ARG:HD2	56:AT:139:ARG:HH22	1.69	0.58
6:BH:44:LYS:HG3	6:BH:63:PRO:HD3	1.86	0.57
23:BQ:113:ASP:HB2	23:BQ:116:LEU:HD23	1.85	0.57
26:BT:77:ASN:HB3	26:BT:95:ASP:HB3	1.86	0.57
38:A1:244:G:H3'	38:A1:245:U:H5''	1.85	0.57
38:A1:1493:G:O6	74:AI:2:ALA:N	2.36	0.57
50:AN:159:ARG:HB2	50:AN:164:LEU:HB2	1.84	0.57
54:AR:136:ARG:O	54:AR:140:GLU:HG3	2.04	0.57
55:AS:77:VAL:HG13	55:AS:126:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:116:ARG:NH1	34:B5:858:G:OP1	2.36	0.57
23:BQ:69:VAL:HG11	23:BQ:81:ILE:HD11	1.86	0.57
38:A1:576:C:OP1	43:AF:241:LYS:NZ	2.37	0.57
83:eI:49:THR:HG22	83:eI:56:LYS:HD3	1.85	0.57
34:B5:58:U:O2'	34:B5:451:A:N3	2.36	0.57
38:A1:567:G:H2'	38:A1:568:G:C8	2.39	0.57
48:AL:9:ILE:HD12	63:Aa:34:MET:HE1	1.86	0.57
34:B5:579:A:N6	34:B5:1438:G:O2'	2.37	0.57
34:B5:953:G:H2'	34:B5:954:G:H8	1.70	0.57
38:A1:1110:PSU:H2'	38:A1:1111:U:C6	2.39	0.57
54:AR:170:ARG:HH21	54:AR:173:ARG:HH21	1.51	0.57
7:BI:104:ILE:HG13	7:BI:105:ASP:H	1.69	0.57
8:BJ:132:ARG:NH2	34:B5:532:U:OP1	2.37	0.57
15:BY:29:HIS:HB2	15:BY:32:ARG:HB3	1.85	0.57
26:BT:57:ARG:NE	34:B5:1479:A:OP1	2.36	0.57
36:AB:71:GLU:OE1	59:AW:1:MET:N	2.38	0.57
36:AB:93:VAL:HG12	36:AB:155:ALA:H	1.69	0.57
58:AV:10:LYS:HB2	58:AV:125:LEU:HD11	1.87	0.57
34:B5:1237:G:H2'	34:B5:1238:A:H8	1.70	0.57
6:BH:14:THR:OG1	6:BH:15:GLU:OE1	2.23	0.57
8:BJ:8:TYR:O	34:B5:25:C:N4	2.38	0.57
51:AO:65[A]:ASN:HB3	51:AO:68[A]:ARG:HG2	1.85	0.57
52:AP:122:ALA:HB3	52:AP:143:PRO:HB2	1.85	0.57
4:BE:108:ARG:NH2	34:B5:788:A:OP2	2.37	0.57
34:B5:1434:U:O2'	34:B5:1436:A:OP1	2.20	0.57
38:A1:664:U:H2'	38:A1:665:A:C8	2.40	0.57
38:A1:3182:G:H4'	51:AO:161[A]:LYS:HG2	1.85	0.57
46:AI:30:LYS:HG3	46:AI:63:GLU:HG3	1.85	0.57
19:BD:55:THR:HA	19:BD:58:VAL:HG12	1.87	0.57
33:BM:68:GLU:HG3	33:BM:70:ASN:H	1.69	0.57
34:B5:895:G:H1	34:B5:917:U:H3	1.53	0.57
38:A1:1657:C:O2'	38:A1:1797:A:OP2	2.20	0.57
79:E:67:ILE:HB	79:E:84:ALA:HA	1.87	0.57
10:BN:5:HIS:HB3	10:BN:117:LEU:HD23	1.87	0.57
1:BA:13:ASP:OD2	1:BA:179:ARG:NH2	2.33	0.56
14:BX:6:PRO:HG3	14:BX:14:LYS:HG2	1.87	0.56
31:Bg:8:VAL:O	31:Bg:10:ARG:NH1	2.38	0.56
31:Bg:274:LEU:HD23	31:Bg:313:TRP:HZ3	1.70	0.56
34:B5:973:A:H4'	38:A1:848:A:H8	1.69	0.56
38:A1:1805:C:H2'	38:A1:1806:A:H8	1.70	0.56
83:eI:90:TYR:HB3	83:eI:102:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BM:42:ALA:N	33:BM:122:VAL:O	2.36	0.56
34:B5:894:U:H2'	34:B5:895:G:C8	2.41	0.56
38:A1:1831:U:O2'	40:A4:114:G:OP1	2.18	0.56
38:A1:2794:G:OP1	77:Ao:61:LYS:NZ	2.37	0.56
7:BI:10:LYS:NZ	34:B5:322:G:O2'	2.38	0.56
23:BQ:100:GLN:HE21	31:Bg:56:VAL:HG22	1.70	0.56
38:A1:533:A:O2'	38:A1:535:G:OP2	2.24	0.56
38:A1:1211:U:O2'	55:AS:113:ARG:NH1	2.38	0.56
38:A1:1504:A:H5''	52:AP:125:GLN:HE22	1.70	0.56
38:A1:2767:U:O2'	77:Ao:30:ALA:O	2.23	0.56
42:AE:43:LEU:HD11	42:AE:85:ILE:HG13	1.87	0.56
79:E:54:LYS:HA	79:E:154:THR:HG22	1.87	0.56
38:A1:1214:U:OP2	55:AS:137:ARG:NH2	2.39	0.56
38:A1:2768:U:H2'	38:A1:2769:A:H8	1.69	0.56
38:A1:2966:G:H2'	38:A1:2967:A:C8	2.40	0.56
73:Ak:27:ILE:HG23	73:Ak:39:ARG:HD2	1.86	0.56
6:BH:104:ARG:NH1	34:B5:803:A:N3	2.52	0.56
28:BZ:95:HIS:ND1	28:BZ:96:SER:O	2.38	0.56
34:B5:1355:C:N4	34:B5:1369:U:O4	2.39	0.56
36:AB:250:ALA:HB3	38:A1:2880:PSU:H1'	1.87	0.56
38:A1:2573:G:OP2	62:AZ:58:GLY:N	2.33	0.56
44:AG:148:ALA:HA	44:AG:201:THR:HG22	1.86	0.56
3:BC:145:GLY:O	13:BW:98:GLN:NE2	2.35	0.56
7:BI:101:ILE:HD12	7:BI:184:LEU:HD11	1.87	0.56
38:A1:2895:G:O2'	75:Am:100:TYR:O	2.23	0.56
55:AS:125:LYS:HE3	55:AS:127:ALA:HB2	1.87	0.56
1:BA:107:PHE:HB3	1:BA:139:VAL:HG11	1.88	0.56
24:BR:3:ARG:NH2	34:B5:1414:U:OP2	2.37	0.56
27:BU:101:LYS:O	27:BU:105:GLN:NE2	2.39	0.56
47:AJ:23:VAL:HG13	47:AJ:29:ARG:HH11	1.71	0.56
81:tA:53:G:H2'	81:tA:54:A:C8	2.41	0.56
7:BI:178:ARG:NH1	34:B5:207:U:O2	2.39	0.56
8:BJ:21:SER:HA	8:BJ:24:LEU:HB2	1.87	0.56
36:AB:30:LYS:NZ	38:A1:3139:A:OP2	2.25	0.56
37:AC:170:LYS:HG2	37:AC:175:HIS:CD2	2.41	0.56
38:A1:1737:U:O2	69:Ag:52:GLN:NE2	2.39	0.56
38:A1:2838:A:N6	38:A1:2850:G:O2'	2.38	0.56
5:BG:136:LYS:NZ	34:B5:65:A:O5'	2.35	0.56
14:BX:51:GLY:HA2	14:BX:77:ILE:HG13	1.88	0.56
34:B5:52:U:H2'	34:B5:53:G:C8	2.41	0.56
41:AD:211:LEU:HG	41:AD:219:PHE:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ad:55:LEU:HB2	66:Ad:95:PRO:HD3	1.88	0.56
74:Al:25:GLN:OE1	74:Al:28:ARG:NH1	2.39	0.56
4:BE:3:ARG:HG2	34:B5:399:A:H4'	1.87	0.56
5:BG:72:ARG:NH2	34:B5:418:G:O2'	2.36	0.56
25:BS:25:ASN:O	25:BS:57:ARG:NH2	2.31	0.56
36:AB:28:ARG:NH2	38:A1:3140:G:N7	2.46	0.56
37:AC:271:LYS:NZ	38:A1:695:C:OP1	2.39	0.56
38:A1:170:G:H5''	70:Ah:109:ILE:HD12	1.87	0.56
40:A4:150:G:OP1	60:AX:27:ARG:NH2	2.38	0.56
63:Aa:24:LYS:O	63:Aa:26:ARG:HG2	2.06	0.56
1:BA:27:ARG:NH1	1:BA:43:ASP:O	2.39	0.55
35:AA:152:SER:OG	38:A1:2157:G:N7	2.36	0.55
45:AH:8:GLN:HB3	45:AH:72:LYS:HD2	1.87	0.55
57:AU:53:ALA:O	57:AU:68:THR:N	2.37	0.55
83:eI:130:GLU:OE2	83:eI:132:LYS:NZ	2.39	0.55
27:BU:36:ASN:OD1	27:BU:37:VAL:N	2.39	0.55
34:B5:1588:G:O6	34:B5:1608:U:O4	2.24	0.55
35:AA:80:GLU:HG3	78:Ap:66:GLY:HA2	1.88	0.55
38:A1:627:U:H2'	38:A1:628:A:C8	2.41	0.55
38:A1:775:A:O2'	38:A1:777:U:OP2	2.23	0.55
45:AH:151:VAL:O	45:AH:155:SER:OG	2.20	0.55
54:AR:23:TRP:HB3	54:AR:51:VAL:HG22	1.88	0.55
62:AZ:50:PRO:HD3	62:AZ:68:ILE:HG12	1.87	0.55
11:BO:80:HIS:HA	11:BO:113:GLY:O	2.06	0.55
35:AA:109:GLU:HG2	35:AA:138:GLY:HA2	1.88	0.55
38:A1:2836:C:H5	38:A1:2852:C:H42	1.54	0.55
2:BB:61:LEU:HG	2:BB:96:LEU:HD21	1.88	0.55
19:BD:204:ASP:OD2	34:B5:1330:G:N2	2.34	0.55
34:B5:1727:G:H2'	34:B5:1728:A:C8	2.42	0.55
42:AE:13:GLU:HA	67:Ae:4:LEU:HD11	1.89	0.55
4:BE:38:LEU:HD23	34:B5:298:C:H5''	1.89	0.55
17:Bb:67:THR:OG1	17:Bb:70:LYS:O	2.24	0.55
38:A1:1108:U:H2'	38:A1:1109:U:C6	2.41	0.55
38:A1:2697:A:H2'	38:A1:2698:G:C8	2.42	0.55
3:BC:81:MET:HG3	3:BC:211:LEU:HD11	1.87	0.55
31:Bg:10:ARG:NH2	31:Bg:314:GLN:OE1	2.39	0.55
38:A1:1667:A:H2'	38:A1:1668:G:C8	2.42	0.55
38:A1:3225:C:H2'	38:A1:3226:A:H8	1.72	0.55
48:AL:106:GLN:HB3	71:Ai:18:THR:HB	1.87	0.55
79:E:188:ASN:HA	79:E:191:VAL:HG22	1.87	0.55
23:BQ:90:VAL:HG21	23:BQ:117:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Bf:108:VAL:HG23	33:BM:74:LEU:HD23	1.86	0.55
34:B5:924:A:H2'	34:B5:925:G:C8	2.42	0.55
38:A1:2805:G:OP1	83:eI:54:HIS:NE2	2.39	0.55
38:A1:3252:G:H2'	38:A1:3253:G:H8	1.72	0.55
50:AN:147:ARG:HG3	70:Ah:101:THR:HG21	1.89	0.55
83:eI:32:VAL:HG11	83:eI:59:LEU:HD21	1.89	0.55
11:BO:72:LYS:NZ	11:BO:108:SER:O	2.40	0.55
17:Bb:56:CYS:SG	17:Bb:57:GLU:N	2.78	0.55
31:Bg:88:THR:HG22	31:Bg:104:VAL:HG12	1.88	0.55
34:B5:1125:A:O2'	34:B5:1776:A:OP1	2.14	0.55
8:BJ:106:GLU:HG2	8:BJ:111:THR:HG21	1.89	0.55
38:A1:68:C:OP2	38:A1:301:G:N2	2.40	0.55
38:A1:3261:C:OP1	49:AM:126:GLN:NE2	2.40	0.55
39:A3:112:G:H2'	39:A3:113:C:C6	2.42	0.55
79:E:96:ASN:HB2	79:E:99:LEU:HG	1.89	0.55
8:BJ:171:ARG:NH2	34:B5:513:U:O4	2.39	0.55
9:BL:125:VAL:HG12	9:BL:139:VAL:HA	1.89	0.55
22:BP:52:LYS:HG3	22:BP:53:PRO:HD3	1.88	0.55
34:B5:538:A:H5'	34:B5:543:C:H41	1.71	0.55
37:AC:347:THR:O	38:A1:520:U:N3	2.38	0.55
1:BA:120:LEU:HD11	1:BA:144:ILE:HG13	1.89	0.54
16:Ba:8:ASN:HB3	34:B5:1791:A:H3'	1.89	0.54
52:AP:116:HIS:HB3	52:AP:149:VAL:HB	1.88	0.54
25:BS:112:ASP:OD1	25:BS:115:ARG:NH2	2.34	0.54
26:BT:72:GLY:HA3	34:B5:1498:G:H5''	1.88	0.54
38:A1:401:U:H5''	38:A1:402:A:H5''	1.88	0.54
14:BX:70:LYS:NZ	34:B5:567:A:OP1	2.40	0.54
21:BK:77:ARG:NH2	21:BK:83:PRO:O	2.41	0.54
28:BZ:55:PRO:O	28:BZ:56:THR:HG22	2.07	0.54
34:B5:205:U:H2'	34:B5:206:A:H8	1.72	0.54
34:B5:1227:A:H5'	34:B5:1229:G:H5'	1.88	0.54
37:AC:317:PRO:C	37:AC:319:LYS:H	2.14	0.54
38:A1:2356:A:H61	38:A1:2983:C:H5	1.53	0.54
3:BC:78:ASP:HB3	3:BC:104:VAL:HG12	1.89	0.54
38:A1:1323:G:H4'	55:AS:2:ALA:HB2	1.89	0.54
34:B5:828:U:O2'	34:B5:829:A:O5'	2.26	0.54
37:AC:98:ARG:NH2	38:A1:804:C:OP1	2.39	0.54
38:A1:3322:A:H2'	38:A1:3323:A:C8	2.42	0.54
48:AL:124:ILE:HD11	70:Ah:119:LYS:HG3	1.89	0.54
15:BY:78:SER:OG	15:BY:81:GLU:OE1	2.19	0.54
33:BM:59:LEU:HD13	33:BM:137:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:82:ARG:NH2	2:BB:188:LEU:O	2.32	0.54
15:BY:128:LYS:NZ	34:B5:154:G:N7	2.55	0.54
26:BT:77:ASN:OD1	26:BT:101:ASN:ND2	2.40	0.54
27:BU:26:LEU:HB3	27:BU:34:LEU:HD11	1.89	0.54
34:B5:647:G:H21	34:B5:687:G:H1	1.54	0.54
55:AS:22:PRO:O	56:AT:146:ASN:ND2	2.36	0.54
80:tP:16:U:H3	83:eI:89:GLU:HG2	1.72	0.54
32:Bf:141:CYS:O	34:B5:1252:C:O2'	2.26	0.54
38:A1:3210:A:OP1	49:AM:109:ARG:NH1	2.35	0.54
44:AG:183:LYS:HB2	44:AG:194:THR:HG23	1.90	0.54
49:AM:48:GLY:HA3	49:AM:53:VAL:HB	1.89	0.54
61:AY:74:TYR:CD2	61:AY:77:LYS:HG2	2.43	0.54
70:Ah:5:LYS:HB2	70:Ah:8:GLU:OE1	2.08	0.54
26:BT:86:ARG:NH1	34:B5:1601:G:OP1	2.41	0.54
27:BU:74:GLU:OE1	34:B5:1428:G:N2	2.41	0.54
31:Bg:205:SER:HA	31:Bg:245:PHE:HD2	1.73	0.54
33:BM:93:ASP:HB3	33:BM:96:GLN:HB2	1.89	0.54
35:AA:47:GLN:HB2	35:AA:60:LYS:HB2	1.90	0.54
43:AF:31:ALA:HA	43:AF:34:LYS:HG2	1.90	0.54
53:AQ:122:ILE:HG23	53:AQ:126:GLN:HB2	1.90	0.54
27:BU:62:VAL:HA	27:BU:84:MET:O	2.09	0.53
38:A1:2464:U:H2'	38:A1:2465:G:C8	2.42	0.53
47:AJ:109:HIS:CD2	47:AJ:112:LEU:HD13	2.43	0.53
7:BI:119:GLN:HG3	7:BI:150:ALA:HB1	1.90	0.53
38:A1:1696:A:H2'	38:A1:1697:A:C8	2.43	0.53
67:Ae:96:ILE:HG21	67:Ae:105:ARG:HG2	1.90	0.53
15:BY:58:PHE:HB2	15:BY:72:PHE:HB3	1.91	0.53
38:A1:364:G:OP2	72:Aj:52:LYS:NZ	2.36	0.53
38:A1:2899:C:O2'	38:A1:2901:G:OP2	2.24	0.53
40:A4:58:G:O6	72:Aj:63:ARG:NH1	2.41	0.53
5:BG:220:LYS:HG2	5:BG:223:LYS:HE3	1.91	0.53
38:A1:1786:G:H2'	38:A1:1787:A:C8	2.44	0.53
38:A1:3092:C:O2'	38:A1:3094:A:OP2	2.19	0.53
40:A4:9:A:H2'	40:A4:10:A:C8	2.44	0.53
75:Am:79:GLU:OE1	75:Am:82:LEU:HD23	2.09	0.53
4:BE:100:ARG:HB2	4:BE:114:ILE:HD13	1.90	0.53
6:BH:64:VAL:HB	6:BH:94:ALA:HB1	1.90	0.53
27:BU:20:ILE:HD11	27:BU:97:VAL:HG12	1.90	0.53
31:Bg:131:ILE:HB	31:Bg:144:LEU:HB2	1.90	0.53
4:BE:123:LEU:HD12	4:BE:159:THR:HG22	1.90	0.53
23:BQ:41:PRO:HB2	23:BQ:43:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BT:44:GLU:O	26:BT:45:MET:HE2	2.08	0.53
28:BZ:60:VAL:HB	28:BZ:101:TYR:HB2	1.90	0.53
38:A1:307:A:H2'	38:A1:308:A:C8	2.44	0.53
72:Aj:25:ARG:HD2	74:Al:51:ILE:HB	1.89	0.53
81:tA:10:A:H61	81:tA:25:C:H42	1.55	0.53
34:B5:1202:A:N6	34:B5:1457:C:OP1	2.40	0.53
34:B5:1628:U:H2'	34:B5:1629:G:C8	2.43	0.53
38:A1:1873:U:OP1	54:AR:21:LYS:NZ	2.40	0.53
7:BI:11:ARG:NH1	7:BI:15:GLY:O	2.42	0.53
7:BI:84:HIS:NE2	7:BI:97:THR:OG1	2.40	0.53
23:BQ:42:GLU:HB2	23:BQ:45:ARG:HE	1.73	0.53
24:BR:41:ILE:HD13	24:BR:47:ARG:HG3	1.91	0.53
34:B5:615:A:O2'	34:B5:621:A:N1	2.37	0.53
37:AC:112:LYS:HE2	50:AN:202:TYR:HB3	1.90	0.53
27:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.91	0.53
34:B5:12:U:H2'	34:B5:13:C:C6	2.44	0.53
34:B5:1158:C:H5	34:B5:1163:A:H61	1.56	0.53
38:A1:716:A:C6	63:Aa:117:ARG:HG3	2.44	0.53
73:Ak:59:ALA:HA	73:Ak:62:ALA:HB3	1.91	0.53
5:BG:177:ARG:NH1	34:B5:143:G:N7	2.51	0.53
23:BQ:87:LYS:HG2	23:BQ:117:LEU:HD13	1.91	0.53
46:AI:208:ASN:HA	46:AI:211:ARG:HG2	1.91	0.53
35:AA:52:SER:HB3	35:AA:191:LEU:HD12	1.91	0.52
38:A1:2507:C:H2'	38:A1:2508:U:C6	2.43	0.52
50:AN:18:VAL:HG13	50:AN:19:LEU:HD12	1.91	0.52
19:BD:170:THR:HG22	19:BD:187:LYS:HG3	1.90	0.52
34:B5:520:A:H2'	34:B5:521:A:C8	2.45	0.52
35:AA:9:ARG:NH2	38:A1:912:G:OP2	2.41	0.52
38:A1:19:U:H2'	38:A1:20:A:C8	2.44	0.52
58:AV:23:MET:HE3	58:AV:100:GLY:HA3	1.91	0.52
59:AW:46:PRO:HB2	59:AW:54:LEU:HD12	1.90	0.52
65:Ac:16:LEU:HB3	65:Ac:98:SER:HB2	1.90	0.52
2:BB:146:GLN:HG3	2:BB:206:PRO:HG3	1.90	0.52
34:B5:187:G:H21	34:B5:198:A:H62	1.57	0.52
61:AY:74:TYR:HD2	61:AY:77:LYS:HG2	1.74	0.52
20:BF:80:LYS:HB2	20:BF:83:ARG:HB2	1.92	0.52
20:BF:189:THR:HB	20:BF:192:GLU:HG3	1.91	0.52
38:A1:1221:A:H3'	38:A1:1222:G:H4'	1.90	0.52
38:A1:1404:G:N2	38:A1:1407:A:OP2	2.37	0.52
54:AR:105:LEU:HD23	54:AR:138:LEU:HD23	1.91	0.52
8:BJ:129:ILE:HG13	8:BJ:134:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2481:G:N7	38:A1:2482:U:N3	2.58	0.52
32:Bf:106:TYR:HE2	33:BM:49:THR:HB	1.75	0.52
38:A1:1678:G:O6	57:AU:74:LYS:NZ	2.43	0.52
38:A1:2108:C:H1'	38:A1:3344:A:C8	2.44	0.52
38:A1:2284:C:N4	38:A1:2308:C:OP2	2.42	0.52
4:BE:87:MET:HE1	4:BE:236:ILE:HG12	1.92	0.52
38:A1:1223:A:OP1	38:A1:1285:G:N2	2.43	0.52
38:A1:2465:G:H1'	79:E:166:ALA:HB3	1.91	0.52
54:AR:134:HIS:CD2	54:AR:136:ARG:HG2	2.45	0.52
4:BE:77:ARG:NH2	34:B5:122:U:O3'	2.43	0.52
4:BE:166:SER:OG	4:BE:168:LYS:NZ	2.42	0.52
5:BG:164:LYS:NZ	34:B5:71:A:OP2	2.42	0.52
38:A1:316:U:O2'	71:Ai:30:LYS:NZ	2.40	0.52
38:A1:1093:A:OP1	56:AT:120:LYS:NZ	2.43	0.52
38:A1:3343:G:H21	38:A1:3362:A:H2	1.58	0.52
54:AR:105:LEU:HD13	54:AR:135:LYS:HE3	1.92	0.52
55:AS:81:TYR:HE1	55:AS:90:MET:HE3	1.75	0.52
81:tA:22:G:O6	81:tA:46:G:N1	2.41	0.52
2:BB:88:VAL:HG21	2:BB:96:LEU:HD23	1.90	0.52
23:BQ:13:LYS:HG2	23:BQ:76:SER:HA	1.92	0.52
25:BS:87:ASN:OD1	34:B5:1546:G:N2	2.43	0.52
38:A1:2383:C:OP2	51:AO:85[A]:ARG:NH2	2.42	0.52
38:A1:3016:A:H2'	38:A1:3017:A:H8	1.74	0.52
42:AE:146:ILE:HG22	42:AE:150:LYS:HE2	1.90	0.52
46:AI:93:PRO:HB2	46:AI:125:LEU:HB3	1.91	0.52
58:AV:18:PRO:HA	58:AV:51:ALA:HA	1.91	0.52
2:BB:127:VAL:HG11	2:BB:173:THR:HG22	1.92	0.52
7:BI:41:LYS:NZ	34:B5:260:U:OP2	2.29	0.52
8:BJ:78:ARG:NH2	34:B5:764:U:OP1	2.35	0.52
19:BD:135:GLU:HB3	19:BD:187:LYS:HB3	1.91	0.52
19:BD:191:ASP:HB3	19:BD:194:LYS:HD2	1.92	0.52
20:BF:22:PRO:HB3	20:BF:34:GLN:HG2	1.92	0.52
20:BF:185:ARG:HH12	34:B5:1572:G:H21	1.57	0.52
31:Bg:295:SER:OG	31:Bg:300:THR:OG1	2.20	0.52
34:B5:16:G:H2'	34:B5:17:C:C6	2.45	0.52
34:B5:490:C:N4	34:B5:492:A:O2'	2.42	0.52
35:AA:117:GLU:HG2	35:AA:124:GLY:H	1.73	0.52
38:A1:2160:G:H2'	38:A1:2161:G:H8	1.74	0.52
65:Ac:14:LEU:O	65:Ac:18:ILE:HG12	2.09	0.52
5:BG:137:ARG:HB3	5:BG:140:ASN:HB2	1.92	0.51
12:BV:32:VAL:HG22	12:BV:60:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BQ:43:ILE:HG23	23:BQ:44:LEU:HD12	1.93	0.51
31:Bg:89:LEU:HB2	31:Bg:103:PHE:HB2	1.92	0.51
34:B5:1125:A:OP1	76:An:18:ARG:NH2	2.43	0.51
35:AA:68:LYS:HE3	38:A1:1579:C:H5''	1.91	0.51
38:A1:649:A:OP2	38:A1:2868:U:O2'	2.29	0.51
38:A1:900:G:H1'	38:A1:1589:A:N6	2.25	0.51
38:A1:1940:G:H21	38:A1:3362:A:H8	1.56	0.51
45:AH:31:ARG:NH1	45:AH:83:THR:O	2.43	0.51
52:AP:60:PHE:HB3	52:AP:64:ASN:HB3	1.90	0.51
65:Ac:55:GLU:HB3	69:Ag:94:LEU:HD11	1.92	0.51
30:Bd:22:ARG:NH1	30:Bd:36:LEU:O	2.43	0.51
35:AA:68:LYS:HD3	35:AA:70:ARG:HH11	1.76	0.51
38:A1:3295:A:H2'	38:A1:3296:A:C8	2.45	0.51
45:AH:90:MET:HG2	45:AH:181:VAL:HA	1.93	0.51
79:E:91:LYS:HA	79:E:123:LEU:HD11	1.91	0.51
31:Bg:131:ILE:HD11	31:Bg:151:VAL:HG21	1.92	0.51
33:BM:27:ALA:HB3	33:BM:136:ILE:HD11	1.92	0.51
33:BM:62:LEU:HB3	33:BM:88:LEU:HD11	1.91	0.51
36:AB:316:GLU:HG3	36:AB:318:LYS:HE3	1.92	0.51
47:AJ:18:VAL:HG22	47:AJ:70:THR:HG22	1.92	0.51
58:AV:87:ARG:HH22	58:AV:137:VAL:HG21	1.76	0.51
6:BH:147:ASN:OD1	6:BH:148:LYS:N	2.43	0.51
31:Bg:220:ILE:HD13	31:Bg:243:LEU:HD21	1.93	0.51
34:B5:751:G:H2'	34:B5:752:A:C8	2.46	0.51
34:B5:972:G:O2'	38:A1:847:A:N6	2.44	0.51
34:B5:1533:C:H4'	34:B5:1539:G:C6	2.46	0.51
3:BC:188:LEU:HD13	3:BC:196:VAL:HG11	1.92	0.51
4:BE:87:MET:HE2	4:BE:123:LEU:HB2	1.92	0.51
34:B5:434:G:O2'	34:B5:436:A:N7	2.39	0.51
34:B5:1198:G:OP1	34:B5:1199:G:O2'	2.20	0.51
34:B5:1355:C:C2	34:B5:1368:G:N2	2.78	0.51
38:A1:1019:G:N2	38:A1:1035:G:N7	2.47	0.51
38:A1:1534:A:H2'	38:A1:1535:A:C8	2.45	0.51
53:AQ:92:ARG:HG3	63:Aa:76:ASP:HB2	1.92	0.51
8:BJ:172:VAL:O	8:BJ:176:ASN:ND2	2.44	0.51
16:Ba:82:ARG:HB2	16:Ba:85:ARG:HH21	1.75	0.51
20:BF:99:MET:HB3	20:BF:100:ASN:HA	1.92	0.51
31:Bg:201:THR:OG1	31:Bg:241:PHE:O	2.24	0.51
34:B5:108:A:H2'	34:B5:109:G:C8	2.45	0.51
38:A1:1609:C:OP1	60:AX:125:ARG:NH1	2.41	0.51
38:A1:1798:A:H2'	38:A1:1799:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A3:39:C:H4'	47:AJ:44:THR:HG23	1.92	0.51
40:A4:57:C:H4'	40:A4:63:G:N7	2.25	0.51
43:AF:156:ILE:HD12	43:AF:161:VAL:HB	1.92	0.51
4:BE:7:LYS:HD2	34:B5:94:U:H1'	1.92	0.51
6:BH:14:THR:HG23	6:BH:16:LEU:H	1.75	0.51
7:BI:81:VAL:HG22	7:BI:102:VAL:HG12	1.91	0.51
35:AA:69:TYR:OH	38:A1:2557:A:OP1	2.26	0.51
38:A1:528:U:H2'	38:A1:529:A:C8	2.45	0.51
38:A1:792:G:H2'	38:A1:793:C:C6	2.46	0.51
38:A1:3231:U:H2'	38:A1:3232:G:H8	1.76	0.51
10:BN:114:ARG:NH2	34:B5:939:A:OP1	2.43	0.51
19:BD:27:ARG:NH2	34:B5:1436:A:OP2	2.34	0.51
25:BS:36:LYS:HB2	25:BS:102:ALA:HA	1.93	0.51
34:B5:218:A:N1	34:B5:843:U:C4	2.78	0.51
38:A1:443:G:H2'	38:A1:491:A:H61	1.74	0.51
38:A1:675:C:O2'	38:A1:679:U:OP1	2.25	0.51
70:Ah:27:GLU:OE2	70:Ah:43:LYS:NZ	2.41	0.51
4:BE:68:ARG:HD2	4:BE:76:VAL:HG11	1.92	0.51
7:BI:152:ILE:HG13	7:BI:153:GLU:H	1.76	0.51
10:BN:142:GLU:OE2	10:BN:145:THR:OG1	2.19	0.51
14:BX:128:SER:OG	14:BX:142:LYS:NZ	2.44	0.51
34:B5:591:A:H2'	34:B5:592:A:C8	2.45	0.51
34:B5:1477:G:H2'	34:B5:1478:G:H8	1.74	0.51
34:B5:1592:A:H2'	34:B5:1593:A:C8	2.46	0.51
38:A1:412:G:OP1	52:AP:62:ARG:NH1	2.43	0.51
38:A1:2376:G:H2'	38:A1:2377:G:C8	2.46	0.51
81:tA:43:G:H2'	81:tA:44:A:C8	2.46	0.51
6:BH:155:ASP:OD1	6:BH:155:ASP:N	2.44	0.51
38:A1:2457:G:H2'	38:A1:2458:A:H8	1.76	0.51
38:A1:2664:C:OP2	47:AJ:142:LYS:NZ	2.42	0.51
38:A1:2768:U:H2'	38:A1:2769:A:C8	2.46	0.51
43:AF:186:HIS:HA	43:AF:189:ILE:HG22	1.92	0.51
8:BJ:139:GLN:NE2	15:BY:64:PHE:O	2.44	0.50
34:B5:130:C:H1'	34:B5:136:C:H41	1.76	0.50
38:A1:655:C:H2'	38:A1:656:A:C8	2.45	0.50
47:AJ:77:GLU:OE2	47:AJ:167:TYR:OH	2.24	0.50
69:Ag:98:GLN:HA	69:Ag:101:VAL:HG12	1.93	0.50
4:BE:246:LEU:HD22	4:BE:254:ARG:HH21	1.76	0.50
18:Be:29:LYS:O	18:Be:31:LYS:NZ	2.45	0.50
33:BM:41:LEU:HD21	33:BM:121:VAL:HG13	1.93	0.50
34:B5:273:G:N7	34:B5:284:G:N2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:303:GLY:H	38:A1:1347:U:H5''	1.76	0.50
38:A1:417:A:H2'	38:A1:418:A:C8	2.47	0.50
38:A1:1003:A:N1	38:A1:1049:C:O2'	2.42	0.50
38:A1:1129:A:H2'	38:A1:1130:A:C8	2.46	0.50
38:A1:1863:G:N1	38:A1:1866:C:OP2	2.36	0.50
31:Bg:238:ASP:HB2	31:Bg:257:ALA:HB3	1.94	0.50
34:B5:1524:A:H2'	34:B5:1525:A:C8	2.46	0.50
38:A1:394:G:N1	38:A1:397:A:OP2	2.42	0.50
38:A1:2810:C:OP2	38:A1:2955:U:O2'	2.29	0.50
51:AO:75[A]:ALA:HB3	51:AO:78[A]:ARG:HG2	1.93	0.50
1:BA:76:ILE:HD13	1:BA:98:ILE:HB	1.93	0.50
4:BE:108:ARG:NH1	34:B5:789:A:OP1	2.43	0.50
10:BN:26:PHE:CZ	10:BN:28:LEU:HB2	2.47	0.50
34:B5:71:A:N6	34:B5:81:G:O6	2.45	0.50
34:B5:197:A:H2'	34:B5:198:A:H8	1.76	0.50
38:A1:651:G:O2'	38:A1:1435:A:OP1	2.29	0.50
34:B5:953:G:H2'	34:B5:954:G:C8	2.46	0.50
34:B5:1575:G7M:H2'	34:B5:1576:A:C8	2.46	0.50
38:A1:1351:U:H2'	38:A1:1352:A:N9	2.26	0.50
75:Am:78:ILE:HB	75:Am:83:LYS:HE2	1.94	0.50
16:Ba:44:ILE:HG23	16:Ba:45:VAL:HG13	1.93	0.50
32:Bf:128:ALA:H	33:BM:54:ARG:HH12	1.58	0.50
38:A1:1751:G:H5'	73:Ak:26:LYS:HE2	1.93	0.50
38:A1:2152:A:H2'	38:A1:2153:U:H6	1.77	0.50
38:A1:3175:U:OP1	68:Af:10:LYS:NZ	2.42	0.50
38:A1:3271:G:C2	42:AE:108:LYS:HG3	2.46	0.50
15:BY:78:SER:N	15:BY:81:GLU:OE2	2.37	0.50
20:BF:72:HIS:NE2	34:B5:1610:G:OP1	2.42	0.50
34:B5:1380:U:O2'	34:B5:1516:A:N1	2.44	0.50
34:B5:1591:C:H2'	34:B5:1592:A:C8	2.47	0.50
38:A1:1779:C:N4	38:A1:2102:U:OP1	2.44	0.50
38:A1:2116:G:OP1	38:A1:2118:C:N4	2.45	0.50
83:eI:21:MET:SD	83:eI:22:GLN:N	2.85	0.50
5:BG:181:PRO:HA	5:BG:184:LEU:HD12	1.93	0.50
31:Bg:250:TYR:HE2	31:Bg:265:LEU:HB3	1.76	0.50
34:B5:107:C:H2'	34:B5:108:A:H8	1.75	0.50
34:B5:1387:G:H21	34:B5:1410:A:H61	1.60	0.50
38:A1:1719:G:N7	54:AR:121:HIS:HE1	2.10	0.50
38:A1:2683:U:H2'	38:A1:2684:C:C6	2.47	0.50
44:AG:186:LEU:HB3	44:AG:195:SER:HB3	1.93	0.50
46:AI:192:ASP:HA	46:AI:197:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:246:LEU:HD23	4:BE:250:GLU:HG2	1.93	0.50
23:BQ:14:LYS:NZ	34:B5:1610:G:N7	2.59	0.50
24:BR:60:ARG:HD2	34:B5:1400:A:H5'	1.94	0.50
29:BC:41:VAL:HG12	29:BC:63:ALA:HB3	1.94	0.50
34:B5:751:G:H2'	34:B5:752:A:H8	1.77	0.50
37:AC:332:LYS:NZ	38:A1:599:C:OP1	2.32	0.50
38:A1:1119:C:H2'	38:A1:1120:A:H8	1.77	0.50
50:AN:36:ILE:HD11	50:AN:105:ARG:HB3	1.93	0.50
53:AQ:123:THR:OG1	53:AQ:125:ASP:OD1	2.29	0.50
57:AU:33:TYR:OH	57:AU:80:THR:OG1	2.22	0.50
3:BC:116:LYS:HG2	3:BC:127:ALA:HB3	1.94	0.49
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.94	0.49
6:BH:138:LYS:HD3	6:BH:150:GLN:HE21	1.75	0.49
31:Bg:273:ASP:OD1	31:Bg:275:ARG:NH2	2.45	0.49
38:A1:494:G:O2'	38:A1:495:G:OP2	2.28	0.49
38:A1:1560:G:H2'	38:A1:1561:G:C8	2.46	0.49
38:A1:1596:C:H2'	38:A1:1597:C:C6	2.47	0.49
38:A1:2268:U:H3	38:A1:2272:G:H22	1.59	0.49
44:AG:178:ALA:HB2	44:AG:218:ILE:HD12	1.93	0.49
70:Ah:2:ALA:HB3	70:Ah:46:THR:HG21	1.93	0.49
3:BC:90:THR:OG1	3:BC:93:GLY:O	2.28	0.49
5:BG:175:ILE:HD11	5:BG:178:LEU:HD22	1.94	0.49
21:BK:24:LYS:O	21:BK:39:ASN:ND2	2.45	0.49
22:BP:32:ASP:HA	22:BP:35:LYS:HZ3	1.77	0.49
36:AB:194:TRP:O	36:AB:198:HIS:ND1	2.41	0.49
38:A1:129:U:H2'	38:A1:130:A:C8	2.47	0.49
38:A1:2467:G:N2	38:A1:2488:A:H62	2.07	0.49
9:BL:2:SER:OG	9:BL:3:THR:N	2.45	0.49
16:Ba:2:PRO:HB3	34:B5:1142:A:H5''	1.94	0.49
34:B5:197:A:H2'	34:B5:198:A:C8	2.47	0.49
34:B5:980:G:H4'	34:B5:1776:A:H4'	1.92	0.49
38:A1:152:U:OP1	70:Ah:106:LYS:NZ	2.35	0.49
38:A1:1621:A:H2'	38:A1:1622:U:C6	2.48	0.49
52:AP:113:TYR:HB3	52:AP:153:LYS:HE3	1.94	0.49
55:AS:81:TYR:CE1	55:AS:90:MET:HE3	2.47	0.49
2:BB:85:LYS:HE2	2:BB:101:HIS:HD2	1.77	0.49
34:B5:733:A:OP2	34:B5:735:C:N4	2.45	0.49
38:A1:2160:G:H2'	38:A1:2161:G:C8	2.47	0.49
38:A1:3070:A:OP1	54:AR:62:ARG:NH1	2.44	0.49
44:AG:74:THR:HG22	44:AG:164:VAL:HG22	1.95	0.49
45:AH:101:VAL:HG22	45:AH:114:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AZ:41:ALA:HB2	62:AZ:77:TYR:HE1	1.77	0.49
5:BG:66:GLY:HA2	34:B5:1681:A:H1'	1.93	0.49
9:BL:123:VAL:HG12	9:BL:142:VAL:HG22	1.95	0.49
30:Bd:30:LEU:O	34:B5:1199:G:N2	2.40	0.49
30:Bd:47:ALA:HB1	30:Bd:52:PHE:HB2	1.95	0.49
34:B5:52:U:H2'	34:B5:53:G:H8	1.77	0.49
34:B5:1114:G:O2'	34:B5:1130:G:O6	2.24	0.49
38:A1:2228:A:H2'	38:A1:2229:A:C8	2.48	0.49
40:A4:26:U:H2'	40:A4:27:U:C6	2.48	0.49
2:BB:81:PHE:CD2	2:BB:82:ARG:HG3	2.47	0.49
12:BV:33:GLN:HE21	12:BV:52:THR:HG21	1.77	0.49
34:B5:126:A:H8	34:B5:204:G:H21	1.60	0.49
38:A1:2369:G:H2'	38:A1:2370:G:C8	2.48	0.49
46:AI:49:CYS:HB3	46:AI:168:SER:HB3	1.95	0.49
50:AN:5:LYS:O	50:AN:8:GLU:HB3	2.12	0.49
69:Ag:76:TYR:HB3	69:Ag:80:ARG:HB2	1.94	0.49
79:E:31:THR:O	79:E:209:SER:N	2.46	0.49
79:E:31:THR:H	79:E:209:SER:HB2	1.78	0.49
6:BH:64:VAL:HG23	6:BH:67:LEU:HD23	1.95	0.49
10:BN:64:ARG:HD2	10:BN:70:LYS:HE2	1.94	0.49
34:B5:1041:G:H2'	34:B5:1042:G:C8	2.48	0.49
34:B5:1202:A:H1'	34:B5:1207:C:N4	2.26	0.49
36:AB:124:LYS:NZ	38:A1:3297:U:O4	2.45	0.49
38:A1:2433:U:H1'	50:AN:125:SER:HB3	1.94	0.49
46:AI:36:LEU:HD21	46:AI:69:ARG:HD3	1.95	0.49
58:AV:86:ARG:HB2	58:AV:92:PHE:CE2	2.47	0.49
79:E:65:ILE:HG22	79:E:109:ALA:HB3	1.95	0.49
25:BS:134:ARG:NH2	34:B5:1546:G:N7	2.60	0.49
26:BT:102:ARG:NH1	34:B5:1502:G:O6	2.38	0.49
26:BT:105:LEU:HD22	26:BT:122:ARG:HG2	1.94	0.49
27:BU:62:VAL:HG12	27:BU:85:ARG:HG3	1.95	0.49
34:B5:472:U:H2'	34:B5:473:A:C8	2.48	0.49
38:A1:411:U:H2'	38:A1:412:G:H8	1.77	0.49
38:A1:1283:C:O2'	38:A1:1284:C:H5''	2.12	0.49
38:A1:2407:C:H2'	38:A1:2408:U:C6	2.48	0.49
38:A1:2674:A:H5''	47:AJ:105:GLY:HA3	1.94	0.49
48:AL:115:ARG:NH2	48:AL:145:PHE:O	2.43	0.49
68:Af:49:ILE:HD11	68:Af:71:VAL:HG22	1.95	0.49
81:tA:60:A:H5'	81:tA:61:C:H5	1.78	0.49
4:BE:198:LYS:HG3	4:BE:208:VAL:HG22	1.94	0.49
19:BD:141:LYS:NZ	34:B5:1275:A:N3	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1229:G:H1'	34:B5:1230:A:H5'	1.95	0.49
34:B5:1776:A:H2'	34:B5:1777:G:C8	2.48	0.49
36:AB:316:GLU:N	36:AB:316:GLU:OE1	2.46	0.49
38:A1:612:U:OP1	42:AE:21:THR:OG1	2.22	0.49
65:Ac:10:ILE:HD12	65:Ac:13:LYS:HD3	1.95	0.49
70:Ah:56:THR:O	70:Ah:60:GLU:HG3	2.13	0.49
73:Ak:26:LYS:HD2	73:Ak:78:LEU:HD13	1.95	0.49
77:Ao:72:LEU:O	77:Ao:80:ARG:HA	2.13	0.49
2:BB:35:PRO:HG3	2:BB:99:ASN:HA	1.95	0.49
2:BB:104:ASP:N	2:BB:104:ASP:OD1	2.46	0.49
6:BH:104:ARG:NH2	34:B5:805:U:O4	2.43	0.49
34:B5:898:A:H8	34:B5:899:G:H1'	1.78	0.49
34:B5:1591:C:H2'	34:B5:1592:A:H8	1.78	0.49
34:B5:1641:C:H2'	34:B5:1642:G:C8	2.48	0.49
36:AB:261:MET:HB2	36:AB:264:VAL:HG23	1.95	0.49
37:AC:7:THR:OG1	37:AC:147:GLU:OE2	2.26	0.49
38:A1:1947:G:OP1	54:AR:136:ARG:NH1	2.45	0.49
43:AF:147:LEU:HD11	43:AF:207:LEU:HD21	1.94	0.49
45:AH:48:VAL:HB	45:AH:52:LEU:HB2	1.94	0.49
48:AL:163:GLY:HA2	63:Aa:139:ARG:NH2	2.28	0.49
80:tP:10:A:H61	80:tP:25:C:H42	1.61	0.49
1:BA:111:ILE:HD11	34:B5:1292:G:H21	1.78	0.48
2:BB:82:ARG:HG2	2:BB:105:PHE:CE1	2.48	0.48
4:BE:23:LEU:HD22	8:BJ:3:ARG:NH2	2.28	0.48
7:BI:56:ARG:HH22	34:B5:332:U:P	2.35	0.48
25:BS:91:ASP:OD1	25:BS:91:ASP:N	2.45	0.48
34:B5:1502:G:N2	34:B5:1505:A:OP2	2.39	0.48
45:AH:86:TYR:CE2	45:AH:151:VAL:HB	2.48	0.48
53:AQ:22:ASP:HA	53:AQ:27:LYS:HE2	1.95	0.48
66:Ad:96:VAL:HG12	66:Ad:98:VAL:HG13	1.95	0.48
81:tA:23:C:H2'	81:tA:24:G:H8	1.78	0.48
2:BB:176:VAL:O	2:BB:177:GLN:HG3	2.13	0.48
4:BE:246:LEU:HD22	4:BE:254:ARG:NH2	2.29	0.48
6:BH:9:LEU:HD13	6:BH:21:ALA:HB2	1.93	0.48
8:BJ:119:ALA:O	8:BJ:124:HIS:ND1	2.37	0.48
18:Be:42:ARG:NH2	34:B5:590:C:OP2	2.46	0.48
21:BK:83:PRO:HB2	21:BK:86:ILE:HD12	1.94	0.48
23:BQ:101:SER:O	23:BQ:105:LEU:HG	2.13	0.48
34:B5:147:A:OP2	34:B5:166:C:N4	2.45	0.48
34:B5:1218:G:N2	34:B5:1444:A:OP2	2.40	0.48
35:AA:149:ARG:NH1	35:AA:150:LEU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AA:181:LYS:HB2	38:A1:860:G:C5	2.48	0.48
42:AE:64:LEU:HD11	42:AE:76:LEU:HD12	1.95	0.48
51:AO:121[A]:PRO:HA	51:AO:124[A]:LEU:HD12	1.95	0.48
1:BA:107:PHE:N	1:BA:135:GLU:OE2	2.37	0.48
1:BA:175:TYR:HE1	1:BA:195:TRP:HD1	1.61	0.48
7:BI:114:GLU:HA	7:BI:118:GLY:HA2	1.96	0.48
20:BF:42:LEU:N	20:BF:46:TRP:O	2.46	0.48
21:BK:20:VAL:HG12	21:BK:67:THR:HG23	1.95	0.48
31:Bg:243:LEU:HA	31:Bg:253:ALA:O	2.13	0.48
34:B5:142:G:N2	34:B5:142:G:OP2	2.46	0.48
34:B5:828:U:O2'	34:B5:829:A:O4'	2.31	0.48
38:A1:655:C:H2'	38:A1:656:A:H8	1.77	0.48
38:A1:945:C:H2'	38:A1:946:U:C6	2.48	0.48
38:A1:3056:U:O2	66:Ad:28:ARG:NH2	2.46	0.48
73:Ak:32:ASN:ND2	73:Ak:36:LYS:O	2.46	0.48
83:eI:108:ASP:N	83:eI:108:ASP:OD1	2.46	0.48
14:BX:53:VAL:HA	14:BX:74:VAL:HG22	1.93	0.48
27:BU:50:LEU:HD21	27:BU:93:LEU:HD11	1.95	0.48
31:Bg:243:LEU:HD22	31:Bg:252:LEU:HD11	1.94	0.48
32:Bf:128:ALA:H	33:BM:54:ARG:NH1	2.11	0.48
33:BM:31:VAL:HG22	33:BM:133:LEU:HD13	1.96	0.48
33:BM:60:VAL:HA	33:BM:122:VAL:HG22	1.95	0.48
34:B5:412:A:H2'	34:B5:413:U:O2	2.13	0.48
34:B5:472:U:H2'	34:B5:473:A:H8	1.77	0.48
34:B5:819:G:N7	34:B5:853:G:N2	2.61	0.48
34:B5:891:A:H2'	34:B5:892:A:H8	1.79	0.48
34:B5:1226:A:O2'	34:B5:1229:G:N3	2.45	0.48
43:AF:138:TYR:CD2	43:AF:233:GLU:HB2	2.48	0.48
44:AG:143:ILE:HG23	44:AG:175:VAL:HG21	1.95	0.48
54:AR:180:LYS:HA	54:AR:184:LEU:HB3	1.95	0.48
80:tP:26:G:O6	80:tP:44:A:N1	2.46	0.48
83:eI:43:ASP:HB3	83:eI:60:VAL:HB	1.95	0.48
2:BB:116:LYS:HG3	34:B5:931:C:H5''	1.94	0.48
2:BB:149:GLN:HE22	2:BB:154:SER:HB3	1.78	0.48
8:BJ:37:LYS:NZ	34:B5:594:A:OP2	2.47	0.48
20:BF:63:GLN:HB3	20:BF:88:PRO:HA	1.95	0.48
34:B5:1346:A:H62	34:B5:1369:U:H3'	1.79	0.48
34:B5:1413:U:O2'	34:B5:1416:G:OP1	2.31	0.48
34:B5:1474:G:H2'	34:B5:1475:A:H8	1.79	0.48
55:AS:93:GLU:HG3	55:AS:140:VAL:HG21	1.96	0.48
1:BA:92:HIS:ND1	1:BA:202:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:212:LYS:NZ	34:B5:1298:U:O3'	2.45	0.48
5:BG:102:VAL:HG13	5:BG:106:LEU:HD12	1.96	0.48
7:BI:138:ASN:HA	7:BI:141:ARG:NH1	2.29	0.48
10:BN:11:ILE:HD12	17:Bb:21:LEU:HD23	1.94	0.48
12:BV:30:ALA:O	12:BV:60:ARG:NH1	2.39	0.48
34:B5:546:U:H2'	34:B5:547:U:C6	2.48	0.48
34:B5:872:G:H2'	34:B5:873:U:O4'	2.13	0.48
34:B5:1525:A:H2'	34:B5:1526:A:C8	2.48	0.48
38:A1:662:U:H2'	38:A1:663:C:C6	2.49	0.48
44:AG:154:ALA:HB2	44:AG:186:LEU:HD12	1.95	0.48
8:BJ:18:PRO:O	8:BJ:23:ARG:NH2	2.47	0.48
14:BX:46:SER:OG	14:BX:48:HIS:O	2.30	0.48
20:BF:82:PHE:HB2	29:Bc:49:ARG:NH2	2.29	0.48
26:BT:127:ASN:OD1	26:BT:128:GLY:N	2.46	0.48
30:Bd:32:ARG:NH1	34:B5:1597:A:OP2	2.33	0.48
34:B5:74:U:H1'	34:B5:76:A:H5''	1.95	0.48
34:B5:381:C:O2'	34:B5:755:A:N1	2.44	0.48
38:A1:3268:A:OP1	42:AE:46:ARG:NH2	2.41	0.48
55:AS:90:MET:HE1	55:AS:114:HIS:CE1	2.48	0.48
80:tP:53:G:H2'	80:tP:54:A:H8	1.79	0.48
7:BI:110:ARG:NH2	7:BI:160:PHE:O	2.46	0.48
19:BD:141:LYS:HG3	19:BD:179:GLN:HG3	1.96	0.48
20:BF:72:HIS:CD2	20:BF:107:LYS:HD2	2.49	0.48
34:B5:15:U:H2'	34:B5:16:G:O4'	2.13	0.48
34:B5:1474:G:H2'	34:B5:1475:A:C8	2.48	0.48
36:AB:284:ARG:NH1	36:AB:293:ASN:O	2.46	0.48
38:A1:700:C:OP1	48:AL:65:TYR:OH	2.26	0.48
38:A1:1575:A:N6	38:A1:1576:G:O6	2.47	0.48
38:A1:1951:C:H2'	38:A1:1952:G:C8	2.48	0.48
41:AD:182:GLY:HA2	41:AD:194:LEU:HD23	1.95	0.48
44:AG:75:ILE:HD11	50:AN:18:VAL:HG23	1.95	0.48
47:AJ:81:GLU:OE2	47:AJ:89:TYR:OH	2.31	0.48
49:AM:23:ILE:O	49:AM:30:GLY:N	2.47	0.48
63:Aa:90:TYR:CG	63:Aa:100:PRO:HG3	2.49	0.48
65:Ac:81:VAL:HG11	65:Ac:90:VAL:HG21	1.95	0.48
12:BV:74:GLN:NE2	12:BV:80:LYS:O	2.32	0.48
19:BD:29:LEU:HB3	19:BD:32:GLU:HB2	1.95	0.48
38:A1:538:G:H2'	38:A1:539:C:H5'	1.96	0.48
38:A1:2806:U:OP1	83:eI:49:THR:OG1	2.21	0.48
