



## Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 04:31 AM EDT

PDB ID : 7N8B / pdb\_00007n8b  
EMDB ID : EMD-24235  
Title : Cycloheximide bound vacant 80S structure isolated from cbf5-D95A  
Authors : Rai, J.; Zhao, Y.; Li, H.  
Deposited on : 2021-06-14  
Resolution : 3.05 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

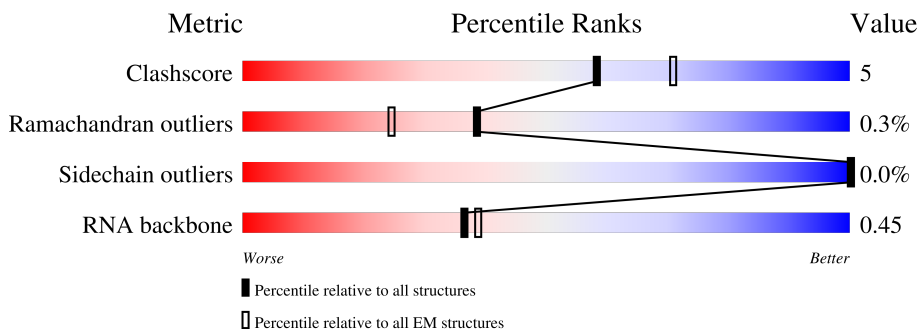
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.05 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.














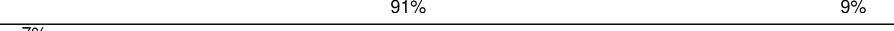







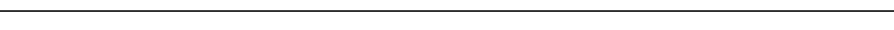

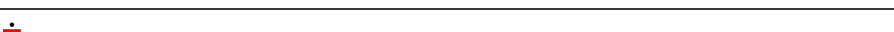
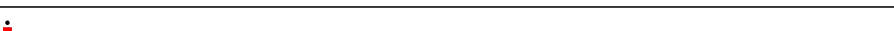


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	A1	3156	
2	A3	121	
3	A4	158	
4	AA	247	
5	AB	386	
6	AC	361	
7	AD	292	

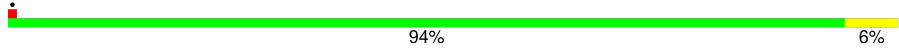
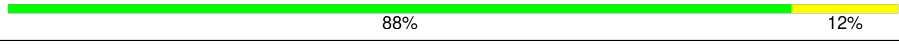
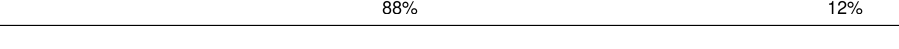
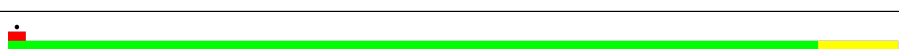


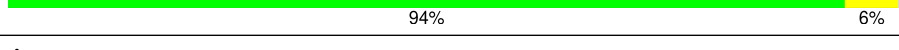
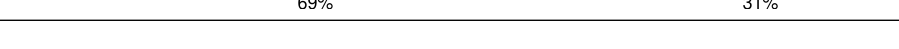



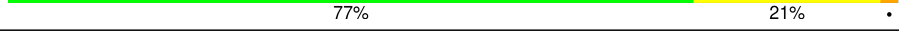

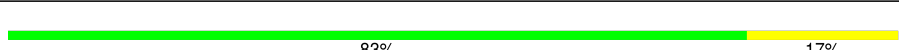


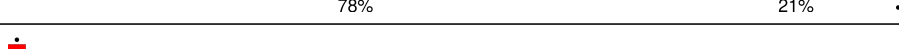


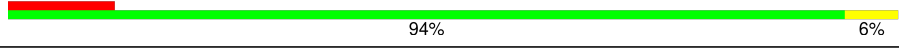




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Mol	Chain	Length	Quality of chain
8	AE	156	 90% 10%
9	AF	222	 82% 17%
10	AG	230	 88% 11%
11	AH	190	 87% 13%
12	AI	205	 80% 20%
13	AJ	169	 5% 83% 17%
14	AL	193	 84% 14% ..
15	AM	136	 93% 7%
16	AN	203	 81% 18%
17	AO	197	 88% 11%
18	AP	175	 89% 11%
19	AQ	185	 91% 9%
20	AR	188	 7% 89% 11%
21	AS	172	 87% 12%
22	AT	159	 79% 20%
23	AU	100	 92% 7%
24	AV	136	 88% 12%
25	AW	63	 90% 10%
26	AX	121	 90% 10%
27	AY	126	 80% 20%
28	AZ	135	 82% 18%
29	Aa	148	 78% 21%
30	Ab	58	 95% 5%
31	Ac	97	 84% 16%
32	Ad	109	 90% 10%





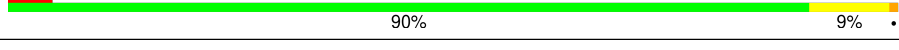

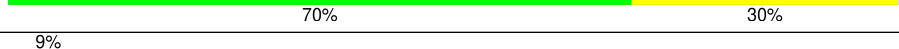
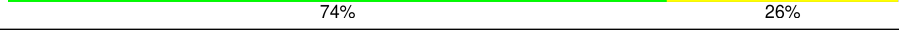
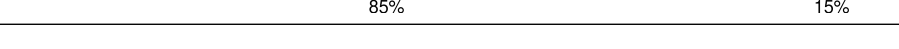
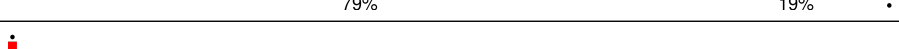
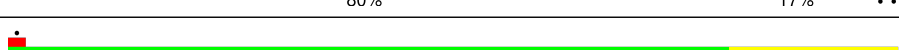

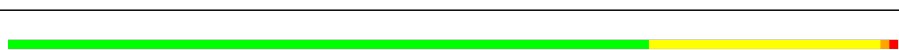

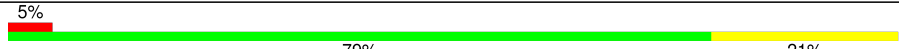





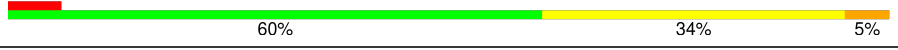
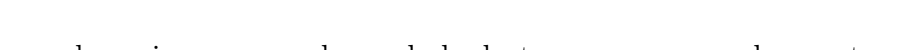
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Mol	Chain	Length	Quality of chain
33	Ae	127	
34	Af	106	
35	Ag	112	
36	Ah	119	
37	Ai	99	
38	Aj	87	
39	Ak	77	
40	Al	50	
41	Am	52	
42	An	25	
43	Ao	105	
44	Ap	91	
45	BA	206	
46	BB	214	
47	BC	217	
48	BD	223	
49	BE	260	
50	BF	206	
51	BG	226	
52	BH	184	
53	BI	188	
54	BJ	185	
55	BK	96	
56	BL	155	
57	BM	121	

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Mol	Chain	Length	Quality of chain
58	BN	150	
59	BO	127	
60	BP	124	
61	BQ	141	
62	BR	121	
63	BS	145	
64	BT	141	
65	BU	107	
66	BV	87	
67	BW	129	
68	BX	144	
69	BY	134	
70	BZ	69	
71	Ba	97	
72	Bb	81	
73	Bc	63	
74	Bd	53	
75	Be	60	
76	Bf	57	
77	Bg	312	
78	Bh	89	
79	B5	1783	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
79	3AU	B5	1191	X	-	-	-
79	G7M	B5	1575	X	-	-	-

## 2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 199900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	3156	Total	C	N	O	P	0	0
			67535	30189	12152	22038	3156		

- Molecule 2 is a RNA chain called 5S.

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

- Molecule 3 is a RNA chain called 5.8S.

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

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AB	386	Total	C	N	O	S	0	0
			3079	1954	584	533	8		

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

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	LEU	deletion	UNP Q02326
AE	?	-	THR	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	GLU	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326
AE	?	-	GLU	deletion	UNP Q02326
AE	?	-	ALA	deletion	UNP Q02326
AE	?	-	ASN	deletion	UNP Q02326
AE	?	-	LEU	deletion	UNP Q02326
AE	?	-	PHE	deletion	UNP Q02326
AE	?	-	PRO	deletion	UNP Q02326
AE	?	-	GLU	deletion	UNP Q02326
AE	?	-	GLN	deletion	UNP Q02326
AE	?	-	GLN	deletion	UNP Q02326
AE	?	-	ASN	deletion	UNP Q02326
AE	?	-	LYS	deletion	UNP Q02326

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

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

- Molecule 10 is a protein called 60S ribosomal protein L8-A.



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

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

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	?	-	MET	deletion	UNP P41805
AI	?	-	LEU	deletion	UNP P41805
AI	?	-	SER	deletion	UNP P41805
AI	?	-	CYS	deletion	UNP P41805
AI	?	-	ALA	deletion	UNP P41805
AI	?	-	GLY	deletion	UNP P41805
AI	?	-	ALA	deletion	UNP P41805
AI	?	-	ASP	deletion	UNP P41805
AI	?	-	ARG	deletion	UNP P41805
AI	?	-	LEU	deletion	UNP P41805
AI	?	-	GLN	deletion	UNP P41805
AI	?	-	GLN	deletion	UNP P41805

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	VAL	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	LYS	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	ALA	deletion	UNP P05740
AP	?	-	GLU	deletion	UNP P05740
AP	?	-	LYS	deletion	UNP P05740

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

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

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

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

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called 60S ribosomal protein L25.

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

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

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

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

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

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

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

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

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

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

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

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

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 46 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 47 is a protein called 40S ribosomal protein S2.

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

- Molecule 48 is a protein called 40S ribosomal protein S3.

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

- Molecule 49 is a protein called 40S ribosomal protein S4-A.

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

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

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

- Molecule 51 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 52 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 53 is a protein called 40S ribosomal protein S8-A.

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

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	ASN	deletion	UNP P0CX39
BI	?	-	VAL	deletion	UNP P0CX39
BI	?	-	LYS	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39

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Chain	Residue	Modelled	Actual	Comment	Reference
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	GLU	deletion	UNP P0CX39
BI	?	-	THR	deletion	UNP P0CX39
BI	?	-	VAL	deletion	UNP P0CX39
BI	?	-	ALA	deletion	UNP P0CX39

- Molecule 54 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BM	121	Total	C	N	O	S	0	0
			913	574	162	175	2		

- Molecule 58 is a protein called 40S ribosomal protein S13.

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

- Molecule 59 is a protein called 40S ribosomal protein S14-A.

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



- Molecule 60 is a protein called 40S ribosomal protein S15.

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

- Molecule 61 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BR	121	Total	C	N	O	S	0	0
			975	611	183	179	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	?	-	SER	deletion	UNP P02407
BR	?	-	ASN	deletion	UNP P02407
BR	?	-	GLY	deletion	UNP P02407
BR	?	-	VAL	deletion	UNP P02407

- Molecule 63 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 64 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S20.

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

- Molecule 66 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BZ	69	Total	C	N	O		0	0
			558	357	103	98			

- Molecule 71 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 72 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bf	57	Total	C	N	O	S	0	0
			454	288	86	77	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bf	97	ALA	LYS	conflict	UNP P05759
Bf	?	-	CYS	deletion	UNP P05759
Bf	?	-	GLY	deletion	UNP P05759
Bf	?	-	ALA	deletion	UNP P05759

- Molecule 77 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

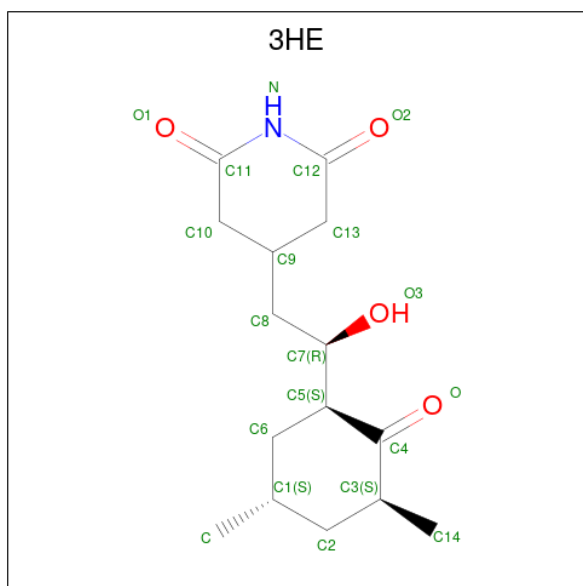
- Molecule 78 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bh	89	Total	C	N	O		0	0
			675	391	137	147			

- Molecule 79 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	B5	1783	Total	C	N	O	P	1	0
			37891	16950	6664	12494	1783		

- Molecule 80 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>).