4:BE:121:TYR:CG	4:BE:161:LYS:HE3	2.49	0.48
36:AB:220:VAL:O	36:AB:334:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1784:G:OP1	69:Ag:19:LYS:NZ	2.38	0.48
38:A1:2152:A:H2'	38:A1:2153:U:C6	2.48	0.48
38:A1:2544:U:H2'	38:A1:2545:C:C6	2.49	0.48
63:Aa:112:ILE:HB	63:Aa:130:VAL:HG23	1.96	0.48
1:BA:55:GLU:HG3	12:BV:79:LEU:HG	1.96	0.47
13:BW:114:GLU:OE1	13:BW:117:ARG:NH2	2.47	0.47
34:B5:511:A:H2'	34:B5:512:A:H8	1.79	0.47
34:B5:629:U:OP2	34:B5:969:C:N4	2.39	0.47
38:A1:1176:C:H2'	38:A1:1177:G:N2	2.29	0.47
38:A1:1475:A:H4'	66:Ad:57:GLN:HG2	1.96	0.47
42:AE:66:SER:HB2	42:AE:76:LEU:HD13	1.95	0.47
7:BI:76:THR:HB	7:BI:108:PRO:HG2	1.96	0.47
8:BJ:133:HIS:HE2	34:B5:513:U:H5'	1.79	0.47
16:Ba:84:VAL:O	34:B5:1797:A:N6	2.47	0.47
33:BM:97:LEU:HA	33:BM:100:TRP:HE1	1.78	0.47
34:B5:1297:G:N2	34:B5:1300:A:OP2	2.34	0.47
35:AA:140:ASN:OD1	35:AA:147:ARG:NH1	2.47	0.47
38:A1:99:A:H5'	50:AN:194:GLN:HG2	1.96	0.47
38:A1:2864:A:H5''	46:AI:114:GLY:HA2	1.96	0.47
19:BD:141:LYS:HD2	19:BD:179:GLN:HB2	1.96	0.47
34:B5:163:G:OP2	34:B5:163:G:N2	2.40	0.47
34:B5:219:A:H2'	34:B5:220:A:C8	2.49	0.47
34:B5:968:U:H2'	34:B5:969:C:O4'	2.13	0.47
37:AC:4:PRO:HG2	37:AC:22:LEU:HD22	1.95	0.47
38:A1:525:C:OP2	49:AM:77:ARG:NH2	2.47	0.47
39:A3:89:G:H4'	55:AS:84:ARG:HD3	1.95	0.47
11:BO:42:VAL:HA	11:BO:46:MET:HE2	1.96	0.47
23:BQ:49:TYR:HB3	23:BQ:53:LEU:HD13	1.97	0.47
25:BS:46:VAL:HG11	25:BS:73:MET:HG3	1.97	0.47
38:A1:1829:G:H5''	38:A1:1830:G:H5'	1.96	0.47
38:A1:3348:G:O6	38:A1:3357:U:O4	2.32	0.47
56:AT:48:ILE:HD13	56:AT:94:GLU:HG2	1.97	0.47
8:BJ:83:VAL:HA	8:BJ:149:ARG:HA	1.97	0.47
15:BY:3:ASP:OD2	15:BY:32:ARG:NH1	2.41	0.47
34:B5:1524:A:N3	34:B5:1590:G:O2'	2.37	0.47
35:AA:28:LYS:HB2	35:AA:123:ARG:HB3	1.97	0.47
35:AA:127:ALA:HB2	35:AA:134:VAL:HG23	1.96	0.47
36:AB:85:VAL:HG22	36:AB:202:THR:HG22	1.96	0.47
38:A1:178:U:H2'	38:A1:179:C:C6	2.49	0.47
38:A1:595:G:OP1	43:AF:33:ARG:NH2	2.36	0.47
38:A1:1228:C:N4	38:A1:1282:G:O6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:AF:221:LYS:HB2	43:AF:227:GLY:HA3	1.97	0.47
47:AJ:95:ASN:HB3	47:AJ:103:GLY:O	2.15	0.47
63:Aa:132:LYS:HG2	63:Aa:136:GLU:OE1	2.14	0.47
79:E:143:ASP:OD1	79:E:143:ASP:N	2.48	0.47
81:tA:23:C:H2'	81:tA:24:G:C8	2.49	0.47
23:BQ:95:LYS:O	31:Bg:59:ARG:NH1	2.46	0.47
28:BZ:80:LEU:HD21	28:BZ:101:TYR:CE1	2.50	0.47
34:B5:140:A:H4'	34:B5:141:U:H5'	1.97	0.47
34:B5:182:A:H2'	34:B5:183:U:H6	1.80	0.47
38:A1:266:A:H2'	71:Ai:30:LYS:HE3	1.95	0.47
38:A1:3225:C:H2'	38:A1:3226:A:C8	2.48	0.47
40:A4:65:A:O2'	70:Ah:10:ARG:NH2	2.48	0.47
47:AJ:133:ARG:NH2	47:AJ:153:LYS:O	2.41	0.47
2:BB:181:LEU:HD12	2:BB:184:LEU:HD23	1.97	0.47
11:BO:61:MET:HG3	11:BO:104:ALA:HB2	1.97	0.47
14:BX:107:PHE:HE2	14:BX:120:VAL:HG12	1.80	0.47
19:BD:72:LEU:HG	21:BK:20:VAL:HG21	1.97	0.47
25:BS:16:ARG:CZ	47:AJ:111:ASP:HB3	2.44	0.47
31:Bg:191:ASP:OD1	31:Bg:191:ASP:N	2.44	0.47
34:B5:648:G:O6	34:B5:686:C:N4	2.37	0.47
34:B5:1175:U:H2'	34:B5:1176:G:C8	2.49	0.47
34:B5:1261:G:H2'	34:B5:1262:U:C6	2.50	0.47
34:B5:1669:U:H3	34:B5:1732:A:H62	1.62	0.47
34:B5:1689:A:N6	34:B5:1707:A:N1	2.63	0.47
38:A1:943:U:H3'	63:Aa:13:GLY:HA2	1.97	0.47
38:A1:2464:U:H2'	38:A1:2465:G:H8	1.79	0.47
38:A1:3291:G:H2'	38:A1:3292:A:C8	2.50	0.47
50:AN:65:ARG:HD2	50:AN:127:TYR:CG	2.50	0.47
51:AO:119[A]:VAL:HG23	55:AS:164:SER:HB3	1.96	0.47
58:AV:108:GLU:HG3	58:AV:128:ARG:HG3	1.96	0.47
65:Ac:13:LYS:O	65:Ac:17:VAL:HG23	2.14	0.47
73:Ak:14:LEU:HD21	73:Ak:52:TYR:CG	2.49	0.47
79:E:55:LEU:HD23	79:E:59:PRO:HD3	1.96	0.47
79:E:145:TYR:HA	79:E:148:VAL:HG22	1.97	0.47
80:tP:53:G:H2'	80:tP:54:A:C8	2.49	0.47
25:BS:14:ILE:HD11	47:AJ:117:ASP:HA	1.96	0.47
25:BS:39:GLY:H	34:B5:1566:U:H5''	1.80	0.47
34:B5:1351:G:H2'	34:B5:1352:G:H8	1.79	0.47
38:A1:29:C:H4'	38:A1:62:A:H4'	1.97	0.47
38:A1:1694:U:H5	38:A1:1752:A:N1	2.13	0.47
38:A1:2427:U:H2'	38:A1:2428:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3013:U:H2'	38:A1:3014:U:C6	2.50	0.47
39:A3:36:C:H2'	39:A3:37:G:C8	2.50	0.47
40:A4:142:C:H2'	40:A4:143:U:C6	2.49	0.47
44:AG:107:GLU:O	44:AG:111:LYS:HG2	2.15	0.47
81:tA:67:G:H2'	81:tA:68:G:C8	2.50	0.47
26:BT:66:TYR:HD2	26:BT:67:MET:HE2	1.79	0.47
34:B5:156:A:H2'	34:B5:157:A:O4'	2.14	0.47
34:B5:1477:G:H2'	34:B5:1478:G:C8	2.50	0.47
34:B5:1609:U:H2'	34:B5:1610:G:O4'	2.14	0.47
38:A1:8:C:H2'	38:A1:9:U:C6	2.50	0.47
38:A1:785:G:N2	53:AQ:89:ASP:O	2.36	0.47
38:A1:1119:C:H2'	38:A1:1120:A:C8	2.50	0.47
39:A3:118:A:H5''	41:AD:253:PHE:HZ	1.80	0.47
41:AD:60:ILE:HB	41:AD:80:SER:HB2	1.97	0.47
42:AE:166:LYS:O	68:Af:6:ARG:NH2	2.48	0.47
65:Ac:17:VAL:HG11	65:Ac:92:ILE:HD12	1.97	0.47
3:BC:95:ARG:HH22	3:BC:97:ARG:HD3	1.80	0.47
4:BE:180:LEU:N	4:BE:229:GLY:O	2.48	0.47
7:BI:5:ARG:NH1	34:B5:336:G:O6	2.43	0.47
11:BO:43:THR:OG1	34:B5:900:A:OP1	2.26	0.47
37:AC:304:GLN:HE22	38:A1:594:U:H3	1.63	0.47
38:A1:526:C:H2'	38:A1:527:A:H8	1.80	0.47
38:A1:631:U:H2'	38:A1:632:G:C8	2.49	0.47
38:A1:1243:G:H22	38:A1:1269:U:H3	1.63	0.47
51:AO:166[A]:GLU:OE2	51:AO:170[A]:LYS:NZ	2.47	0.47
53:AQ:125:ASP:OD1	53:AQ:126:GLN:N	2.47	0.47
6:BH:15:GLU:HA	6:BH:18:LEU:HB2	1.97	0.46
26:BT:68:ARG:NE	34:B5:1521:G:O6	2.47	0.46
34:B5:1336:A:H2'	34:B5:1337:A:O4'	2.15	0.46
34:B5:1484:G:H21	34:B5:1606:C:H1'	1.80	0.46
35:AA:107:VAL:O	35:AA:139:HIS:NE2	2.41	0.46
38:A1:110:G:OP2	48:AL:73:ARG:NH2	2.38	0.46
38:A1:758:C:OP1	77:Ao:15:LYS:NZ	2.48	0.46
38:A1:1239:C:H5	38:A1:1244:A:H2'	1.80	0.46
38:A1:1578:C:H2'	38:A1:1579:C:C6	2.50	0.46
38:A1:1622:U:H2'	38:A1:1623:G:H8	1.79	0.46
38:A1:1791:C:H2'	38:A1:1792:C:C6	2.50	0.46
38:A1:2357:A:H2'	38:A1:2358:A:C8	2.50	0.46
41:AD:83:LEU:HD13	41:AD:88:ILE:HD12	1.96	0.46
54:AR:23:TRP:HB2	54:AR:53:LYS:HD2	1.96	0.46
72:Aj:47:TYR:O	72:Aj:54:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:6:SER:HB2	34:B5:1514:U:H1'	1.97	0.46
25:BS:42:TYR:HA	25:BS:85:PHE:HE2	1.80	0.46
38:A1:1616:U:H2'	38:A1:1617:G:C8	2.50	0.46
41:AD:68:THR:OG1	41:AD:71:GLY:O	2.30	0.46
47:AJ:37:LEU:HD12	47:AJ:67:VAL:HG22	1.97	0.46
2:BB:204:ILE:O	34:B5:1064:G:O2'	2.29	0.46
6:BH:30:SER:O	6:BH:34:LEU:N	2.47	0.46
7:BI:191:PHE:O	7:BI:195:ARG:HG2	2.15	0.46
10:BN:99:ARG:NH2	10:BN:119:GLU:OE2	2.49	0.46
25:BS:140:THR:HA	25:BS:143:ARG:HH21	1.80	0.46
34:B5:413:U:H5	34:B5:420:A:N1	2.14	0.46
34:B5:973:A:H4'	38:A1:848:A:C8	2.50	0.46
34:B5:1260:U:H2'	34:B5:1261:G:C8	2.49	0.46
34:B5:1374:C:H2'	34:B5:1375:A:H8	1.80	0.46
38:A1:235:A:H2'	38:A1:236:G:C8	2.51	0.46
38:A1:411:U:H2'	38:A1:412:G:C8	2.50	0.46
38:A1:422:A:C2	38:A1:2363:A:H4'	2.51	0.46
41:AD:65:ILE:HG12	41:AD:74:VAL:HG22	1.97	0.46
44:AG:78:PHE:O	44:AG:79:GLN:HG3	2.16	0.46
53:AQ:170:ARG:HD2	63:Aa:57:GLY:HA3	1.97	0.46
4:BE:176:ASP:HB3	4:BE:179:LYS:HE2	1.98	0.46
5:BG:49:VAL:HB	5:BG:115:LYS:HB3	1.98	0.46
20:BF:82:PHE:HB2	29:Bc:49:ARG:HH21	1.79	0.46
23:BQ:101:SER:HA	23:BQ:104:GLU:HG3	1.98	0.46
25:BS:127:HIS:CD2	25:BS:133:VAL:HG11	2.50	0.46
29:Bc:8:THR:HB	29:Bc:56:LEU:HB2	1.96	0.46
38:A1:2767:U:H2'	38:A1:2768:U:C6	2.50	0.46
54:AR:109:TYR:HB3	54:AR:115:ILE:HG12	1.97	0.46
55:AS:13:ARG:NH2	55:AS:50:LYS:O	2.49	0.46
62:AZ:26:VAL:HG11	62:AZ:96:VAL:HB	1.97	0.46
79:E:32:VAL:HA	79:E:208:SER:HA	1.96	0.46
79:E:33:GLU:HB3	79:E:207:LYS:HE3	1.96	0.46
83:eI:122:ASP:O	83:eI:126:THR:HG23	2.15	0.46
8:BJ:112:GLN:HG3	8:BJ:148:VAL:HG21	1.97	0.46
25:BS:66:LEU:O	25:BS:69:ILE:HG22	2.16	0.46
28:BZ:77:ARG:NH1	34:B5:1533:C:OP2	2.41	0.46
38:A1:176:G:C2	38:A1:177:U:H1'	2.51	0.46
38:A1:2406:C:H2'	38:A1:2407:C:C6	2.51	0.46
56:AT:151:LEU:HG	56:AT:152:ALA:H	1.80	0.46
15:BY:93:ARG:NH2	34:B5:526:A:OP2	2.37	0.46
20:BF:120:ILE:HA	20:BF:123:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BK:23:ALA:O	21:BK:64:TYR:HB2	2.14	0.46
34:B5:1689:A:H2'	34:B5:1690:G:C8	2.51	0.46
38:A1:3119:U:H4'	75:Am:104:PRO:HG3	1.96	0.46
43:AF:102:VAL:HG13	43:AF:126:LEU:HD22	1.98	0.46
4:BE:103:TYR:O	4:BE:182:TYR:OH	2.34	0.46
4:BE:131:LEU:HD12	34:B5:251:A:H2	1.81	0.46
14:BX:19:ARG:O	14:BX:23:ARG:HB2	2.16	0.46
31:Bg:245:PHE:HE1	31:Bg:252:LEU:HD22	1.81	0.46
34:B5:182:A:H2'	34:B5:183:U:C6	2.51	0.46
38:A1:156:G:OP2	71:Ai:27:SER:OG	2.24	0.46
38:A1:3084:C:OP1	59:AW:38:SER:OG	2.32	0.46
48:AL:119:TYR:O	48:AL:123:ILE:HG12	2.16	0.46
52:AP:67:ILE:HD11	52:AP:80:LYS:HB3	1.97	0.46
67:Ae:90:LYS:HB2	67:Ae:90:LYS:HE2	1.68	0.46
71:Ai:5:THR:HG23	71:Ai:12:ASN:HB2	1.98	0.46
72:Aj:2:GLY:O	72:Aj:7:SER:OG	2.25	0.46
81:tA:75:C:H2'	81:tA:76:A:C8	2.51	0.46
4:BE:152:PRO:HD2	5:BG:215:ARG:HH12	1.80	0.46
20:BF:117:THR:O	20:BF:121:ILE:HG13	2.16	0.46
34:B5:1358:G:H2'	34:B5:1359:C:C6	2.50	0.46
34:B5:1483:A:H2'	34:B5:1484:G:C8	2.51	0.46
38:A1:269:G:H5''	50:AN:14:LYS:HE2	1.97	0.46
38:A1:1495:U:H5	38:A1:1835:A:N1	2.14	0.46
38:A1:2180:G:H2'	38:A1:2181:C:C6	2.50	0.46
38:A1:2478:C:N3	38:A1:2479:C:N4	2.64	0.46
38:A1:3302:U:H3	38:A1:3312:U:H3	1.64	0.46
39:A3:28:C:H1'	39:A3:55:A:H61	1.80	0.46
41:AD:95:TRP:HZ3	41:AD:199:ILE:HG13	1.81	0.46
52:AP:131:ARG:HB2	52:AP:135:ARG:HB3	1.97	0.46
55:AS:93:GLU:OE2	55:AS:137:ARG:HB2	2.16	0.46
62:AZ:70:PRO:HG3	62:AZ:115:LYS:HB2	1.98	0.46
79:E:194:LEU:HD13	79:E:200:ASN:HB2	1.97	0.46
3:BC:45:VAL:HG21	3:BC:68:ILE:HG12	1.96	0.46
10:BN:11:ILE:HG13	10:BN:12:SER:H	1.80	0.46
22:BP:102:PHE:CZ	34:B5:1241:G:H5'	2.51	0.46
28:BZ:81:ARG:O	28:BZ:85:LYS:HG2	2.15	0.46
31:Bg:16:HIS:CD2	31:Bg:45:TRP:HZ2	2.34	0.46
31:Bg:198:ASN:HB2	31:Bg:216:LYS:HB2	1.97	0.46
34:B5:625:C:H2'	34:B5:626:U:C6	2.51	0.46
36:AB:17:LEU:HD21	36:AB:233:TRP:HH2	1.80	0.46
36:AB:148:LEU:HD22	36:AB:192:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:179:LEU:HD11	37:AC:183:LYS:HE2	1.98	0.46
38:A1:616:G:H2'	38:A1:617:G:C8	2.51	0.46
38:A1:682:U:H5''	38:A1:683:U:H5	1.81	0.46
38:A1:963:G:O2'	63:Aa:29:PRO:O	2.34	0.46
38:A1:2762:A:H2'	38:A1:2763:U:H6	1.80	0.46
2:BB:67:GLU:OE2	2:BB:83:LYS:HB2	2.16	0.46
7:BI:137:LYS:HA	7:BI:140:GLU:HB3	1.98	0.46
8:BJ:87:SER:H	8:BJ:90:LYS:NZ	2.14	0.46
19:BD:224:ASP:HB2	31:Bg:228:LYS:HE2	1.98	0.46
31:Bg:289:ALA:HA	31:Bg:305:TYR:HA	1.98	0.46
34:B5:17:C:H2'	34:B5:18:C:C6	2.50	0.46
34:B5:107:C:H2'	34:B5:108:A:C8	2.51	0.46
34:B5:447:U:H2'	34:B5:448:C:O4'	2.16	0.46
34:B5:1350:U:H2'	34:B5:1351:G:C8	2.50	0.46
34:B5:1354:G:O6	34:B5:1369:U:C4	2.69	0.46
34:B5:1588:G:N2	34:B5:1608:U:O2	2.33	0.46
38:A1:428:A:H2'	38:A1:429:U:C6	2.51	0.46
38:A1:974:G:H5'	53:AQ:16:ARG:HG3	1.97	0.46
38:A1:2266:PSU:H2'	38:A1:2267:C:C6	2.51	0.46
42:AE:56:LYS:HB3	42:AE:64:LEU:HB3	1.98	0.46
46:AI:206:LEU:O	46:AI:210:ILE:HD12	2.16	0.46
51:AO:143[A]:THR:OG1	51:AO:150[A]:GLU:OE1	2.28	0.46
1:BA:15:GLN:HE22	24:BR:118:PRO:HD2	1.81	0.45
1:BA:29:VAL:HG13	1:BA:149:LEU:HB3	1.98	0.45
34:B5:699:U:O2'	34:B5:740:A:N6	2.49	0.45
34:B5:1236:A:H2'	34:B5:1237:G:H8	1.80	0.45
38:A1:47:C:OP2	38:A1:48:A:O2'	2.26	0.45
38:A1:710:A:H2'	38:A1:711:A:C8	2.51	0.45
38:A1:1141:C:O2'	38:A1:1153:A:N3	2.49	0.45
38:A1:3217:C:C2	52:AP:182:ILE:HD11	2.51	0.45
45:AH:21:LYS:HD3	45:AH:21:LYS:HA	1.75	0.45
52:AP:25:SER:O	52:AP:29:THR:OG1	2.22	0.45
78:Ap:32:GLN:NE2	78:Ap:70:THR:OG1	2.49	0.45
7:BI:83:TYR:HB3	7:BI:101:ILE:HB	1.98	0.45
10:BN:14:SER:HB3	34:B5:959:U:H5''	1.98	0.45
13:BW:30:SER:HB2	13:BW:61:ILE:HG13	1.97	0.45
21:BK:50:THR:OG1	21:BK:55:VAL:O	2.27	0.45
26:BT:137:ALA:O	26:BT:141:GLU:HG2	2.17	0.45
29:Bc:12:VAL:HG12	29:Bc:52:ASP:H	1.81	0.45
29:Bc:16:LEU:N	29:Bc:27:GLN:O	2.48	0.45
31:Bg:297:ASP:N	31:Bg:297:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:26:A:H2'	34:B5:27:U:C6	2.52	0.45
34:B5:393:C:H2'	34:B5:394:C:C6	2.50	0.45
38:A1:2426:U:H2'	38:A1:2427:U:C6	2.51	0.45
38:A1:3066:U:H2'	38:A1:3067:C:C6	2.50	0.45
38:A1:3294:A:H2'	38:A1:3295:A:O4'	2.16	0.45
49:AM:32:LEU:HD11	49:AM:94:TRP:CD1	2.51	0.45
53:AQ:62:VAL:HG13	53:AQ:66:ARG:HD2	1.98	0.45
83:eI:124:LEU:HD12	83:eI:150:PHE:CD1	2.51	0.45
2:BB:99:ASN:OD1	2:BB:100:PHE:N	2.48	0.45
3:BC:222:TYR:OH	12:BV:10:GLU:OE2	2.34	0.45
23:BQ:93:HIS:CE1	23:BQ:105:LEU:HD11	2.50	0.45
25:BS:41:ARG:NH1	26:BT:46:PRO:HG3	2.31	0.45
35:AA:104:LEU:HD22	35:AA:136:ILE:HD11	1.99	0.45
36:AB:57:VAL:HG22	36:AB:73:VAL:HG22	1.98	0.45
38:A1:1659:U:H2'	38:A1:1660:C:C6	2.51	0.45
80:tP:21:A:N6	80:tP:46:G:H2'	2.31	0.45
2:BB:171:ILE:O	2:BB:175:GLU:HG2	2.16	0.45
19:BD:106:LYS:HG3	19:BD:175:VAL:HG22	1.97	0.45
27:BU:63:LEU:O	27:BU:83:GLU:HA	2.16	0.45
30:Bd:24:CYS:HB2	34:B5:1434:U:H4'	1.98	0.45
34:B5:1147:A:H2'	34:B5:1148:C:C6	2.52	0.45
38:A1:1017:C:H5	38:A1:1035:G:H1	1.65	0.45
38:A1:2197:C:N4	38:A1:2241:U:H2'	2.32	0.45
38:A1:2447:A:N1	38:A1:2500:A:N6	2.65	0.45
39:A3:16:U:H2'	39:A3:17:A:H8	1.81	0.45
41:AD:119:TYR:OH	41:AD:139:PRO:O	2.24	0.45
44:AG:152:LEU:HD12	44:AG:180:VAL:HB	1.98	0.45
46:AI:31:ILE:HG22	46:AI:62:SER:HB2	1.97	0.45
79:E:91:LYS:HA	79:E:91:LYS:HD2	1.75	0.45
3:BC:185:LYS:O	3:BC:189:GLN:HG3	2.16	0.45
5:BG:186:ARG:NH1	34:B5:268:C:OP2	2.50	0.45
14:BX:69:ARG:HG3	14:BX:117:ILE:HG12	1.97	0.45
22:BP:60:LEU:HD22	22:BP:76:VAL:HG11	1.97	0.45
24:BR:15:ALA:HA	24:BR:18:GLU:HG2	1.97	0.45
35:AA:47:GLN:HB3	35:AA:49:VAL:HG13	1.99	0.45
36:AB:5:LYS:HE2	38:A1:2878:G:H5''	1.98	0.45
38:A1:30:G:H5'	50:AN:172:ARG:HG2	1.99	0.45
38:A1:2540:A:H4'	38:A1:2541:U:H5'	1.99	0.45
38:A1:2930:A:H2'	38:A1:2931:C:C6	2.51	0.45
58:AV:81:GLN:HG2	58:AV:83:LYS:H	1.81	0.45
81:tA:18:G:O2'	81:tA:57:G:N2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:87:GLN:OE1	34:B5:10:G:O2'	2.31	0.45
7:BI:110:ARG:O	7:BI:114:GLU:HG2	2.16	0.45
23:BQ:82:ARG:HH22	23:BQ:116:LEU:HD21	1.80	0.45
30:Bd:4:GLU:HB2	34:B5:1244:A:H4'	1.99	0.45
38:A1:691:A:N1	40:A4:28:C:O2'	2.44	0.45
50:AN:104:GLU:OE2	50:AN:161:ALA:HA	2.16	0.45
55:AS:139:TYR:CD1	55:AS:140:VAL:HG23	2.52	0.45
2:BB:157:GLN:HB2	2:BB:160:HIS:CE1	2.52	0.45
38:A1:316:U:O4	71:AI:28:TYR:HA	2.17	0.45
38:A1:1364:C:H5''	53:AQ:3:ILE:HD13	1.98	0.45
44:AG:152:LEU:HD13	44:AG:178:ALA:HB3	1.98	0.45
49:AM:65:LEU:HG	55:AS:172:TYR:OH	2.16	0.45
4:BE:93:ASP:OD1	4:BE:94:ALA:N	2.50	0.45
7:BI:39:GLY:HA2	7:BI:61:GLU:HB3	1.97	0.45
20:BF:145:ASP:HB3	20:BF:217:LEU:HD21	1.99	0.45
22:BP:49:MET:HA	22:BP:52:LYS:HZ3	1.81	0.45
26:BT:134:ARG:HH12	34:B5:1360:A:H5'	1.82	0.45
34:B5:472:U:O2'	34:B5:769:A:N3	2.42	0.45
34:B5:607:G:H5'	34:B5:613:G:N2	2.32	0.45
36:AB:250:ALA:HB1	38:A1:2947:G:C2	2.52	0.45
38:A1:674:G:O6	53:AQ:56:LYS:NZ	2.50	0.45
38:A1:708:G:N2	38:A1:711:A:OP2	2.44	0.45
38:A1:1184:A:H5''	49:AM:59:ASN:HD22	1.82	0.45
38:A1:1194:G:H2'	38:A1:1195:A:C8	2.52	0.45
39:A3:35:C:O2	39:A3:45:A:O2'	2.34	0.45
79:E:41:TYR:CE1	79:E:195:LYS:HE3	2.52	0.45
80:tP:28:A:H2'	80:tP:29:G:H8	1.81	0.45
6:BH:5:GLN:O	6:BH:9:LEU:HB2	2.17	0.45
20:BF:125:THR:HG22	20:BF:127:GLN:HB2	1.99	0.45
23:BQ:37:THR:HG23	23:BQ:38:LEU:HD22	1.99	0.45
27:BU:23:ARG:NH2	27:BU:92:ASP:OD2	2.42	0.45
31:Bg:13:LEU:HB2	31:Bg:310:ILE:HB	1.98	0.45
32:Bf:121:CYS:H	32:Bf:130:VAL:HG11	1.81	0.45
34:B5:1146:G:H2'	34:B5:1147:A:C8	2.52	0.45
34:B5:1351:G:H2'	34:B5:1352:G:C8	2.51	0.45
34:B5:1692:G:H5''	34:B5:1693:A:N7	2.31	0.45
38:A1:120:G:H1	44:AG:124:ASP:HB3	1.82	0.45
38:A1:1497:C:H2'	38:A1:1498:A:C8	2.51	0.45
47:AJ:93:ASP:OD1	47:AJ:94:ARG:N	2.50	0.45
51:AO:18[A]:ARG:O	51:AO:22[A]:VAL:HG23	2.16	0.45
2:BB:48:VAL:HG13	2:BB:49:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:32:ILE:H	5:BG:32:ILE:HD12	1.82	0.45
23:BQ:46:PHE:O	23:BQ:50:GLU:HG3	2.17	0.45
24:BR:33:ARG:NH2	34:B5:1387:G:OP1	2.39	0.45
24:BR:52:GLY:HA3	34:B5:1389:C:O2'	2.17	0.45
34:B5:416:A:H3'	34:B5:417:A:H8	1.82	0.45
34:B5:816:G:H2'	34:B5:817:A:H8	1.82	0.45
38:A1:1157:G:O2'	38:A1:1169:A:N3	2.45	0.45
38:A1:2697:A:H2'	38:A1:2698:G:H8	1.79	0.45
38:A1:3183:A:OP1	51:AO:37[A]:ARG:NH1	2.44	0.45
46:AI:99:ILE:HG22	46:AI:123:HIS:HB2	1.99	0.45
54:AR:11:ALA:HA	54:AR:14:VAL:HG12	1.97	0.45
58:AV:54:LEU:HD21	58:AV:119:GLY:HA3	1.99	0.45
69:Ag:58:ARG:HB2	69:Ag:61:GLN:NE2	2.32	0.45
70:Ah:12:LYS:NZ	70:Ah:20:GLN:OE1	2.47	0.45
83:eI:97:ASP:OD1	83:eI:97:ASP:N	2.49	0.45
2:BB:36:SER:HA	2:BB:41:ARG:HD3	1.99	0.44
11:BO:89:THR:HG21	11:BO:126:THR:O	2.18	0.44
13:BW:14:ILE:HG12	13:BW:25:VAL:HG11	1.99	0.44
13:BW:27:ILE:HB	13:BW:61:ILE:HB	1.99	0.44
13:BW:110:ILE:HD12	13:BW:126:LEU:HD11	1.98	0.44
20:BF:109:LYS:HB2	20:BF:109:LYS:HE2	1.79	0.44
25:BS:36:LYS:HE2	25:BS:36:LYS:HB3	1.74	0.44
34:B5:1393:C:H2'	34:B5:1394:G:H8	1.82	0.44
34:B5:1579:U:H2'	34:B5:1580:C:C6	2.52	0.44
37:AC:157:GLU:OE2	37:AC:211:GLU:N	2.31	0.44
38:A1:1073:U:H2'	38:A1:1074:U:C6	2.53	0.44
38:A1:1597:C:P	69:Ag:8:ARG:HH12	2.40	0.44
38:A1:1915:A:H2'	38:A1:1916:U:C6	2.52	0.44
69:Ag:58:ARG:HB2	69:Ag:61:GLN:HE21	1.82	0.44
6:BH:34:LEU:HB3	6:BH:39:ARG:HH12	1.82	0.44
8:BJ:73:GLY:O	8:BJ:77:ILE:HG12	2.18	0.44
11:BO:28:VAL:HG12	11:BO:67:VAL:HG11	2.00	0.44
11:BO:80:HIS:ND1	11:BO:114:ARG:HB2	2.31	0.44
14:BX:116:ASP:OD1	34:B5:570:A:N6	2.47	0.44
15:BY:81:GLU:HA	15:BY:84:LYS:HG2	1.99	0.44
20:BF:152:GLY:HA2	82:MR:-2:A:C5	2.52	0.44
24:BR:22:PRO:O	31:Bg:216:LYS:NZ	2.47	0.44
33:BM:61:VAL:HG12	33:BM:89:ILE:HB	1.99	0.44
34:B5:107:C:OP1	34:B5:383:G:O2'	2.27	0.44
34:B5:809:A:H2'	34:B5:810:G:C8	2.53	0.44
38:A1:531:G:H2'	38:A1:532:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:698:U:H2'	38:A1:699:A:O4'	2.16	0.44
38:A1:3094:A:OP1	58:AV:14:SER:OG	2.32	0.44
57:AU:18:ASP:HB3	57:AU:104:ARG:HB2	1.99	0.44
3:BC:156:THR:HG23	13:BW:95:PRO:HB2	1.99	0.44
7:BI:56:ARG:NH1	7:BI:174:GLY:O	2.50	0.44
9:BL:109:VAL:HG21	9:BL:125:VAL:HG11	1.99	0.44
19:BD:29:LEU:HB2	19:BD:34:TYR:HB2	1.98	0.44
26:BT:105:LEU:HD23	26:BT:108:LEU:HD12	1.99	0.44
34:B5:1469:A:H4'	34:B5:1541:G:H4'	1.98	0.44
34:B5:1684:U:O2	34:B5:1717:G:O6	2.36	0.44
37:AC:322:GLN:HE22	38:A1:598:A:H1'	1.82	0.44
38:A1:1490:A:O2'	72:Aj:12:HIS:O	2.34	0.44
38:A1:1497:C:O2'	38:A1:1602:A:N3	2.47	0.44
38:A1:1556:C:H2'	38:A1:2169:G:N2	2.32	0.44
38:A1:3160:U:H2'	38:A1:3161:C:C6	2.53	0.44
42:AE:39:VAL:O	42:AE:87:THR:OG1	2.28	0.44
56:AT:41:ASP:OD1	56:AT:61:THR:OG1	2.24	0.44
58:AV:15:LEU:HD13	58:AV:51:ALA:HB3	1.98	0.44
4:BE:22:LYS:NZ	34:B5:758:U:OP1	2.50	0.44
9:BL:46:LYS:O	9:BL:50:GLU:HG2	2.17	0.44
19:BD:168:ILE:HD13	19:BD:168:ILE:HA	1.89	0.44
21:BK:11:ILE:HD11	21:BK:37:THR:HG21	1.99	0.44
26:BT:64:HIS:HE1	34:B5:1523:G:N7	2.15	0.44
31:Bg:40:LYS:HA	31:Bg:68:VAL:HG23	1.99	0.44
34:B5:477:A:H2'	34:B5:478:A:H8	1.82	0.44
34:B5:825:U:H2'	34:B5:826:U:O4'	2.18	0.44
34:B5:1175:U:H2'	34:B5:1176:G:H8	1.82	0.44
38:A1:973:A:N1	38:A1:1108:U:H5	2.15	0.44
38:A1:1065:A:O4'	64:Ab:28:LYS:HE2	2.18	0.44
38:A1:2413:A:H2'	38:A1:2414:G:H8	1.83	0.44
38:A1:2621:G:O2'	83:eI:53:GLY:O	2.33	0.44
43:AF:138:TYR:CE2	43:AF:233:GLU:HB2	2.51	0.44
46:AI:66:GLU:OE2	46:AI:69:ARG:NH2	2.50	0.44
50:AN:110:ALA:HB1	50:AN:113:LEU:HD12	2.00	0.44
53:AQ:40:THR:OG1	53:AQ:45:ASN:ND2	2.50	0.44
61:AY:101:PRO:HA	61:AY:104:LEU:HD12	1.99	0.44
63:Aa:82:ILE:HD11	63:Aa:102:ILE:HD11	2.00	0.44
34:B5:407:A:H2'	34:B5:408:C:C6	2.53	0.44
34:B5:752:A:H2	34:B5:797:G:H22	1.64	0.44
34:B5:1429:G:H2'	34:B5:1430:U:C6	2.53	0.44
34:B5:1489:U:OP2	34:B5:1515:A:N6	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3322:A:H2'	38:A1:3323:A:H8	1.81	0.44
39:A3:16:U:H2'	39:A3:17:A:C8	2.52	0.44
41:AD:164:LYS:HE2	41:AD:195:LEU:HD21	1.99	0.44
41:AD:196:ARG:NH2	41:AD:237:GLU:OE2	2.43	0.44
44:AG:144:GLU:HA	44:AG:173:MET:HE3	1.98	0.44
47:AJ:90:GLN:NE2	47:AJ:173:ASP:OD1	2.47	0.44
67:Ae:79:VAL:O	67:Ae:83:GLU:HG2	2.18	0.44
80:tP:7:G:O2'	80:tP:49:C:H5'	2.17	0.44
4:BE:137:PRO:HG2	4:BE:150:PRO:HD2	2.00	0.44
9:BL:79:LYS:HD3	34:B5:346:G:H5'	2.00	0.44
20:BF:41:LYS:HE3	20:BF:41:LYS:HB2	1.88	0.44
21:BK:25:LYS:HD2	21:BK:59:PHE:HZ	1.83	0.44
31:Bg:153:GLN:HG3	31:Bg:201:THR:HA	2.00	0.44
34:B5:86:A:H2'	34:B5:87:C:H6	1.82	0.44
34:B5:119:A:H1'	34:B5:397:A:C5	2.53	0.44
34:B5:273:G:O6	34:B5:283:U:O2	2.35	0.44
36:AB:35:ASP:OD2	36:AB:37:ARG:NH1	2.51	0.44
38:A1:1471:U:H2'	38:A1:1472:U:C6	2.53	0.44
38:A1:1717:U:H2'	38:A1:1718:G:H8	1.81	0.44
38:A1:2148:U:H2'	38:A1:2149:A:C5	2.53	0.44
38:A1:3334:U:H4'	38:A1:3335:A:H5'	2.00	0.44
48:AL:106:GLN:NE2	48:AL:110:ASP:OD1	2.51	0.44
78:Ap:59:CYS:C	78:Ap:61:LYS:H	2.25	0.44
83:eI:23:CYS:SG	83:eI:80:MET:HE2	2.57	0.44
1:BA:59:LEU:O	1:BA:63:ILE:HG12	2.17	0.44
1:BA:198:MET:HE1	1:BA:200:ASP:HB2	1.99	0.44
8:BJ:141:VAL:HG12	8:BJ:143:ILE:H	1.81	0.44
23:BQ:137:ARG:HB2	34:B5:1580:C:H4'	2.00	0.44
34:B5:1348:A:H2'	34:B5:1349:G:O4'	2.18	0.44
34:B5:1469:A:H2'	34:B5:1470:C:C6	2.53	0.44
34:B5:1550:A:H2'	34:B5:1551:U:C6	2.53	0.44
35:AA:178:PRO:HG2	78:Ap:26:VAL:HG23	2.00	0.44
37:AC:52:VAL:HG21	37:AC:99:MET:HE3	2.00	0.44
38:A1:874:U:OP2	38:A1:1907:C:O2'	2.33	0.44
38:A1:1334:U:H2'	38:A1:1335:C:C6	2.52	0.44
38:A1:2407:C:H2'	38:A1:2408:U:H6	1.82	0.44
38:A1:3068:U:OP2	54:AR:62:ARG:NH2	2.36	0.44
40:A4:149:A:H2'	40:A4:150:G:C8	2.52	0.44
45:AH:41:ILE:HG21	45:AH:71:VAL:HG21	1.99	0.44
46:AI:182:LEU:HD23	46:AI:185:ARG:HH21	1.83	0.44
69:Ag:58:ARG:HD2	69:Ag:58:ARG:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Ap:7:LYS:O	78:Ap:27:LYS:NZ	2.41	0.44
1:BA:64:ILE:HG23	1:BA:73:VAL:HG11	2.00	0.44
7:BI:153:GLU:O	7:BI:157:GLU:HG2	2.18	0.44
8:BJ:133:HIS:NE2	34:B5:512:A:O3'	2.46	0.44
9:BL:7:VAL:HG13	9:BL:8:GLN:HG2	1.98	0.44
11:BO:82:LYS:HG2	11:BO:118:VAL:HG21	1.99	0.44
25:BS:40:ARG:NH2	34:B5:1540:G:OP2	2.50	0.44
27:BU:55:PRO:HA	27:BU:91:ILE:HG12	1.99	0.44
34:B5:17:C:H2'	34:B5:18:C:H6	1.82	0.44
34:B5:1160:A:H2'	34:B5:1161:C:C6	2.53	0.44
34:B5:1374:C:H2'	34:B5:1375:A:C8	2.53	0.44
36:AB:292:ALA:HB2	36:AB:302:LYS:HD2	1.99	0.44
37:AC:138:ARG:NH1	38:A1:1384:U:H5'	2.33	0.44
38:A1:1807:G:O2'	38:A1:2559:U:O4	2.35	0.44
38:A1:2611:U:H2'	38:A1:2612:U:C6	2.53	0.44
38:A1:2801:A:O2'	38:A1:2802:A:H2'	2.17	0.44
38:A1:3150:A:H2'	38:A1:3151:U:O4'	2.18	0.44
38:A1:3343:G:O2'	38:A1:3362:A:N6	2.51	0.44
39:A3:44:C:OP2	47:AJ:137:ARG:NH2	2.51	0.44
65:Ac:16:LEU:HD12	65:Ac:16:LEU:HA	1.80	0.44
79:E:37:GLY:HA3	79:E:203:SER:HB2	2.00	0.44
4:BE:92:LEU:HD23	15:BY:17:LEU:HD21	1.98	0.44
5:BG:155:ASP:OD1	5:BG:155:ASP:N	2.51	0.44
21:BK:81:ASN:ND2	33:BM:37:VAL:HG13	2.33	0.44
34:B5:424:C:O2'	34:B5:426:G:OP1	2.26	0.44
34:B5:700:C:H2'	34:B5:701:U:C6	2.52	0.44
34:B5:1290:PSU:H2'	34:B5:1291:G:C8	2.53	0.44
34:B5:1479:A:H2'	34:B5:1480:G:H8	1.83	0.44
36:AB:232:ARG:NH1	36:AB:266:ARG:O	2.47	0.44
38:A1:351:A:N6	74:Al:37:TYR:O	2.43	0.44
38:A1:656:A:H2'	38:A1:657:A:C8	2.53	0.44
39:A3:7:G:OP1	41:AD:33:ARG:NH1	2.47	0.44
42:AE:30:LEU:HD23	42:AE:30:LEU:HA	1.85	0.44
50:AN:180:PHE:O	50:AN:184:LYS:HG3	2.18	0.44
52:AP:126:ARG:HG3	52:AP:140:GLU:HG2	2.00	0.44
83:eI:18:THR:HB	83:eI:81:GLU:HB3	1.99	0.44
31:Bg:148:ASN:N	31:Bg:175:ASP:OD2	2.50	0.43
35:AA:2:GLY:HA2	38:A1:2608:G:OP1	2.18	0.43
38:A1:385:A:H2'	38:A1:386:A:C8	2.53	0.43
38:A1:1129:A:OP1	46:AI:13:LYS:NZ	2.31	0.43
38:A1:1228:C:H2'	38:A1:1229:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1699:A:H2'	38:A1:1700:G:C8	2.53	0.43
38:A1:1766:G:N7	54:AR:46:LYS:NZ	2.46	0.43
38:A1:3121:U:H1'	38:A1:3122:A:H5''	1.99	0.43
47:AJ:80:LEU:HD22	47:AJ:167:TYR:HE2	1.83	0.43
48:AL:87:ALA:HB1	48:AL:97:VAL:HG11	2.00	0.43
49:AM:135:LEU:HD21	51:AO:178[A]:VAL:HG22	1.99	0.43
51:AO:127[A]:LEU:HD22	55:AS:156:VAL:HG13	2.00	0.43
55:AS:152:LEU:HB2	55:AS:172:TYR:CE2	2.53	0.43
61:AY:55:GLU:HB2	61:AY:108:LYS:HB3	2.00	0.43
83:eI:26:LEU:O	83:eI:27:ARG:NH1	2.51	0.43
6:BH:17:GLU:HB3	6:BH:46:ILE:HG12	1.99	0.43
6:BH:144:VAL:HA	13:BW:42:GLN:HE21	1.83	0.43
15:BY:57:VAL:HB	15:BY:60:PHE:CE2	2.53	0.43
27:BU:24:ILE:HG13	27:BU:116:VAL:HG22	2.00	0.43
34:B5:168:A:H2'	34:B5:169:A:C8	2.53	0.43
34:B5:844:A:H2'	34:B5:845:G:C2	2.53	0.43
38:A1:1264:G:N2	38:A1:1276:U:O4	2.52	0.43
54:AR:86:GLU:HG2	54:AR:90:PRO:HA	1.98	0.43
56:AT:126:VAL:HG13	56:AT:128:LEU:HD22	1.99	0.43
6:BH:122:HIS:HA	6:BH:125:ILE:HD12	2.01	0.43
13:BW:28:ARG:HD3	13:BW:60:LYS:HE2	1.99	0.43
14:BX:112:LYS:NZ	34:B5:19:A:OP1	2.52	0.43
20:BF:142:PRO:O	20:BF:167:ARG:HG2	2.19	0.43
21:BK:52:LYS:HE3	34:B5:1220:C:H5''	1.99	0.43
34:B5:846:G:H2'	34:B5:847:A:C8	2.53	0.43
34:B5:1071:U:H2'	34:B5:1072:C:C6	2.53	0.43
34:B5:1518:C:H2'	34:B5:1519:U:C6	2.52	0.43
38:A1:1095:U:N3	56:AT:127:GLN:OE1	2.52	0.43
40:A4:69:U:H2'	40:A4:70:G:O4'	2.18	0.43
41:AD:41:LYS:HB2	56:AT:68:THR:O	2.18	0.43
46:AI:55:ASN:HB3	46:AI:162:GLN:HB2	2.00	0.43
47:AJ:106:ILE:HD11	47:AJ:109:HIS:HD2	1.84	0.43
54:AR:105:LEU:HD22	54:AR:135:LYS:HG3	1.99	0.43
2:BB:156:ALA:HB3	2:BB:161:ILE:HD11	2.00	0.43
21:BK:52:LYS:NZ	34:B5:1221:A:OP1	2.51	0.43
31:Bg:240:VAL:HG12	31:Bg:256:THR:HA	1.98	0.43
34:B5:888:U:H2'	34:B5:889:U:C6	2.53	0.43
34:B5:923:A:H2'	34:B5:924:A:C8	2.53	0.43
34:B5:1346:A:N6	34:B5:1370:U:OP2	2.52	0.43
35:AA:226:SER:HB3	38:A1:2202:C:H5''	2.00	0.43
38:A1:1622:U:H2'	38:A1:1623:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2167:A:H2'	38:A1:2168:A:C8	2.53	0.43
38:A1:2568:C:O2'	38:A1:2569:A:O5'	2.30	0.43
38:A1:3176:G:N2	38:A1:3213:A:H1'	2.34	0.43
47:AJ:106:ILE:HD11	47:AJ:109:HIS:CD2	2.54	0.43
53:AQ:176:ARG:HA	53:AQ:182:LYS:O	2.18	0.43
62:AZ:23:VAL:HG12	62:AZ:45:GLY:HA3	2.00	0.43
63:Aa:19:LYS:HB3	63:Aa:25:HIS:HB2	2.00	0.43
1:BA:6:THR:HB	1:BA:191:ARG:HG2	2.01	0.43
2:BB:144:ARG:HB2	2:BB:208:GLN:HG3	2.00	0.43
4:BE:12:LEU:HD21	4:BE:22:LYS:HG2	1.99	0.43
5:BG:2:LYS:HG2	5:BG:17:GLU:HG3	2.00	0.43
10:BN:17:PRO:HG3	17:Bb:28:PRO:HG3	2.00	0.43
20:BF:195:ALA:O	20:BF:199:ILE:HG12	2.19	0.43
34:B5:593:U:H4'	34:B5:595:G:H4'	1.99	0.43
38:A1:2271:A:H2'	38:A1:2272:G:O4'	2.19	0.43
38:A1:3318:G:O2'	38:A1:3320:A:OP2	2.36	0.43
42:AE:45:GLY:O	42:AE:48:ARG:NH1	2.52	0.43
43:AF:178:ILE:HG23	43:AF:183:ASP:HB3	2.01	0.43
47:AJ:99:THR:O	47:AJ:154:THR:OG1	2.37	0.43
77:Ao:27:GLN:HE21	77:Ao:68:VAL:HG13	1.83	0.43
79:E:137:PRO:O	79:E:147:LYS:NZ	2.51	0.43
4:BE:19:LEU:HB2	4:BE:51:ARG:HH22	1.84	0.43
7:BI:67:TRP:HE3	7:BI:72:ILE:HD11	1.84	0.43
34:B5:884:A:H2'	34:B5:885:G:C8	2.54	0.43
34:B5:1561:U:H2'	34:B5:1562:G:H8	1.83	0.43
34:B5:1689:A:H2'	34:B5:1690:G:H8	1.83	0.43
36:AB:173:GLN:HG2	36:AB:175:LYS:H	1.84	0.43
37:AC:231:ALA:O	38:A1:694:C:O2'	2.35	0.43
38:A1:871:U:H2'	38:A1:872:U:C6	2.53	0.43
38:A1:1060:U:H2'	38:A1:1061:A:C8	2.53	0.43
38:A1:2461:A:H62	38:A1:2486:A:H2	1.66	0.43
42:AE:149:ILE:HG23	42:AE:155:LEU:HB2	1.99	0.43
43:AF:34:LYS:O	43:AF:38:LYS:HG2	2.19	0.43
62:AZ:104:PRO:O	62:AZ:108:GLU:HG2	2.19	0.43
70:Ah:85:THR:HG22	70:Ah:87:ALA:H	1.84	0.43
81:tA:28:A:H2'	81:tA:29:G:C8	2.53	0.43
6:BH:121:VAL:O	6:BH:125:ILE:HG13	2.19	0.43
13:BW:25:VAL:HG12	13:BW:63:VAL:HB	2.00	0.43
19:BD:12:VAL:HG21	30:Bd:34:TYR:HB3	2.00	0.43
25:BS:64:GLU:O	25:BS:68:ARG:HG3	2.18	0.43
35:AA:68:LYS:HD3	35:AA:70:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:143:GLU:HG2	37:AC:144:LYS:HG3	2.00	0.43
37:AC:286:VAL:HA	37:AC:289:ILE:HD12	2.01	0.43
38:A1:370:U:H4'	38:A1:404:G:H5'	2.01	0.43
38:A1:2367:A:H2'	38:A1:2368:A:C8	2.54	0.43
40:A4:63:G:H22	40:A4:97:A:H2	1.67	0.43
45:AH:87:LYS:HG3	45:AH:145:VAL:HG13	1.99	0.43
56:AT:73:GLY:HA2	56:AT:89:LEU:O	2.19	0.43
70:Ah:102:GLU:HA	70:Ah:105:ARG:HB3	2.01	0.43
4:BE:44:LEU:HD12	4:BE:82:TYR:HB3	2.01	0.43
4:BE:141:THR:OG1	4:BE:143:ASP:OD1	2.28	0.43
6:BH:49:ILE:O	6:BH:57:ALA:N	2.43	0.43
7:BI:138:ASN:ND2	34:B5:187:G:H3'	2.34	0.43
8:BJ:87:SER:H	8:BJ:90:LYS:HZ3	1.66	0.43
13:BW:24:GLN:HA	13:BW:63:VAL:O	2.17	0.43
19:BD:18:TYR:OH	19:BD:37:VAL:O	2.23	0.43
23:BQ:82:ARG:HA	23:BQ:85:ILE:HG22	2.01	0.43
24:BR:34:LEU:HD12	31:Bg:150:TRP:HH2	1.83	0.43
25:BS:81:ILE:HG22	25:BS:83:ALA:H	1.83	0.43
34:B5:602:U:H2'	34:B5:603:U:C6	2.54	0.43
35:AA:65:ASP:HB3	35:AA:68:LYS:O	2.18	0.43
35:AA:143:GLU:OE1	35:AA:143:GLU:N	2.51	0.43
37:AC:170:LYS:HG2	37:AC:175:HIS:HD2	1.82	0.43
38:A1:20:A:H2'	38:A1:21:G:C8	2.53	0.43
38:A1:622:A:O4'	68:Af:60:ARG:NH2	2.51	0.43
38:A1:1597:C:H5'	38:A1:1696:A:H1'	1.99	0.43
38:A1:2724:U:OP2	38:A1:2726:C:N4	2.51	0.43
38:A1:3214:U:C6	49:AM:121:MET:HE2	2.54	0.43
49:AM:31:LYS:HB3	49:AM:51:ALA:HB1	2.00	0.43
56:AT:136:ARG:HD2	56:AT:139:ARG:NH2	2.34	0.43
80:tP:69:C:H2'	80:tP:70:G:O4'	2.19	0.43
2:BB:169:SER:O	2:BB:173:THR:HG23	2.19	0.43
5:BG:57:ASP:HA	5:BG:106:LEU:HA	2.01	0.43
8:BJ:149:ARG:HG2	34:B5:765:G:O6	2.19	0.43
17:Bb:20:LYS:NZ	34:B5:958:U:OP2	2.43	0.43
34:B5:221:A:OP2	34:B5:832:U:O2'	2.28	0.43
34:B5:688:G:H2'	34:B5:689:G:C8	2.54	0.43
34:B5:885:G:H2'	34:B5:886:U:C6	2.54	0.43
34:B5:1062:A:H3'	34:B5:1063:U:H6	1.84	0.43
38:A1:585:A:H2'	38:A1:586:C:C6	2.53	0.43
38:A1:1083:G:H2'	38:A1:1084:A:C8	2.54	0.43
38:A1:1219:C:O2'	38:A1:1223:A:OP2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2413:A:H2'	38:A1:2414:G:C8	2.54	0.43
38:A1:2897:A:H5''	75:Am:125:LYS:HD2	2.00	0.43
46:AI:48:LEU:O	46:AI:139:ARG:HA	2.19	0.43
66:Ad:26:LYS:HA	66:Ad:26:LYS:HD3	1.71	0.43
79:E:64:SER:O	79:E:108:ASN:N	2.51	0.43
1:BA:83:GLN:HE22	1:BA:100:GLY:N	2.17	0.43
2:BB:103:MET:HE1	2:BB:212:VAL:HG23	2.01	0.43
24:BR:3:ARG:NH1	34:B5:1390:U:O4'	2.52	0.43
34:B5:250:C:H2'	34:B5:251:A:H8	1.83	0.43
34:B5:1223:A:H2'	34:B5:1224:A:H8	1.83	0.43
34:B5:1426:C:O2'	34:B5:1428:G:H5'	2.18	0.43
37:AC:64:SER:HA	37:AC:75:PRO:HA	2.01	0.43
38:A1:235:A:H2'	38:A1:236:G:H8	1.84	0.43
38:A1:238:A:H2'	38:A1:239:G:O4'	2.19	0.43
38:A1:371:G:N1	38:A1:374:A:OP2	2.46	0.43
38:A1:887:G:H2'	38:A1:888:A:C8	2.54	0.43
38:A1:1621:A:H2'	38:A1:1622:U:H6	1.84	0.43
38:A1:2680:A:C2	47:AJ:24:GLY:HA2	2.54	0.43
50:AN:9:GLU:OE2	50:AN:13:LYS:NZ	2.37	0.43
54:AR:14:VAL:HG11	54:AR:41:ILE:HG22	2.01	0.43
62:AZ:115:LYS:HE3	62:AZ:119:GLU:OE1	2.19	0.43
2:BB:98:THR:O	2:BB:232:HIS:NE2	2.43	0.42
4:BE:105:VAL:HG21	4:BE:245:LYS:N	2.33	0.42
5:BG:121:LEU:HD22	5:BG:124:LEU:HD12	2.00	0.42
25:BS:20:THR:HG21	25:BS:35:ILE:HA	2.00	0.42
25:BS:40:ARG:CZ	34:B5:1539:G:H4'	2.49	0.42
30:Bd:10:HIS:ND1	34:B5:1452:U:OP1	2.43	0.42
30:Bd:19:ARG:O	30:Bd:27:HIS:ND1	2.51	0.42
34:B5:183:U:H2'	34:B5:184:C:H6	1.84	0.42
36:AB:308:MET:HE3	36:AB:373:PRO:HD3	2.01	0.42
38:A1:90:C:OP1	63:Aa:59:ARG:NH1	2.51	0.42
38:A1:1011:A:H2'	38:A1:1012:G:C8	2.54	0.42
38:A1:2471:U:N3	38:A1:2473:C:OP1	2.52	0.42
42:AE:148:GLU:CD	42:AE:151:LYS:HZ3	2.27	0.42
43:AF:86:VAL:O	43:AF:114:GLY:HA2	2.19	0.42
79:E:21:ASN:O	79:E:25:LYS:NZ	2.48	0.42
79:E:86:SER:OG	79:E:87:VAL:N	2.52	0.42
8:BJ:28:LEU:HD23	18:Be:44:PHE:HE1	1.83	0.42
15:BY:27:VAL:HG21	15:BY:35:VAL:HG11	2.01	0.42
18:Be:51:ASN:N	18:Be:51:ASN:OD1	2.51	0.42
20:BF:121:ILE:HG23	20:BF:199:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BM:62:LEU:HD13	33:BM:120:VAL:HB	2.00	0.42
35:AA:183:GLY:HA2	38:A1:896:A:H5''	2.01	0.42
38:A1:716:A:N6	63:Aa:117:ARG:HG3	2.33	0.42
38:A1:1035:G:H3'	38:A1:1036:A:H8	1.84	0.42
38:A1:1899:G:O2'	38:A1:2334:U:O4	2.28	0.42
38:A1:2806:U:H2'	38:A1:2807:U:C6	2.54	0.42
66:Ad:6:ASP:OD1	66:Ad:7:VAL:N	2.52	0.42
72:Aj:17:THR:O	72:Aj:25:ARG:HA	2.19	0.42
83:eI:38:PRO:HG3	83:eI:142:MET:SD	2.59	0.42
3:BC:211:LEU:HD23	3:BC:211:LEU:HA	1.87	0.42
4:BE:57:ASN:O	4:BE:61:VAL:HG23	2.19	0.42
5:BG:3:LEU:O	5:BG:15:THR:HA	2.19	0.42
6:BH:5:GLN:HE22	6:BH:25:VAL:HG21	1.83	0.42
6:BH:122:HIS:HD2	6:BH:125:ILE:HD12	1.84	0.42
25:BS:119:ILE:HD12	25:BS:119:ILE:HA	1.91	0.42
32:Bf:78:LYS:HB3	34:B5:1271:G:H5''	2.00	0.42
34:B5:895:G:H2'	34:B5:896:U:C6	2.55	0.42
34:B5:968:U:OP1	34:B5:1033:C:O2'	2.37	0.42
36:AB:95:THR:OG1	36:AB:98:GLY:O	2.22	0.42
36:AB:128:LYS:HG3	38:A1:3294:A:H5'	2.00	0.42
37:AC:23:PRO:HD2	37:AC:26:PHE:CD2	2.55	0.42
38:A1:1290:A:H2'	38:A1:1291:A:C8	2.54	0.42
38:A1:1635:G:N2	38:A1:1638:A:OP2	2.37	0.42
38:A1:1688:U:H2'	38:A1:1689:U:C6	2.54	0.42
38:A1:2232:A:H2'	38:A1:2233:A:C8	2.53	0.42
38:A1:2251:G:O2'	80:tP:12:G:H5''	2.19	0.42
44:AG:178:ALA:HB2	44:AG:218:ILE:HG23	2.01	0.42
56:AT:143:THR:HG23	56:AT:148:PRO:HD3	2.01	0.42
73:Ak:27:ILE:HB	73:Ak:78:LEU:HD21	2.00	0.42
1:BA:180:GLU:OE2	1:BA:191:ARG:NH1	2.43	0.42
20:BF:101:GLY:HA2	34:B5:1166:A:H5''	2.01	0.42
22:BP:30:THR:HA	22:BP:33:PHE:HB3	2.02	0.42
26:BT:117:SER:HB3	26:BT:121:GLY:O	2.20	0.42
33:BM:29:LYS:HD3	33:BM:100:TRP:CE2	2.54	0.42
34:B5:181:A:H2'	34:B5:182:A:C8	2.54	0.42
34:B5:406:U:H2'	34:B5:407:A:C8	2.54	0.42
34:B5:448:C:H2'	34:B5:449:C:C6	2.55	0.42
34:B5:800:U:H2'	34:B5:801:G:C8	2.55	0.42
35:AA:33:ASP:O	35:AA:37:ARG:HB2	2.19	0.42
37:AC:304:GLN:NE2	38:A1:594:U:H3	2.17	0.42
38:A1:120:G:H4'	38:A1:121:A:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2909:U:H2'	38:A1:2910:A:O4'	2.19	0.42
39:A3:64:A:N7	46:A1:209:ASN:ND2	2.62	0.42
8:BJ:123:HIS:HB3	18:Be:33:ARG:NH1	2.34	0.42
10:BN:25:TRP:CD1	17:Bb:82:LYS:HE2	2.55	0.42
15:BY:60:PHE:HA	15:BY:70:VAL:O	2.19	0.42
20:BF:189:THR:HG22	20:BF:191:ALA:H	1.84	0.42
22:BP:45:PHE:HA	22:BP:49:MET:HE3	2.02	0.42
22:BP:48:GLY:O	22:BP:52:LYS:NZ	2.52	0.42
34:B5:1081:A:O2'	34:B5:1083:G:N7	2.47	0.42
34:B5:1182:U:O2'	34:B5:1184:A:N7	2.49	0.42
36:AB:148:LEU:HD11	36:AB:196:ARG:HD3	2.01	0.42
38:A1:3072:C:H2'	38:A1:3073:A:O4'	2.19	0.42
41:AD:125:VAL:HG11	41:AD:199:ILE:HG21	2.01	0.42
44:AG:34:PHE:CD1	44:AG:42:PRO:HD3	2.55	0.42
46:A1:54:SER:HB2	46:A1:135:ILE:HD11	2.02	0.42
52:AP:33:ALA:HB1	52:AP:117:ILE:HG12	2.01	0.42
66:Ad:31:ARG:O	66:Ad:35:GLU:HG2	2.19	0.42
7:BI:25:ARG:HA	34:B5:400:A:H5''	2.01	0.42
15:BY:20:ARG:HD2	15:BY:76:TYR:CZ	2.55	0.42
23:BQ:13:LYS:HG3	23:BQ:14:LYS:HG3	2.02	0.42
26:BT:105:LEU:HD13	26:BT:122:ARG:HH11	1.84	0.42
27:BU:23:ARG:NH2	34:B5:1347:U:OP2	2.35	0.42
31:Bg:211:ILE:O	31:Bg:222:LEU:HA	2.19	0.42
34:B5:86:A:O2'	34:B5:147:A:N3	2.44	0.42
34:B5:1001:A:H2'	34:B5:1002:G:C8	2.53	0.42
34:B5:1079:U:H2'	34:B5:1080:U:C6	2.55	0.42
37:AC:159:ILE:HG23	37:AC:164:GLU:HG3	2.02	0.42
38:A1:73:C:C2	71:Ai:15:LYS:HD3	2.55	0.42
38:A1:1203:A:H2'	38:A1:1204:A:C8	2.55	0.42
38:A1:2257:C:H2'	38:A1:2258:PSU:C6	2.55	0.42
38:A1:2941:A:O5'	38:A1:2943:G:H4'	2.19	0.42
38:A1:3272:C:P	42:AE:78:ARG:HH21	2.43	0.42
38:A1:3298:C:C2	38:A1:3299:A:C8	3.07	0.42
40:A4:8:C:H2'	40:A4:9:A:C8	2.55	0.42
51:AO:10[A]:ASP:HB2	51:AO:117[A]:ARG:HB3	2.02	0.42
4:BE:151:ASP:HB3	4:BE:154:ILE:HG13	2.02	0.42
6:BH:17:GLU:HA	6:BH:20:VAL:HG22	2.02	0.42
25:BS:38:VAL:HG23	25:BS:42:TYR:CD2	2.52	0.42
34:B5:5:U:H2'	34:B5:6:G:H8	1.84	0.42
35:AA:118:GLU:OE2	38:A1:2177:G:N2	2.51	0.42
36:AB:2:SER:OG	38:A1:2943:G:OP2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:67:PHE:CD1	58:AV:88:ARG:HD2	2.55	0.42
36:AB:250:ALA:HB1	38:A1:2947:G:N3	2.35	0.42
38:A1:786:A:H4'	38:A1:787:G:H5'	2.02	0.42
38:A1:1157:G:H2'	38:A1:1158:A:O4'	2.19	0.42
38:A1:1351:U:H2'	38:A1:1352:A:C8	2.54	0.42
38:A1:2106:A:H2'	38:A1:2107:A:C8	2.54	0.42
38:A1:2150:G:O2'	38:A1:2189:U:OP1	2.31	0.42
38:A1:2592:G:H4'	38:A1:2594:C:C2	2.54	0.42
38:A1:3113:A:H2'	38:A1:3114:A:O4'	2.19	0.42
45:AH:41:ILE:HG22	45:AH:43:VAL:HG13	2.01	0.42
51:AO:14[A]:HIS:HE1	51:AO:119[A]:VAL:HG12	1.84	0.42
61:AY:115:ARG:O	61:AY:119:ILE:HG12	2.20	0.42
66:Ad:44:MET:HB3	66:Ad:77:ARG:HD3	2.01	0.42
76:An:17:ARG:HA	76:An:20:VAL:HG12	2.01	0.42
1:BA:206:ASP:OD1	1:BA:206:ASP:N	2.52	0.42
5:BG:25:ARG:HA	5:BG:28:PHE:CG	2.54	0.42
8:BJ:35:GLY:HA2	8:BJ:123:HIS:CE1	2.55	0.42
8:BJ:64:GLU:HG3	8:BJ:65:LYS:HG3	2.01	0.42
8:BJ:90:LYS:HB2	8:BJ:95:TYR:CD2	2.55	0.42
15:BY:45:ALA:HA	15:BY:50:ALA:HB3	2.02	0.42
16:Ba:92:ARG:HB3	34:B5:1796:C:O2	2.19	0.42
31:Bg:10:ARG:HH22	31:Bg:314:GLN:HB2	1.85	0.42
31:Bg:16:HIS:NE2	31:Bg:35:SER:OG	2.50	0.42
33:BM:32:LEU:HD11	33:BM:121:VAL:HG11	2.02	0.42
34:B5:739:G:O2'	34:B5:740:A:H5'	2.20	0.42
34:B5:1089:U:O2'	34:B5:1093:A:N1	2.48	0.42
38:A1:275:U:H2'	38:A1:276:U:C6	2.55	0.42
38:A1:1146:C:H4'	38:A1:1331:U:C4	2.55	0.42
38:A1:1264:G:H1'	38:A1:1265:U:H5	1.85	0.42
38:A1:1699:A:H2'	38:A1:1700:G:H8	1.84	0.42
38:A1:2724:U:H4'	56:AT:54:HIS:CD2	2.55	0.42
42:AE:70:LYS:HA	42:AE:70:LYS:HD2	1.78	0.42
43:AF:77:VAL:HB	56:AT:139:ARG:HG2	2.02	0.42
49:AM:23:ILE:HG21	49:AM:28:SER:HB2	2.02	0.42
81:tA:58:A:C2	81:tA:60:A:H2'	2.55	0.42
83:eI:99:PHE:CE1	83:eI:114:LYS:HG2	2.54	0.42
1:BA:107:PHE:HB2	1:BA:135:GLU:HG2	2.00	0.42
2:BB:49:ASN:OD1	2:BB:50:LYS:N	2.53	0.42
3:BC:165:VAL:HG11	3:BC:210:THR:HA	2.02	0.42
7:BI:138:ASN:HA	7:BI:141:ARG:HH12	1.85	0.42
19:BD:207:THR:OG1	24:BR:40:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BF:42:LEU:HD22	20:BF:130:ILE:HD11	2.02	0.42
24:BR:33:ARG:HD3	24:BR:33:ARG:HA	1.78	0.42
31:Bg:209:THR:HG23	31:Bg:210:LEU:HD23	2.02	0.42
34:B5:103:A:H4'	34:B5:105:A:C8	2.55	0.42
34:B5:367:A:H2'	34:B5:368:U:O4'	2.20	0.42
34:B5:1488:G:H3'	34:B5:1515:A:H61	1.85	0.42
34:B5:1511:U:H2'	34:B5:1512:G:H8	1.85	0.42
37:AC:22:LEU:HA	37:AC:23:PRO:HD3	1.77	0.42
38:A1:12:A:H2'	38:A1:13:A:C8	2.55	0.42
38:A1:172:G:H2'	38:A1:173:G:C8	2.55	0.42
38:A1:516:A:H2'	38:A1:517:G:C8	2.55	0.42
38:A1:627:U:H4'	38:A1:1399:A:H1'	2.01	0.42
38:A1:2572:C:H5'	62:AZ:60:LYS:HB3	2.00	0.42
66:Ad:20:LEU:HD11	66:Ad:32:ALA:HB2	2.01	0.42
66:Ad:44:MET:SD	66:Ad:77:ARG:HB2	2.59	0.42
67:Ae:9:ILE:HG12	67:Ae:63:THR:HB	2.00	0.42
7:BI:77:ARG:NH1	38:A1:3354:U:O2	2.53	0.42
33:BM:59:LEU:HB3	33:BM:123:VAL:HG22	2.02	0.42
34:B5:124:A:H2'	34:B5:125:U:O4'	2.19	0.42
34:B5:925:G:H2'	34:B5:926:A:C8	2.55	0.42
37:AC:233:LEU:HD23	37:AC:233:LEU:HA	1.79	0.42
38:A1:4:U:H2'	38:A1:5:G:C8	2.55	0.42
38:A1:92:G:H5'	38:A1:94:G:N7	2.35	0.42
38:A1:985:U:H2'	38:A1:986:PSU:H6	1.84	0.42
38:A1:2534:G:O6	38:A1:2545:C:N4	2.53	0.42
48:AL:149:GLN:HA	48:AL:150:PRO:HD3	1.95	0.42
53:AQ:50:LYS:HB3	53:AQ:50:LYS:HE2	1.89	0.42
58:AV:15:LEU:HD23	58:AV:53:SER:HB3	2.00	0.42
63:Aa:36:GLY:HA3	63:Aa:40:HIS:CE1	2.55	0.42
4:BE:117:GLU:O	4:BE:120:SER:OG	2.36	0.41
6:BH:173:TYR:HE1	6:BH:179:LYS:HB2	1.84	0.41
7:BI:153:GLU:HB2	7:BI:156:VAL:HG22	2.01	0.41
13:BW:57:ARG:NE	17:Bb:26:GLN:HE21	2.18	0.41
19:BD:22:ASN:O	19:BD:26:THR:OG1	2.26	0.41
21:BK:16:PHE:HB2	21:BK:76:LEU:HD22	2.01	0.41
25:BS:36:LYS:HB3	25:BS:105:VAL:HG21	2.02	0.41
31:Bg:127:ARG:HA	31:Bg:150:TRP:HB2	2.02	0.41
34:B5:1196:A:OP2	34:B5:1464:G:N2	2.40	0.41
34:B5:1338:C:H2'	34:B5:1339:C:C6	2.55	0.41
34:B5:1350:U:H2'	34:B5:1351:G:H8	1.84	0.41
34:B5:1560:U:H2'	34:B5:1561:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AA:181:LYS:HB2	38:A1:860:G:C6	2.55	0.41
38:A1:80:G:H2'	38:A1:81:C:H6	1.84	0.41
38:A1:1223:A:OP2	38:A1:1223:A:H8	2.04	0.41
38:A1:1334:U:H5''	43:AF:206:LYS:HB3	2.02	0.41
38:A1:1571:A:H2'	38:A1:1572:U:O4'	2.20	0.41
38:A1:1941:C:H2'	38:A1:1942:U:C6	2.55	0.41
38:A1:2379:U:H2'	38:A1:2380:U:C6	2.55	0.41
38:A1:2770:G:H2'	38:A1:2771:U:C6	2.55	0.41
42:AE:68:PRO:HB2	42:AE:71:VAL:HB	2.01	0.41
45:AH:86:TYR:CD2	45:AH:151:VAL:HB	2.55	0.41
55:AS:73:LYS:NZ	55:AS:97:VAL:O	2.46	0.41
59:AW:5:ILE:HD13	59:AW:5:ILE:HA	1.89	0.41
80:tP:60:A:OP2	80:tP:60:A:H8	2.03	0.41
1:BA:190:ASP:OD1	1:BA:190:ASP:N	2.52	0.41
4:BE:251:GLU:HA	4:BE:254:ARG:HG2	2.01	0.41
5:BG:21:GLU:HA	5:BG:24:ILE:HG12	2.02	0.41
5:BG:174:LYS:HG3	34:B5:78:A:H2	1.84	0.41
6:BH:64:VAL:HA	6:BH:67:LEU:HD23	2.02	0.41
21:BK:32:HIS:HB2	21:BK:39:ASN:HA	2.02	0.41
28:BZ:34:ASP:OD1	28:BZ:34:ASP:N	2.49	0.41
31:Bg:126:SER:OG	31:Bg:127:ARG:N	2.53	0.41
34:B5:297:U:H2'	34:B5:298:C:C6	2.55	0.41
34:B5:891:A:H2'	34:B5:892:A:C8	2.54	0.41
34:B5:1534:G:O2'	34:B5:1535:U:OP2	2.36	0.41
37:AC:51:ALA:O	40:A4:26:U:O2'	2.37	0.41
38:A1:38:U:H2'	38:A1:39:A:O4'	2.21	0.41
38:A1:407:A:C2	40:A4:17:A:H1'	2.55	0.41
38:A1:649:A:H2'	38:A1:650:C:C6	2.55	0.41
38:A1:1486:G:H21	69:Ag:6:THR:HG22	1.85	0.41
38:A1:2225:U:H2'	38:A1:2226:U:C6	2.55	0.41
38:A1:2520:A:H2'	38:A1:2521:U:C6	2.55	0.41
38:A1:3320:A:H2'	38:A1:3321:C:C6	2.55	0.41
40:A4:146:U:H2'	40:A4:147:U:C6	2.55	0.41
55:AS:8:GLN:HB3	55:AS:64:ILE:HD11	2.03	0.41
63:Aa:76:ASP:OD1	63:Aa:77:LYS:N	2.53	0.41
65:Ac:51:LEU:HD11	69:Ag:91:ARG:HA	2.02	0.41
5:BG:5:ILE:HG22	5:BG:113:ILE:HD11	2.02	0.41
5:BG:132:ARG:HD2	5:BG:132:ARG:HA	1.88	0.41
16:Ba:90:GLU:OE1	16:Ba:90:GLU:N	2.54	0.41
20:BF:84:LYS:NZ	34:B5:1614:A:OP2	2.42	0.41
25:BS:38:VAL:HG23	25:BS:42:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:271:VAL:HG23	31:Bg:272:ASP:H	1.85	0.41
33:BM:58:LEU:HD21	33:BM:126:TRP:HE1	1.84	0.41
34:B5:158:U:O2'	34:B5:159:U:H3'	2.20	0.41
34:B5:640:U:H2'	34:B5:641:G:O4'	2.19	0.41
34:B5:1087:A:H2'	34:B5:1088:A:C8	2.55	0.41
34:B5:1592:A:H2'	34:B5:1593:A:H8	1.84	0.41
35:AA:21:ARG:HD3	38:A1:824:C:H5''	2.03	0.41
37:AC:125:ALA:O	37:AC:129:THR:HG23	2.20	0.41
37:AC:169:LEU:HB3	37:AC:174:ALA:HB3	2.02	0.41
38:A1:293:C:H2'	38:A1:294:U:O4'	2.21	0.41
38:A1:1120:A:H2'	38:A1:1121:U:H6	1.84	0.41
38:A1:1580:A:H2	60:AX:33:ARG:HD3	1.85	0.41
38:A1:2111:G:H1'	59:AW:44:LYS:HD2	2.01	0.41
38:A1:3166:C:H2'	38:A1:3167:A:H8	1.85	0.41
39:A3:71:G:H2'	39:A3:72:A:C8	2.55	0.41
41:AD:108:ARG:NE	41:AD:253:PHE:HB2	2.35	0.41
51:AO:7[A]:VAL:HB	51:AO:33[A]:ILE:HD13	2.01	0.41
51:AO:188[A]:SER:O	51:AO:192[A]:LYS:HG2	2.19	0.41
54:AR:167:ARG:NE	54:AR:171:ASP:OD2	2.53	0.41
62:AZ:75:VAL:HG12	62:AZ:76:ASN:O	2.20	0.41
79:E:32:VAL:HG21	79:E:179:LEU:HD11	2.02	0.41
24:BR:16:LEU:HD22	24:BR:38:ILE:HD12	2.02	0.41
31:Bg:20:VAL:HG13	31:Bg:36:ALA:O	2.20	0.41
31:Bg:61:PHE:HB3	31:Bg:92:TRP:CE3	2.56	0.41
35:AA:10:LYS:HA	35:AA:16:PHE:CD2	2.55	0.41
37:AC:120:TYR:CE2	37:AC:277:PRO:HB3	2.56	0.41
38:A1:39:A:H5''	63:Aa:35:ALA:HB2	2.02	0.41
38:A1:251:G:O2'	38:A1:253:A:O4'	2.35	0.41
38:A1:314:U:H2'	38:A1:315:C:C6	2.55	0.41
38:A1:2512:C:H5'	44:AG:249:ARG:HH12	1.83	0.41
38:A1:2842:U:OP1	38:A1:2844:C:N4	2.48	0.41
45:AH:23:ARG:HB2	45:AH:39:LYS:HG2	2.01	0.41
62:AZ:9:LYS:HA	62:AZ:9:LYS:HD3	1.79	0.41
1:BA:33:GLN:NE2	1:BA:153:SER:HG	2.17	0.41
4:BE:181:VAL:HG12	4:BE:227:VAL:HA	2.02	0.41
5:BG:2:LYS:NZ	5:BG:17:GLU:OE2	2.43	0.41
8:BJ:135:ALA:HA	8:BJ:140:ILE:HA	2.01	0.41
11:BO:42:VAL:HG13	11:BO:63:ALA:HB1	2.02	0.41
24:BR:58:MET:HB2	24:BR:58:MET:HE2	1.59	0.41
25:BS:117:LYS:HE3	25:BS:128:PHE:HB2	2.02	0.41
25:BS:144:ARG:NH2	34:B5:1461:C:H5''	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BZ:75:LEU:HA	28:BZ:78:ILE:HG22	2.02	0.41
31:Bg:123:ILE:HG12	31:Bg:133:VAL:HG22	2.01	0.41
34:B5:925:G:H2'	34:B5:926:A:H8	1.85	0.41
34:B5:1223:A:H2'	34:B5:1224:A:C8	2.55	0.41
36:AB:252:ILE:HG12	38:A1:2393:G:H4'	2.02	0.41
38:A1:94:G:H2'	38:A1:95:A:C8	2.56	0.41
38:A1:209:A:H4'	38:A1:211:A:C8	2.56	0.41
38:A1:571:U:H2'	38:A1:572:A:C8	2.52	0.41
38:A1:1348:U:O4'	38:A1:1351:U:H1'	2.20	0.41
39:A3:95:A:N3	55:AS:119:ARG:HD2	2.35	0.41
55:AS:43:TYR:CZ	55:AS:47:LYS:HD2	2.56	0.41
59:AW:8:PHE:CD1	59:AW:46:PRO:HG3	2.56	0.41
81:tA:28:A:H2'	81:tA:29:G:H8	1.85	0.41
3:BC:208:GLU:OE2	3:BC:212:LYS:HD2	2.20	0.41
5:BG:74:LYS:HA	5:BG:96:SER:HA	2.03	0.41
5:BG:92:ARG:NH1	34:B5:1674:C:OP1	2.47	0.41
7:BI:135:LYS:HD2	7:BI:135:LYS:HA	1.84	0.41
9:BL:99:ARG:HG2	14:BX:9:LEU:HA	2.03	0.41
23:BQ:86:ALA:HB2	23:BQ:116:LEU:HD12	2.02	0.41
24:BR:24:LEU:HD13	24:BR:58:MET:HE1	2.01	0.41
25:BS:138:THR:HG22	34:B5:1459:C:H2'	2.02	0.41
34:B5:1259:U:H2'	34:B5:1260:U:C6	2.55	0.41
34:B5:1363:U:O2'	34:B5:1364:G:OP2	2.28	0.41
36:AB:28:ARG:H	36:AB:28:ARG:HG2	1.70	0.41
38:A1:359:U:H2'	38:A1:360:G:O4'	2.20	0.41
38:A1:737:G:H2'	38:A1:738:A:H8	1.86	0.41
38:A1:1579:C:H2'	38:A1:1580:A:O4'	2.21	0.41
38:A1:1666:G:H2'	38:A1:1667:A:C8	2.56	0.41
38:A1:2273:G:N2	38:A1:2311:G:H2'	2.35	0.41
38:A1:2364:G:H22	38:A1:2396:G:H1'	1.86	0.41
38:A1:2816:G:N2	38:A1:2819:A:OP2	2.52	0.41
38:A1:3094:A:H2'	38:A1:3095:U:C6	2.56	0.41
38:A1:3215:A:H5''	68:Af:2:ALA:HB2	2.02	0.41
39:A3:44:C:H2'	39:A3:45:A:H8	1.86	0.41
39:A3:96:U:H2'	39:A3:97:A:H8	1.86	0.41
46:AI:68:ALA:HB2	46:AI:158:LYS:HB2	2.02	0.41
48:AL:86:THR:HG22	48:AL:88:ALA:H	1.85	0.41
48:AL:174:ARG:HB2	71:AI:9:ILE:HD12	2.03	0.41
55:AS:139:TYR:HD1	55:AS:140:VAL:HG23	1.86	0.41
62:AZ:77:TYR:CD2	65:Ac:35:ARG:HD3	2.56	0.41
69:Ag:74:ARG:CZ	69:Ag:82:ALA:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:137:ILE:HG21	2:BB:172:LEU:HD22	2.03	0.41
3:BC:235:LEU:HD21	12:BV:54:ALA:HB2	2.02	0.41
5:BG:160:ARG:O	5:BG:170:THR:HA	2.21	0.41
8:BJ:123:HIS:CD2	18:Be:37:ARG:HH11	2.38	0.41
14:BX:69:ARG:HD3	14:BX:69:ARG:HA	1.86	0.41
15:BY:65:GLY:H	34:B5:532:U:P	2.42	0.41
34:B5:1587:A:H2'	34:B5:1588:G:H8	1.86	0.41
38:A1:209:A:H4'	38:A1:211:A:N7	2.36	0.41
38:A1:761:A:H2'	38:A1:762:U:H6	1.86	0.41
38:A1:1473:G:H5''	54:AR:23:TRP:CD1	2.56	0.41
38:A1:1770:G:H2'	38:A1:1771:C:C6	2.55	0.41
38:A1:2450:G:H22	38:A1:2496:C:H42	1.68	0.41
38:A1:3109:G:H1'	45:AH:163:GLN:HE22	1.85	0.41
47:AJ:110:ILE:H	47:AJ:110:ILE:HD12	1.86	0.41
58:AV:10:LYS:HD3	58:AV:125:LEU:HD11	2.02	0.41
65:Ac:50:VAL:HA	65:Ac:53:LYS:HG2	2.02	0.41
6:BH:51:VAL:HG23	6:BH:53:GLY:H	1.85	0.41
18:Be:36:LYS:HA	18:Be:36:LYS:HD3	1.84	0.41
20:BF:126:ASP:OD1	20:BF:126:ASP:N	2.53	0.41
20:BF:185:ARG:HH12	34:B5:1572:G:N2	2.16	0.41
23:BQ:87:LYS:HB3	23:BQ:87:LYS:HE2	1.78	0.41
26:BT:39:THR:HA	26:BT:100:ILE:HD12	2.03	0.41
29:Bc:12:VAL:HA	29:Bc:30:VAL:HG12	2.03	0.41
34:B5:86:A:H2'	34:B5:87:C:C6	2.55	0.41
34:B5:1787:C:H2'	34:B5:1788:G:C8	2.56	0.41
36:AB:123:TYR:CZ	36:AB:124:LYS:HG3	2.56	0.41
36:AB:286:GLY:HA3	36:AB:321:PHE:CE1	2.56	0.41
38:A1:68:C:O3'	50:AN:177:GLY:HA2	2.20	0.41
38:A1:1184:A:H2'	38:A1:1185:C:C6	2.55	0.41
38:A1:2418:G:N7	83:eI:73:LEU:HD21	2.36	0.41
38:A1:3006:A:H2'	38:A1:3007:U:O4'	2.21	0.41
38:A1:3083:G:H2'	38:A1:3084:C:O4'	2.21	0.41
44:AG:121:SER:OG	44:AG:122:LYS:N	2.53	0.41
46:AI:70:ILE:HG12	81:tA:54:A:H4'	2.02	0.41
51:AO:186[A]:ALA:O	51:AO:187[A]:GLU:HG2	2.21	0.41
56:AT:57:TYR:HA	56:AT:60:LYS:HG2	2.03	0.41
59:AW:13:ILE:HD12	59:AW:30:ARG:HB3	2.03	0.41
1:BA:205:ARG:NH2	24:BR:84:TYR:HB3	2.36	0.41
2:BB:45:LYS:HB2	2:BB:45:LYS:HE2	1.84	0.41
4:BE:100:ARG:NH2	4:BE:118:GLU:O	2.53	0.41
4:BE:199:GLU:OE1	4:BE:201:HIS:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:14:LYS:HD3	5:BG:16:PHE:CZ	2.56	0.41
5:BG:197:ASN:OD1	5:BG:198:ALA:N	2.54	0.41
7:BI:60:ILE:HD11	7:BI:179:CYS:HB2	2.03	0.41
8:BJ:144:PRO:HD2	34:B5:474:A:H5''	2.03	0.41
11:BO:121:VAL:O	34:B5:886:U:O2'	2.39	0.41
20:BF:45:LYS:HD3	20:BF:46:TRP:CH2	2.55	0.41
20:BF:70:VAL:HG13	20:BF:72:HIS:H	1.86	0.41
20:BF:100:ASN:HB2	20:BF:180:ARG:HD3	2.03	0.41
20:BF:114:ILE:HD13	20:BF:114:ILE:HA	1.94	0.41
21:BK:49:LEU:O	21:BK:52:LYS:HB2	2.21	0.41
24:BR:31:ASN:HD22	24:BR:55:THR:HB	1.85	0.41
28:BZ:99:ALA:HB1	28:BZ:101:TYR:HE1	1.86	0.41
31:Bg:9:LEU:HD23	31:Bg:9:LEU:H	1.85	0.41
34:B5:183:U:H2'	34:B5:184:C:C6	2.56	0.41
34:B5:510:G:H2'	34:B5:511:A:C8	2.55	0.41
34:B5:604:A:H2'	34:B5:605:A:O4'	2.21	0.41
34:B5:1236:A:H2'	34:B5:1237:G:C8	2.56	0.41
34:B5:1299:G:H2'	34:B5:1300:A:C8	2.56	0.41
34:B5:1556:A:H1'	34:B5:1560:U:OP2	2.21	0.41
34:B5:1650:U:H2'	34:B5:1651:A:C8	2.56	0.41
36:AB:180:GLU:OE2	38:A1:3002:C:O2'	2.33	0.41
37:AC:74:ILE:HD12	37:AC:75:PRO:HD2	2.02	0.41
38:A1:975:C:H2'	38:A1:976:U:C6	2.56	0.41
38:A1:1108:U:H2'	38:A1:1109:U:H6	1.86	0.41
38:A1:1237:G:H3'	38:A1:1238:C:H5''	2.03	0.41
38:A1:1246:G:N2	38:A1:1274:A:OP1	2.54	0.41
38:A1:1498:A:H2'	38:A1:1499:C:C6	2.56	0.41
38:A1:1553:U:H4'	38:A1:1554:U:H5'	2.03	0.41
38:A1:3192:U:H2'	38:A1:3193:C:C6	2.56	0.41
39:A3:90:U:H2'	39:A3:91:G:O4'	2.21	0.41
50:AN:45:PRO:O	50:AN:49:ARG:HG3	2.21	0.41
62:AZ:103:GLN:NE2	62:AZ:106:GLN:OE1	2.53	0.41
63:Aa:35:ALA:O	63:Aa:41:HIS:ND1	2.50	0.41
5:BG:4:ASN:ND2	34:B5:152:U:O2	2.50	0.41
5:BG:154:ARG:O	5:BG:157:VAL:HG12	2.21	0.41
6:BH:137:GLY:HA3	6:BH:153:LEU:HD12	2.02	0.41
7:BI:84:HIS:CE1	7:BI:86:SER:HB2	2.56	0.41
13:BW:113:HIS:HD2	13:BW:117:ARG:NH1	2.19	0.41
23:BQ:22:VAL:HG12	23:BQ:63:ILE:HD11	2.02	0.41
23:BQ:60:PHE:HA	23:BQ:63:ILE:HG22	2.02	0.41
30:Bd:41:GLN:O	30:Bd:45:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:8:VAL:HG13	31:Bg:10:ARG:NH1	2.36	0.41
34:B5:223:U:H2'	34:B5:224:C:H4'	2.02	0.41
34:B5:737:A:O2'	34:B5:738:G:H5''	2.21	0.41
38:A1:955:U:H2'	38:A1:956:U:C6	2.56	0.41
38:A1:1836:C:O2'	38:A1:1842:A:N1	2.48	0.41
38:A1:2813:A:H2'	38:A1:2814:G:O4'	2.21	0.41
44:AG:108:ARG:O	44:AG:112:GLU:HG3	2.21	0.41
48:AL:156:ALA:HA	63:Aa:101:VAL:HG23	2.02	0.41
50:AN:22:LEU:HD23	50:AN:22:LEU:HA	1.89	0.41
55:AS:75:PHE:O	55:AS:93:GLU:HA	2.21	0.41
61:AY:109:LEU:HD22	61:AY:115:ARG:NH2	2.35	0.41
77:Ao:72:LEU:HD11	77:Ao:83:LEU:HD12	2.02	0.41
1:BA:180:GLU:O	1:BA:184:LEU:HG	2.21	0.40
2:BB:108:ASP:OD1	2:BB:109:LYS:N	2.53	0.40
19:BD:70:THR:O	19:BD:74:GLN:HB2	2.20	0.40
28:BZ:52:LYS:HE3	28:BZ:53:GLU:HB3	2.03	0.40
31:Bg:300:THR:HB	31:Bg:314:GLN:HE21	1.85	0.40
33:BM:59:LEU:O	33:BM:122:VAL:HA	2.21	0.40
34:B5:973:A:H5''	34:B5:973:A:H8	1.86	0.40
34:B5:1144:U:H2'	34:B5:1145:U:C6	2.56	0.40
34:B5:1291:G:H22	34:B5:1324:G:N2	2.19	0.40
38:A1:759:U:H2'	38:A1:760:G:O4'	2.22	0.40
38:A1:2430:A:H2'	38:A1:2431:C:C6	2.56	0.40
38:A1:3359:A:H2'	38:A1:3360:C:C6	2.56	0.40
44:AG:185:ARG:O	44:AG:188:THR:HG22	2.21	0.40
46:AI:189:GLU:HA	46:AI:200:LEU:HB3	2.03	0.40
50:AN:8:GLU:OE1	50:AN:50:ARG:NH2	2.53	0.40
51:AO:174[A]:PHE:O	51:AO:178[A]:VAL:HG23	2.21	0.40
73:Ak:24:THR:HG22	73:Ak:76:ASN:HB3	2.02	0.40
77:Ao:99:GLN:HB3	77:Ao:102:GLN:HG3	2.03	0.40
3:BC:148:LEU:HD23	3:BC:148:LEU:HA	1.87	0.40
4:BE:27:TYR:O	34:B5:447:U:O2'	2.37	0.40
8:BJ:63:ASP:OD1	8:BJ:63:ASP:N	2.54	0.40
23:BQ:10:PHE:HA	23:BQ:18:ALA:O	2.22	0.40
31:Bg:149:ASP:H	31:Bg:175:ASP:HB3	1.86	0.40
34:B5:236:A:H3'	34:B5:237:C:H6	1.86	0.40
34:B5:250:C:H2'	34:B5:251:A:C8	2.55	0.40
34:B5:791:A:H2'	34:B5:792:U:C6	2.56	0.40
34:B5:1466:G:O2'	34:B5:1602:C:OP1	2.34	0.40
35:AA:147:ARG:HG2	35:AA:157:VAL:HG22	2.02	0.40
38:A1:141:C:H2'	38:A1:142:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:650:C:H2'	38:A1:651:G:C8	2.57	0.40
38:A1:2452:G:H8	38:A1:2452:G:OP2	2.04	0.40
38:A1:2609:A:H2'	38:A1:2610:G:C8	2.56	0.40
38:A1:2881:C:H2'	38:A1:2882:U:C6	2.56	0.40
38:A1:3017:A:N1	38:A1:3037:U:H5	2.19	0.40
38:A1:3166:C:H2'	38:A1:3167:A:C8	2.55	0.40
38:A1:3201:C:H2'	38:A1:3202:G:H8	1.86	0.40
38:A1:3371:G:H2'	38:A1:3372:A:C8	2.56	0.40
46:AI:72:ALA:HB2	46:AI:155:ALA:HB2	2.03	0.40
47:AJ:83:GLY:HA3	47:AJ:127:PHE:HE2	1.85	0.40
60:AX:63:ILE:HD13	60:AX:86:VAL:HG12	2.02	0.40
74:AI:44:TRP:CE2	74:AI:45:ARG:HG3	2.56	0.40
79:E:179:LEU:HD12	79:E:179:LEU:HA	1.94	0.40
2:BB:97:LEU:HB3	2:BB:232:HIS:CD2	2.56	0.40
9:BL:53:TYR:CG	9:BL:113:PRO:HG2	2.56	0.40
11:BO:72:LYS:O	11:BO:73:GLU:HG3	2.21	0.40
11:BO:131:GLY:O	16:Ba:22:ARG:NH2	2.54	0.40
15:BY:12:VAL:HG23	34:B5:783:G:H5'	2.04	0.40
31:Bg:10:ARG:NH2	31:Bg:314:GLN:HB2	2.36	0.40
34:B5:97:C:H2'	34:B5:98:U:C6	2.56	0.40
34:B5:688:G:H2'	34:B5:689:G:H8	1.87	0.40
34:B5:939:A:H2'	34:B5:940:A:C8	2.56	0.40
38:A1:1351:U:H5'	38:A1:1352:A:C8	2.56	0.40
38:A1:2106:A:H2'	38:A1:2107:A:H8	1.86	0.40
39:A3:94:C:H2'	39:A3:95:A:C8	2.56	0.40
40:A4:63:G:OP1	40:A4:90:U:H5''	2.21	0.40
40:A4:78:G:H2'	40:A4:79:A:C8	2.56	0.40
45:AH:10:ILE:HB	45:AH:53:ILE:HB	2.04	0.40
45:AH:36:LYS:HE2	45:AH:36:LYS:HB2	1.97	0.40
47:AJ:28:ASP:OD2	47:AJ:32:ARG:NE	2.54	0.40
57:AU:93:ILE:HA	57:AU:106:ALA:O	2.21	0.40
59:AW:18:GLY:HA3	59:AW:31:PHE:O	2.20	0.40
79:E:23:THR:OG1	79:E:24:LYS:N	2.54	0.40
80:tP:1:A:H2'	80:tP:2:G:C8	2.56	0.40
81:tA:21:A:N6	81:tA:46:G:H2'	2.31	0.40
1:BA:31:VAL:HA	1:BA:34:GLU:HG2	2.02	0.40
1:BA:117:GLU:HG3	3:BC:40:LYS:NZ	2.35	0.40
5:BG:65:GLN:HG3	34:B5:1681:A:C8	2.50	0.40
7:BI:37:LYS:C	7:BI:59:ARG:HA	2.46	0.40
10:BN:87:ASP:N	10:BN:87:ASP:OD1	2.53	0.40
13:BW:2:THR:N	34:B5:1034:C:O2'	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:142:LEU:HD12	19:BD:148:LYS:HE3	2.03	0.40
20:BF:57:SER:HA	29:Bc:53:ILE:HB	2.02	0.40
25:BS:13:HIS:ND1	25:BS:14:ILE:HG12	2.36	0.40
28:BZ:50:ILE:HD13	28:BZ:69:LEU:HD13	2.04	0.40
28:BZ:97:LYS:HE3	28:BZ:97:LYS:HB2	1.90	0.40
31:Bg:255:ALA:HB2	31:Bg:292:LEU:HD23	2.02	0.40
34:B5:976:G:N1	34:B5:1023:A:O2'	2.49	0.40
36:AB:346:THR:HA	36:AB:351:LEU:HD22	2.02	0.40
38:A1:516:A:H2'	38:A1:517:G:H8	1.85	0.40
38:A1:2737:C:O2'	64:Ab:36:ASP:OD1	2.33	0.40
38:A1:2747:A:H2'	38:A1:2748:A:C8	2.57	0.40
38:A1:2812:C:H2'	38:A1:2813:A:C8	2.57	0.40
38:A1:2961:G:H2'	38:A1:2962:U:C6	2.57	0.40
38:A1:3165:A:H61	38:A1:3285:C:H42	1.69	0.40
43:AF:120:THR:HB	56:AT:132:PRO:HB2	2.02	0.40
52:AP:112:LEU:HD23	52:AP:112:LEU:HA	1.94	0.40
55:AS:46:GLN:HE22	55:AS:52:LYS:HB3	1.87	0.40
70:Ah:86:ARG:O	70:Ah:90:ARG:HG2	2.22	0.40
76:An:9:ARG:HA	76:An:12:ARG:HE	1.87	0.40
79:E:10:ARG:HA	79:E:10:ARG:HD3	1.94	0.40
1:BA:140:ASN:HD22	3:BC:62:PRO:HD3	1.86	0.40
6:BH:81:LEU:HD23	6:BH:81:LEU:HA	1.94	0.40
8:BJ:62:ARG:HD3	8:BJ:66:ASP:OD2	2.21	0.40
10:BN:47:PRO:HG3	10:BN:75:LEU:HD12	2.03	0.40
22:BP:116:LEU:HD23	22:BP:116:LEU:HA	1.86	0.40
23:BQ:95:LYS:C	31:Bg:59:ARG:HH12	2.30	0.40
25:BS:13:HIS:CE1	25:BS:14:ILE:HG23	2.56	0.40
28:BZ:85:LYS:HA	28:BZ:85:LYS:HD3	1.89	0.40
29:Bc:35:ASP:OD1	29:Bc:35:ASP:N	2.55	0.40
32:Bf:137:ASP:OD1	32:Bf:137:ASP:N	2.50	0.40
33:BM:60:VAL:HG12	33:BM:122:VAL:HG22	2.03	0.40
34:B5:536:C:H2'	34:B5:537:G:O4'	2.21	0.40
34:B5:729:G:H3'	34:B5:730:G:O4'	2.22	0.40
34:B5:861:U:O2'	34:B5:862:A:OP1	2.38	0.40
34:B5:1017:U:H2'	34:B5:1018:U:C6	2.56	0.40
34:B5:1669:U:H2'	34:B5:1670:G:O4'	2.20	0.40
36:AB:39:LYS:HZ1	36:AB:184:ASN:HB3	1.87	0.40
38:A1:830:A:H2'	38:A1:831:G:O4'	2.21	0.40
38:A1:993:G:N3	38:A1:2637:A:H2'	2.36	0.40
38:A1:1555:U:H5'	38:A1:1556:C:OP2	2.21	0.40
38:A1:1827:C:H2'	38:A1:1828:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3252:G:H2'	38:A1:3253:G:C8	2.55	0.40
52:AP:113:TYR:CD1	52:AP:153:LYS:HG2	2.57	0.40
56:AT:137:GLU:HG3	56:AT:138:SER:H	1.86	0.40
61:AY:51:ARG:HD2	61:AY:115:ARG:HH11	1.87	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%)	186 (91%)	18 (9%)	0	100	100
2	BB	212/255 (83%)	182 (86%)	30 (14%)	0	100	100
3	BC	215/254 (85%)	203 (94%)	12 (6%)	0	100	100
4	BE	258/261 (99%)	238 (92%)	20 (8%)	0	100	100
5	BG	224/236 (95%)	216 (96%)	8 (4%)	0	100	100
6	BH	182/190 (96%)	167 (92%)	15 (8%)	0	100	100
7	BI	184/200 (92%)	166 (90%)	18 (10%)	0	100	100
8	BJ	183/197 (93%)	171 (93%)	12 (7%)	0	100	100
9	BL	153/156 (98%)	140 (92%)	13 (8%)	0	100	100
10	BN	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
11	BO	125/137 (91%)	110 (88%)	15 (12%)	0	100	100
12	BV	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
13	BW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
14	BX	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
15	BY	132/135 (98%)	122 (92%)	10 (8%)	0	100	100
16	Ba	95/119 (80%)	85 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Bb	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
18	Be	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
19	BD	221/240 (92%)	207 (94%)	14 (6%)	0	100	100
20	BF	204/225 (91%)	189 (93%)	15 (7%)	0	100	100
21	BK	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
22	BP	122/142 (86%)	113 (93%)	9 (7%)	0	100	100
23	BQ	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
24	BR	117/136 (86%)	113 (97%)	4 (3%)	0	100	100
25	BS	143/146 (98%)	134 (94%)	9 (6%)	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	100/108 (93%)	98 (98%)	2 (2%)	0	100	100
29	Bc	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	284 (92%)	26 (8%)	0	100	100
32	Bf	73/152 (48%)	69 (94%)	4 (6%)	0	100	100
33	BM	122/143 (85%)	108 (88%)	14 (12%)	0	100	100
35	AA	245/254 (96%)	236 (96%)	9 (4%)	0	100	100
36	AB	383/387 (99%)	369 (96%)	14 (4%)	0	100	100
37	AC	359/362 (99%)	339 (94%)	20 (6%)	0	100	100
41	AD	290/297 (98%)	274 (94%)	16 (6%)	0	100	100
42	AE	163/176 (93%)	152 (93%)	11 (7%)	0	100	100
43	AF	220/244 (90%)	212 (96%)	8 (4%)	0	100	100
44	AG	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
45	AH	188/191 (98%)	172 (92%)	16 (8%)	0	100	100
46	AI	215/221 (97%)	207 (96%)	8 (4%)	0	100	100
47	AJ	167/174 (96%)	156 (93%)	11 (7%)	0	100	100
48	AL	191/199 (96%)	183 (96%)	8 (4%)	0	100	100
49	AM	134/138 (97%)	126 (94%)	8 (6%)	0	100	100
50	AN	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	181 (97%)	5 (3%)	0	100	100
55	AS	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
56	AT	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
57	AU	98/121 (81%)	94 (96%)	4 (4%)	0	100	100
58	AV	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
59	AW	61/155 (39%)	61 (100%)	0	0	100	100
60	AX	119/142 (84%)	116 (98%)	3 (2%)	0	100	100
61	AY	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
62	AZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
63	Aa	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
64	Ab	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
67	Ae	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
68	Af	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
69	Ag	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
70	Ah	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
71	Ai	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
72	Aj	85/88 (97%)	84 (99%)	1 (1%)	0	100	100
73	Ak	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
74	Al	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
75	Am	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	92 (89%)	11 (11%)	0	100	100
78	Ap	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
79	E	215/217 (99%)	199 (93%)	16 (7%)	0	100	100
83	eI	152/155 (98%)	131 (86%)	21 (14%)	0	100	100
All	All	11319/12258 (92%)	10641 (94%)	678 (6%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	84/89 (94%)	84 (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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
79	E	198/198 (100%)	198 (100%)	0	100	100
83	eI	118/129 (92%)	118 (100%)	0	100	100
All	All	9631/10315 (93%)	9631 (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 (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	15	GLN
1	BA	32	HIS
2	BB	146	GLN
2	BB	149	GLN
3	BC	94	GLN
3	BC	110	HIS
3	BC	189	GLN
4	BE	17	HIS
4	BE	188	ASN