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

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	A1	247	Total	Mg	0
			247	247	
81	A3	5	Total	Mg	0
			5	5	
81	A4	9	Total	Mg	0
			9	9	
81	AB	4	Total	Mg	0
			4	4	
81	AC	1	Total	Mg	0
			1	1	
81	AG	1	Total	Mg	0
			1	1	
81	AL	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
81	AN	1	Total 1	Mg 1	0
81	AO	1	Total 1	Mg 1	0
81	AP	1	Total 1	Mg 1	0
81	AR	1	Total 1	Mg 1	0
81	AV	1	Total 1	Mg 1	0
81	Aa	1	Total 1	Mg 1	0
81	Ae	2	Total 2	Mg 2	0
81	Af	1	Total 1	Mg 1	0
81	Aj	1	Total 1	Mg 1	0
81	BE	1	Total 1	Mg 1	0
81	BG	1	Total 1	Mg 1	0
81	BJ	1	Total 1	Mg 1	0
81	Ba	1	Total 1	Mg 1	0
81	B5	90	Total 90	Mg 90	0

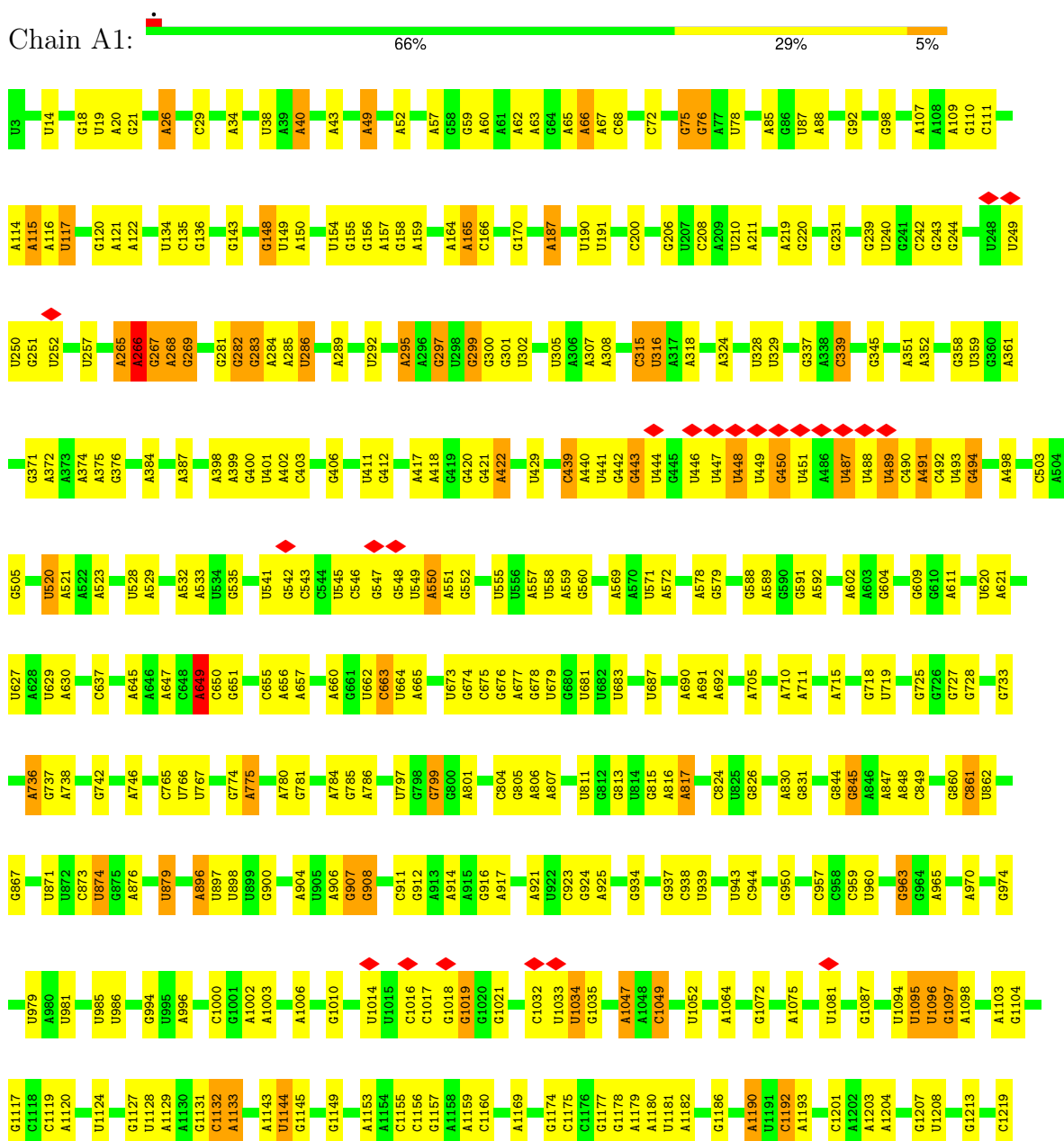
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	Ao	1	Total 1	Zn 1	0
82	Bb	1	Total 1	Zn 1	0

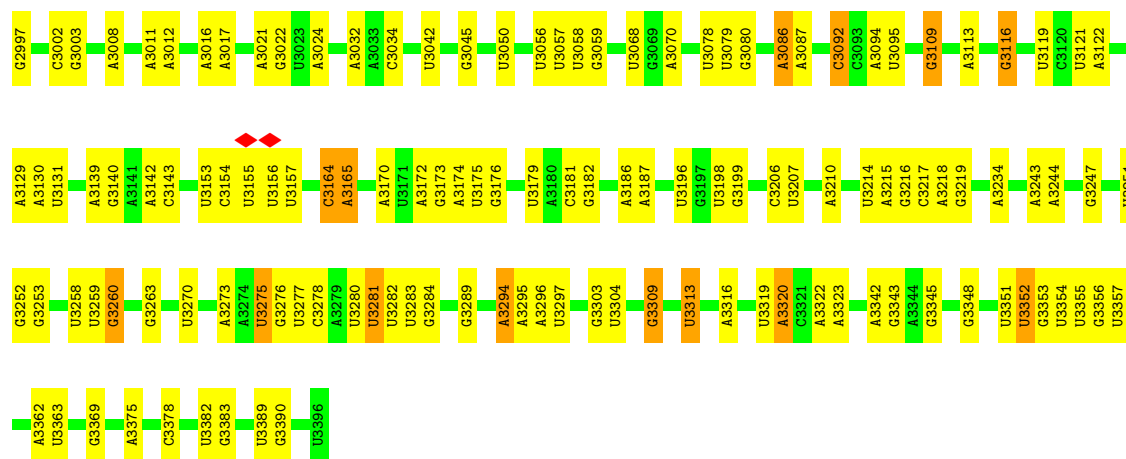
### 3 Residue-property plots

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: 25S







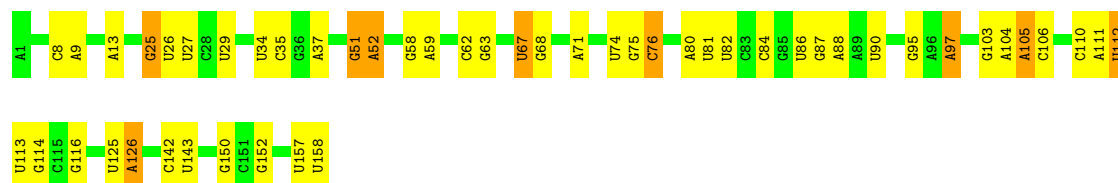
- Molecule 2: 5S

Chain A3: 79% 20%



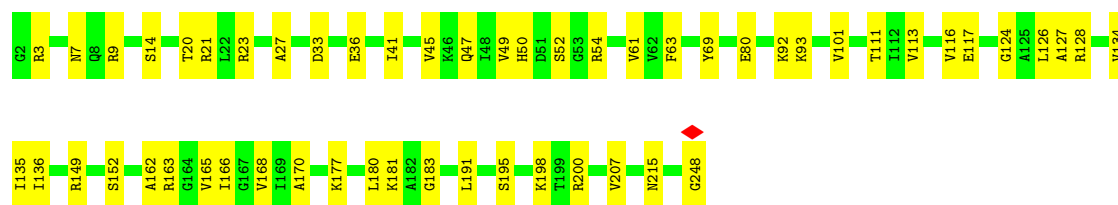
- Molecule 3: 5.8S

Chain A4: 68% 26% 6%



- Molecule 4: 60S ribosomal protein L2-A

Chain AA: 78% 22%

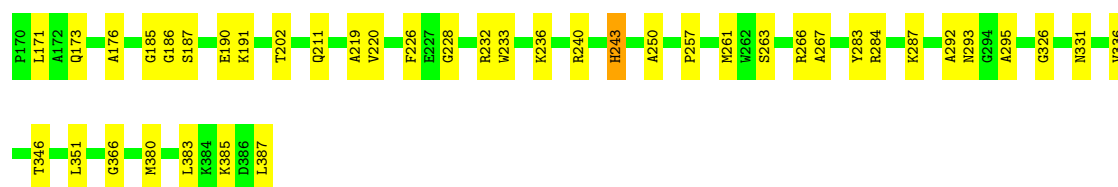


- Molecule 5: 60S ribosomal protein L3

Chain AB: 81% 19%

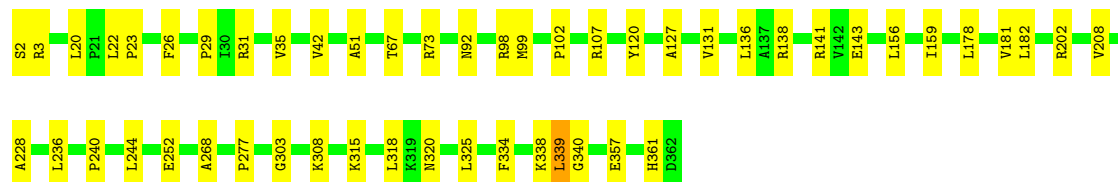






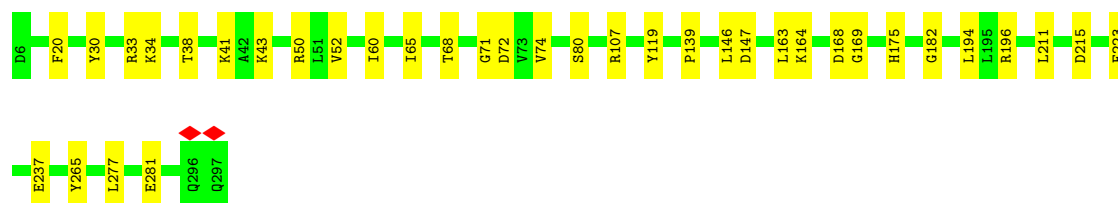
• Molecule 6: 60S ribosomal protein L4-A

Chain AC: 86% 14%



• Molecule 7: 60S ribosomal protein L5

Chain AD: 88% 12%



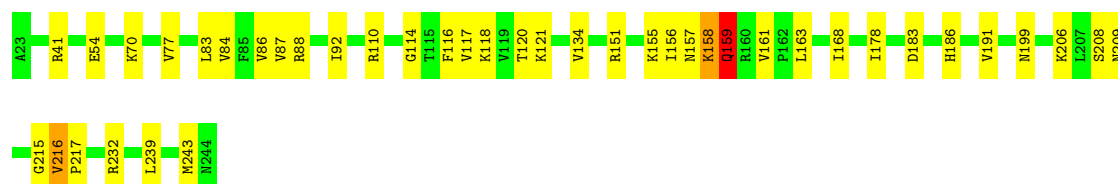
• Molecule 8: 60S ribosomal protein L6-A

Chain AE: 90% 10%



• Molecule 9: 60S ribosomal protein L7-A

Chain AF: 82% 17%

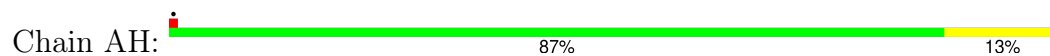


• Molecule 10: 60S ribosomal protein L8-A

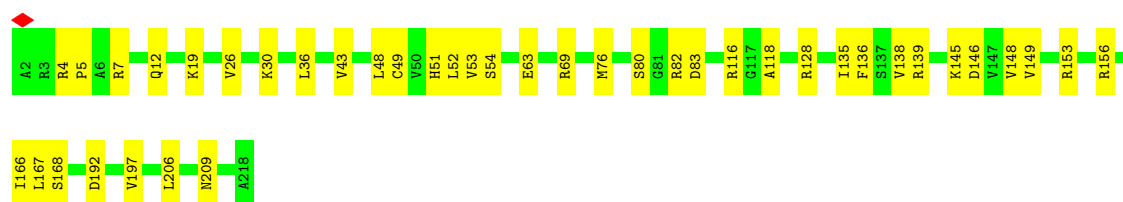
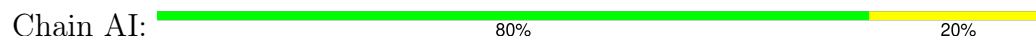
Chain AG: 88% 11%



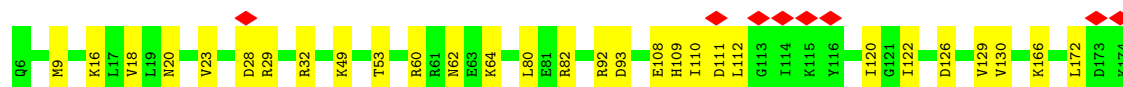
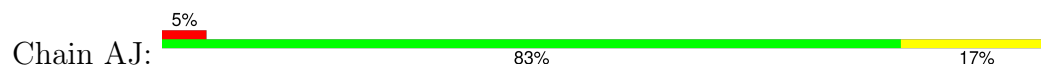
- Molecule 11: 60S ribosomal protein L9-A



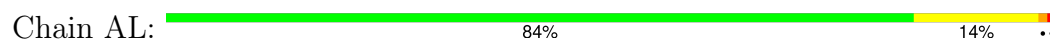
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-A



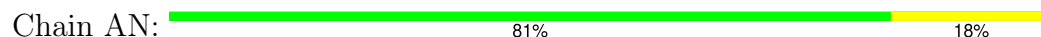
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A



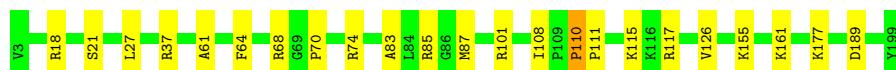
- Molecule 16: 60S ribosomal protein L15-A





- Molecule 17: 60S ribosomal protein L16-A

Chain AO: 88% 11%



- Molecule 18: 60S ribosomal protein L17-A

Chain AP: 89% 11%



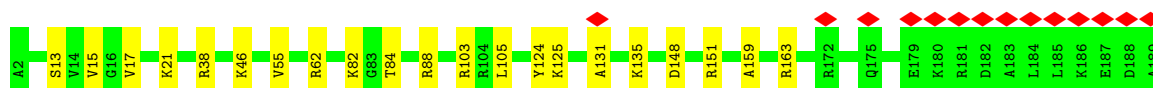
- Molecule 19: 60S ribosomal protein L18-A

Chain AQ: 91% 9%



- Molecule 20: 60S ribosomal protein L19-A

Chain AR: 7% 89% 11%



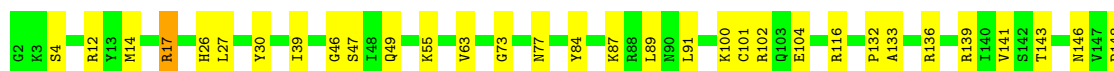
- Molecule 21: 60S ribosomal protein L20-A

Chain AS: 87% 12%

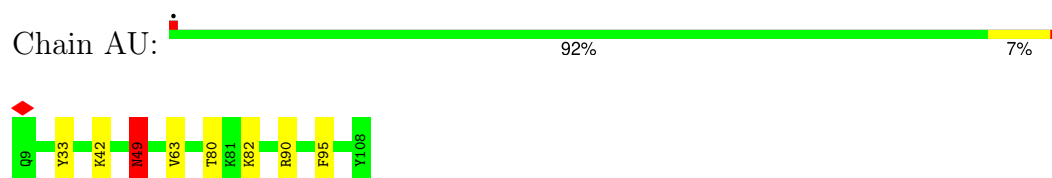


- Molecule 22: 60S ribosomal protein L21-A

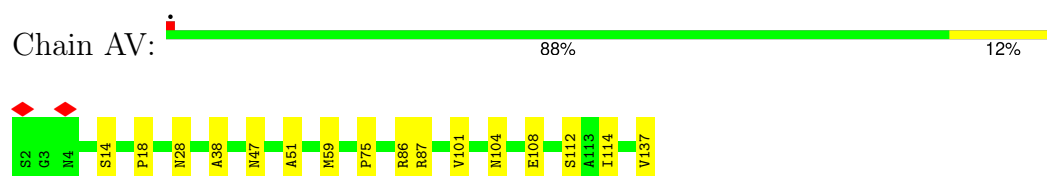
Chain AT: 79% 20%



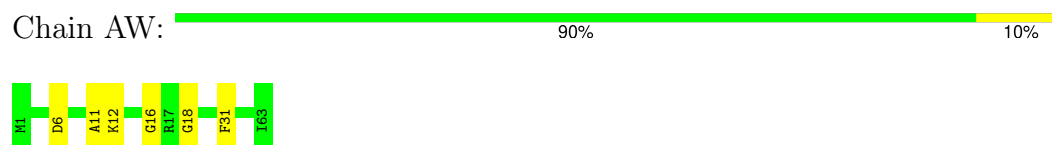
- Molecule 23: 60S ribosomal protein L22-A



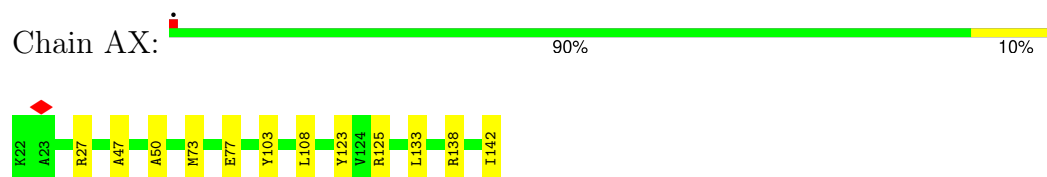
- Molecule 24: 60S ribosomal protein L23-A



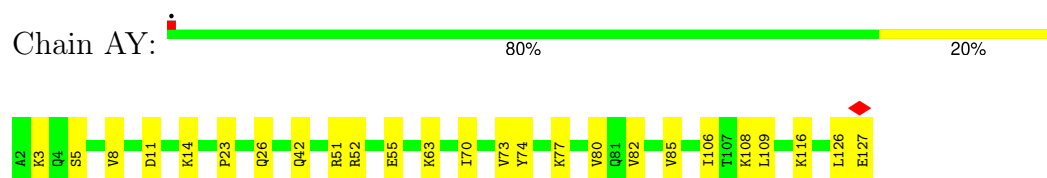
- Molecule 25: 60S ribosomal protein L24-A



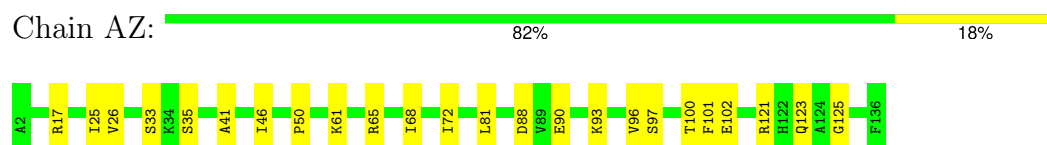
- Molecule 26: 60S ribosomal protein L25



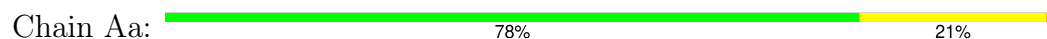
- Molecule 27: 60S ribosomal protein L26-A




- Molecule 28: 60S ribosomal protein L27-A



- Molecule 29: 60S ribosomal protein L28





Chain Ah:  88% 11%




- Molecule 37: 60S ribosomal protein L36-A

Chain Ai:  91% 9%




- Molecule 38: 60S ribosomal protein L37-A

Chain Aj:  84% 16%



- Molecule 39: 60S ribosomal protein L38

Chain Ak:  84% 16%



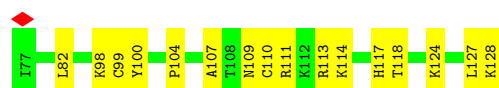
- Molecule 40: 60S ribosomal protein L39

Chain Al:  94% 6%



- Molecule 41: 60S ribosomal protein L40-A

Chain Am:  69% 31%




- Molecule 42: 60S ribosomal protein L41-A

Chain An:  96%




- Molecule 43: 60S ribosomal protein L42-A

Chain Ao:  89% 11%




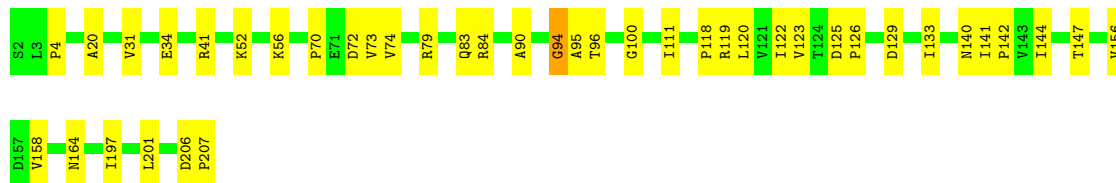
- Molecule 44: 60S ribosomal protein L43-A

Chain Ap:  80% 20%




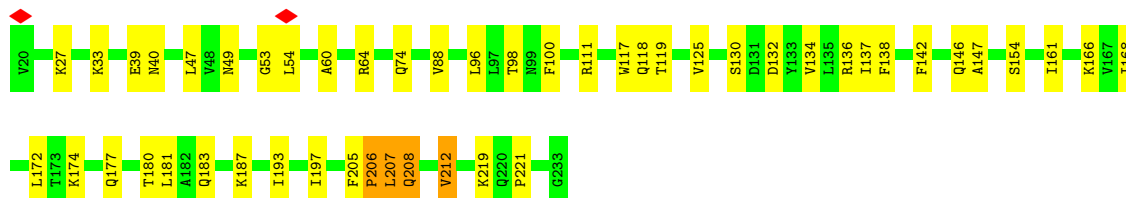
- Molecule 45: 40S ribosomal protein S0-A

Chain BA:  80% 19%




- Molecule 46: 40S ribosomal protein S1-A

Chain BB:  77% 21%




- Molecule 47: 40S ribosomal protein S2

Chain BC:  83% 16%



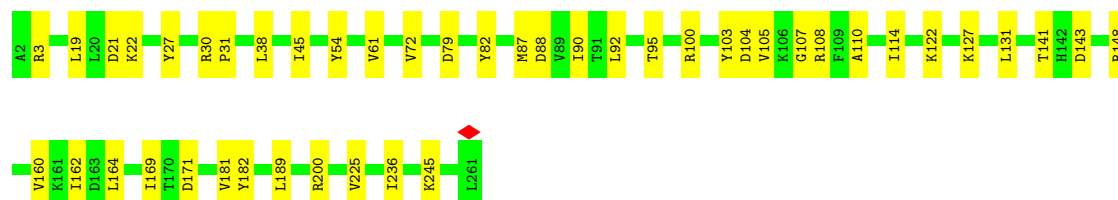
- Molecule 48: 40S ribosomal protein S3

Chain BD:  85% 15%



- Molecule 49: 40S ribosomal protein S4-A

Chain BE: 83% 17%



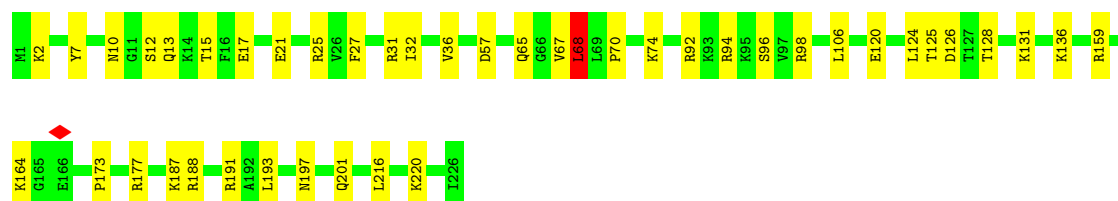
- Molecule 50: 40S ribosomal protein S5

Chain BF: 87% 13%



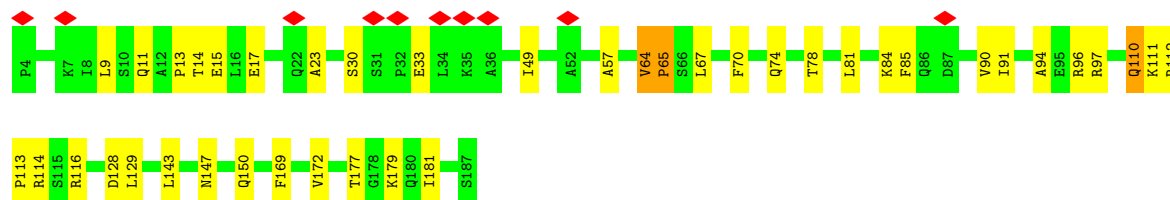
- Molecule 51: 40S ribosomal protein S6-A

Chain BG: 81% 19%



- Molecule 52: 40S ribosomal protein S7-A

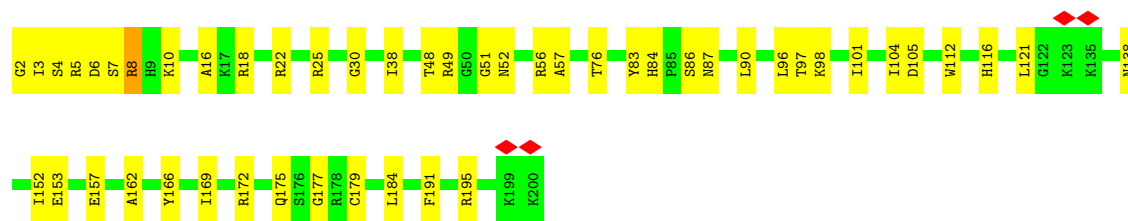
Chain BH: 5% 78% 21%



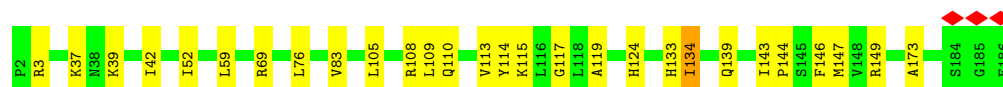
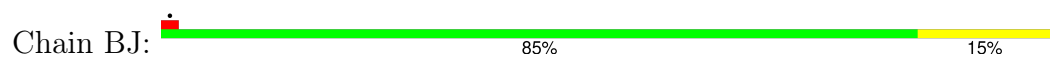
- Molecule 53: 40S ribosomal protein S8-A

Chain BI: 74% 26%

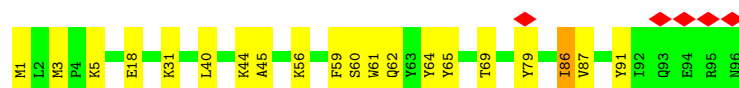
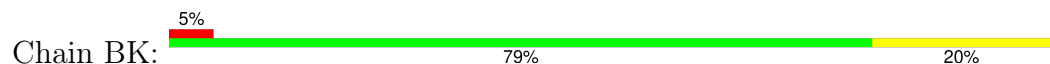




- Molecule 54: 40S ribosomal protein S9-A



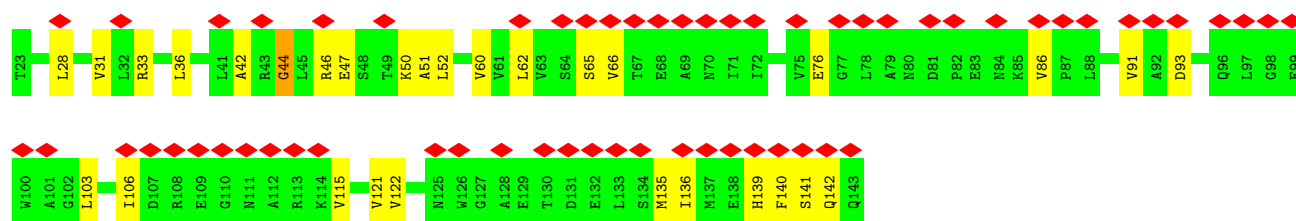
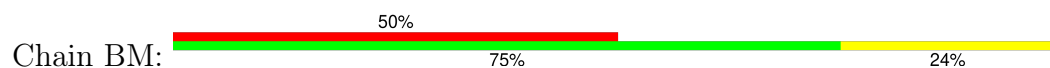
- Molecule 55: 40S ribosomal protein S10-A



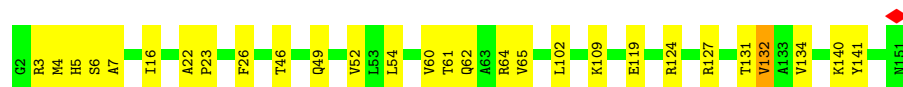
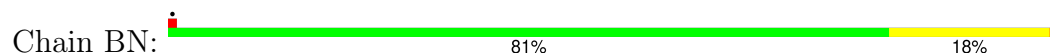
- Molecule 56: 40S ribosomal protein S11-A



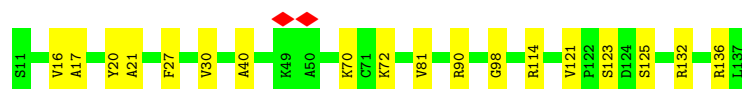
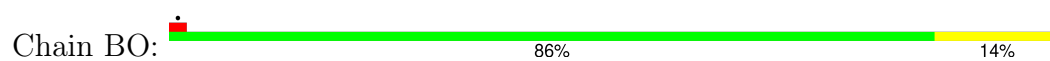
- Molecule 57: 40S ribosomal protein S12



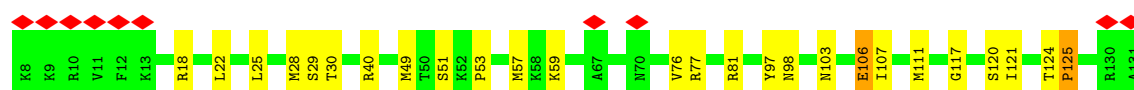
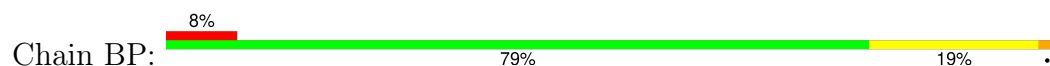
- Molecule 58: 40S ribosomal protein S13