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Mol	Chain	Res	Type
4	BE	216	ASN
4	BE	223	ASN
5	BG	22	HIS
5	BG	176	GLN
5	BG	185	GLN
5	BG	189	HIS
6	BH	5	GLN
6	BH	150	GLN
6	BH	170	GLN
6	BH	180	GLN
7	BI	35	ASN
7	BI	119	GLN
8	BJ	48	GLN
8	BJ	112	GLN
8	BJ	176	ASN
9	BL	14	GLN
9	BL	21	ASN
9	BL	127	GLN
10	BN	5	HIS
10	BN	138	ASN
12	BV	33	GLN
13	BW	42	GLN
14	BX	22	ASN
14	BX	27	ASN
14	BX	89	ASN
15	BY	63	GLN
15	BY	107	GLN
16	Ba	80	HIS
18	Be	17	GLN
19	BD	22	ASN
20	BF	34	GLN
20	BF	104	ASN
20	BF	127	GLN
20	BF	224	ASN
21	BK	47	GLN
21	BK	81	ASN
23	BQ	62	ASN
23	BQ	74	HIS
25	BS	12	GLN
25	BS	21	ASN
25	BS	25	ASN
25	BS	89	GLN

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Mol	Chain	Res	Type
26	BT	64	HIS
27	BU	105	GLN
30	Bd	53	ASN
31	Bg	101	GLN
31	Bg	159	ASN
31	Bg	268	GLN
33	BM	125	ASN
35	AA	47	GLN
36	AB	121	ASN
36	AB	224	HIS
37	AC	5	GLN
37	AC	175	HIS
37	AC	260	GLN
37	AC	304	GLN
37	AC	361	HIS
41	AD	151	GLN
43	AF	64	GLN
44	AG	77	GLN
46	AI	73	ASN
47	AJ	20	ASN
47	AJ	43	GLN
47	AJ	62	ASN
47	AJ	95	ASN
47	AJ	109	HIS
48	AL	99	HIS
48	AL	102	GLN
49	AM	56	GLN
50	AN	15	GLN
50	AN	95	GLN
51	AO	26[A]	GLN
51	AO	31[A]	GLN
52	AP	54	HIS
52	AP	96	GLN
52	AP	121	GLN
52	AP	125	GLN
54	AR	34	GLN
54	AR	39	ASN
54	AR	141	HIS
54	AR	144	GLN
54	AR	166	ASN
55	AS	63	GLN
55	AS	88	HIS