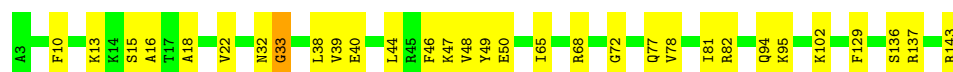
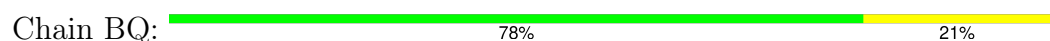
- Molecule 59: 40S ribosomal protein S14-A



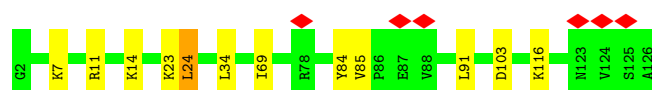
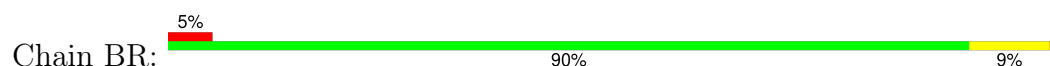
- Molecule 60: 40S ribosomal protein S15



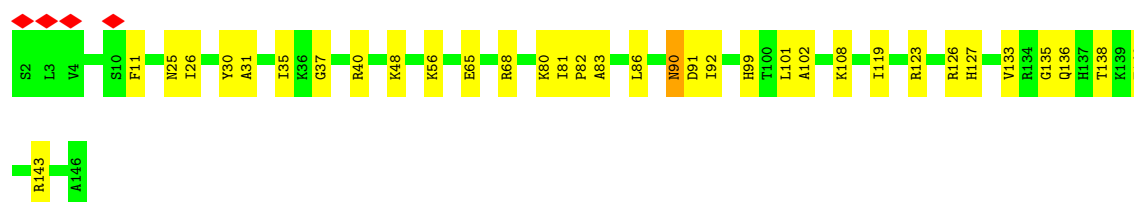
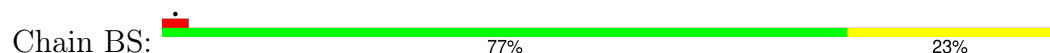
- Molecule 61: 40S ribosomal protein S16-A



- Molecule 62: 40S ribosomal protein S17-A



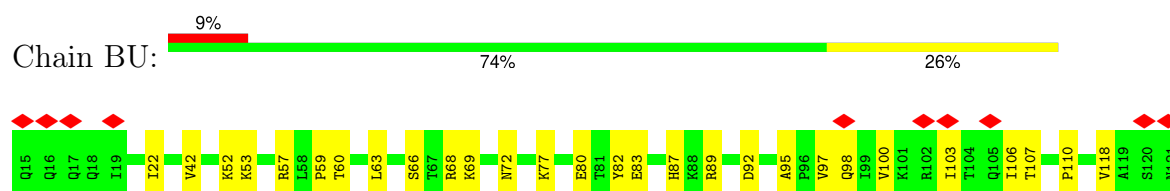
- Molecule 63: 40S ribosomal protein S18-A



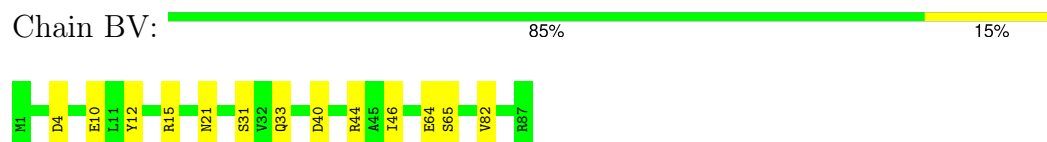
- Molecule 64: 40S ribosomal protein S19-A



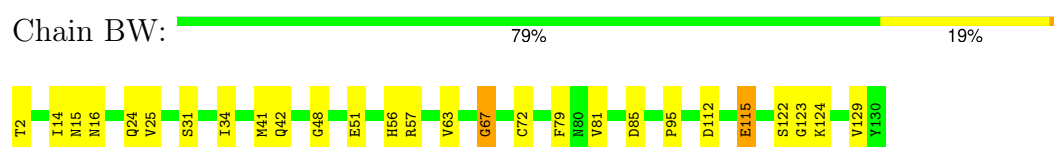
- Molecule 65: 40S ribosomal protein S20



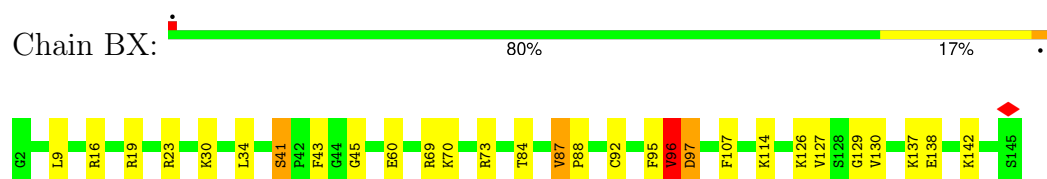
- Molecule 66: 40S ribosomal protein S21-A



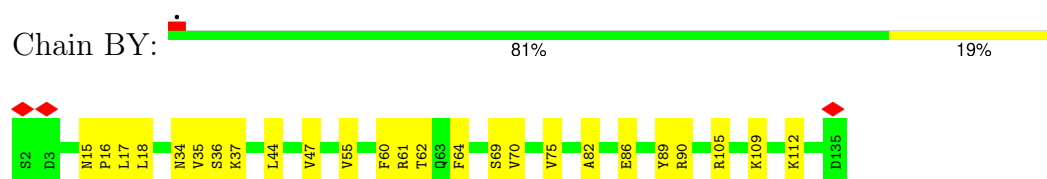
- Molecule 67: 40S ribosomal protein S22-A



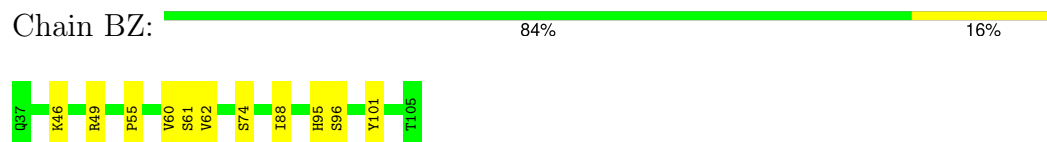
- Molecule 68: 40S ribosomal protein S23-A



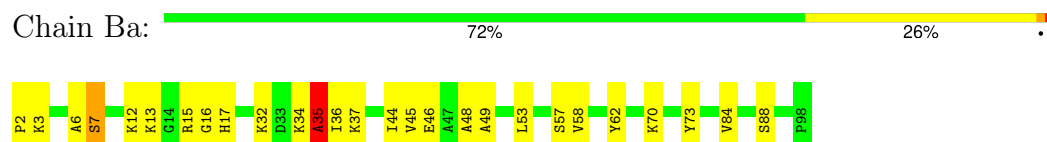
- Molecule 69: 40S ribosomal protein S24-A




- Molecule 70: 40S ribosomal protein S25-A



- Molecule 71: 40S ribosomal protein S26-B




- Molecule 72: 40S ribosomal protein S27-A

Chain Bb:  80% 19%



- Molecule 73: 40S ribosomal protein S28-A

Chain Bc:  5% 79% 21%




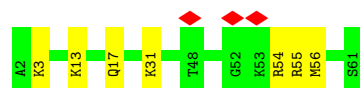
- Molecule 74: 40S ribosomal protein S29-A

Chain Bd:  68% 32%




- Molecule 75: 40S ribosomal protein S30-A

Chain Be:  5% 88% 12%




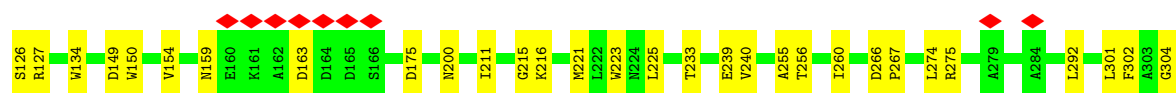
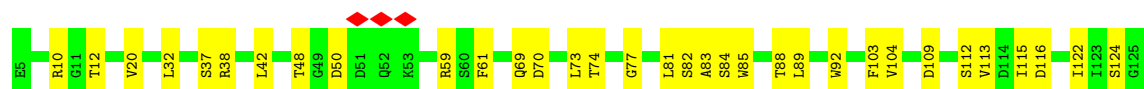
- Molecule 76: 40S ribosomal protein S31

Chain Bf:  42% 86% 14%

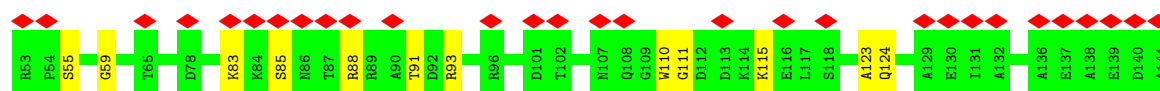
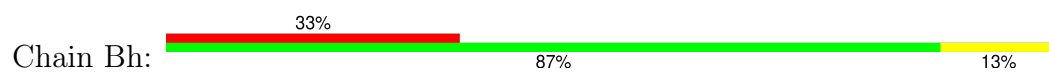


- Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein

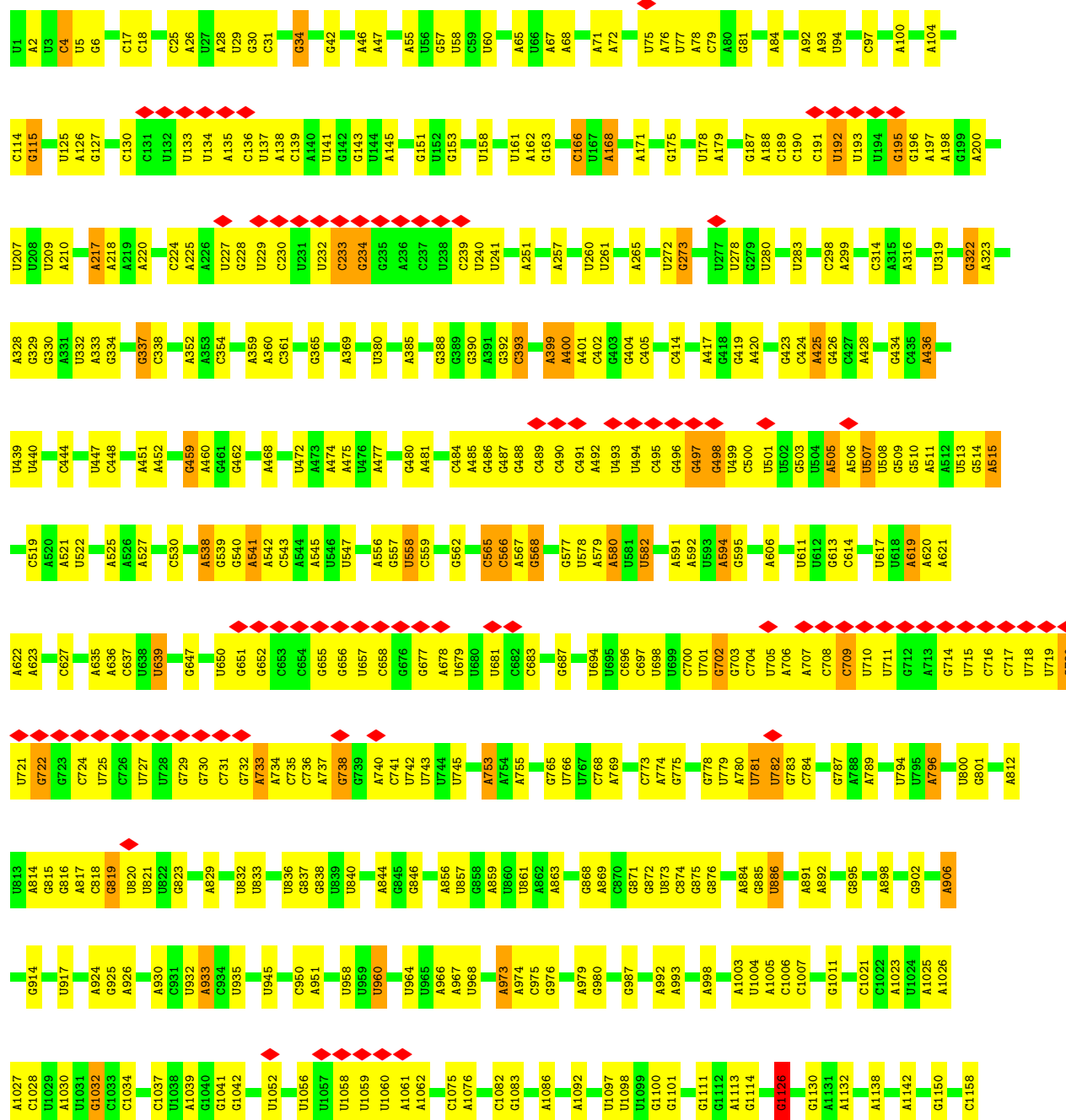
Chain Bg:  79% 21%

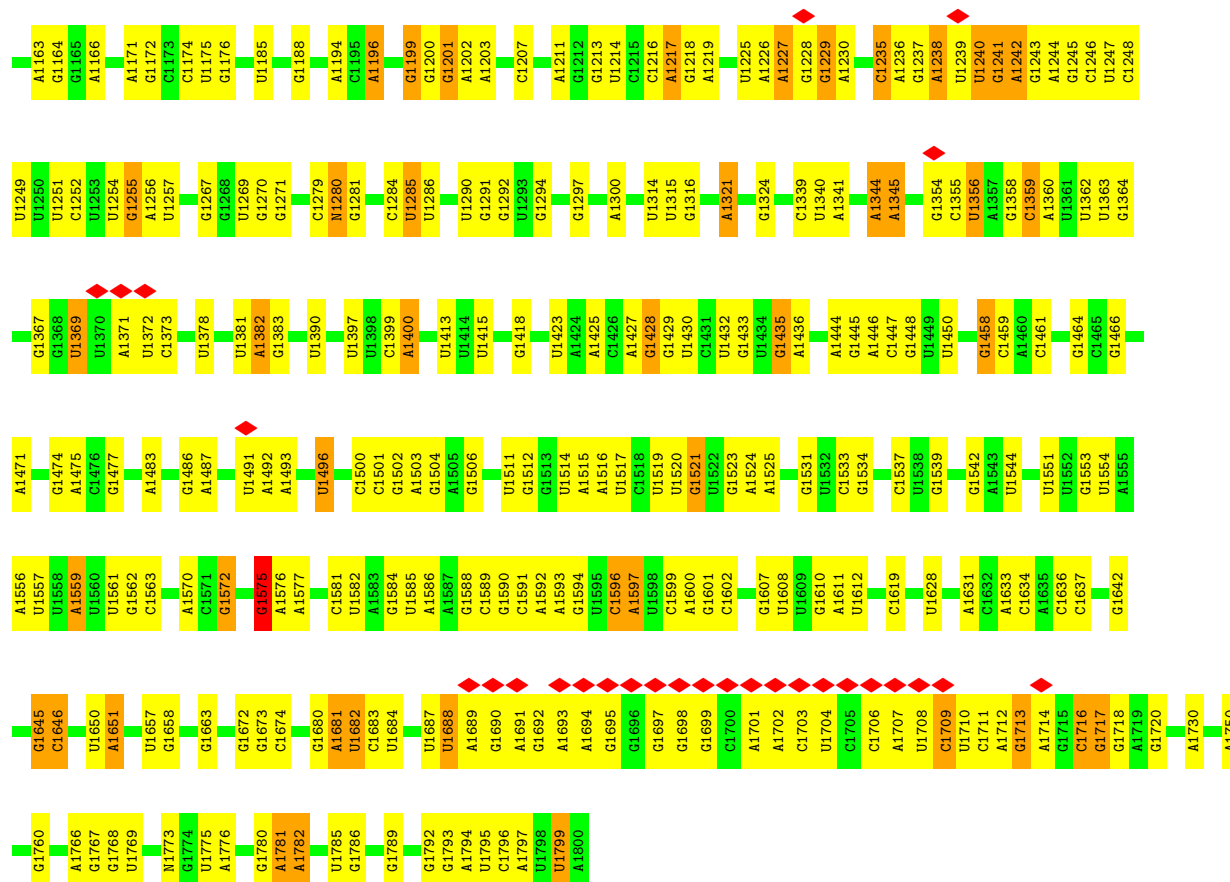


- Molecule 78: Suppressor protein STM1



• Molecule 79: 18S RIBOSOMAL RNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178990	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.233	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	455.75998, 455.75998, 455.75998	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, ZN, G7M, UR3, MA6, 3AU, OMC, A2M, 3HE, 1MA, OMU, HIC, OMG, MG, 4AC

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	A1	0.51	0/74562	0.46	10/116239 (0.0%)
2	A3	0.43	0/2883	0.38	0/4491
3	A4	0.54	0/3745	0.49	1/5828 (0.0%)
4	AA	0.49	0/1912	0.59	0/2569
5	AB	0.54	0/3137	0.66	4/4215 (0.1%)
6	AC	0.49	0/2800	0.69	1/3790 (0.0%)
7	AD	0.37	0/2390	0.62	0/3225
8	AE	0.45	0/1260	0.58	0/1694
9	AF	0.49	0/1821	0.70	3/2451 (0.1%)
10	AG	0.44	0/1830	0.66	1/2469 (0.0%)
11	AH	0.45	0/1531	0.61	0/2062
12	AI	0.35	0/1708	0.55	0/2290
13	AJ	0.33	0/1374	0.70	0/1842
14	AL	0.49	0/1568	0.73	1/2106 (0.0%)
15	AM	0.49	0/1068	0.60	0/1438
16	AN	0.56	0/1757	0.71	0/2354
17	AO	0.50	0/1585	0.59	0/2128
18	AP	0.49	0/1410	0.58	0/1893
19	AQ	0.47	0/1465	0.61	1/1965 (0.1%)
20	AR	0.42	0/1538	0.61	0/2050
21	AS	0.54	0/1481	0.67	0/1990
22	AT	0.46	0/1300	0.66	0/1743
23	AU	0.39	0/812	0.69	2/1099 (0.2%)
24	AV	0.48	0/1018	0.58	0/1369
25	AW	0.46	0/533	0.62	0/707
26	AX	0.49	0/983	0.59	0/1325
27	AY	0.49	0/1004	0.63	0/1341
28	AZ	0.44	0/1118	0.71	2/1497 (0.1%)
29	Aa	0.51	0/1204	0.79	3/1612 (0.2%)
30	Ab	0.36	0/473	0.64	0/629
31	Ac	0.40	0/751	0.57	0/1008
32	Ad	0.49	0/904	0.56	0/1213



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Ae	0.49	0/1041	0.55	0/1394
34	Af	0.54	0/868	0.51	0/1168
35	Ag	0.53	0/890	0.68	0/1189
36	Ah	0.44	0/978	0.61	0/1301
37	Ai	0.44	0/778	0.72	0/1034
38	Aj	0.55	0/696	0.62	0/923
39	Ak	0.48	0/618	0.60	0/826
40	Al	0.55	0/443	0.71	0/588
41	Am	0.46	0/423	0.55	0/562
42	An	0.30	0/234	0.62	0/300
43	Ao	0.39	0/860	0.61	0/1136
44	Ap	0.44	0/701	0.71	0/934
45	BA	0.37	0/1653	0.58	0/2261
46	BB	0.40	0/1735	0.80	4/2335 (0.2%)
47	BC	0.42	0/1665	0.69	3/2263 (0.1%)
48	BD	0.36	0/1759	0.62	0/2368
49	BE	0.42	0/2109	0.64	0/2839
50	BF	0.37	0/1629	0.67	0/2202
51	BG	0.36	0/1844	0.67	3/2464 (0.1%)
52	BH	0.36	0/1506	0.70	0/2028
53	BI	0.41	0/1514	0.69	0/2021
54	BJ	0.40	0/1519	0.69	0/2035
55	BK	0.40	0/837	0.82	1/1131 (0.1%)
56	BL	0.38	0/1272	0.53	0/1712
57	BM	0.26	0/921	0.75	1/1245 (0.1%)
58	BN	0.41	0/1215	0.72	1/1638 (0.1%)
59	BO	0.39	0/952	0.77	0/1279
60	BP	0.41	0/1012	0.78	4/1356 (0.3%)
61	BQ	0.40	0/1125	0.65	1/1510 (0.1%)
62	BR	0.31	0/984	0.68	0/1318
63	BS	0.41	0/1211	0.71	0/1628
64	BT	0.44	0/1113	0.78	3/1494 (0.2%)
65	BU	0.37	0/865	0.63	0/1169
66	BV	0.40	0/692	0.58	0/932
67	BW	0.48	0/1038	0.68	1/1395 (0.1%)
68	BX	0.44	0/1139	0.79	2/1518 (0.1%)
69	BY	0.39	0/1087	0.71	0/1449
70	BZ	0.35	0/566	0.70	0/761
71	Ba	0.44	0/782	0.86	2/1047 (0.2%)
72	Bb	0.36	0/620	0.62	0/838
73	Bc	0.35	0/499	0.65	0/670
74	Bd	0.42	0/452	0.66	0/600
75	Be	0.34	0/483	0.55	0/643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
76	Bf	0.30	0/462	0.70	0/617
77	Bg	0.36	0/2454	0.63	0/3340
78	Bh	0.26	0/678	0.65	0/905
79	B5	0.41	0/41746	0.44	1/65032 (0.0%)
All	All	0.46	0/212593	0.54	56/312030 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	AC	0	2
7	AD	0	1
8	AE	0	1
9	AF	0	3
10	AG	0	4
13	AJ	0	2
14	AL	0	2
16	AN	0	1
17	AO	0	1
20	AR	0	1
21	AS	0	1
22	AT	0	1
28	AZ	0	1
36	Ah	0	1
37	Ai	0	1
45	BA	0	1
46	BB	0	4
47	BC	0	1
50	BF	0	2
51	BG	0	1
52	BH	0	3
53	BI	0	2
54	BJ	0	2
59	BO	0	1
60	BP	0	4
61	BQ	0	3
63	BS	0	3
67	BW	0	1
68	BX	0	5
71	Ba	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
76	Bf	0	1
78	Bh	0	1
79	B5	4	0
All	All	4	61

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	266	A	OP1-P-OP2	-14.25	76.86	119.60
1	A1	266	A	O5'-P-OP1	-10.95	75.14	108.00
1	A1	265	A	OP2-P-O3'	-10.59	76.24	108.00
1	A1	1947	G	OP2-P-O3'	-9.65	79.06	108.00
1	A1	265	A	OP1-P-O3'	8.62	133.87	108.00
1	A1	266	A	O5'-P-OP2	8.27	132.82	108.00
57	BM	44	GLY	N-CA-C	7.85	122.61	111.00
51	BG	67	VAL	CA-C-N	7.69	136.24	121.54
51	BG	67	VAL	C-N-CA	7.69	136.24	121.54
9	AF	157	ASN	CA-C-N	7.65	136.15	121.54
9	AF	157	ASN	C-N-CA	7.65	136.15	121.54
29	Aa	47	LYS	CA-C-N	7.46	135.78	121.54
29	Aa	47	LYS	C-N-CA	7.46	135.78	121.54
71	Ba	35	ALA	CA-C-N	7.32	135.15	121.97
71	Ba	35	ALA	C-N-CA	7.32	135.15	121.97
46	BB	147	ALA	CA-C-N	6.97	134.86	121.54
46	BB	147	ALA	C-N-CA	6.97	134.86	121.54
1	A1	1947	G	OP1-P-O3'	-6.70	87.90	108.00
1	A1	1948	G	OP1-P-OP2	6.70	139.70	119.60
55	BK	86	ILE	N-CA-C	-6.70	107.35	113.71
46	BB	212	VAL	CA-C-N	6.56	134.08	121.54
46	BB	212	VAL	C-N-CA	6.56	134.08	121.54
47	BC	146	THR	N-CA-C	-6.52	97.70	108.07
58	BN	132	VAL	N-CA-C	-6.50	106.18	112.29
23	AU	49	ASN	CA-CB-CG	6.22	118.82	112.60
64	BT	7	ARG	N-CA-C	-6.21	106.93	114.75
29	Aa	56	VAL	N-CA-C	-6.15	96.55	109.34
28	AZ	102	GLU	CA-C-N	-5.99	112.71	122.65
28	AZ	102	GLU	C-N-CA	-5.99	112.71	122.65
68	BX	96	VAL	CA-C-N	5.87	132.76	121.54
68	BX	96	VAL	C-N-CA	5.87	132.76	121.54
14	AL	48	PRO	N-CA-C	5.86	124.54	112.47
9	AF	159	GLN	N-CA-C	5.86	123.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	BW	115	GLU	CA-CB-CG	5.83	125.77	114.10
1	A1	1385	C	C2'-C3'-O3'	5.79	122.39	113.70
10	AG	79	GLN	CA-CB-CG	5.63	125.36	114.10
19	AQ	180	ARG	CA-CB-CG	5.57	125.24	114.10
5	AB	138	ALA	CA-C-N	5.55	132.14	121.54
5	AB	138	ALA	C-N-CA	5.55	132.14	121.54
60	BP	106	GLU	CA-CB-CG	5.48	125.06	114.10
5	AB	4	ARG	CA-C-N	5.48	132.00	121.54
5	AB	4	ARG	C-N-CA	5.48	132.00	121.54
60	BP	28	MET	CA-C-N	5.45	131.94	121.54
60	BP	28	MET	C-N-CA	5.45	131.94	121.54
64	BT	52	GLY	CA-C-N	5.38	131.82	121.54
64	BT	52	GLY	C-N-CA	5.38	131.82	121.54
3	A4	67	U	C2'-C3'-O3'	5.28	121.61	113.70
79	B5	1285	U	P-O3'-C3'	5.27	128.10	120.20
60	BP	30	THR	N-CA-C	5.23	119.13	112.34
47	BC	145	GLY	CA-C-N	5.22	134.21	122.19
47	BC	145	GLY	C-N-CA	5.22	134.21	122.19
23	AU	49	ASN	CB-CA-C	5.07	118.91	111.06
61	BQ	38	LEU	CA-CB-CG	5.03	133.91	116.30
51	BG	68	LEU	N-CA-C	-5.03	100.09	110.80
6	AC	182	LEU	CA-CB-CG	5.02	133.87	116.30
1	A1	406	G	O4'-C1'-N9	5.01	115.71	108.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	B5	1191	3AU	C12
79	B5	1575	G7M	C4',C3',C2'

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AC	131	VAL	Peptide
6	AC	318	LEU	Peptide
7	AD	43	LYS	Peptide
8	AE	67	GLY	Peptide
9	AF	158	LYS	Peptide
9	AF	215	GLY	Peptide
9	AF	232	ARG	Peptide
10	AG	30	THR	Peptide
10	AG	74	THR	Peptide

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Mol	Chain	Res	Type	Group
10	AG	76	ALA	Peptide
10	AG	79	GLN	Peptide
13	AJ	109	HIS	Peptide
13	AJ	166	LYS	Peptide
14	AL	47	ALA	Peptide
14	AL	75	PHE	Peptide
16	AN	80	THR	Peptide
17	AO	110[A]	PRO	Peptide
20	AR	131	ALA	Peptide
21	AS	22	PRO	Peptide
22	AT	17	ARG	Peptide
28	AZ	123	GLN	Peptide
36	Ah	90	ARG	Peptide
37	Ai	27	SER	Peptide
45	BA	94	GLY	Peptide
46	BB	177	GLN	Peptide
46	BB	205	PHE	Peptide
46	BB	206	PRO	Peptide
46	BB	208	GLN	Peptide
47	BC	148	LEU	Peptide
50	BF	42	LEU	Peptide
50	BF	43	PHE	Peptide
51	BG	68	LEU	Peptide
52	BH	110	GLN	Peptide
52	BH	64	VAL	Peptide
52	BH	65	PRO	Peptide
53	BI	51	GLY	Peptide
53	BI	8	ARG	Peptide
54	BJ	117	GLY	Peptide
54	BJ	133	HIS	Peptide
59	BO	123	SER	Peptide
60	BP	106	GLU	Peptide
60	BP	124	THR	Peptide
60	BP	125	PRO	Peptide
60	BP	29	SER	Peptide
61	BQ	32	ASN	Peptide
61	BQ	33	GLY	Peptide
61	BQ	40	GLU	Peptide
63	BS	56	LYS	Peptide
63	BS	81	ILE	Peptide
63	BS	90	ASN	Peptide
67	BW	115	GLU	Peptide

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Mol	Chain	Res	Type	Group
68	BX	137	LYS	Peptide
68	BX	138	GLU	Peptide
68	BX	41	SER	Peptide
68	BX	87	VAL	Peptide
68	BX	97	ASP	Peptide
71	Ba	34	LYS	Peptide
71	Ba	35	ALA	Peptide
71	Ba	7	SER	Peptide
76	Bf	105	TYR	Peptide
78	Bh	85	SER	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	A1	67535	0	33991	368	0
2	A3	2579	0	1303	11	0
3	A4	3353	0	1695	19	0
4	AA	1878	0	1946	40	0
5	AB	3079	0	3154	51	0
6	AC	2748	0	2859	34	0
7	AD	2341	0	2290	23	0
8	AE	1239	0	1326	10	0
9	AF	1784	0	1862	25	0
10	AG	1798	0	1894	16	0
11	AH	1510	0	1576	17	0
12	AI	1672	0	1711	27	0
13	AJ	1353	0	1383	18	0
14	AL	1543	0	1608	23	0
15	AM	1053	0	1149	6	0
16	AN	1720	0	1779	35	0
17	AO	1555	0	1659	19	0
18	AP	1388	0	1423	13	0
19	AQ	1441	0	1543	12	0
20	AR	1521	0	1617	16	0
21	AS	1445	0	1487	17	0
22	AT	1276	0	1323	26	0
23	AU	796	0	812	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	AV	1003	0	1048	10	0
25	AW	521	0	551	4	0
26	AX	968	0	1036	7	0
27	AY	993	0	1081	14	0
28	AZ	1092	0	1155	14	0
29	Aa	1173	0	1215	26	0
30	Ab	462	0	491	3	0
31	Ac	743	0	797	12	0
32	Ad	890	0	938	7	0
33	Ae	1020	0	1090	6	0
34	Af	850	0	880	9	0
35	Ag	880	0	945	11	0
36	Ah	969	0	1078	9	0
37	Ai	771	0	849	5	0
38	Aj	681	0	687	9	0
39	Ak	612	0	682	10	0
40	Al	436	0	475	3	0
41	Am	417	0	459	12	0
42	An	233	0	284	1	0
43	Ao	847	0	914	9	0
44	Ap	694	0	738	14	0
45	BA	1612	0	1623	27	0
46	BB	1709	0	1784	29	0
47	BC	1635	0	1723	21	0
48	BD	1734	0	1817	25	0
49	BE	2068	0	2154	30	0
50	BF	1609	0	1675	18	0
51	BG	1820	0	1918	31	0
52	BH	1481	0	1572	24	0
53	BI	1489	0	1525	33	0
54	BJ	1494	0	1573	19	0
55	BK	817	0	804	15	0
56	BL	1244	0	1314	8	0
57	BM	913	0	955	22	0
58	BN	1192	0	1255	19	0
59	BO	941	0	979	13	0
60	BP	991	0	1035	13	0
61	BQ	1105	0	1166	20	0
62	BR	975	0	1039	11	0
63	BS	1192	0	1222	22	0
64	BT	1095	0	1114	28	0
65	BU	855	0	917	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	BV	684	0	671	10	0
67	BW	1021	0	1060	19	0
68	BX	1121	0	1196	18	0
69	BY	1073	0	1132	19	0
70	BZ	558	0	598	6	0
71	Ba	769	0	818	18	0
72	Bb	610	0	630	10	0
73	Bc	497	0	535	9	0
74	Bd	442	0	432	13	0
75	Be	475	0	525	5	0
76	Bf	454	0	468	5	0
77	Bg	2401	0	2356	41	0
78	Bh	675	0	654	10	0
79	B5	37891	0	19102	265	0
80	A1	20	0	23	0	0
81	A1	247	0	0	0	0
81	A3	5	0	0	0	0
81	A4	9	0	0	0	0
81	AB	4	0	0	0	0
81	AC	1	0	0	0	0
81	AG	1	0	0	0	0
81	AL	3	0	0	0	0
81	AN	1	0	0	0	0
81	AO	1	0	0	0	0
81	AP	1	0	0	0	0
81	AR	1	0	0	0	0
81	AV	1	0	0	0	0
81	Aa	1	0	0	0	0
81	Ae	2	0	0	0	0
81	Af	1	0	0	0	0
81	Aj	1	0	0	0	0
81	B5	90	0	0	0	0
81	BE	1	0	0	0	0
81	BG	1	0	0	0	0
81	BJ	1	0	0	0	0
81	Ba	1	0	0	0	0
82	Ao	1	0	0	0	0
82	Bb	1	0	0	0	0
All	All	199900	0	148147	1521	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 5.