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Mol	Chain	Res	Type
57	AU	25	ASN
57	AU	40	HIS
58	AV	98	ASN
60	AX	137	ASN
61	AY	42	GLN
68	Af	5	HIS
69	Ag	33	GLN
69	Ag	61	GLN
69	Ag	108	GLN
70	Ah	16	GLN
72	Aj	69	HIS
77	Ao	22	GLN
78	Ap	32	GLN
79	E	181	ASN
79	E	197	ASN
83	eI	22	GLN
83	eI	58	HIS
83	eI	88	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1780/1798 (98%)	445 (25%)	22 (1%)
38	A1	3212/3395 (94%)	600 (18%)	23 (0%)
39	A3	120/121 (99%)	12 (10%)	0
40	A4	157/158 (99%)	26 (16%)	0
80	tP	74/75 (98%)	19 (25%)	0
81	tA	75/76 (98%)	16 (21%)	0
82	MR	11/12 (91%)	1 (9%)	0
All	All	5429/5635 (96%)	1119 (20%)	45 (0%)

All (1119) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	25	C
34	B5	26	A
34	B5	34	G
34	B5	47	A
34	B5	57	G

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Mol	Chain	Res	Type
34	B5	60	U
34	B5	61	A
34	B5	68	A
34	B5	71	A
34	B5	72	A
34	B5	73	U
34	B5	75	U
34	B5	76	A
34	B5	77	U
34	B5	78	A
34	B5	79	C
34	B5	94	U
34	B5	104	A
34	B5	114	C
34	B5	115	G
34	B5	116	U
34	B5	126	A
34	B5	127	G
34	B5	128	U
34	B5	130	C
34	B5	131	C
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U
34	B5	138	A
34	B5	140	A
34	B5	141	U
34	B5	144	U
34	B5	145	A
34	B5	149	C
34	B5	153	G
34	B5	156	A
34	B5	158	U
34	B5	160	C
34	B5	161	U
34	B5	176	C
34	B5	178	U
34	B5	179	A
34	B5	188	A
34	B5	190	C

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Mol	Chain	Res	Type
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	195	G
34	B5	196	G
34	B5	197	A
34	B5	199	G
34	B5	200	A
34	B5	211	PSU
34	B5	217	A
34	B5	221	A
34	B5	224	C
34	B5	225	A
34	B5	226	A
34	B5	229	U
34	B5	231	U
34	B5	233	C
34	B5	235	G
34	B5	237	C
34	B5	238	U
34	B5	239	C
34	B5	240	U
34	B5	241	U
34	B5	257	A
34	B5	260	U
34	B5	261	U
34	B5	270	C
34	B5	276	C
34	B5	278	U
34	B5	280	U
34	B5	281	G
34	B5	299	A
34	B5	309	C
34	B5	313	U
34	B5	314	C
34	B5	316	A
34	B5	321	C
34	B5	322	G
34	B5	326	G
34	B5	337	G
34	B5	338	C
34	B5	352	A

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Mol	Chain	Res	Type
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	365	G
34	B5	380	U
34	B5	390	G
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	434	G
34	B5	435	C
34	B5	439	U
34	B5	444	C
34	B5	445	A
34	B5	448	C
34	B5	460	A
34	B5	461	G
34	B5	475	A
34	B5	477	A
34	B5	479	C
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	490	C
34	B5	491	C
34	B5	492	A
34	B5	493	U
34	B5	494	U
34	B5	496	G
34	B5	497	G
34	B5	499	U
34	B5	500	C
34	B5	501	U
34	B5	504	U
34	B5	506	A

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Mol	Chain	Res	Type
34	B5	508	U
34	B5	515	A
34	B5	518	A
34	B5	519	C
34	B5	524	U
34	B5	525	A
34	B5	526	A
34	B5	527	A
34	B5	534	A
34	B5	539	G
34	B5	541	A
34	B5	542	A
34	B5	544	A
34	B5	555	A
34	B5	558	U
34	B5	559	C
34	B5	565	C
34	B5	568	G
34	B5	576	G
34	B5	577	G
34	B5	578	U
34	B5	579	A
34	B5	582	U
34	B5	583	C
34	B5	594	A
34	B5	595	G
34	B5	608	U
34	B5	610	G
34	B5	611	U
34	B5	619	A
34	B5	620	A
34	B5	622	A
34	B5	623	A
34	B5	635	A
34	B5	638	U
34	B5	639	U
34	B5	643	G
34	B5	648	G
34	B5	650	U
34	B5	651	G
34	B5	652	G
34	B5	654	C

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Mol	Chain	Res	Type
34	B5	655	G
34	B5	656	G
34	B5	657	U
34	B5	658	C
34	B5	677	G
34	B5	679	U
34	B5	681	U
34	B5	683	C
34	B5	684	A
34	B5	688	G
34	B5	694	U
34	B5	696	C
34	B5	697	C
34	B5	698	U
34	B5	699	U
34	B5	702	G
34	B5	704	C
34	B5	705	U
34	B5	706	A
34	B5	707	A
34	B5	708	C
34	B5	709	C
34	B5	711	U
34	B5	712	G
34	B5	714	G
34	B5	715	U
34	B5	716	C
34	B5	717	C
34	B5	718	U
34	B5	719	U
34	B5	720	G
34	B5	722	G
34	B5	727	U
34	B5	728	U
34	B5	730	G
34	B5	732	G
34	B5	733	A
34	B5	735	C
34	B5	736	C
34	B5	737	A
34	B5	739	G
34	B5	740	A

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Mol	Chain	Res	Type
34	B5	765	G
34	B5	766	PSU
34	B5	771	A
34	B5	774	A
34	B5	778	G
34	B5	782	U
34	B5	783	G
34	B5	784	C
34	B5	787	G
34	B5	789	A
34	B5	794	U
34	B5	799	A
34	B5	804	A
34	B5	812	A
34	B5	821	U
34	B5	822	U
34	B5	823	G
34	B5	824	G
34	B5	825	U
34	B5	827	C
34	B5	829	A
34	B5	832	U
34	B5	833	U
34	B5	834	G
34	B5	837	G
34	B5	838	G
34	B5	839	U
34	B5	840	U
34	B5	842	C
34	B5	843	U
34	B5	844	A
34	B5	845	G
34	B5	851	U
34	B5	853	G
34	B5	860	U
34	B5	862	A
34	B5	863	A
34	B5	876	G
34	B5	898	A
34	B5	901	G
34	B5	902	G
34	B5	913	G

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Mol	Chain	Res	Type
34	B5	914	G
34	B5	921	U
34	B5	933	A
34	B5	935	U
34	B5	951	A
34	B5	960	U
34	B5	966	A
34	B5	992	A
34	B5	993	A
34	B5	1003	A
34	B5	1004	U
34	B5	1005	A
34	B5	1020	A
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	1043	A
34	B5	1052	U
34	B5	1053	G
34	B5	1054	U
34	B5	1056	U
34	B5	1058	U
34	B5	1059	U
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1070	C
34	B5	1076	A
34	B5	1081	A
34	B5	1082	C
34	B5	1092	A
34	B5	1093	A
34	B5	1097	U
34	B5	1098	U
34	B5	1100	G
34	B5	1124	A
34	B5	1126	G
34	B5	1138	A
34	B5	1150	G

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Mol	Chain	Res	Type
34	B5	1158	C
34	B5	1159	C
34	B5	1164	G
34	B5	1170	G
34	B5	1180	C
34	B5	1183	A
34	B5	1185	U
34	B5	1186	U
34	B5	1194	A
34	B5	1196	A
34	B5	1197	C
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1202	A
34	B5	1209	C
34	B5	1217	A
34	B5	1218	G
34	B5	1219	A
34	B5	1228	G
34	B5	1229	G
34	B5	1230	A
34	B5	1237	G
34	B5	1239	U
34	B5	1240	U
34	B5	1242	A
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1248	C
34	B5	1250	U
34	B5	1253	U
34	B5	1255	G
34	B5	1257	U
34	B5	1270	G
34	B5	1286	U
34	B5	1307	U
34	B5	1314	U
34	B5	1315	U
34	B5	1318	G
34	B5	1321	A

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Mol	Chain	Res	Type
34	B5	1324	G
34	B5	1338	C
34	B5	1340	U
34	B5	1344	A
34	B5	1345	A
34	B5	1346	A
34	B5	1347	U
34	B5	1353	U
34	B5	1356	U
34	B5	1357	A
34	B5	1358	G
34	B5	1360	A
34	B5	1361	U
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1369	U
34	B5	1370	U
34	B5	1372	U
34	B5	1378	U
34	B5	1390	U
34	B5	1398	U
34	B5	1399	C
34	B5	1413	U
34	B5	1414	U
34	B5	1415	PSU
34	B5	1425	A
34	B5	1427	A
34	B5	1428	G
34	B5	1432	U
34	B5	1433	G
34	B5	1435	G
34	B5	1446	A
34	B5	1459	C
34	B5	1460	A
34	B5	1466	G
34	B5	1471	A
34	B5	1472	C
34	B5	1486	G
34	B5	1489	U
34	B5	1491	U
34	B5	1492	A

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Mol	Chain	Res	Type
34	B5	1493	A
34	B5	1516	A
34	B5	1521	G
34	B5	1522	U
34	B5	1523	G
34	B5	1524	A
34	B5	1536	G
34	B5	1537	C
34	B5	1542	G
34	B5	1554	U
34	B5	1557	U
34	B5	1559	A
34	B5	1573	A
34	B5	1575	G7M
34	B5	1576	A
34	B5	1584	G
34	B5	1590	G
34	B5	1597	A
34	B5	1601	G
34	B5	1607	G
34	B5	1616	G
34	B5	1622	G
34	B5	1635	A
34	B5	1636	C
34	B5	1657	U
34	B5	1658	G
34	B5	1681	A
34	B5	1682	U
34	B5	1683	C
34	B5	1684	U
34	B5	1686	C
34	B5	1687	U
34	B5	1689	A
34	B5	1693	A
34	B5	1695	G
34	B5	1696	G
34	B5	1699	G
34	B5	1700	C
34	B5	1702	A
34	B5	1703	C
34	B5	1705	C
34	B5	1710	U

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Mol	Chain	Res	Type
34	B5	1712	A
34	B5	1713	G
34	B5	1717	G
34	B5	1755	A
34	B5	1756[A]	A
34	B5	1757	G
34	B5	1760	G
34	B5	1762	A
34	B5	1767	G
34	B5	1768	G
34	B5	1769	U
34	B5	1780	G
34	B5	1782	MA6
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1796	C
34	B5	1799	U
38	A1	6	A
38	A1	26	A
38	A1	30	G
38	A1	40	A
38	A1	43	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	93	C
38	A1	99	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	118	U
38	A1	119	U
38	A1	120	G
38	A1	121	A
38	A1	122	A
38	A1	133	U
38	A1	135	C

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Mol	Chain	Res	Type
38	A1	136	G
38	A1	148	G
38	A1	156	G
38	A1	157	A
38	A1	161	G
38	A1	162	G
38	A1	164	A
38	A1	165	A
38	A1	173	G
38	A1	174	C
38	A1	175	C
38	A1	177	U
38	A1	178	U
38	A1	187	A
38	A1	190	U
38	A1	200	C
38	A1	206	G
38	A1	210	U
38	A1	219	A
38	A1	234	G
38	A1	239	G
38	A1	240	U
38	A1	242	C
38	A1	245	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	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	315	C
38	A1	329	U
38	A1	337	G
38	A1	376	G

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Mol	Chain	Res	Type
38	A1	387	A
38	A1	398	A
38	A1	399	A
38	A1	402	A
38	A1	403	C
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	441	U
38	A1	442	G
38	A1	443	G
38	A1	444	U
38	A1	445	G
38	A1	446	U
38	A1	448	U
38	A1	450	G
38	A1	487	U
38	A1	488	U
38	A1	489	U
38	A1	491	A
38	A1	492	C
38	A1	493	U
38	A1	494	G
38	A1	495	G
38	A1	521	A
38	A1	535	G
38	A1	539	C
38	A1	541	U
38	A1	542	G
38	A1	544	C
38	A1	545	U
38	A1	546	C
38	A1	547	G
38	A1	548	G
38	A1	549	U
38	A1	550	A
38	A1	551	A
38	A1	555	U
38	A1	557	A
38	A1	559	A
38	A1	560	G

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Mol	Chain	Res	Type
38	A1	578	A
38	A1	579	G
38	A1	597	G
38	A1	603	A
38	A1	611	A
38	A1	612	U
38	A1	620	U
38	A1	621	A
38	A1	622	A
38	A1	636	C
38	A1	649	A
38	A1	660	A
38	A1	677	A
38	A1	681	U
38	A1	690	A
38	A1	705	A
38	A1	715	A
38	A1	719	U
38	A1	720	A
38	A1	725	G
38	A1	733	G
38	A1	735	A
38	A1	739	G
38	A1	766	U
38	A1	767	U
38	A1	771	A
38	A1	777	U
38	A1	780	A
38	A1	781	G
38	A1	784	A
38	A1	785	G
38	A1	786	A
38	A1	799	G
38	A1	806	A
38	A1	817	A
38	A1	830	A
38	A1	837	A
38	A1	844	G
38	A1	849	C
38	A1	857	G
38	A1	861	C
38	A1	874	U

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Mol	Chain	Res	Type
38	A1	879	U
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	924	G
38	A1	925	A
38	A1	937	G
38	A1	944	C
38	A1	953	G
38	A1	959	C
38	A1	960	PSU
38	A1	977	C
38	A1	980	A
38	A1	982	C
38	A1	991	G
38	A1	994	G
38	A1	1010	G
38	A1	1015	U
38	A1	1016	C
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1021	G
38	A1	1031	C
38	A1	1034	U
38	A1	1045	C
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1081	U
38	A1	1082	U
38	A1	1087	G
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1096	U
38	A1	1097	G

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Mol	Chain	Res	Type
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1131	G
38	A1	1144	U
38	A1	1153	A
38	A1	1154	A
38	A1	1155	C
38	A1	1159	A
38	A1	1160	C
38	A1	1178	G
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1196	C
38	A1	1201	C
38	A1	1208	U
38	A1	1219	C
38	A1	1221	A
38	A1	1222	G
38	A1	1223	A
38	A1	1226	G
38	A1	1227	C
38	A1	1230	G
38	A1	1231	A
38	A1	1232	C
38	A1	1235	U
38	A1	1236	G
38	A1	1237	G
38	A1	1238	C
38	A1	1239	C
38	A1	1241	U
38	A1	1242	G
38	A1	1243	G
38	A1	1245	A
38	A1	1246	G
38	A1	1247	U
38	A1	1249	G
38	A1	1250	G

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Mol	Chain	Res	Type
38	A1	1251	A
38	A1	1252	A
38	A1	1253	U
38	A1	1255	C
38	A1	1256	G
38	A1	1259	A
38	A1	1260	A
38	A1	1261	G
38	A1	1262	G
38	A1	1263	A
38	A1	1264	G
38	A1	1265	U
38	A1	1268	G
38	A1	1270	A
38	A1	1271	A
38	A1	1273	A
38	A1	1275	C
38	A1	1276	U
38	A1	1278	A
38	A1	1279	C
38	A1	1281	G
38	A1	1284	C
38	A1	1285	G
38	A1	1293	U
38	A1	1307	G
38	A1	1309	U
38	A1	1317	A
38	A1	1330	A
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1354	G
38	A1	1355	A
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1399	A
38	A1	1400	G
38	A1	1418	A
38	A1	1419	A

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Mol	Chain	Res	Type
38	A1	1431	G
38	A1	1434	G
38	A1	1437	C
38	A1	1446	A
38	A1	1448	U
38	A1	1449	A
38	A1	1481	A
38	A1	1482	A
38	A1	1483	G
38	A1	1487	G
38	A1	1496	C
38	A1	1525	G
38	A1	1527	C
38	A1	1539	A
38	A1	1555	U
38	A1	1560	G
38	A1	1562	C
38	A1	1567	U
38	A1	1568	U
38	A1	1570	U
38	A1	1572	U
38	A1	1574	C
38	A1	1576	G
38	A1	1578	C
38	A1	1587	A
38	A1	1593	A
38	A1	1605	A
38	A1	1613	A
38	A1	1629	U
38	A1	1630	U
38	A1	1642	A
38	A1	1643	A
38	A1	1657	C
38	A1	1683	A
38	A1	1704	A
38	A1	1715	A
38	A1	1724	U
38	A1	1750	A
38	A1	1751	G
38	A1	1756	C
38	A1	1760	A
38	A1	1762	C

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Mol	Chain	Res	Type
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1778	G
38	A1	1797	A
38	A1	1808	G
38	A1	1809	A
38	A1	1813	A
38	A1	1815	U
38	A1	1816	A
38	A1	1817	G
38	A1	1820	U
38	A1	1821	U
38	A1	1842	A
38	A1	1849	C
38	A1	1867	A
38	A1	1878	G
38	A1	1880	U
38	A1	1886	A
38	A1	1893	A
38	A1	1906	G
38	A1	1943	C
38	A1	1950	U
38	A1	1952	G
38	A1	1953	G
38	A1	1954	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	2188	A
38	A1	2206	G
38	A1	2220	A
38	A1	2225	U
38	A1	2249	G

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Mol	Chain	Res	Type
38	A1	2256	A
38	A1	2257	C
38	A1	2266	PSU
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
38	A1	2279	A
38	A1	2281	A
38	A1	2288	G
38	A1	2307	G
38	A1	2310	U
38	A1	2313	A
38	A1	2315	G
38	A1	2318	U
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2366	C
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2385	G
38	A1	2388	U
38	A1	2391	G
38	A1	2393	G
38	A1	2394	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2421	U
38	A1	2437	G
38	A1	2438	A
38	A1	2439	A
38	A1	2441	A
38	A1	2446	U
38	A1	2449	A
38	A1	2451	G
38	A1	2452	G
38	A1	2453	U

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Mol	Chain	Res	Type
38	A1	2454	G
38	A1	2455	U
38	A1	2458	A
38	A1	2459	A
38	A1	2461	A
38	A1	2462	A
38	A1	2463	G
38	A1	2464	U
38	A1	2468	A
38	A1	2469	G
38	A1	2470	C
38	A1	2473	C
38	A1	2474	G
38	A1	2475	G
38	A1	2478	C
38	A1	2479	C
38	A1	2480	A
38	A1	2481	G
38	A1	2482	U
38	A1	2487	U
38	A1	2488	A
38	A1	2489	C
38	A1	2490	C
38	A1	2492	C
38	A1	2493	U
38	A1	2494	A
38	A1	2500	A
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	2510	U
38	A1	2514	U
38	A1	2515	A
38	A1	2522	G
38	A1	2523	A
38	A1	2524	A
38	A1	2535	A

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Mol	Chain	Res	Type
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
38	A1	2552	C
38	A1	2566	C
38	A1	2569	A
38	A1	2570	U
38	A1	2585	G
38	A1	2593	A
38	A1	2595	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2652	U
38	A1	2656	A
38	A1	2657	A
38	A1	2672	G
38	A1	2674	A
38	A1	2677	G
38	A1	2680	A
38	A1	2681	U
38	A1	2689	A
38	A1	2690	G
38	A1	2691	A
38	A1	2704	A
38	A1	2719	U
38	A1	2724	U
38	A1	2725	U
38	A1	2727	A
38	A1	2728	G
38	A1	2729	U
38	A1	2749	G
38	A1	2752	U
38	A1	2753	G

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Mol	Chain	Res	Type
38	A1	2755	C
38	A1	2762	A
38	A1	2772	C
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2780	A
38	A1	2796	G
38	A1	2799	A
38	A1	2800	G
38	A1	2801	A
38	A1	2802	A
38	A1	2803	A
38	A1	2810	C
38	A1	2814	G
38	A1	2817	A
38	A1	2822	U
38	A1	2842	U
38	A1	2845	A
38	A1	2849	C
38	A1	2860	U
38	A1	2861	U
38	A1	2867	C
38	A1	2871	G
38	A1	2887	A
38	A1	2898	G
38	A1	2923	PSU
38	A1	2935	U
38	A1	2936	A
38	A1	2942	C
38	A1	2947	G
38	A1	2971	A
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3012	A
38	A1	3022	G
38	A1	3032	A
38	A1	3046	A
38	A1	3055	U
38	A1	3056	U
38	A1	3059	G

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Mol	Chain	Res	Type
38	A1	3078	U
38	A1	3079	U
38	A1	3080	G
38	A1	3086	A
38	A1	3092	C
38	A1	3130	A
38	A1	3131	U
38	A1	3142	A
38	A1	3143	C
38	A1	3144	G
38	A1	3151	U
38	A1	3153	U
38	A1	3154	C
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3165	A
38	A1	3169	U
38	A1	3170	A
38	A1	3173	G
38	A1	3174	A
38	A1	3175	U
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3196	U
38	A1	3207	U
38	A1	3213	A
38	A1	3214	U
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3227	A
38	A1	3231	U
38	A1	3234	A
38	A1	3236	U
38	A1	3238	G
38	A1	3242	G
38	A1	3243	A
38	A1	3244	A

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Mol	Chain	Res	Type
38	A1	3247	G
38	A1	3250	U
38	A1	3259	U
38	A1	3263	G
38	A1	3275	U
38	A1	3276	G
38	A1	3279	A
38	A1	3281	U
38	A1	3287	U
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U
38	A1	3313	U
38	A1	3316	A
38	A1	3317	U
38	A1	3318	G
38	A1	3319	U
38	A1	3320	A
38	A1	3341	U
38	A1	3345	G
38	A1	3348	G
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3369	G
38	A1	3378	C
38	A1	3382	U
38	A1	3386	G
38	A1	3390	G
39	A3	7	G
39	A3	33	U
39	A3	52	G
39	A3	54	U
39	A3	55	A
39	A3	60	G
39	A3	65	G
39	A3	76	A
39	A3	102	A
39	A3	109	G
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	70	G
40	A4	81	U
40	A4	82	U
40	A4	83	C
40	A4	84	C
40	A4	86	U
40	A4	90	U
40	A4	95	G
40	A4	104	A
40	A4	106	C
40	A4	111	A
40	A4	112	U
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	127	U
40	A4	152	G
40	A4	158	U
80	tP	9	G
80	tP	13	C
80	tP	16	U
80	tP	18	G
80	tP	19	G
80	tP	20	A
80	tP	21	A
80	tP	23	C
80	tP	25	C
80	tP	46	G
80	tP	47	U
80	tP	48	C
80	tP	49	C
80	tP	51	C
80	tP	60	A
80	tP	64	A

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Mol	Chain	Res	Type
80	tP	68	G
80	tP	70	G
80	tP	76	A
81	tA	2	G
81	tA	5	C
81	tA	9	G
81	tA	15	G
81	tA	16	U
81	tA	17	A
81	tA	18	G
81	tA	19	G
81	tA	20	A
81	tA	38	A
81	tA	46	G
81	tA	47	U
81	tA	48	C
81	tA	49	C
81	tA	74	C
81	tA	76	A
82	MR	8	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	71	A
34	B5	143	G
34	B5	577	G
34	B5	695	U
34	B5	698	U
34	B5	821	U
34	B5	828	U
34	B5	861	U
34	B5	862	A
34	B5	1003	A
34	B5	1055	U
34	B5	1228	G
34	B5	1236	A
34	B5	1239	U
34	B5	1256	A
34	B5	1285	U
34	B5	1344	A
34	B5	1357	A

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Mol	Chain	Res	Type
34	B5	1362	U
34	B5	1363	U
34	B5	1458	G
34	B5	1755	A
38	A1	251	G
38	A1	602	A
38	A1	843	A
38	A1	873	C
38	A1	916	G
38	A1	1094	U
38	A1	1225	A
38	A1	1292	C
38	A1	1356	U
38	A1	1571	A
38	A1	1577	G
38	A1	2372	A
38	A1	2445	A
38	A1	2461	A
38	A1	2468	A
38	A1	2474	G
38	A1	2479	C
38	A1	2487	U
38	A1	2500	A
38	A1	2506	U
38	A1	2544	U
38	A1	2772	C
38	A1	2801	A

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

60 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	$\# Z > 2$
38	PSU	A1	2266	38	18,21,22	1.54	5 (27%)	21,30,33	2.21	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	PSU	A1	2416	38,84	18,21,22	1.66	5 (27%)	21,30,33	2.07	4 (19%)
36	HIC	AB	243	36	10,11,12	1.30	1 (10%)	9,14,16	1.36	2 (22%)
38	PSU	A1	966	38	18,21,22	1.69	5 (27%)	21,30,33	2.09	5 (23%)
38	PSU	A1	2129	38	18,21,22	1.61	4 (22%)	21,30,33	2.15	3 (14%)
38	PSU	A1	990	38	18,21,22	1.47	4 (22%)	21,30,33	2.20	4 (19%)
38	PSU	A1	2880	38	18,21,22	1.62	5 (27%)	21,30,33	2.23	6 (28%)
34	PSU	B5	999	34	18,21,22	1.41	4 (22%)	21,30,33	2.17	5 (23%)
38	PSU	A1	776	38	18,21,22	1.50	4 (22%)	21,30,33	2.00	5 (23%)
38	PSU	A1	1004	38	18,21,22	1.48	4 (22%)	21,30,33	2.12	5 (23%)
38	PSU	A1	2191	38	18,21,22	1.55	4 (22%)	21,30,33	2.17	5 (23%)
38	PSU	A1	1052	38	18,21,22	1.43	4 (22%)	21,30,33	2.03	4 (19%)
40	PSU	A4	73	40	18,21,22	1.45	4 (22%)	21,30,33	2.02	3 (14%)
38	PSU	A1	1124	38	18,21,22	1.51	5 (27%)	21,30,33	2.27	4 (19%)
38	PSU	A1	2264	38	18,21,22	1.44	3 (16%)	21,30,33	2.17	5 (23%)
38	PSU	A1	2351	38	18,21,22	1.52	4 (22%)	21,30,33	2.16	4 (19%)
38	OMU	A1	2921	38,84	19,22,23	1.32	3 (15%)	25,31,34	1.89	6 (24%)
34	B8N	B5	1191	34	25,29,30	1.38	3 (12%)	28,42,45	3.04	6 (21%)
38	PSU	A1	2133	38	18,21,22	1.46	3 (16%)	21,30,33	2.20	5 (23%)
38	PSU	A1	2260	38	18,21,22	1.51	4 (22%)	21,30,33	2.15	3 (14%)
38	UR3	A1	2634	38	19,22,23	0.91	1 (5%)	26,32,35	1.74	4 (15%)
38	PSU	A1	2349	38,84	18,21,22	1.50	4 (22%)	21,30,33	1.97	4 (19%)
38	PSU	A1	2826	38	18,21,22	1.59	6 (33%)	21,30,33	2.26	6 (28%)
38	PSU	A1	2865	38	18,21,22	1.48	6 (33%)	21,30,33	2.19	4 (19%)
34	PSU	B5	302	34	18,21,22	1.48	4 (22%)	21,30,33	2.01	3 (14%)
34	PSU	B5	759	34	18,21,22	1.37	3 (16%)	21,30,33	2.00	3 (14%)
38	PSU	A1	2735	38	18,21,22	1.44	4 (22%)	21,30,33	2.16	4 (19%)
38	PSU	A1	2944	38,84	18,21,22	1.56	5 (27%)	21,30,33	2.23	4 (19%)
38	PSU	A1	1110	38	18,21,22	1.51	5 (27%)	21,30,33	2.01	5 (23%)
34	G7M	B5	1575	80,34	23,26,27	2.45	6 (26%)	34,39,42	3.29	15 (44%)
34	PSU	B5	1290	34	18,21,22	1.40	3 (16%)	21,30,33	2.02	3 (14%)
34	PSU	B5	632	34	18,21,22	1.45	4 (22%)	21,30,33	2.02	3 (14%)
34	4AC	B5	1773	34	21,24,25	1.02	2 (9%)	28,34,37	2.47	6 (21%)
34	MA6	B5	1781	34	23,26,27	1.45	5 (21%)	33,38,41	2.07	10 (30%)
38	PSU	A1	2340	38	18,21,22	1.57	4 (22%)	21,30,33	2.11	4 (19%)
83	5CT	eI	51	-	13,14,15	0.66	0	8,15,17	1.53	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PSU	B5	106	34	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
34	PSU	B5	1415	34	18,21,22	1.44	3 (16%)	21,30,33	2.04	4 (19%)
38	5MC	A1	2870	38	19,22,23	1.27	3 (15%)	26,32,35	1.39	4 (15%)
38	PSU	A1	986	38	18,21,22	1.45	4 (22%)	21,30,33	2.05	4 (19%)
38	5MC	A1	2278	38,84	19,22,23	1.51	3 (15%)	26,32,35	1.35	4 (15%)
34	PSU	B5	120	34	18,21,22	1.40	3 (16%)	21,30,33	2.13	3 (14%)
34	PSU	B5	1187	34	18,21,22	1.47	4 (22%)	21,30,33	2.07	3 (14%)
38	PSU	A1	2314	38	18,21,22	1.50	4 (22%)	21,30,33	2.12	4 (19%)
34	MA6	B5	1782	34	23,26,27	1.46	5 (21%)	33,38,41	2.14	10 (30%)
38	PSU	A1	2258	38	18,21,22	1.43	4 (22%)	21,30,33	2.11	4 (19%)
34	PSU	B5	466	34	18,21,22	1.40	3 (16%)	21,30,33	2.16	4 (19%)
34	4AC	B5	1280	34	21,24,25	1.06	1 (4%)	28,34,37	1.08	3 (10%)
34	PSU	B5	211	34	18,21,22	1.45	4 (22%)	21,30,33	2.10	4 (19%)
34	PSU	B5	1181	34	18,21,22	1.42	4 (22%)	21,30,33	2.15	4 (19%)
38	PSU	A1	1042	38	18,21,22	1.45	3 (16%)	21,30,33	2.12	4 (19%)
38	PSU	A1	1056	38	18,21,22	1.43	4 (22%)	21,30,33	2.07	4 (19%)
39	PSU	A3	50	39	18,21,22	1.38	3 (16%)	21,30,33	2.00	3 (14%)
38	OMG	A1	2922	38,81	23,26,27	1.19	4 (17%)	32,38,41	2.07	7 (21%)
38	PSU	A1	2975	38	18,21,22	1.57	5 (27%)	21,30,33	2.27	4 (19%)
38	1MA	A1	645	38,84	21,25,26	1.33	4 (19%)	30,37,40	1.69	6 (20%)
38	1MA	A1	2142	38	21,25,26	1.30	4 (19%)	30,37,40	1.81	4 (13%)
38	PSU	A1	960	38	18,21,22	1.55	5 (27%)	21,30,33	2.19	4 (19%)
34	PSU	B5	766	34	18,21,22	1.47	4 (22%)	21,30,33	2.09	5 (23%)
38	PSU	A1	2923	38,81	18,21,22	1.53	5 (27%)	21,30,33	2.14	3 (14%)

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
38	PSU	A1	2266	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2416	38,84	-	0/7/25/26	0/2/2/2
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
38	PSU	A1	966	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2129	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	990	38	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	2880	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	999	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	776	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	1004	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2191	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1052	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	1124	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	2351	38	-	0/7/25/26	0/2/2/2
38	OMU	A1	2921	38,84	-	0/9/27/28	0/2/2/2
34	B8N	B5	1191	34	-	4/16/34/35	0/2/2/2
38	PSU	A1	2133	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2260	38	-	2/7/25/26	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2349	38,84	-	0/7/25/26	0/2/2/2
38	PSU	A1	2826	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2865	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	302	34	-	2/7/25/26	0/2/2/2
34	PSU	B5	759	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2735	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2944	38,84	-	0/7/25/26	0/2/2/2
38	PSU	A1	1110	38	-	0/7/25/26	0/2/2/2
34	G7M	B5	1575	80,34	-	0/7/25/26	0/3/3/3
34	PSU	B5	1290	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	632	34	-	0/7/25/26	0/2/2/2
34	4AC	B5	1773	34	-	3/11/29/30	0/2/2/2
34	MA6	B5	1781	34	-	0/11/29/30	0/3/3/3
38	PSU	A1	2340	38	-	1/7/25/26	0/2/2/2
83	5CT	eI	51	-	-	7/13/14/16	-
34	PSU	B5	106	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	1415	34	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
38	PSU	A1	986	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2278	38,84	-	0/7/25/26	0/2/2/2
34	PSU	B5	120	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	2314	38	-	1/7/25/26	0/2/2/2
34	MA6	B5	1782	34	-	3/11/29/30	0/3/3/3
38	PSU	A1	2258	38	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PSU	B5	466	34	-	0/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	4/11/29/30	0/2/2/2
34	PSU	B5	211	34	-	2/7/25/26	0/2/2/2
34	PSU	B5	1181	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	1042	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1056	38	-	0/7/25/26	0/2/2/2
39	PSU	A3	50	39	-	1/7/25/26	0/2/2/2
38	OMG	A1	2922	38,81	-	0/9/27/28	0/3/3/3
38	PSU	A1	2975	38	-	0/7/25/26	0/2/2/2
38	1MA	A1	645	38,84	-	2/7/25/26	0/3/3/3
38	1MA	A1	2142	38	-	0/7/25/26	0/3/3/3
38	PSU	A1	960	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	766	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2923	38,81	-	3/7/25/26	0/2/2/2

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N7	7.10	1.45	1.33
34	B5	1575	G7M	C5-N7	-5.63	1.32	1.39
38	A1	2278	5MC	C5-C4	5.17	1.48	1.44
34	B5	1782	MA6	C5-C4	4.26	1.46	1.39
34	B5	1781	MA6	C5-C4	3.99	1.46	1.39
34	B5	1191	B8N	C4-C5	-3.96	1.38	1.47
34	B5	1575	G7M	C8-N9	3.89	1.46	1.35
38	A1	2416	PSU	C4-N3	-3.65	1.32	1.38
38	A1	2826	PSU	C4-N3	-3.61	1.32	1.38
38	A1	2880	PSU	C4-N3	-3.54	1.32	1.38
38	A1	2191	PSU	C4-N3	-3.52	1.32	1.38
34	B5	1575	G7M	C5-C4	3.49	1.47	1.38
38	A1	966	PSU	C4-N3	-3.43	1.32	1.38
38	A1	2944	PSU	C4-N3	-3.38	1.32	1.38
38	A1	2129	PSU	C4-N3	-3.37	1.32	1.38
38	A1	2870	5MC	C5-C4	3.36	1.46	1.44
34	B5	1415	PSU	C6-C5	3.36	1.39	1.35
38	A1	2923	PSU	C6-C5	3.35	1.39	1.35
38	A1	2975	PSU	C6-C5	3.31	1.39	1.35
38	A1	2260	PSU	C4-N3	-3.28	1.32	1.38
38	A1	1124	PSU	C4-N3	-3.28	1.32	1.38
34	B5	1187	PSU	C6-C5	3.26	1.38	1.35
38	A1	2314	PSU	C4-N3	-3.22	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2349	PSU	C4-N3	-3.21	1.32	1.38
38	A1	1110	PSU	C4-N3	-3.20	1.32	1.38
38	A1	1004	PSU	C4-N3	-3.19	1.32	1.38
38	A1	2351	PSU	C4-N3	-3.19	1.32	1.38
38	A1	2340	PSU	C4-N3	-3.19	1.32	1.38
38	A1	2921	OMU	C4-N3	-3.18	1.33	1.38
39	A3	50	PSU	C6-C5	3.15	1.38	1.35
34	B5	1290	PSU	C6-C5	3.15	1.38	1.35
38	A1	986	PSU	C4-N3	-3.12	1.33	1.38
38	A1	1042	PSU	C4-N3	-3.12	1.33	1.38
38	A1	966	PSU	C6-C5	3.10	1.38	1.35
38	A1	776	PSU	C6-C5	3.07	1.38	1.35
34	B5	999	PSU	C4-N3	-3.07	1.33	1.38
38	A1	960	PSU	C4-N3	-3.07	1.33	1.38
38	A1	2133	PSU	C4-N3	-3.07	1.33	1.38
34	B5	632	PSU	C4-N3	-3.06	1.33	1.38
38	A1	2416	PSU	C2-N3	-3.06	1.32	1.37
38	A1	2264	PSU	C4-N3	-3.06	1.33	1.38
34	B5	120	PSU	C6-C5	3.05	1.38	1.35
38	A1	1052	PSU	C4-N3	-3.05	1.33	1.38
34	B5	766	PSU	C6-C5	3.05	1.38	1.35
34	B5	1187	PSU	C4-N3	-3.04	1.33	1.38
38	A1	2865	PSU	C4-N3	-3.03	1.33	1.38
38	A1	990	PSU	C4-N3	-3.03	1.33	1.38
34	B5	1181	PSU	C4-N3	-3.03	1.33	1.38
38	A1	966	PSU	C2-N3	-3.02	1.32	1.37
38	A1	2921	OMU	C2-N3	-3.02	1.32	1.38
38	A1	2416	PSU	C2-N1	-3.02	1.32	1.36
38	A1	2735	PSU	C4-N3	-3.01	1.33	1.38
34	B5	759	PSU	C6-C5	3.01	1.38	1.35
38	A1	2266	PSU	C4-N3	-3.01	1.33	1.38
38	A1	2880	PSU	C2-N3	-3.01	1.32	1.37
38	A1	776	PSU	C4-N3	-3.00	1.33	1.38
34	B5	211	PSU	C6-C5	2.99	1.38	1.35
34	B5	302	PSU	C4-N3	-2.99	1.33	1.38
38	A1	2129	PSU	C6-C5	2.98	1.38	1.35
38	A1	2191	PSU	C2-N3	-2.97	1.32	1.37
34	B5	466	PSU	C4-N3	-2.97	1.33	1.38
34	B5	1280	4AC	C4-N4	-2.95	1.35	1.39
38	A1	1042	PSU	C6-C5	2.94	1.38	1.35
34	B5	302	PSU	C6-C5	2.93	1.38	1.35
38	A1	2340	PSU	C6-C5	2.93	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	1056	PSU	C4-N3	-2.93	1.33	1.38
38	A1	2923	PSU	C4-N3	-2.93	1.33	1.38
34	B5	1782	MA6	C5-C6	2.91	1.48	1.41
40	A4	73	PSU	C4-N3	-2.91	1.33	1.38
38	A1	2266	PSU	C6-C5	2.91	1.38	1.35
34	B5	466	PSU	C6-C5	2.90	1.38	1.35
38	A1	1056	PSU	C6-C5	2.89	1.38	1.35
38	A1	2975	PSU	C4-N3	-2.89	1.33	1.38
34	B5	106	PSU	C4-N3	-2.88	1.33	1.38
38	A1	2191	PSU	C6-C5	2.87	1.38	1.35
38	A1	2264	PSU	C6-C5	2.87	1.38	1.35
34	B5	766	PSU	C4-N3	-2.86	1.33	1.38
38	A1	2944	PSU	C6-C5	2.86	1.38	1.35
34	B5	759	PSU	C4-N3	-2.86	1.33	1.38
34	B5	1290	PSU	C4-N3	-2.86	1.33	1.38
38	A1	1004	PSU	C6-C5	2.84	1.38	1.35
38	A1	2129	PSU	C2-N3	-2.84	1.32	1.37
38	A1	645	1MA	C5-N7	-2.84	1.33	1.39
38	A1	2826	PSU	C2-N3	-2.84	1.32	1.37
38	A1	960	PSU	O4'-C1'	-2.84	1.39	1.43
38	A1	1124	PSU	C6-C5	2.83	1.38	1.35
38	A1	2133	PSU	C6-C5	2.81	1.38	1.35
34	B5	1415	PSU	C4-N3	-2.80	1.33	1.38
34	B5	106	PSU	C6-C5	2.80	1.38	1.35
38	A1	2922	OMG	C6-N1	-2.78	1.33	1.38
38	A1	2314	PSU	C6-C5	2.78	1.38	1.35
38	A1	645	1MA	C5-C4	2.78	1.46	1.38
38	A1	2351	PSU	C2-N3	-2.77	1.32	1.37
38	A1	2266	PSU	C2-N1	-2.77	1.33	1.36
38	A1	2944	PSU	C2-N3	-2.77	1.32	1.37
39	A3	50	PSU	C4-N3	-2.76	1.33	1.38
34	B5	1781	MA6	C5-C6	2.76	1.48	1.41
34	B5	211	PSU	C4-N3	-2.75	1.33	1.38
38	A1	2258	PSU	C4-N3	-2.75	1.33	1.38
38	A1	2142	1MA	C5-N7	-2.74	1.33	1.39
38	A1	2351	PSU	C6-C5	2.73	1.38	1.35
38	A1	2340	PSU	C2-N3	-2.73	1.33	1.37
38	A1	1052	PSU	C6-C5	2.71	1.38	1.35
34	B5	1181	PSU	C6-C5	2.71	1.38	1.35
40	A4	73	PSU	C6-C5	2.70	1.38	1.35
38	A1	990	PSU	C6-C5	2.70	1.38	1.35
38	A1	2258	PSU	C6-C5	2.70	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2735	PSU	C6-C5	2.69	1.38	1.35
34	B5	120	PSU	C4-N3	-2.69	1.33	1.38
38	A1	966	PSU	C2-N1	-2.69	1.33	1.36
38	A1	645	1MA	C6-N6	2.69	1.34	1.28
38	A1	2278	5MC	C6-N1	-2.68	1.33	1.38
38	A1	2880	PSU	C6-C5	2.67	1.38	1.35
38	A1	2129	PSU	C2-N1	-2.67	1.33	1.36
38	A1	986	PSU	C6-C5	2.67	1.38	1.35
38	A1	2349	PSU	C2-N3	-2.64	1.33	1.37
34	B5	1773	4AC	C4-N4	-2.64	1.35	1.39
38	A1	960	PSU	C6-C5	2.64	1.38	1.35
38	A1	2870	5MC	C6-C5	2.62	1.38	1.34
38	A1	2133	PSU	C2-N3	-2.62	1.33	1.37
38	A1	2314	PSU	C2-N3	-2.62	1.33	1.37
38	A1	2975	PSU	C2-N3	-2.62	1.33	1.37
38	A1	2349	PSU	C6-C5	2.61	1.38	1.35
38	A1	2260	PSU	C2-N3	-2.61	1.33	1.37
38	A1	2870	5MC	C6-N1	-2.60	1.33	1.38
38	A1	2142	1MA	C6-N6	2.60	1.34	1.28
38	A1	2921	OMU	C5-C4	-2.59	1.38	1.43
38	A1	2975	PSU	C2-N1	-2.58	1.33	1.36
38	A1	2922	OMG	C5-C4	2.56	1.45	1.38
34	B5	1781	MA6	C4-N9	-2.56	1.32	1.37
38	A1	2340	PSU	C2-N1	-2.53	1.33	1.36
38	A1	2826	PSU	C2-N1	-2.52	1.33	1.36
34	B5	1781	MA6	C5-N7	-2.51	1.34	1.39
38	A1	2142	1MA	C5-C4	2.51	1.45	1.38
34	B5	1782	MA6	C4-N9	-2.50	1.32	1.37
38	A1	966	PSU	C6-N1	-2.48	1.32	1.36
38	A1	1052	PSU	C2-N3	-2.48	1.33	1.37
38	A1	776	PSU	C2-N3	-2.47	1.33	1.37
34	B5	999	PSU	C2-N3	-2.47	1.33	1.37
34	B5	632	PSU	C2-N3	-2.46	1.33	1.37
38	A1	1110	PSU	C2-N3	-2.44	1.33	1.37
38	A1	1110	PSU	C6-C5	2.44	1.38	1.35
38	A1	1004	PSU	C2-N3	-2.44	1.33	1.37
38	A1	986	PSU	C2-N3	-2.43	1.33	1.37
38	A1	2264	PSU	C2-N3	-2.43	1.33	1.37
34	B5	1782	MA6	C5-N7	-2.43	1.34	1.39
38	A1	1124	PSU	C2-N1	-2.42	1.33	1.36
34	B5	632	PSU	C6-C5	2.42	1.38	1.35
38	A1	2923	PSU	C2-N1	-2.42	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1191	B8N	C6-C5	2.41	1.38	1.35
38	A1	2922	OMG	C5-N7	-2.41	1.34	1.39
34	B5	1575	G7M	C6-N1	-2.40	1.34	1.38
38	A1	2278	5MC	C6-C5	2.40	1.38	1.34
38	A1	960	PSU	C2-N3	-2.39	1.33	1.37
38	A1	2880	PSU	C2-N1	-2.39	1.33	1.36
34	B5	999	PSU	C6-C5	2.39	1.37	1.35
40	A4	73	PSU	C2-N3	-2.38	1.33	1.37
38	A1	2260	PSU	C6-C5	2.37	1.37	1.35
38	A1	1042	PSU	C2-N3	-2.37	1.33	1.37
38	A1	990	PSU	C2-N3	-2.37	1.33	1.37
38	A1	1056	PSU	C2-N3	-2.35	1.33	1.37
38	A1	2351	PSU	C2-N1	-2.35	1.33	1.36
34	B5	766	PSU	O4'-C1'	-2.34	1.40	1.43
38	A1	2865	PSU	C6-N1	-2.33	1.32	1.36
38	A1	990	PSU	C2-N1	-2.33	1.33	1.36
38	A1	2258	PSU	C2-N1	-2.32	1.33	1.36
38	A1	2260	PSU	C2-N1	-2.32	1.33	1.36
38	A1	2944	PSU	C2-N1	-2.32	1.33	1.36
38	A1	2349	PSU	C2-N1	-2.32	1.33	1.36
38	A1	2416	PSU	C6-C5	2.32	1.37	1.35
38	A1	776	PSU	C2-N1	-2.31	1.33	1.36
34	B5	302	PSU	C2-N3	-2.31	1.33	1.37
38	A1	2735	PSU	C2-N3	-2.30	1.33	1.37
38	A1	2416	PSU	C6-N1	-2.28	1.32	1.36
38	A1	2258	PSU	C2-N3	-2.27	1.33	1.37
36	AB	243	HIC	CD2-CG	2.27	1.40	1.36
34	B5	1181	PSU	C2-N3	-2.27	1.33	1.37
40	A4	73	PSU	C2-N1	-2.27	1.33	1.36
38	A1	2865	PSU	C2-N1	-2.26	1.33	1.36
34	B5	211	PSU	C2-N3	-2.25	1.33	1.37
38	A1	2266	PSU	C2-N3	-2.25	1.33	1.37
38	A1	2865	PSU	C2-N3	-2.25	1.33	1.37
34	B5	302	PSU	C2-N1	-2.24	1.33	1.36
38	A1	2314	PSU	C2-N1	-2.23	1.33	1.36
34	B5	1187	PSU	C2-N3	-2.22	1.33	1.37
38	A1	1124	PSU	C2-N3	-2.22	1.33	1.37
38	A1	986	PSU	C2-N1	-2.22	1.33	1.36
34	B5	466	PSU	C2-N3	-2.21	1.33	1.37
38	A1	2922	OMG	C4-N9	-2.21	1.32	1.38
34	B5	1181	PSU	C2-N1	-2.21	1.33	1.36
34	B5	106	PSU	C2-N3	-2.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1781	MA6	C8-N9	-2.20	1.33	1.37
38	A1	1110	PSU	C2-N1	-2.20	1.33	1.36
38	A1	1056	PSU	C2-N1	-2.20	1.33	1.36
38	A1	960	PSU	C2-N1	-2.19	1.33	1.36
34	B5	120	PSU	C2-N3	-2.18	1.33	1.37
38	A1	2865	PSU	C6-C5	2.18	1.37	1.35
38	A1	2142	1MA	C4-N9	-2.17	1.32	1.38
38	A1	2865	PSU	O4'-C1'	-2.17	1.40	1.43
38	A1	2826	PSU	O4'-C1'	-2.17	1.40	1.43
34	B5	766	PSU	C2-N3	-2.16	1.33	1.37
38	A1	2880	PSU	C6-N1	-2.16	1.32	1.36
38	A1	2735	PSU	C2-N1	-2.15	1.33	1.36
34	B5	1187	PSU	C2-N1	-2.15	1.33	1.36
34	B5	1290	PSU	C2-N3	-2.15	1.33	1.37
34	B5	632	PSU	C2-N1	-2.15	1.33	1.36
38	A1	2191	PSU	C2-N1	-2.15	1.33	1.36
34	B5	759	PSU	C2-N3	-2.14	1.33	1.37
38	A1	1052	PSU	C2-N1	-2.14	1.33	1.36
38	A1	2923	PSU	C2-N3	-2.13	1.34	1.37
34	B5	1575	G7M	C2'-C3'	-2.11	1.47	1.53
34	B5	1773	4AC	C6-N1	-2.11	1.33	1.38
38	A1	2944	PSU	O4'-C1'	-2.10	1.40	1.43
38	A1	2923	PSU	O4'-C1'	-2.10	1.40	1.43
38	A1	2826	PSU	C6-N1	-2.09	1.32	1.36
38	A1	2975	PSU	C6-N1	-2.09	1.32	1.36
38	A1	645	1MA	C4-N9	-2.09	1.32	1.38
38	A1	1110	PSU	O4'-C1'	-2.09	1.41	1.43
34	B5	999	PSU	C2-N1	-2.08	1.33	1.36
38	A1	1124	PSU	C6-N1	-2.06	1.32	1.36
38	A1	2634	UR3	C5-C4	-2.06	1.38	1.43
34	B5	211	PSU	C2-N1	-2.06	1.34	1.36
34	B5	1415	PSU	C2-N3	-2.05	1.34	1.37
34	B5	1782	MA6	C8-N9	-2.05	1.34	1.37
38	A1	1004	PSU	C2-N1	-2.04	1.34	1.36
34	B5	1191	B8N	O4'-C1'	-2.02	1.41	1.43
38	A1	2266	PSU	O4'-C1'	-2.02	1.41	1.43
38	A1	2826	PSU	C6-C5	2.01	1.37	1.35
39	A3	50	PSU	C2-N3	-2.01	1.34	1.37