All (1521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:3348:G:H1	1:A1:3357:U:H3	1.04	0.99
79:B5:1356:U:H3	79:B5:1367:G:H1	0.96	0.95
79:B5:868:G:H1	79:B5:960:U:H3	1.15	0.88
79:B5:1588:G:H1	79:B5:1608:U:H3	1.24	0.86
79:B5:976:G:H1	79:B5:1023:A:HO2'	1.24	0.85
16:AN:16:SER:O	16:AN:20:ARG:HB2	1.79	0.81
2:A3:52:G:H21	13:AJ:9:MET:HE3	1.50	0.76
28:AZ:88:ASP:HB3	28:AZ:121:ARG:HH12	1.54	0.73
79:B5:1213:G:H1	79:B5:1450:U:H3	1.37	0.72
63:BS:48:LYS:HD3	64:BT:35:ASP:HB3	1.72	0.70
79:B5:895:G:H1	79:B5:917:U:H3	1.38	0.70
72:Bb:56:CYS:HB2	72:Bb:59:CYS:H	1.56	0.68
1:A1:2392:C:O2'	5:AB:266:ARG:NH2	2.27	0.68
49:BE:87:MET:HE1	49:BE:236:ILE:HD13	1.76	0.68
62:BR:24:LEU:HB3	62:BR:34:LEU:HD11	1.76	0.67
70:BZ:95:HIS:ND1	70:BZ:96:SER:O	2.26	0.67
1:A1:2987:A:H5''	17:AO:68[A]:ARG:HH12	1.60	0.67
32:Ad:51:LEU:HB3	32:Ad:55:LEU:HD23	1.77	0.66
1:A1:1213:G:H4'	21:AS:90:MET:HG2	1.77	0.66
24:AV:104:ASN:HD21	24:AV:108:GLU:HB2	1.60	0.66
39:Ak:5:ILE:HG22	39:Ak:7:ASP:H	1.58	0.66
1:A1:1766:G:N7	20:AR:46:LYS:NZ	2.43	0.66
1:A1:2721:A:H5''	30:Ab:33:LYS:HE2	1.76	0.66
50:BF:166:ARG:HH12	73:Bc:45:LYS:HE3	1.59	0.65
59:BO:16:VAL:O	59:BO:30:VAL:HA	1.97	0.65
4:AA:27:ALA:O	4:AA:128:ARG:NH2	2.29	0.65
1:A1:687:U:OP2	14:AL:36:ARG:NH2	2.30	0.65
79:B5:737:A:C2	79:B5:738:G:O6	2.50	0.65
5:AB:10:ARG:NH1	5:AB:11:HIS:O	2.30	0.64
52:BH:70:PHE:O	52:BH:74:GLN:HB2	1.97	0.64
79:B5:513:U:H3	79:B5:538:A:H2	1.44	0.64
1:A1:860:G:OP1	44:Ap:17:ARG:NH1	2.29	0.64
47:BC:38:VAL:HG13	47:BC:39:THR:HG23	1.80	0.64
65:BU:82:TYR:HB3	74:Bd:52:PHE:HB3	1.79	0.64
7:AD:50:ARG:NH2	7:AD:72:ASP:OD2	2.31	0.64
1:A1:1682:U:O4	23:AU:90:ARG:NH1	2.31	0.64
50:BF:63:GLN:HE22	50:BF:66:GLN:HG2	1.63	0.64
1:A1:1097:G:N7	22:AT:116:ARG:NH2	2.45	0.63
57:BM:47:GLU:HB2	79:B5:1229:G:H1	1.62	0.63
67:BW:15:ASN:ND2	67:BW:72:CYS:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:912:G:OP2	4:AA:9:ARG:NH1	2.32	0.63
9:AF:87:VAL:HG11	9:AF:243:MET:HE1	1.80	0.63
77:Bg:216:LYS:HA	77:Bg:239:GLU:HG3	1.79	0.63
1:A1:1575:A:O2'	1:A1:1576:G:N3	2.32	0.63
46:BB:132:ASP:HB3	46:BB:221:PRO:HB3	1.80	0.63
67:BW:31:SER:H	67:BW:34:ILE:HD12	1.64	0.62
68:BX:96:VAL:O	68:BX:142:LYS:NZ	2.30	0.62
71:Ba:46:GLU:HB3	71:Ba:49:ALA:H	1.64	0.62
63:BS:135:GLY:HA3	79:B5:1559:A:H5''	1.81	0.62
16:AN:183:THR:HG22	16:AN:187:ARG:HB3	1.80	0.62
44:Ap:46:THR:OG1	44:Ap:57:CYS:SG	2.57	0.62
1:A1:3045:G:OP1	5:AB:19:ARG:NH2	2.33	0.62
72:Bb:48:SER:HG	72:Bb:49:HIS:HD1	1.48	0.62
5:AB:10:ARG:NH2	5:AB:263:SER:O	2.33	0.62
16:AN:155:VAL:O	16:AN:162:ARG:NH2	2.32	0.62
1:A1:299:G:HO2'	1:A1:300:G:H8	1.48	0.62
1:A1:1639:C:OP2	35:Ag:74:ARG:NH2	2.31	0.62
9:AF:163:LEU:HA	9:AF:168:ILE:HD11	1.81	0.61
64:BT:38:LYS:O	64:BT:43:ASN:ND2	2.33	0.61
21:AS:112:ALA:O	21:AS:115:ARG:NH1	2.33	0.61
36:Ah:85:THR:HB	36:Ah:88:LEU:HB2	1.82	0.61
61:BQ:39:VAL:HG21	61:BQ:48:VAL:HG21	1.82	0.61
67:BW:2:THR:N	79:B5:1034:C:HO2'	1.98	0.61
4:AA:101:VAL:HG22	4:AA:165:VAL:HG22	1.82	0.61
26:AX:103:TYR:O	26:AX:138:ARG:NH1	2.34	0.61
41:Am:104:PRO:HG2	41:Am:107:ALA:HB2	1.83	0.61
50:BF:225:ARG:NH1	73:Bc:58:GLU:OE2	2.34	0.61
66:BV:40:ASP:HB3	66:BV:46:ILE:HD11	1.81	0.61
1:A1:1317:A:O2'	17:AO:18[A]:ARG:NH2	2.34	0.61
4:AA:117:GLU:HG2	4:AA:124:GLY:H	1.66	0.61
6:AC:136:LEU:HD11	6:AC:143:GLU:HG3	1.83	0.61
50:BF:72:HIS:NE2	79:B5:1610:G:OP1	2.28	0.60
53:BI:98:LYS:HB3	79:B5:329:G:H5''	1.83	0.60
77:Bg:81:LEU:HD11	77:Bg:122:ILE:HD12	1.83	0.60
1:A1:676:G:HO2'	1:A1:678:G:HO2'	1.46	0.60
1:A1:1348:U:OP1	19:AQ:39:ARG:NH1	2.35	0.60
5:AB:37:ARG:HD3	5:AB:186:GLY:HA2	1.83	0.60
31:Ac:13:LYS:HB3	31:Ac:100:ILE:HG22	1.84	0.60
57:BM:62:LEU:HD22	57:BM:76:GLU:HG2	1.83	0.60
79:B5:1354:G:O6	79:B5:1369:U:O4	2.19	0.60
12:AI:36:LEU:HD11	12:AI:69:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BI:172:ARG:HE	53:BI:175:GLN:HG3	1.65	0.60
74:Bd:14:TYR:HH	79:B5:1553:G:HO2'	1.49	0.60
1:A1:3034:C:H5	11:AH:121:LYS:H	1.49	0.60
12:AI:76:MET:HE1	12:AI:138:VAL:HG21	1.83	0.60
31:Ac:17:VAL:HG11	31:Ac:92:ILE:HD12	1.82	0.60
20:AR:148:ASP:OD1	20:AR:151:ARG:NH1	2.34	0.60
68:BX:70:LYS:NZ	79:B5:567:A:OP1	2.34	0.60
1:A1:2878:G:H5''	5:AB:5:LYS:HE2	1.84	0.60
68:BX:69:ARG:NH2	79:B5:568:G:N7	2.50	0.60
69:BY:61:ARG:NH1	79:B5:530:C:O2	2.35	0.60
3:A4:52:A:H62	40:Al:27:ILE:HD13	1.67	0.60
23:AU:49:ASN:O	23:AU:49:ASN:ND2	2.35	0.60
54:BJ:119:ALA:O	54:BJ:124:HIS:ND1	2.32	0.60
61:BQ:129:PHE:O	61:BQ:137:ARG:NH2	2.35	0.60
3:A4:71:A:O2'	27:AY:52:ARG:NH2	2.35	0.60
5:AB:284:ARG:NH1	5:AB:293:ASN:O	2.35	0.60
65:BU:72:ASN:ND2	79:B5:1429:G:N3	2.50	0.60
78:Bh:93:ARG:HH22	79:B5:1636:C:H5''	1.65	0.60
3:A4:150:G:OP1	26:AX:27:ARG:NH2	2.35	0.59
1:A1:1385:C:OP1	6:AC:141:ARG:NH1	2.34	0.59
51:BG:13:GLN:NE2	79:B5:151:G:N3	2.50	0.59
6:AC:20:LEU:HD11	6:AC:252:GLU:HG3	1.85	0.59
18:AP:118:GLN:NE2	18:AP:120:ASN:OD1	2.35	0.59
66:BV:10:GLU:O	66:BV:12:TYR:N	2.35	0.59
65:BU:95:ALA:HB1	65:BU:100:VAL:HG21	1.82	0.59
1:A1:1390:A:N6	1:A1:1418:A:O2'	2.34	0.59
16:AN:80:THR:HG22	16:AN:82:GLY:H	1.68	0.59
74:Bd:43:PHE:O	74:Bd:47:ALA:HB2	2.02	0.59
1:A1:2901:G:O2'	1:A1:3024:A:N1	2.33	0.59
60:BP:18:ARG:NH1	63:BS:90:ASN:O	2.35	0.59
6:AC:99:MET:HE3	6:AC:102:PRO:HA	1.83	0.59
79:B5:1023:A:OP1	79:B5:1126:OMG:N2	2.35	0.59
1:A1:2779:A:O2'	14:AL:180:ARG:NH2	2.36	0.58
1:A1:2842:U:OP1	1:A1:2844:C:N4	2.33	0.58
3:A4:51:G:OP2	40:Al:21:ARG:NH1	2.34	0.58
54:BJ:139:GLN:NE2	69:BY:64:PHE:O	2.35	0.58
71:Ba:84:VAL:O	79:B5:1797:A:N6	2.36	0.58
17:AO:61[A]:ALA:HA	17:AO:70[A]:PRO:HD2	1.84	0.58
1:A1:1361:U:O2	9:AF:159:GLN:NE2	2.35	0.58
1:A1:439:C:H1'	1:A1:494:G:H21	1.68	0.58
29:Aa:104:THR:HG21	29:Aa:112:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BG:57:ASP:HA	51:BG:106:LEU:HA	1.86	0.58
79:B5:233:C:O2'	79:B5:234:G:N2	2.35	0.58
79:B5:1354:G:O6	79:B5:1369:U:C4	2.56	0.58
1:A1:2406:C:O2'	1:A1:2619:OMG:N2	2.36	0.58
55:BK:40:LEU:O	55:BK:44:LYS:HB2	2.04	0.58
45:BA:72:ASP:HB2	45:BA:118:PRO:HA	1.84	0.58
1:A1:2848:G:OP1	41:Am:100:TYR:OH	2.22	0.58
57:BM:44:GLY:HA2	79:B5:1227:A:H2	1.69	0.58
1:A1:831:G:O2'	1:A1:1864:A:N3	2.32	0.58
79:B5:979:A:N3	79:B5:1775:U:O2'	2.36	0.58
79:B5:1291:G:H1	79:B5:1324:G:H22	1.50	0.58
47:BC:199:GLN:NE2	79:B5:2:A:N3	2.52	0.58
64:BT:102:ARG:NH2	79:B5:1502:G:N7	2.51	0.58
79:B5:730:G:N2	79:B5:733:A:OP1	2.36	0.58
1:A1:3297:U:O4	5:AB:124:LYS:NZ	2.36	0.58
10:AG:81:THR:HG21	10:AG:181:LYS:HB2	1.84	0.58
54:BJ:109:LEU:HB2	54:BJ:146:PHE:HB3	1.86	0.58
79:B5:709:C:N4	79:B5:730:G:O2'	2.37	0.58
1:A1:1669:C:H5'	35:Ag:30:LEU:HD11	1.86	0.57
1:A1:1722:U:OP2	20:AR:103:ARG:NH1	2.37	0.57
6:AC:338:LYS:O	6:AC:340:GLY:N	2.37	0.57
57:BM:47:GLU:OE1	79:B5:1229:G:N2	2.36	0.57
1:A1:443:G:N2	1:A1:492:C:O2'	2.38	0.57
1:A1:799:G:O2'	14:AL:18:TRP:NE1	2.35	0.57
22:AT:73:GLY:HA2	22:AT:89:LEU:O	2.04	0.57
50:BF:76:ARG:O	50:BF:83:ARG:NH1	2.37	0.57
1:A1:38:U:H4'	29:Aa:32:ARG:HD2	1.86	0.57
5:AB:185:GLY:O	5:AB:191:LYS:NZ	2.36	0.57
46:BB:39:GLU:HB3	46:BB:74:GLN:HA	1.85	0.57
77:Bg:149:ASP:H	77:Bg:175:ASP:HB3	1.69	0.57
1:A1:1592:G:OP1	35:Ag:58:ARG:NH2	2.37	0.57
11:AH:57:VAL:HG23	11:AH:68:LEU:HD13	1.87	0.57
16:AN:35:VAL:O	16:AN:64:VAL:HA	2.04	0.57
54:BJ:3:ARG:NH2	79:B5:462:G:OP1	2.37	0.57
58:BN:23:PRO:HD2	58:BN:26:PHE:HB2	1.86	0.57
74:Bd:30:LEU:HA	74:Bd:39:CYS:HA	1.85	0.57
1:A1:1124:U:O2'	1:A1:2635:A:OP1	2.22	0.57
5:AB:113:GLU:HB3	5:AB:176:ALA:HB2	1.87	0.57
6:AC:357:GLU:O	6:AC:361:HIS:HB2	2.04	0.57
1:A1:2890:A:O2'	1:A1:2933:A:N3	2.34	0.57
22:AT:89:LEU:HB3	22:AT:91:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:19:LEU:HD11	49:BE:108:ARG:HD2	1.85	0.57
65:BU:42:VAL:HG13	65:BU:52:LYS:HE2	1.87	0.57
57:BM:135:MET:SD	57:BM:139:HIS:NE2	2.78	0.57
79:B5:220:A:H5''	79:B5:832:U:H1'	1.85	0.57
79:B5:1238:A:H61	79:B5:1246:C:H42	1.51	0.57
1:A1:2631:U:OP2	22:AT:4:SER:OG	2.23	0.57
50:BF:70:VAL:HG12	61:BQ:47:LYS:HE3	1.87	0.57
1:A1:284:A:OP2	43:Ao:41:ARG:NH1	2.34	0.56
1:A1:692:A:OP1	16:AN:201:ARG:NH2	2.33	0.56
1:A1:938:C:OP2	29:Aa:26:ARG:NH1	2.39	0.56
69:BY:105:ARG:NH2	79:B5:459:G:OP2	2.38	0.56
1:A1:541:U:H3	1:A1:550:A:H61	1.51	0.56
4:AA:36:GLU:OE1	4:AA:163:ARG:NH1	2.38	0.56
5:AB:17:LEU:HD11	5:AB:233:TRP:HH2	1.69	0.56
45:BA:144:ILE:HG12	45:BA:158:VAL:HB	1.86	0.56
51:BG:31:ARG:NH1	79:B5:1681:A:O2'	2.38	0.56
79:B5:1339:C:O2'	79:B5:1341:A:N7	2.33	0.56
49:BE:103:TYR:O	49:BE:182:TYR:OH	2.23	0.56
53:BI:172:ARG:NH1	79:B5:330:G:OP2	2.38	0.56
1:A1:939:U:O2'	1:A1:2402:A:N1	2.38	0.56
1:A1:2622:C:H42	12:AI:116:ARG:HH12	1.54	0.56
11:AH:89:LYS:HG2	11:AH:145:VAL:HG22	1.88	0.56
42:An:18:ARG:NH2	79:B5:1126:OMG:OP2	2.38	0.56
56:BL:129:ARG:HD3	79:B5:115:G:H5'	1.87	0.56
62:BR:7:LYS:HD2	62:BR:11:ARG:HH22	1.71	0.56
78:Bh:111:GLY:HA3	78:Bh:115:LYS:HE2	1.88	0.56
1:A1:1322:U:O2	21:AS:108:GLN:NE2	2.39	0.56
1:A1:3343:G:H21	1:A1:3362:A:H2	1.54	0.56
6:AC:35:VAL:HG21	6:AC:244:LEU:HD21	1.88	0.56
7:AD:50:ARG:NH1	7:AD:147:ASP:OD2	2.38	0.56
8:AE:40:LEU:HB3	8:AE:84:VAL:HG13	1.88	0.56
37:AI:70:ARG:HD3	37:AI:84:LYS:HG2	1.88	0.56
53:BI:87:ASN:HB3	53:BI:90:LEU:HG	1.88	0.56
77:Bg:127:ARG:HA	77:Bg:150:TRP:HB2	1.88	0.56
6:AC:29:PRO:HD2	6:AC:277:PRO:HB2	1.87	0.56
9:AF:121:LYS:HB2	22:AT:133:ALA:HB3	1.87	0.56
47:BC:181:SER:HB3	79:B5:4:C:H4'	1.87	0.56
57:BM:66:VAL:HG11	57:BM:93:ASP:HB2	1.88	0.56
57:BM:103:LEU:HD11	57:BM:121:VAL:HG21	1.87	0.56
1:A1:63:A:N3	1:A1:78:U:O2'	2.36	0.56
1:A1:1047:A:N3	1:A1:2633:U:O2'	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:2552:C:H2'	31:Ac:50:VAL:HG11	1.86	0.56
26:AX:77:GLU:HB3	26:AX:133:LEU:HD13	1.88	0.56
63:BS:11:PHE:HZ	63:BS:25:ASN:H	1.53	0.56
14:AL:48:PRO:HA	14:AL:137:GLN:HB2	1.88	0.55
46:BB:111:ARG:NH2	79:B5:930:A:N3	2.50	0.55
51:BG:201:GLN:NE2	79:B5:125:U:OP1	2.39	0.55
50:BF:94:THR:HG22	50:BF:114:ILE:HG13	1.89	0.55
51:BG:10:ASN:HB3	51:BG:128:THR:HA	1.89	0.55
1:A1:1448:U:H2'	1:A1:1449:A2M:H8	1.87	0.55
28:AZ:90:GLU:HA	28:AZ:93:LYS:HG2	1.88	0.55
63:BS:136:GLN:NE2	79:B5:1544:U:OP1	2.37	0.55
64:BT:102:ARG:NH1	79:B5:1501:C:OP2	2.39	0.55
1:A1:1940:G:H21	1:A1:3362:A:H8	1.54	0.55
1:A1:549:U:H3'	1:A1:550:A:H8	1.72	0.55
1:A1:816:A:H5'	1:A1:906:A:H61	1.72	0.55
13:AJ:53:THR:HG23	13:AJ:60:ARG:HA	1.88	0.55