All (270) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	B8N	C32-C31-N3	13.77	136.22	112.16
34	B5	1773	4AC	N4-C4-N3	9.03	128.52	113.87
34	B5	1575	G7M	CN7-N7-C8	-8.46	111.98	124.79
38	A1	1124	PSU	N1-C2-N3	7.27	122.83	115.17
38	A1	2826	PSU	N1-C2-N3	7.12	122.68	115.17
38	A1	2944	PSU	N1-C2-N3	7.02	122.58	115.17
38	A1	2880	PSU	N1-C2-N3	7.00	122.55	115.17
38	A1	990	PSU	N1-C2-N3	6.99	122.55	115.17
38	A1	2634	UR3	C4-N3-C2	-6.95	118.98	124.58
38	A1	1042	PSU	N1-C2-N3	6.83	122.37	115.17
38	A1	2264	PSU	N1-C2-N3	6.81	122.36	115.17
38	A1	2133	PSU	N1-C2-N3	6.81	122.36	115.17
38	A1	2735	PSU	N1-C2-N3	6.81	122.35	115.17
38	A1	2314	PSU	N1-C2-N3	6.80	122.35	115.17
38	A1	2923	PSU	N1-C2-N3	6.80	122.34	115.17
38	A1	2865	PSU	N1-C2-N3	6.79	122.33	115.17
34	B5	466	PSU	N1-C2-N3	6.79	122.33	115.17
38	A1	2129	PSU	N1-C2-N3	6.77	122.31	115.17
38	A1	960	PSU	N1-C2-N3	6.77	122.31	115.17
38	A1	2266	PSU	N1-C2-N3	6.74	122.28	115.17
38	A1	1004	PSU	N1-C2-N3	6.74	122.28	115.17
38	A1	2191	PSU	N1-C2-N3	6.74	122.28	115.17
38	A1	2260	PSU	N1-C2-N3	6.71	122.25	115.17
34	B5	999	PSU	N1-C2-N3	6.71	122.24	115.17
34	B5	120	PSU	N1-C2-N3	6.62	122.15	115.17
38	A1	2351	PSU	N1-C2-N3	6.60	122.13	115.17
34	B5	766	PSU	N1-C2-N3	6.60	122.13	115.17
34	B5	1181	PSU	N1-C2-N3	6.59	122.12	115.17
38	A1	2975	PSU	N1-C2-N3	6.56	122.08	115.17
34	B5	1187	PSU	N1-C2-N3	6.55	122.08	115.17
34	B5	211	PSU	N1-C2-N3	6.54	122.07	115.17
38	A1	966	PSU	N1-C2-N3	6.52	122.04	115.17
34	B5	1290	PSU	N1-C2-N3	6.49	122.02	115.17
38	A1	2416	PSU	N1-C2-N3	6.49	122.02	115.17
34	B5	106	PSU	N1-C2-N3	6.44	121.96	115.17
38	A1	1056	PSU	N1-C2-N3	6.42	121.94	115.17
38	A1	2340	PSU	N1-C2-N3	6.40	121.92	115.17
38	A1	986	PSU	N1-C2-N3	6.36	121.88	115.17
40	A4	73	PSU	N1-C2-N3	6.34	121.86	115.17
34	B5	759	PSU	N1-C2-N3	6.33	121.85	115.17
38	A1	2258	PSU	N1-C2-N3	6.33	121.85	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1415	PSU	N1-C2-N3	6.30	121.81	115.17
34	B5	302	PSU	N1-C2-N3	6.29	121.81	115.17
34	B5	632	PSU	N1-C2-N3	6.29	121.80	115.17
34	B5	1575	G7M	N9-C8-N7	-6.28	97.22	112.48
38	A1	1052	PSU	N1-C2-N3	6.26	121.77	115.17
38	A1	776	PSU	N1-C2-N3	6.24	121.75	115.17
39	A3	50	PSU	N1-C2-N3	6.19	121.69	115.17
38	A1	2349	PSU	N1-C2-N3	6.17	121.67	115.17
34	B5	1575	G7M	C8-N7-C5	6.10	115.40	107.78
38	A1	1110	PSU	N1-C2-N3	6.04	121.54	115.17
38	A1	2922	OMG	C5-C4-N3	-5.86	119.06	128.39
34	B5	1773	4AC	C5-C4-N4	-5.74	113.26	122.94
34	B5	1575	G7M	N9-C4-N3	5.70	137.34	125.95
38	A1	2142	1MA	C5-C4-N3	-5.54	119.12	127.27
38	A1	2922	OMG	C2-N3-C4	5.50	121.78	112.30
34	B5	1191	B8N	C4-N3-C2	-5.41	118.96	125.62
34	B5	1575	G7M	C5-C4-N3	-5.36	118.03	128.15
34	B5	1782	MA6	C5-C4-N3	-5.26	119.47	126.72
38	A1	645	1MA	C5-C4-N3	-4.88	120.09	127.27
38	A1	2133	PSU	C4-N3-C2	-4.85	119.68	126.37
38	A1	2921	OMU	C4-N3-C2	-4.83	120.62	126.61
34	B5	1781	MA6	C5-C4-N3	-4.79	120.12	126.72
38	A1	2921	OMU	N3-C2-N1	4.77	121.10	114.89
38	A1	2266	PSU	O2-C2-N1	-4.75	117.89	122.79
34	B5	1575	G7M	O3'-C3'-C4'	4.74	124.69	111.08
38	A1	2142	1MA	C2-N3-C4	4.72	121.80	112.53
34	B5	1575	G7M	CN7-N7-C5	4.65	132.60	126.80
38	A1	2975	PSU	O2-C2-N1	-4.61	118.04	122.79
34	B5	1781	MA6	C2-N1-C6	4.61	123.08	111.83
38	A1	2944	PSU	C4-N3-C2	-4.60	120.03	126.37
34	B5	1181	PSU	C4-N3-C2	-4.60	120.04	126.37
38	A1	2826	PSU	C4-N3-C2	-4.58	120.06	126.37
38	A1	2975	PSU	C4-N3-C2	-4.57	120.07	126.37
38	A1	2264	PSU	C4-N3-C2	-4.56	120.09	126.37
34	B5	1575	G7M	C2-N3-C4	4.55	120.14	112.30
38	A1	2880	PSU	C4-N3-C2	-4.53	120.13	126.37
34	B5	999	PSU	C4-N3-C2	-4.53	120.13	126.37
34	B5	1782	MA6	C2-N1-C6	4.51	122.85	111.83
38	A1	1124	PSU	O2-C2-N1	-4.50	118.15	122.79
34	B5	466	PSU	C4-N3-C2	-4.48	120.20	126.37
38	A1	990	PSU	C4-N3-C2	-4.48	120.20	126.37
38	A1	960	PSU	C4-N3-C2	-4.47	120.21	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	645	1MA	C2-N3-C4	4.45	121.25	112.53
38	A1	2865	PSU	C4-N3-C2	-4.43	120.28	126.37
34	B5	106	PSU	C4-N3-C2	-4.42	120.28	126.37
38	A1	2735	PSU	C4-N3-C2	-4.41	120.30	126.37
38	A1	2260	PSU	C4-N3-C2	-4.40	120.30	126.37
38	A1	2351	PSU	C4-N3-C2	-4.37	120.35	126.37
38	A1	2922	OMG	N9-C4-N3	4.36	134.66	125.95
38	A1	2191	PSU	C4-N3-C2	-4.35	120.38	126.37
38	A1	2870	5MC	C5-C6-N1	-4.32	118.62	123.31
34	B5	1773	4AC	CM7-C7-N4	4.30	122.21	115.27
38	A1	1124	PSU	C4-N3-C2	-4.28	120.47	126.37
38	A1	2266	PSU	C4-N3-C2	-4.28	120.48	126.37
34	B5	1781	MA6	C4-C5-N7	-4.27	105.69	110.58
38	A1	1042	PSU	C4-N3-C2	-4.27	120.49	126.37
38	A1	2129	PSU	C4-N3-C2	-4.27	120.50	126.37
38	A1	2340	PSU	C4-N3-C2	-4.26	120.51	126.37
34	B5	120	PSU	C4-N3-C2	-4.25	120.51	126.37
38	A1	2923	PSU	O2-C2-N1	-4.22	118.44	122.79
38	A1	986	PSU	C4-N3-C2	-4.19	120.60	126.37
34	B5	1782	MA6	C4-C5-N7	-4.19	105.80	110.58
38	A1	1056	PSU	C4-N3-C2	-4.17	120.63	126.37
38	A1	966	PSU	C4-N3-C2	-4.15	120.65	126.37
38	A1	2314	PSU	C4-N3-C2	-4.15	120.65	126.37
38	A1	2865	PSU	O2-C2-N1	-4.15	118.51	122.79
38	A1	1004	PSU	C4-N3-C2	-4.12	120.69	126.37
34	B5	120	PSU	O2-C2-N1	-4.11	118.55	122.79
38	A1	1052	PSU	C4-N3-C2	-4.10	120.72	126.37
34	B5	759	PSU	C4-N3-C2	-4.10	120.72	126.37
34	B5	632	PSU	C4-N3-C2	-4.09	120.73	126.37
38	A1	2921	OMU	C5-C4-N3	4.09	120.52	114.80
34	B5	766	PSU	C4-N3-C2	-4.08	120.75	126.37
38	A1	2416	PSU	C4-N3-C2	-4.06	120.77	126.37
38	A1	2258	PSU	C4-N3-C2	-4.02	120.83	126.37
38	A1	2278	5MC	C5-C6-N1	-4.01	118.95	123.31
40	A4	73	PSU	C4-N3-C2	-4.01	120.85	126.37
34	B5	1782	MA6	N3-C4-N9	4.01	133.98	127.17
34	B5	1415	PSU	C4-N3-C2	-4.00	120.85	126.37
39	A3	50	PSU	C4-N3-C2	-4.00	120.86	126.37
38	A1	2923	PSU	C4-N3-C2	-4.00	120.86	126.37
34	B5	211	PSU	C4-N3-C2	-3.98	120.88	126.37
38	A1	960	PSU	O2-C2-N1	-3.92	118.74	122.79
38	A1	2258	PSU	O2-C2-N1	-3.92	118.75	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1575	G7M	O2'-C2'-C3'	3.90	124.32	111.82
34	B5	1187	PSU	C4-N3-C2	-3.90	121.00	126.37
38	A1	1110	PSU	C4-N3-C2	-3.89	121.01	126.37
38	A1	2142	1MA	N9-C4-N3	3.89	135.75	126.90
34	B5	302	PSU	C4-N3-C2	-3.89	121.02	126.37
38	A1	1004	PSU	O2-C2-N1	-3.88	118.79	122.79
38	A1	2922	OMG	C6-C5-N7	3.83	137.25	130.29
34	B5	1290	PSU	C4-N3-C2	-3.83	121.10	126.37
34	B5	1782	MA6	C2-N3-C4	3.81	121.13	111.83
34	B5	211	PSU	O2-C2-N1	-3.80	118.87	122.79
38	A1	2735	PSU	O2-C2-N1	-3.79	118.88	122.79
38	A1	2351	PSU	O2-C2-N1	-3.77	118.90	122.79
38	A1	2349	PSU	C4-N3-C2	-3.76	121.19	126.37
38	A1	2340	PSU	O2-C2-N1	-3.76	118.91	122.79
38	A1	990	PSU	O2-C2-N1	-3.75	118.92	122.79
34	B5	1782	MA6	N1-C2-N3	-3.75	122.91	128.58
38	A1	2129	PSU	O2-C2-N1	-3.73	118.95	122.79
34	B5	1187	PSU	O2-C2-N1	-3.72	118.95	122.79
38	A1	2944	PSU	O2-C2-N1	-3.66	119.01	122.79
34	B5	1181	PSU	O2-C2-N1	-3.66	119.02	122.79
34	B5	766	PSU	O2-C2-N1	-3.64	119.03	122.79
38	A1	776	PSU	C4-N3-C2	-3.59	121.42	126.37
34	B5	999	PSU	O2-C2-N1	-3.56	119.12	122.79
38	A1	2260	PSU	O2-C2-N1	-3.55	119.13	122.79
34	B5	1575	G7M	O3'-C3'-C2'	3.55	123.19	111.82
34	B5	1415	PSU	O2-C2-N1	-3.54	119.14	122.79
34	B5	1781	MA6	N3-C4-N9	3.53	133.18	127.17
34	B5	1575	G7M	C8-N9-C4	3.53	115.84	107.09
83	eI	51	5CT	C1-NZ-CE	-3.53	105.67	113.38
39	A3	50	PSU	O2-C2-N1	-3.53	119.15	122.79
34	B5	302	PSU	O2-C2-N1	-3.51	119.17	122.79
34	B5	1781	MA6	C2-N3-C4	3.47	120.31	111.83
34	B5	1781	MA6	N1-C2-N3	-3.47	123.33	128.58
34	B5	106	PSU	O2-C2-N1	-3.46	119.22	122.79
34	B5	466	PSU	O2-C2-N1	-3.45	119.23	122.79
38	A1	2314	PSU	O2-C2-N1	-3.45	119.23	122.79
38	A1	1056	PSU	O2-C2-N1	-3.44	119.24	122.79
38	A1	2416	PSU	O2-C2-N1	-3.44	119.24	122.79
34	B5	1290	PSU	O2-C2-N1	-3.43	119.25	122.79
40	A4	73	PSU	O2-C2-N1	-3.42	119.26	122.79
38	A1	986	PSU	O2-C2-N1	-3.42	119.26	122.79
38	A1	2880	PSU	O2-C2-N1	-3.39	119.29	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1052	PSU	O2-C2-N1	-3.38	119.30	122.79
38	A1	2826	PSU	O2-C2-N1	-3.35	119.33	122.79
38	A1	2258	PSU	C6-C5-C4	-3.31	115.94	118.17
38	A1	2349	PSU	O2-C2-N1	-3.30	119.38	122.79
38	A1	2264	PSU	O2-C2-N1	-3.29	119.40	122.79
38	A1	1042	PSU	O2-C2-N1	-3.29	119.40	122.79
34	B5	1773	4AC	C6-C5-C4	3.26	120.92	117.00
38	A1	2278	5MC	O2-C2-N3	-3.25	117.21	122.33
38	A1	2634	UR3	C5-C4-N3	3.22	119.28	115.04
38	A1	645	1MA	N9-C4-N3	3.22	134.24	126.90
38	A1	2191	PSU	O2-C2-N1	-3.18	119.51	122.79
38	A1	1110	PSU	O2-C2-N1	-3.17	119.52	122.79
34	B5	632	PSU	O2-C2-N1	-3.17	119.52	122.79
38	A1	2133	PSU	O2-C2-N1	-3.16	119.53	122.79
34	B5	1280	4AC	N4-C4-N3	3.15	118.98	113.87
38	A1	966	PSU	O2-C2-N1	-3.13	119.56	122.79
38	A1	2870	5MC	C5-C4-N3	-3.10	118.58	121.75
34	B5	759	PSU	O2-C2-N1	-3.06	119.63	122.79
34	B5	1781	MA6	C4-N9-C8	3.06	108.95	105.74
34	B5	1781	MA6	C5-N7-C8	3.04	108.22	103.45
34	B5	1191	B8N	N3-C2-N1	3.02	120.41	116.72
34	B5	1782	MA6	C4-N9-C8	3.01	108.90	105.74
34	B5	1782	MA6	C5-N7-C8	2.96	108.10	103.45
38	A1	776	PSU	C6-C5-C4	-2.95	116.18	118.17
36	AB	243	HIC	NE2-CE1-ND1	-2.93	111.54	112.66
38	A1	2880	PSU	C5-C6-N1	-2.92	118.09	122.14
34	B5	1782	MA6	C6-C5-N7	2.90	138.06	133.43
38	A1	2133	PSU	C5-C6-N1	-2.83	118.21	122.14
34	B5	1773	4AC	C5-C4-N3	-2.81	118.20	122.60
38	A1	2826	PSU	C5-C6-N1	-2.79	118.26	122.14
34	B5	1575	G7M	O2'-C2'-C1'	2.79	119.72	110.10
38	A1	2921	OMU	O4-C4-C5	-2.76	120.41	125.16
38	A1	2975	PSU	C6-C5-C4	-2.76	116.31	118.17
34	B5	1575	G7M	C1'-N9-C8	-2.69	117.65	126.74
38	A1	2278	5MC	C5-C4-N3	-2.68	119.01	121.75
34	B5	1781	MA6	C6-C5-N7	2.66	137.68	133.43
38	A1	1110	PSU	C6-C5-C4	-2.65	116.39	118.17
38	A1	776	PSU	O2-C2-N1	-2.62	120.09	122.79
34	B5	211	PSU	C6-C5-C4	-2.59	116.43	118.17
38	A1	2922	OMG	C4-C5-N7	-2.58	106.59	110.67
34	B5	1575	G7M	O6-C6-C5	-2.57	122.28	128.01
34	B5	999	PSU	C5-C6-N1	-2.50	118.67	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2870	5MC	O2-C2-N3	-2.49	118.40	122.33
38	A1	2191	PSU	C5-C6-N1	-2.48	118.69	122.14
38	A1	2921	OMU	O2-C2-N1	-2.48	119.56	122.80
34	B5	1781	MA6	N9-C8-N7	-2.47	110.43	113.94
38	A1	645	1MA	C4-C5-N7	-2.45	106.79	110.67
34	B5	1575	G7M	C3'-C2'-C1'	2.45	106.09	101.46
38	A1	2826	PSU	O4'-C1'-C2'	2.42	108.50	105.15
38	A1	2340	PSU	C6-C5-C4	-2.39	116.56	118.17
38	A1	645	1MA	C6-C5-N7	2.39	136.38	132.16
38	A1	2944	PSU	C5-C6-N1	-2.34	118.89	122.14
34	B5	1191	B8N	C31-N3-C2	2.33	121.08	117.64
38	A1	2264	PSU	C5-C6-N1	-2.32	118.92	122.14
34	B5	1782	MA6	N9-C8-N7	-2.31	110.65	113.94
34	B5	1181	PSU	C5-C6-N1	-2.31	118.93	122.14
36	AB	243	HIC	CB-CG-CD2	-2.31	124.40	129.96
38	A1	2142	1MA	C4-C5-N7	-2.29	107.04	110.67
38	A1	2351	PSU	C5-C6-N1	-2.28	118.98	122.14
34	B5	1191	B8N	C1'-C5-C4	2.28	121.06	117.61
38	A1	2634	UR3	C6-N1-C2	-2.26	119.95	121.80
38	A1	966	PSU	C6-C5-C4	-2.25	116.66	118.17
34	B5	1773	4AC	O7-C7-N4	-2.24	118.36	121.90
38	A1	2922	OMG	O6-C6-C5	-2.23	120.65	126.53
34	B5	1191	B8N	O4'-C1'-C2'	2.23	108.23	105.15
38	A1	2314	PSU	C5-C6-N1	-2.19	119.09	122.14
38	A1	2826	PSU	O2-C2-N3	-2.18	117.98	121.86
38	A1	2922	OMG	C5-C6-N1	2.18	118.81	113.25
34	B5	466	PSU	C5-C6-N1	-2.18	119.11	122.14
38	A1	2865	PSU	O4'-C1'-C2'	2.18	108.17	105.15
38	A1	2349	PSU	C6-C5-C4	-2.15	116.72	118.17
38	A1	2278	5MC	N1-C2-N3	2.14	122.52	118.80
34	B5	766	PSU	C5-C6-N1	-2.14	119.17	122.14
38	A1	2735	PSU	C5-C6-N1	-2.14	119.17	122.14
34	B5	1280	4AC	C6-C5-C4	2.13	119.57	117.00
38	A1	2416	PSU	C5-C6-N1	-2.13	119.19	122.14
38	A1	1124	PSU	C5-C6-N1	-2.12	119.20	122.14
38	A1	2133	PSU	O2-C2-N3	-2.11	118.11	121.86
38	A1	1004	PSU	C5-C6-N1	-2.10	119.22	122.14
38	A1	990	PSU	C5-C6-N1	-2.09	119.24	122.14
38	A1	776	PSU	O2-C2-N3	-2.09	118.15	121.86
38	A1	2880	PSU	O2-C2-N3	-2.09	118.16	121.86
38	A1	2921	OMU	C6-N1-C2	-2.08	118.46	121.00
34	B5	106	PSU	C5-C6-N1	-2.08	119.25	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1110	PSU	O4'-C1'-C2'	2.08	108.03	105.15
38	A1	645	1MA	N1-C2-N3	-2.07	123.53	126.00
38	A1	960	PSU	C5-C6-N1	-2.07	119.27	122.14
38	A1	966	PSU	C5-C6-N1	-2.07	119.27	122.14
34	B5	999	PSU	O4'-C1'-C2'	2.06	108.01	105.15
38	A1	2191	PSU	O2-C2-N3	-2.06	118.20	121.86
38	A1	2634	UR3	C3U-N3-C4	2.06	120.73	117.87
38	A1	2266	PSU	C6-C5-C4	-2.06	116.79	118.17
38	A1	2880	PSU	O4'-C1'-C2'	2.05	107.98	105.15
38	A1	1056	PSU	C6-C5-C4	-2.05	116.79	118.17
38	A1	1042	PSU	O2-C2-N3	-2.04	118.23	121.86
34	B5	1415	PSU	C6-C5-C4	-2.04	116.80	118.17
38	A1	2264	PSU	O2-C2-N3	-2.04	118.25	121.86
34	B5	766	PSU	O4'-C1'-C2'	2.03	107.96	105.15
38	A1	1052	PSU	C5-C6-N1	-2.02	119.34	122.14
38	A1	2870	5MC	N1-C2-N3	2.01	122.29	118.80
38	A1	986	PSU	C5-C6-N1	-2.01	119.36	122.14
38	A1	1004	PSU	O4'-C1'-C2'	2.01	107.93	105.15
34	B5	1280	4AC	O2-C2-N3	-2.01	119.17	122.33

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	eI	51	5CT	C1-C2-C3-C4
83	eI	51	5CT	O1-C2-C3-C4
83	eI	51	5CT	C-CA-CB-CG
34	B5	1280	4AC	O7-C7-N4-C4
34	B5	1280	4AC	CM7-C7-N4-C4
34	B5	1773	4AC	N3-C4-N4-C7
38	A1	2923	PSU	C3'-C4'-C5'-O5'
34	B5	211	PSU	O4'-C4'-C5'-O5'
34	B5	1782	MA6	O4'-C4'-C5'-O5'
38	A1	2260	PSU	C3'-C4'-C5'-O5'
38	A1	2260	PSU	O4'-C4'-C5'-O5'
83	eI	51	5CT	CG-CD-CE-NZ
38	A1	776	PSU	O4'-C4'-C5'-O5'
38	A1	2258	PSU	C3'-C4'-C5'-O5'
38	A1	2258	PSU	O4'-C4'-C5'-O5'
38	A1	2923	PSU	O4'-C4'-C5'-O5'
34	B5	1782	MA6	C3'-C4'-C5'-O5'
34	B5	1191	B8N	N34-C33-C34-O36

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Mol	Chain	Res	Type	Atoms
34	B5	211	PSU	C3'-C4'-C5'-O5'
34	B5	302	PSU	C3'-C4'-C5'-O5'
34	B5	1191	B8N	N34-C33-C34-O35
83	eI	51	5CT	CA-CB-CG-CD
38	A1	2870	5MC	C2'-C1'-N1-C6
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	2923	PSU	C4'-C5'-O5'-P
38	A1	2314	PSU	C4'-C5'-O5'-P
34	B5	1191	B8N	O4'-C1'-C5-C4
34	B5	1782	MA6	C5-C6-N6-C9
38	A1	776	PSU	C3'-C4'-C5'-O5'
34	B5	302	PSU	O4'-C4'-C5'-O5'
38	A1	2340	PSU	C4'-C5'-O5'-P
38	A1	645	1MA	C2'-C1'-N9-C8
38	A1	645	1MA	C2'-C1'-N9-C4
34	B5	1191	B8N	O4'-C1'-C5-C6
83	eI	51	5CT	CE-CD-CG-CB
38	A1	2870	5MC	O4'-C1'-N1-C2
34	B5	1280	4AC	C5-C4-N4-C7
39	A3	50	PSU	C3'-C4'-C5'-O5'
34	B5	1280	4AC	N3-C4-N4-C7
38	A1	2870	5MC	C2'-C1'-N1-C2
83	eI	51	5CT	N-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	2266	PSU	1	0
38	A1	2880	PSU	1	0
38	A1	1110	PSU	1	0
34	B5	1575	G7M	2	0
34	B5	1290	PSU	1	0
38	A1	986	PSU	1	0
38	A1	2258	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 207 ligands modelled in this entry, 205 are 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	$\# Z > 2$
86	SPD	A1	3401	-	9,9,9	0.39	0	8,8,8	1.11	0
87	3HE	A1	3402	-	21,21,21	0.42	0	23,30,30	0.70	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
86	SPD	A1	3401	-	-	4/7/7/7	-
87	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 (6) torsion outliers are listed below:

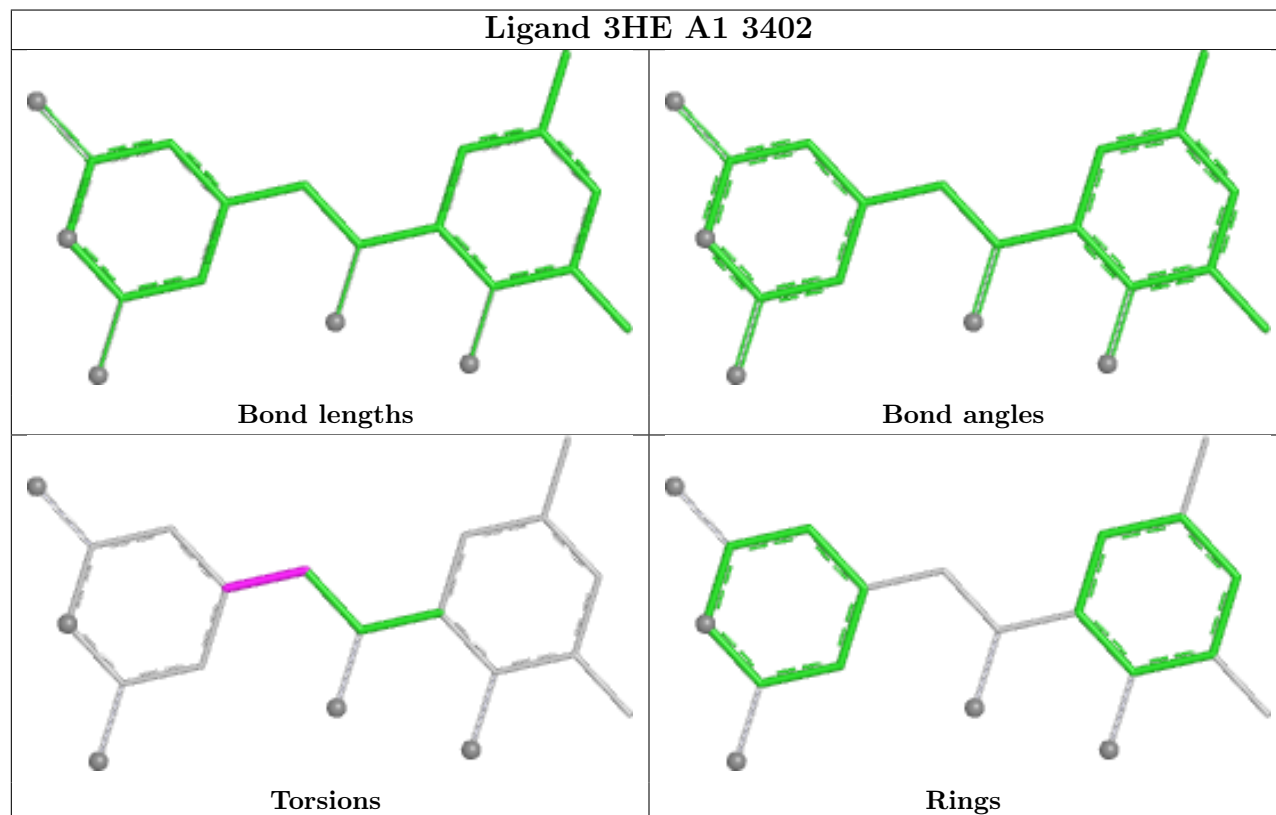
Mol	Chain	Res	Type	Atoms
87	A1	3402	3HE	C7-C8-C9-C10
86	A1	3401	SPD	N6-C7-C8-C9
87	A1	3402	3HE	C7-C8-C9-C13
86	A1	3401	SPD	C2-C3-C4-C5
86	A1	3401	SPD	C4-C5-N6-C7
86	A1	3401	SPD	C8-C7-N6-C5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

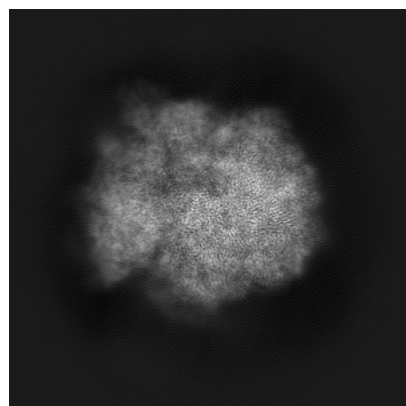
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40990. These allow visual inspection of the internal detail of the map and identification of artifacts.

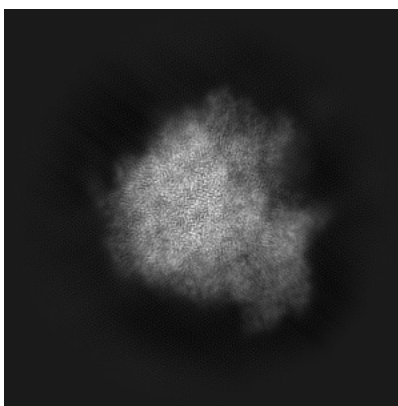
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

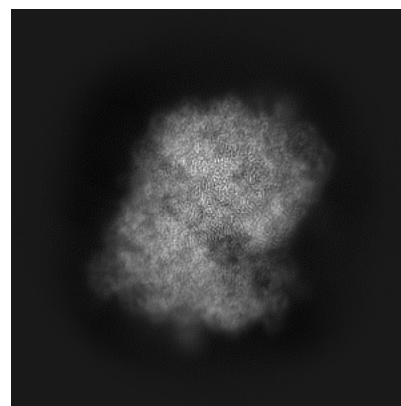
6.1.1 Primary map



X

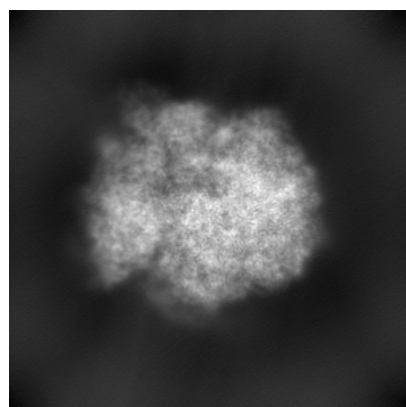


Y

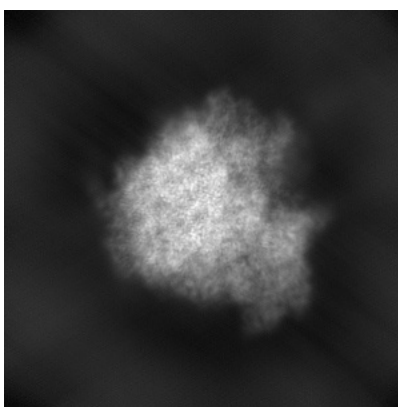


Z

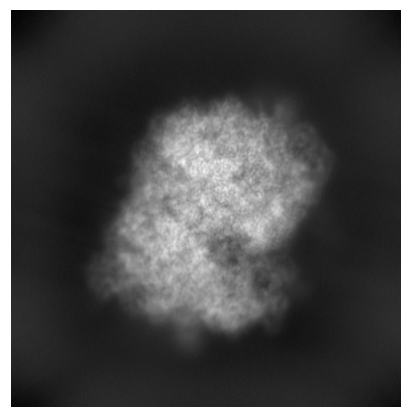
6.1.2 Raw map



X



Y

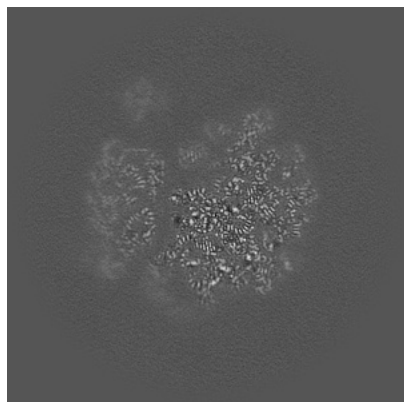


Z

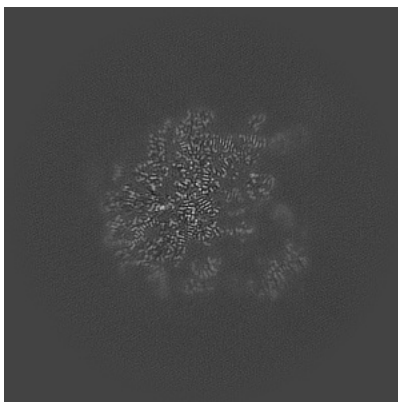
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

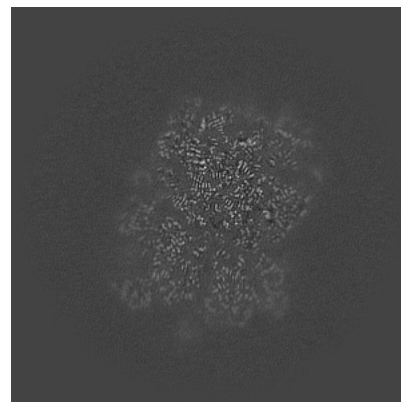
6.2.1 Primary map



X Index: 200

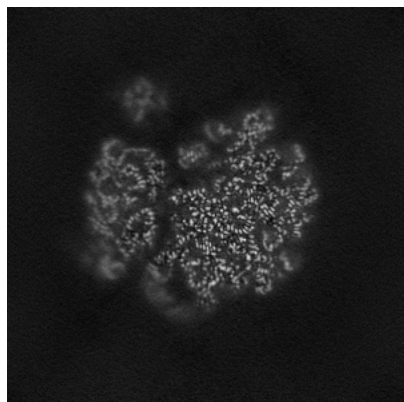


Y Index: 200

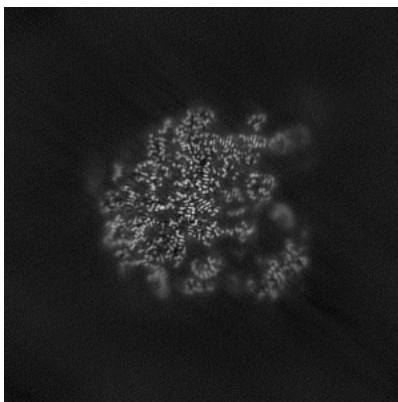


Z Index: 200

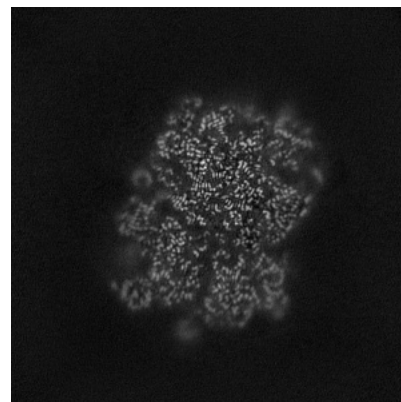
6.2.2 Raw map



X Index: 200



Y Index: 200

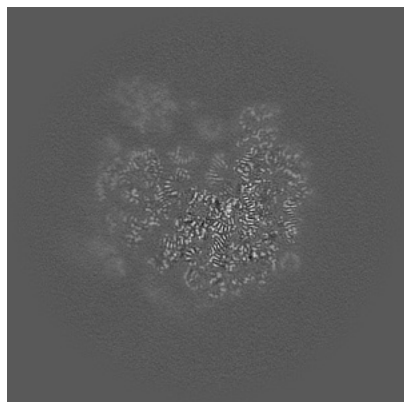


Z Index: 200

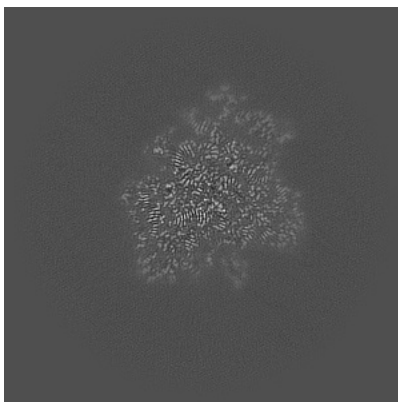
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

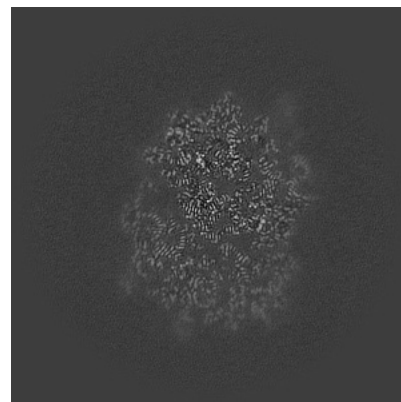
6.3.1 Primary map



X Index: 192

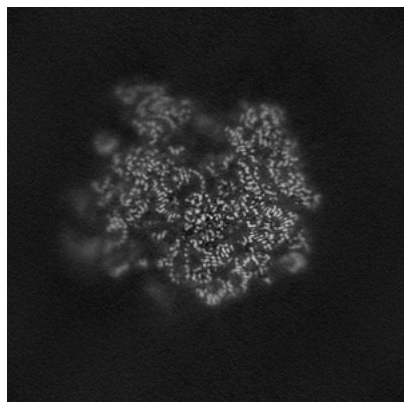


Y Index: 244

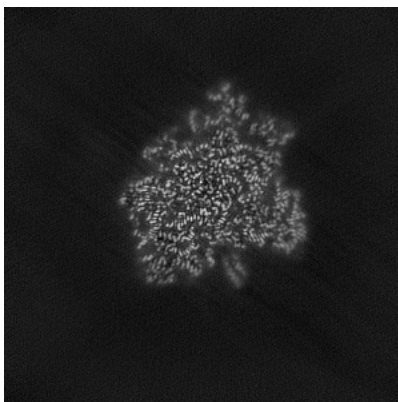


Z Index: 187

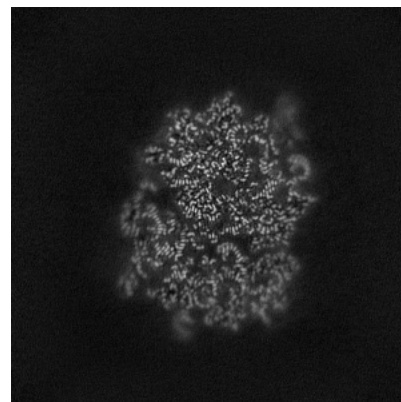
6.3.2 Raw map



X Index: 184



Y Index: 247

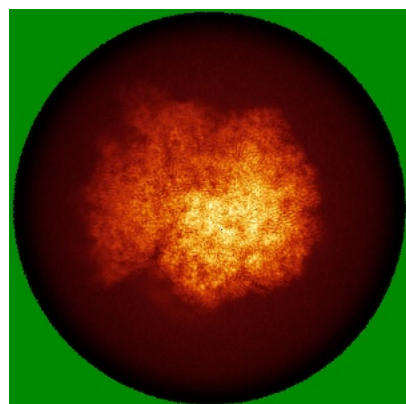


Z Index: 188

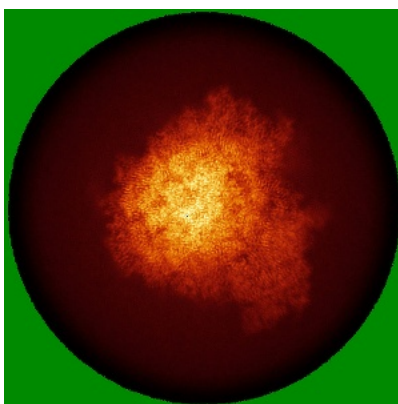
The images above show the largest variance slices of the map in three orthogonal directions.

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

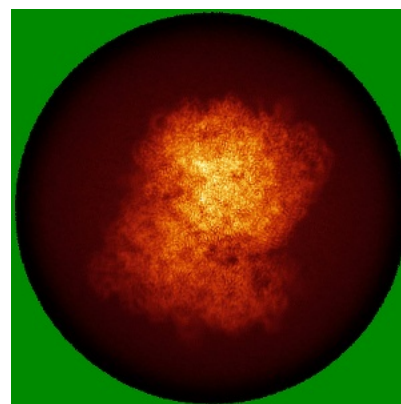
6.4.1 Primary map



X

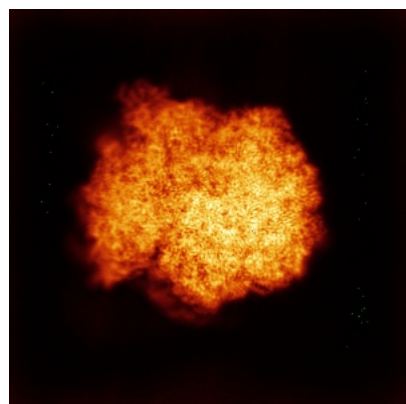


Y

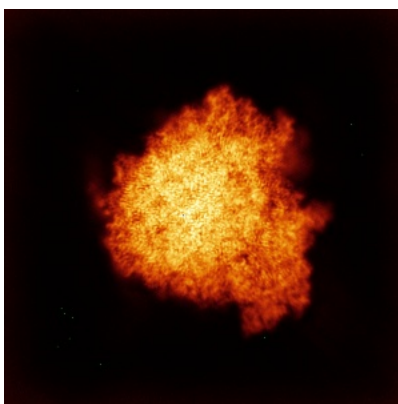


Z

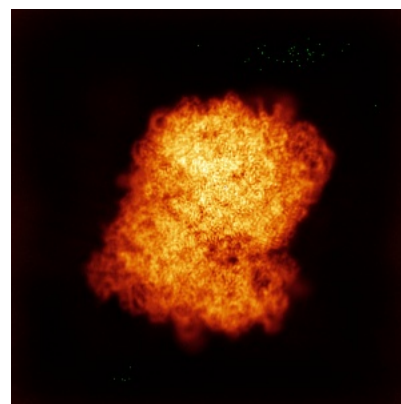
6.4.2 Raw map



X



Y

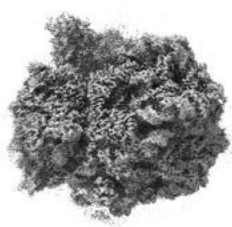


Z

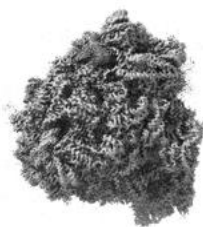
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

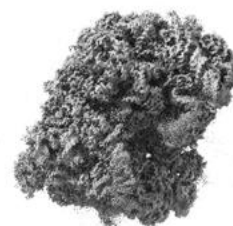
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

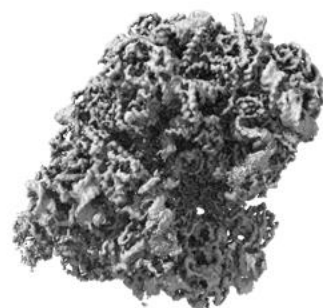
6.5.2 Raw map



X



Y



Z

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

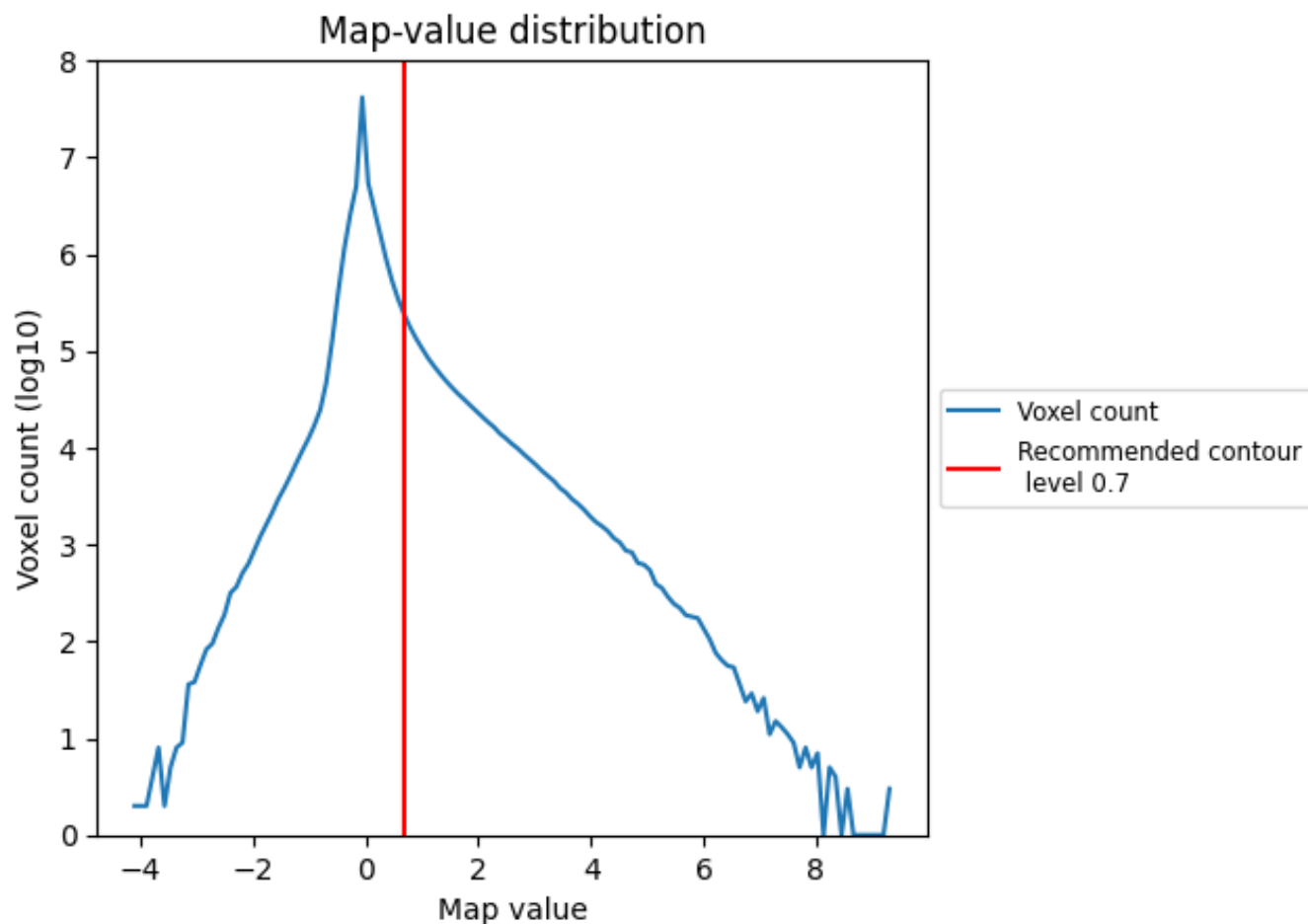
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

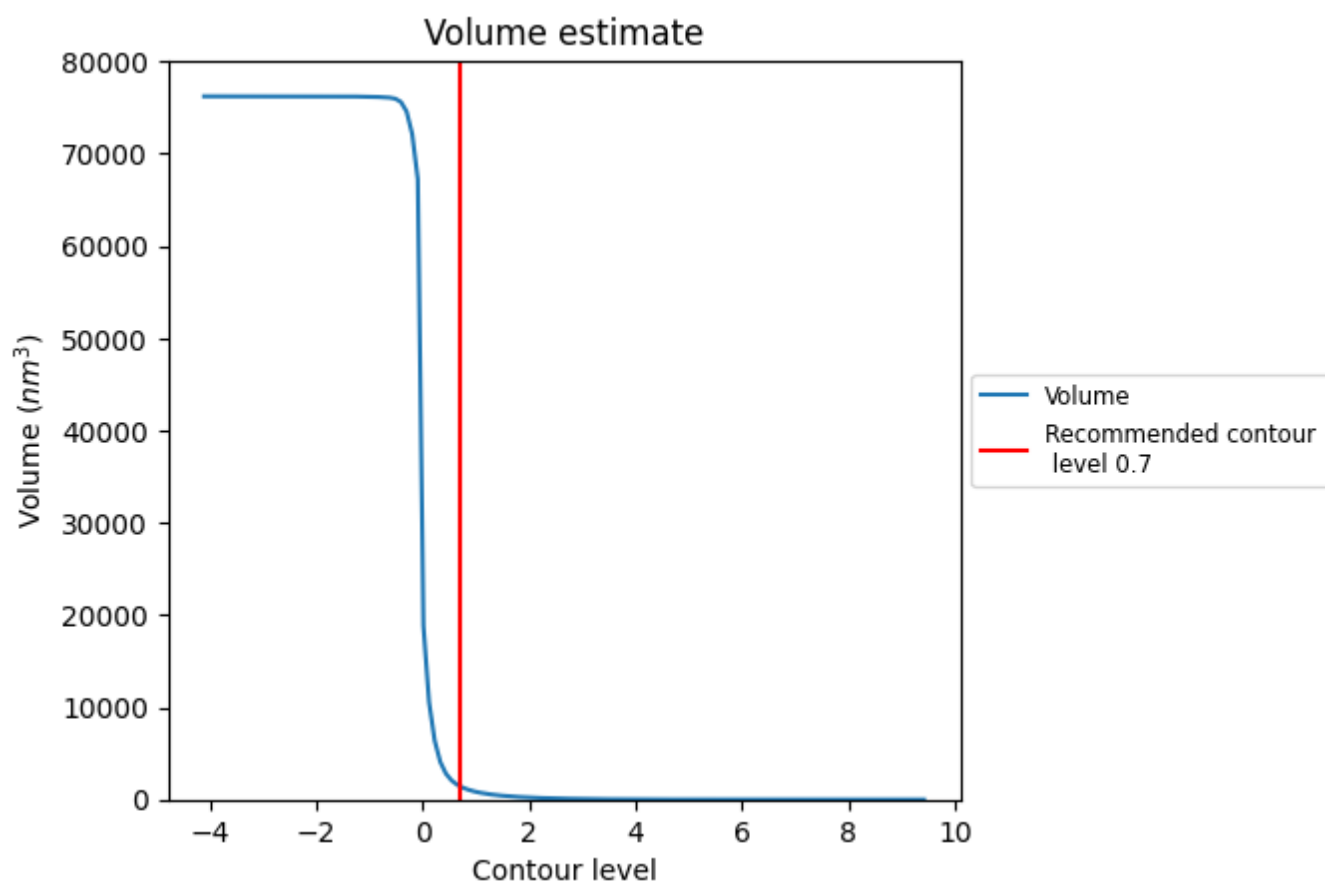
This section contains the results of statistical analysis of the map.

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.

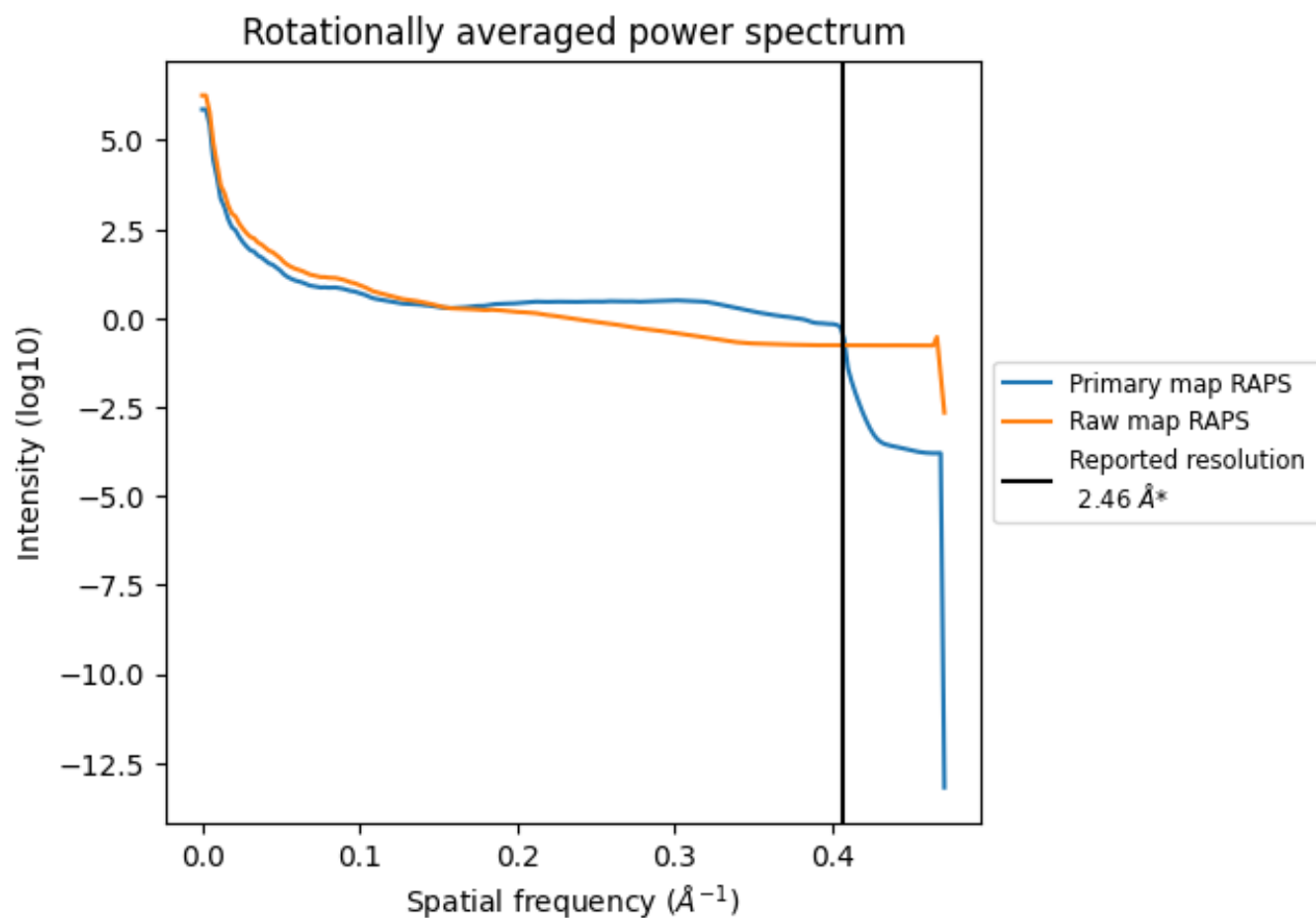
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1445 nm³; this corresponds to an approximate mass of 1305 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 ⓘ

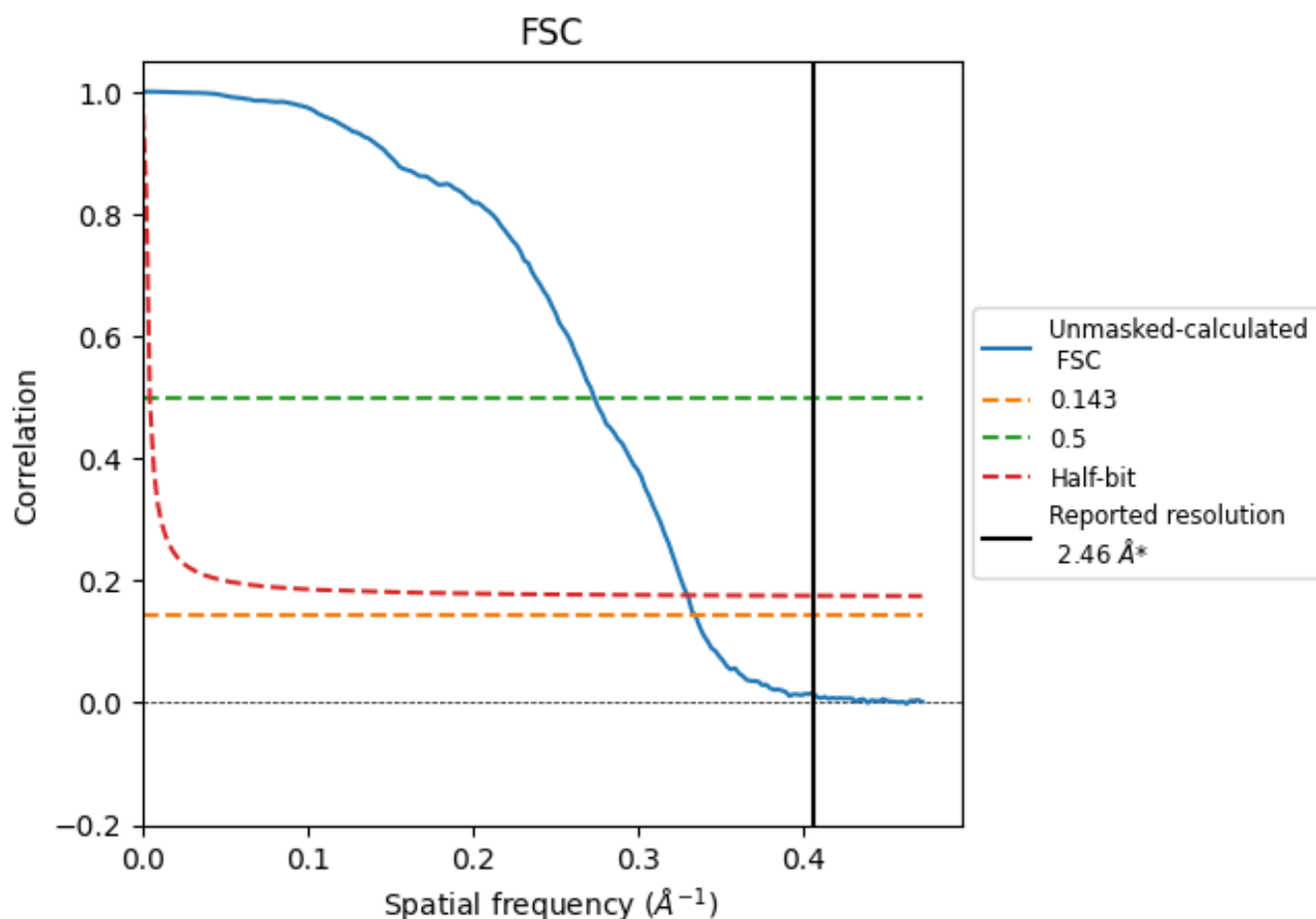


*Reported resolution corresponds to spatial frequency of 0.407 Å⁻¹

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 0.407 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

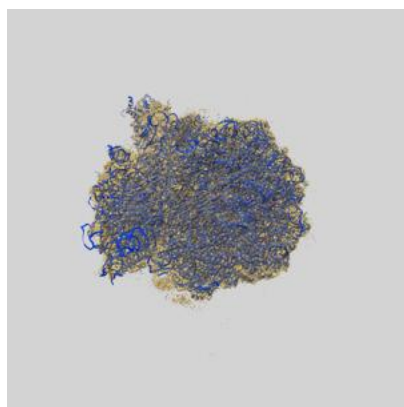
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.66	3.03

*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 2.99 differs from the reported value 2.46 by more than 10 %

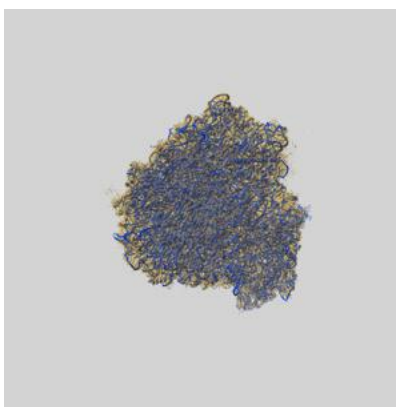
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40990 and PDB model 8T2X. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

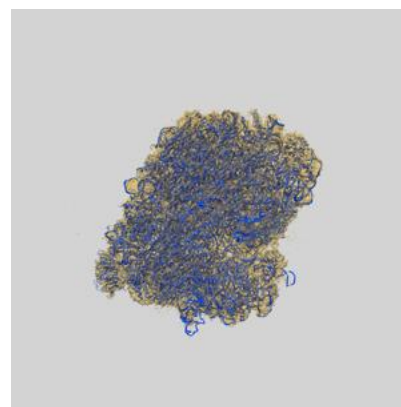
9.1 Map-model overlay [i](#)



X



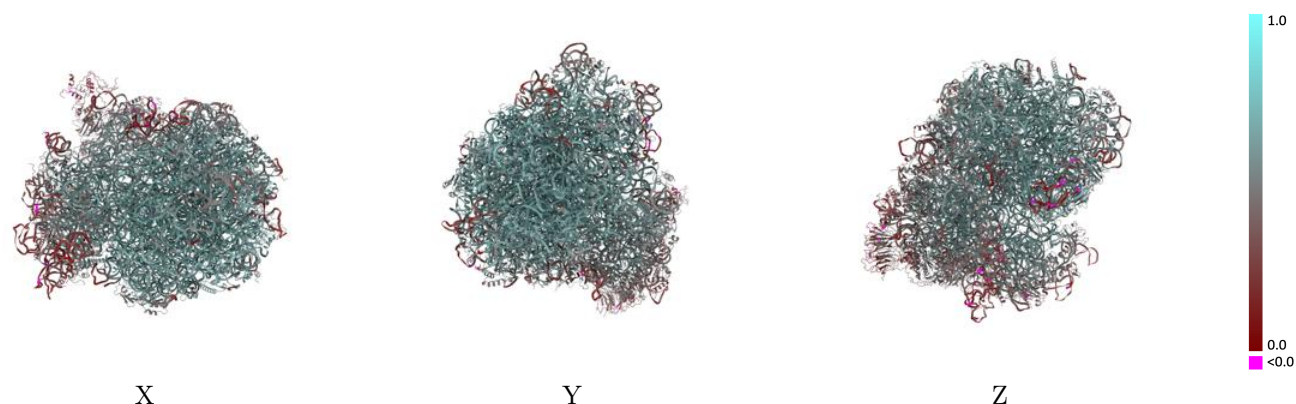
Y



Z

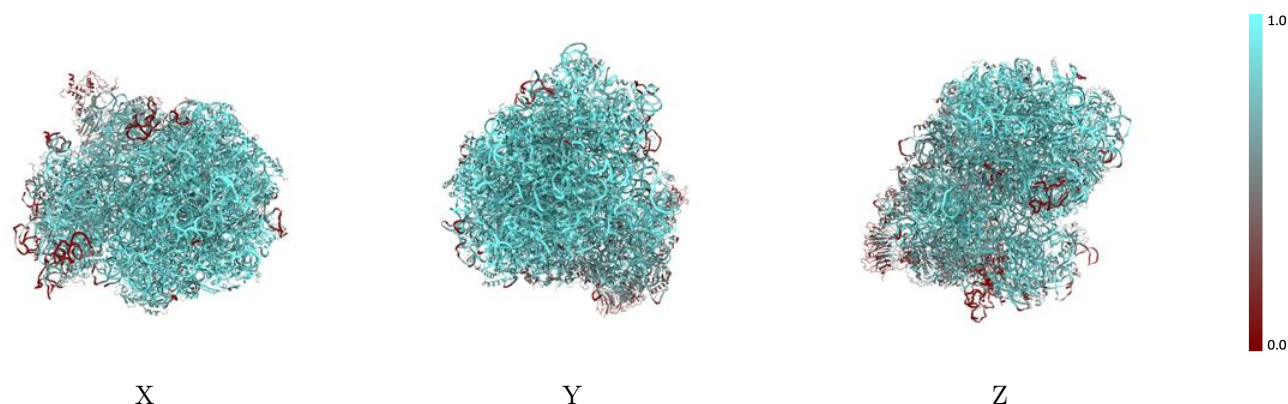
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



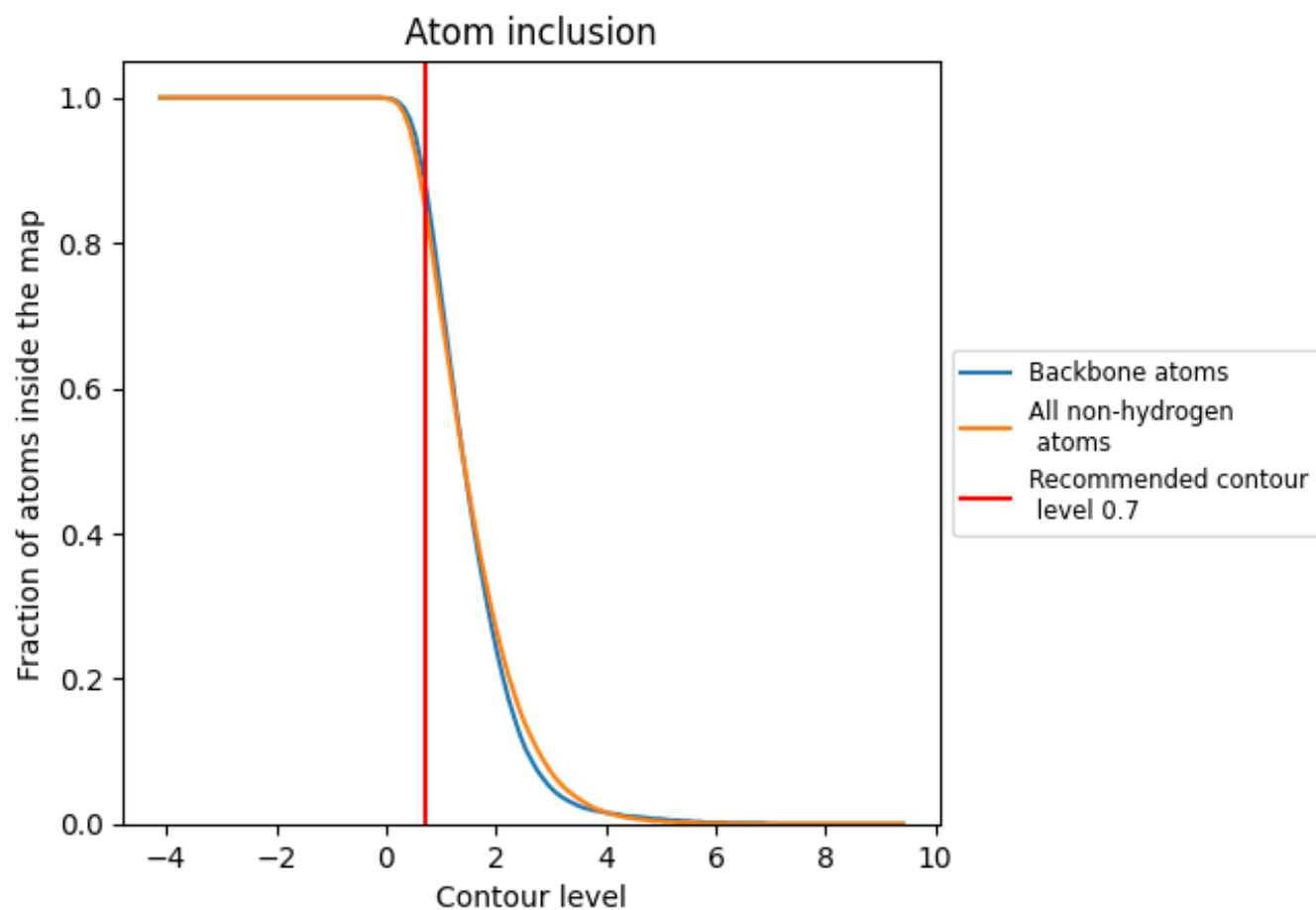
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 89% of all backbone atoms, 86% 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	 0.8550	 0.5590
A1	 0.9320	 0.6040
A3	 0.9650	 0.5760
A4	 0.9710	 0.6290
AA	 0.9830	 0.6780
AB	 0.9420	 0.6350
AC	 0.9310	 0.6200
AD	 0.7820	 0.5130
AE	 0.7990	 0.5210
AF	 0.9260	 0.6110
AG	 0.8400	 0.5510
AH	 0.8410	 0.5690
AI	 0.9160	 0.6210
AJ	 0.7540	 0.5000
AL	 0.9120	 0.6110
AM	 0.8460	 0.5470
AN	 0.9870	 0.6680
AO	 0.9440	 0.6250
AP	 0.9420	 0.6510
AQ	 0.9690	 0.6450
AR	 0.8430	 0.5790
AS	 0.9210	 0.6010
AT	 0.9150	 0.6100
AU	 0.7740	 0.5260
AV	 0.9390	 0.6470
AW	 0.9450	 0.6410
AX	 0.9350	 0.6210
AY	 0.9130	 0.6040
AZ	 0.8510	 0.5560
Aa	 0.9530	 0.6410
Ab	 0.9160	 0.6060
Ac	 0.8950	 0.5950
Ad	 0.8720	 0.6180
Ae	 0.9600	 0.6540
Af	 0.9720	 0.6480



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Chain	Atom inclusion	Q-score
Ag	 0.9120	 0.6310
Ah	 0.9300	 0.6000
Ai	 0.8860	 0.5740
Aj	 0.9680	 0.6740
Ak	 0.7380	 0.5240
Al	 0.9780	 0.6660
Am	 0.8860	 0.6150
An	 0.8540	 0.6240
Ao	 0.9350	 0.6410
Ap	 0.9430	 0.6550
B5	 0.8420	 0.5130
BA	 0.6740	 0.4580
BB	 0.7420	 0.4980
BC	 0.8070	 0.5290
BD	 0.5770	 0.4220
BE	 0.7440	 0.4790
BF	 0.6810	 0.4940
BG	 0.6770	 0.4280
BH	 0.5280	 0.4120
BI	 0.8040	 0.5340
BJ	 0.7050	 0.4560
BK	 0.5150	 0.3590
BL	 0.7920	 0.5520
BM	 0.1240	 0.2170
BN	 0.8450	 0.5560
BO	 0.8540	 0.5640
BP	 0.6080	 0.4390
BQ	 0.6360	 0.4520
BR	 0.5950	 0.4280
BS	 0.6730	 0.4640
BT	 0.6010	 0.4100
BU	 0.5260	 0.3880
BV	 0.7180	 0.4870
BW	 0.8920	 0.5700
BX	 0.9160	 0.6230
BY	 0.6390	 0.4240
BZ	 0.5150	 0.4410
Ba	 0.8690	 0.5840
Bb	 0.7210	 0.4840
Bc	 0.6920	 0.5220
Bd	 0.8230	 0.5140
Be	 0.6860	 0.4750

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Chain	Atom inclusion	Q-score
Bf	 0.2110	 0.2820
Bg	 0.3470	 0.3080
E	 0.6350	 0.4490
MR	 0.9420	 0.6060
eI	 0.7950	 0.5650
tA	 0.8760	 0.5540
tP	 0.9210	 0.5890