21:AS:22:PRO:O	22:AT:146:ASN:ND2	2.33	0.55
1:A1:1128:U:OP1	12:AI:4:ARG:NH2	2.36	0.55
1:A1:1334:U:H5''	9:AF:206:LYS:HB3	1.89	0.55
1:A1:2433:U:H1'	16:AN:125:SER:HB3	1.88	0.55
22:AT:39:ILE:HG12	22:AT:63:VAL:HG22	1.87	0.55
54:BJ:52:ILE:HG23	54:BJ:76:LEU:HD11	1.89	0.55
77:Bg:32:LEU:HD22	77:Bg:73:LEU:HD21	1.89	0.55
41:Am:109:ASN:ND2	41:Am:117:HIS:O	2.38	0.55
47:BC:170:ILE:HB	47:BC:197:TYR:HB2	1.88	0.55
52:BH:143:LEU:HD12	52:BH:147:ASN:HB3	1.89	0.55
1:A1:1192:C:N4	1:A1:1301:A:O2'	2.32	0.55
4:AA:135:ILE:HD12	4:AA:149:ARG:HE	1.71	0.55
16:AN:143:ARG:NH2	36:Ah:90:ARG:O	2.40	0.55
1:A1:68:C:OP2	1:A1:301:G:N2	2.39	0.54
1:A1:117:U:OP2	16:AN:2:GLY:N	2.39	0.54
1:A1:2219:A:H2'	1:A1:2220:A2M:H8	1.90	0.54
5:AB:10:ARG:HH21	5:AB:14:LEU:HD21	1.72	0.54
35:Ag:54:ILE:HG23	35:Ag:70:LYS:HA	1.90	0.54
1:A1:845:G:H21	1:A1:848:A:H2	1.53	0.54
47:BC:40:LYS:HE3	47:BC:248:SER:HB3	1.88	0.54
55:BK:3:MET:HE1	55:BK:45:ALA:HB2	1.89	0.54
1:A1:149:U:OP2	16:AN:49:ARG:NH2	2.40	0.54
1:A1:1618:G:O2'	3:A4:126:A:N1	2.39	0.54
45:BA:41:ARG:NH2	62:BR:103:ASP:OD2	2.40	0.54
1:A1:1178:G:N3	1:A1:1328:C:O2'	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1243:G:H21	1:A1:1244:A:H62	1.56	0.54
52:BH:110:GLN:NE2	79:B5:816:G:N3	2.51	0.54
79:B5:1585:U:H3	79:B5:1611:A:H2	1.54	0.54
1:A1:98:G:N7	14:AL:13:HIS:NE2	2.56	0.54
5:AB:169:THR:HG22	5:AB:171:LEU:HD13	1.89	0.54
7:AD:196:ARG:NH2	7:AD:237:GLU:OE2	2.40	0.54
13:AJ:82:ARG:NH2	13:AJ:112:LEU:O	2.41	0.54
1:A1:1779:C:N4	1:A1:2102:U:OP1	2.39	0.54
5:AB:57:VAL:HG22	5:AB:73:VAL:HG22	1.89	0.54
16:AN:137:PRO:O	16:AN:143:ARG:NH1	2.41	0.54
47:BC:148:LEU:O	47:BC:174:ARG:NH2	2.41	0.54
53:BI:2:GLY:N	79:B5:393:C:OP2	2.41	0.54
53:BI:152:ILE:HG13	53:BI:153:GLU:H	1.73	0.54
57:BM:46:ARG:HH21	79:B5:1229:G:H2'	1.73	0.54
64:BT:49:ASP:HB3	64:BT:53:TRP:HB3	1.90	0.54
79:B5:1594:G:OP2	79:B5:1596:C:N4	2.41	0.54
7:AD:41:LYS:NZ	22:AT:30:TYR:O	2.37	0.54
51:BG:193:LEU:O	51:BG:197:ASN:HB2	2.08	0.54
53:BI:57:ALA:HB2	53:BI:177:GLY:HA2	1.89	0.54
1:A1:358:G:N2	1:A1:361:A:OP2	2.36	0.54
29:Aa:104:THR:HG22	29:Aa:109:TYR:HB2	1.89	0.54
54:BJ:59:LEU:HD22	54:BJ:69:ARG:HA	1.90	0.54
58:BN:54:LEU:HB3	58:BN:60:VAL:HB	1.90	0.54
1:A1:1302:A:N7	1:A1:2857:C:O2'	2.41	0.53
7:AD:146:LEU:HD22	7:AD:163:LEU:HD13	1.89	0.53
49:BE:21:ASP:OD1	49:BE:21:ASP:N	2.40	0.53
61:BQ:10:PHE:HA	61:BQ:18:ALA:O	2.09	0.53
69:BY:89:TYR:OH	69:BY:90:ARG:NH2	2.42	0.53
1:A1:351:A:N6	40:Al:37:TYR:O	2.38	0.53
18:AP:126:ARG:HA	18:AP:140:GLU:HG2	1.89	0.53
26:AX:47:ALA:HB3	26:AX:50:ALA:HB2	1.90	0.53
45:BA:119:ARG:NH1	47:BC:241:ASP:OD1	2.41	0.53
52:BH:11:GLN:HG3	52:BH:13:PRO:HD2	1.90	0.53
1:A1:824:C:H5''	4:AA:21:ARG:HD3	1.90	0.53
12:AI:12:GLN:HG2	12:AI:128:ARG:HG2	1.91	0.53
51:BG:131:LYS:HD2	79:B5:166:C:H4'	1.89	0.53
59:BO:90:ARG:NH1	79:B5:902:G:OP1	2.42	0.53
64:BT:6:VAL:HG22	64:BT:136:ALA:HB2	1.89	0.53
77:Bg:240:VAL:HG22	77:Bg:256:THR:HG22	1.90	0.53
79:B5:1267:G:HO2'	79:B5:1448:G:HO2'	1.55	0.53
6:AC:325:LEU:O	9:AF:41:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AH:22:SER:OG	11:AH:23:ARG:N	2.41	0.53
73:Bc:42:ARG:NH2	73:Bc:58:GLU:O	2.37	0.53
79:B5:1229:G:O2'	79:B5:1255:G:N2	2.37	0.53
1:A1:297:G:O2'	37:Ai:32:ALA:O	2.27	0.53
1:A1:1149:G:OP2	34:Af:21:ARG:NH2	2.42	0.53
1:A1:1348:U:OP2	19:AQ:38:ARG:NH2	2.41	0.53
1:A1:2193:U:H5''	1:A1:2194:G:H5'	1.91	0.53
9:AF:118:LYS:HG3	9:AF:191:VAL:HG11	1.90	0.53
13:AJ:60:ARG:NH2	43:Ao:104:LEU:O	2.41	0.53
52:BH:112:ARG:NH2	79:B5:639:U:OP1	2.40	0.53
67:BW:81:VAL:HB	67:BW:123:GLY:O	2.08	0.53
74:Bd:31:ILE:HG22	79:B5:1199:G:H1	1.74	0.53
1:A1:1565:G:N2	1:A1:1811:G:OP1	2.41	0.53
1:A1:2836:C:H5	1:A1:2852:C:H42	1.56	0.53
24:AV:18:PRO:HA	24:AV:51:ALA:HA	1.89	0.53
46:BB:168:ILE:HG12	46:BB:197:ILE:HD12	1.89	0.53
61:BQ:95:LYS:O	77:Bg:59:ARG:NH1	2.41	0.53
1:A1:449:U:O2'	1:A1:450:G:N2	2.42	0.53
64:BT:40:SER:HB3	64:BT:43:ASN:HB2	1.90	0.53
68:BX:60:GLU:HG2	75:Be:3:LYS:HB2	1.91	0.53
72:Bb:53:ALA:HB1	72:Bb:62:ILE:HD12	1.91	0.53
79:B5:1171:A:H2'	79:B5:1172:G:C8	2.44	0.53
79:B5:1561:U:H2'	79:B5:1562:G:H8	1.73	0.53
79:B5:1600:A:O2'	79:B5:1602:C:N4	2.41	0.53
1:A1:797:U:O2	14:AL:12:ASN:ND2	2.41	0.53
22:AT:17:ARG:HE	22:AT:47:SER:HB3	1.74	0.53
53:BI:5:ARG:NH1	79:B5:332:U:O2'	2.41	0.53
60:BP:40:ARG:NH2	79:B5:1551:U:O4	2.42	0.53
77:Bg:126:SER:OG	77:Bg:127:ARG:N	2.38	0.53
1:A1:165:A:H62	1:A1:257:U:H3	1.57	0.53
1:A1:289:A:O2'	16:AN:93:LYS:O	2.26	0.53
1:A1:2969:A:N7	4:AA:215:ASN:ND2	2.56	0.53
24:AV:38:ALA:HB3	24:AV:59:MET:HB2	1.90	0.53
54:BJ:144:PRO:HD2	79:B5:474:A:H5''	1.89	0.53
56:BL:133:LYS:HB2	79:B5:337:G:H3'	1.91	0.53
1:A1:1132:C:H2'	1:A1:1133:A2M:H8	1.90	0.52
1:A1:2700:G:H5''	22:AT:17:ARG:HB2	1.91	0.52
48:BD:40:ARG:HG2	65:BU:110:PRO:HB3	1.90	0.52
48:BD:138:VAL:HG22	48:BD:184:ILE:HG22	1.91	0.52
79:B5:1474:G:H2'	79:B5:1475:A:H8	1.74	0.52
51:BG:70:PRO:HA	51:BG:98:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BW:112:ASP:OD1	67:BW:112:ASP:N	2.40	0.52
1:A1:503:C:O2	8:AE:23:LYS:NZ	2.40	0.52
1:A1:728:G:H5''	19:AQ:43:PRO:HB2	1.90	0.52
11:AH:129:ARG:NH1	11:AH:160:ASP:OD2	2.38	0.52
37:AI:25:LYS:O	37:AI:29:LYS:NZ	2.42	0.52
41:Am:127:LEU:HG	41:Am:128:LYS:HG3	1.91	0.52
50:BF:96:SER:HB3	50:BF:176:THR:HG21	1.91	0.52
61:BQ:136:SER:HB3	79:B5:1586:A:H5''	1.91	0.52
63:BS:126:ARG:HB2	63:BS:133:VAL:HG12	1.92	0.52
74:Bd:13:ARG:NH2	79:B5:1554:U:OP1	2.38	0.52
21:AS:12:ARG:HD2	21:AS:22:PRO:HD2	1.91	0.52
45:BA:140:ASN:ND2	66:BV:31:SER:O	2.36	0.52
51:BG:32:ILE:HD12	51:BG:65:GLN:HA	1.90	0.52
64:BT:109:GLU:OE1	64:BT:122:ARG:NH1	2.42	0.52
1:A1:444:U:H3	1:A1:491:A:H61	1.58	0.52
1:A1:938:C:O2	1:A1:2813:A:O2'	2.28	0.52
4:AA:92:LYS:HE3	4:AA:93:LYS:HE3	1.91	0.52
62:BR:14:LYS:HG3	62:BR:69:ILE:HD13	1.90	0.52
1:A1:733:G:N2	1:A1:736:A:OP2	2.42	0.52
1:A1:824:C:O2'	1:A1:1534:A:N3	2.40	0.52
1:A1:2383:C:OP2	17:AO:85[A]:ARG:NH2	2.43	0.52
1:A1:3070:A:OP1	20:AR:62:ARG:NH2	2.39	0.52
9:AF:83:LEU:HD11	9:AF:116:PHE:HB3	1.91	0.52
12:AI:82:ARG:NH2	12:AI:83:ASP:OD1	2.39	0.52
1:A1:450:G:N7	1:A1:487:U:O2'	2.42	0.52
1:A1:1174:G:N2	17:AO:87[A]:MET:SD	2.83	0.52
5:AB:187:SER:O	5:AB:190:GLU:N	2.43	0.52
7:AD:107:ARG:NH1	7:AD:169:GLY:O	2.40	0.52
49:BE:95:THR:HG22	69:BY:16:PRO:HD2	1.90	0.52
77:Bg:10:ARG:NH1	77:Bg:314:GLN:OE1	2.42	0.52
1:A1:1315:U:OP1	17:AO:18[A]:ARG:NE	2.33	0.52
1:A1:3119:U:H4'	41:Am:104:PRO:HG3	1.92	0.52
3:A4:37:A:OP1	36:Ah:89:ARG:NH2	2.43	0.52
46:BB:39:GLU:HG3	46:BB:40:ASN:H	1.74	0.52
53:BI:5:ARG:NH2	79:B5:334:G:O6	2.43	0.52
53:BI:8:ARG:HE	53:BI:22:ARG:HH21	1.58	0.52
66:BV:4:ASP:N	66:BV:4:ASP:OD1	2.43	0.52
71:Ba:3:LYS:HE2	71:Ba:6:ALA:HA	1.92	0.52
1:A1:2727:A:OP2	1:A1:2728:G:N2	2.38	0.52
2:A3:101:G:N7	21:AS:52:LYS:NZ	2.57	0.52
10:AG:162:LEU:HA	16:AN:7:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Am:98:LYS:HD3	41:Am:118:THR:HG21	1.91	0.52
44:Ap:38:ASP:HA	44:Ap:45:LYS:HA	1.92	0.52
46:BB:180:THR:O	46:BB:183:GLN:N	2.43	0.52
47:BC:79:GLU:HG3	47:BC:186:LYS:HE3	1.91	0.52
79:B5:720:G:N2	79:B5:722:G:OP2	2.43	0.52
1:A1:3313:U:H4'	5:AB:173:GLN:HG3	1.91	0.51
14:AL:48:PRO:HB2	36:Ah:117:ALA:HB2	1.92	0.51
18:AP:64:ASN:O	18:AP:80:LYS:NZ	2.43	0.51
46:BB:60:ALA:O	46:BB:64:ARG:NH1	2.43	0.51
48:BD:172:THR:HG23	48:BD:185:LYS:HG2	1.92	0.51
64:BT:105:LEU:HD22	64:BT:122:ARG:HG3	1.92	0.51
70:BZ:46:LYS:HE3	70:BZ:49:ARG:HH11	1.75	0.51
1:A1:649:A2M:OP2	1:A1:2868:U:O2'	2.28	0.51
1:A1:1232:C:N4	1:A1:1262:G:OP2	2.43	0.51
1:A1:1729:A:O4'	31:Ac:52:ARG:NH1	2.40	0.51
7:AD:30:TYR:HA	7:AD:33:ARG:HB3	1.92	0.51
13:AJ:28:ASP:OD1	13:AJ:28:ASP:N	2.40	0.51
65:BU:22:ILE:HG22	65:BU:118:VAL:HG12	1.92	0.51
65:BU:59:PRO:HG3	79:B5:1381:U:H4'	1.92	0.51
77:Bg:73:LEU:HD23	77:Bg:77:GLY:HA2	1.91	0.51
77:Bg:255:ALA:HB2	77:Bg:292:LEU:HD22	1.91	0.51
79:B5:472:U:O2'	79:B5:769:A:N3	2.37	0.51
79:B5:701:U:O2	79:B5:738:G:O6	2.28	0.51
79:B5:1027:A:OP1	79:B5:1789:G:O2'	2.28	0.51
1:A1:873:C:H3'	1:A1:874:U:H4'	1.93	0.51
1:A1:1468:A:N1	1:A1:1880:U:O2'	2.37	0.51
12:AI:52:LEU:HB3	12:AI:136:PHE:HB2	1.91	0.51
21:AS:24:LEU:HD21	22:AT:141:VAL:HG11	1.93	0.51
27:AY:55:GLU:HB2	27:AY:108:LYS:HB3	1.91	0.51
53:BI:16:ALA:HB2	79:B5:354:C:H5''	1.92	0.51
54:BJ:173:ALA:HB2	79:B5:511:A:H5'	1.91	0.51
1:A1:115:A:H2'	1:A1:265:A:H2	1.75	0.51
1:A1:2157:G:N7	4:AA:152:SER:OG	2.39	0.51
31:Ac:27:TYR:OH	31:Ac:55:GLU:OE2	2.28	0.51
60:BP:77:ARG:HG3	79:B5:1241:G:H5''	1.91	0.51
65:BU:106:ILE:HG13	65:BU:107:THR:HG23	1.91	0.51
72:Bb:42:ASN:C	72:Bb:42:ASN:HD22	2.17	0.51
72:Bb:67:THR:OG1	72:Bb:70:LYS:O	2.29	0.51
1:A1:3042:U:OP2	1:A1:3092:C:N4	2.41	0.51
28:AZ:33:SER:OG	28:AZ:35:SER:O	2.25	0.51
66:BV:21:ASN:HB3	67:BW:67:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:292:U:OP2	16:AN:68:ARG:NH2	2.41	0.51
7:AD:215:ASP:OD1	7:AD:215:ASP:N	2.44	0.51
11:AH:22:SER:OG	11:AH:39:LYS:NZ	2.43	0.51
12:AI:192:ASP:HA	12:AI:197:VAL:HG23	1.92	0.51
29:Aa:72:VAL:HG12	29:Aa:111:LYS:HB3	1.91	0.51
55:BK:44:LYS:HD2	79:B5:1217:A:H5'	1.93	0.51
60:BP:53:PRO:HB2	60:BP:57:MET:HE2	1.92	0.51
61:BQ:16:ALA:HB2	61:BQ:72:GLY:HA3	1.92	0.51
78:Bh:93:ARG:NH1	79:B5:1636:C:OP1	2.43	0.51
4:AA:180:LEU:HD11	44:Ap:26:VAL:HG11	1.93	0.51
47:BC:83:ILE:HD11	47:BC:125:ILE:HD11	1.92	0.51
1:A1:412:G:OP1	18:AP:62:ARG:NH1	2.43	0.51
3:A4:143:U:OP1	16:AN:38:ARG:NH2	2.38	0.51
6:AC:334:PHE:HA	6:AC:339:LEU:HD12	1.92	0.51
13:AJ:49:LYS:HG2	13:AJ:64:LYS:HG2	1.93	0.51
79:B5:428:A:N3	79:B5:440:U:O2'	2.38	0.51
1:A1:2146:C:OP1	4:AA:200:ARG:NH1	2.40	0.51
3:A4:142:C:OP1	16:AN:38:ARG:NH1	2.43	0.51
11:AH:5:GLN:NE2	11:AH:7:GLU:OE1	2.37	0.51
22:AT:14:MET:HE1	22:AT:55:LYS:HB2	1.93	0.51
51:BG:164:LYS:NZ	79:B5:71:A:OP2	2.38	0.51
4:AA:168:VAL:HG13	44:Ap:79:VAL:HG21	1.93	0.51
51:BG:21:GLU:OE2	51:BG:25:ARG:NH2	2.44	0.51
51:BG:92:ARG:NH2	79:B5:1674:C:OP1	2.42	0.51
64:BT:41:SER:O	64:BT:84:LYS:NZ	2.44	0.51
17:AO:27[A]:LEU:O	17:AO:101[A]:ARG:NH1	2.42	0.50
77:Bg:42:LEU:HB2	77:Bg:61:PHE:HB2	1.92	0.50
79:B5:480:G:O6	79:B5:508:U:O2	2.29	0.50
79:B5:1280:4AC:H2'	79:B5:1281:G:H8	1.76	0.50
1:A1:286:U:O2'	16:AN:179:LYS:O	2.29	0.50
1:A1:1410:U:O2'	33:Ae:95:GLU:OE1	2.27	0.50
51:BG:94:ARG:NH2	79:B5:1673:G:OP1	2.44	0.50
51:BG:159:ARG:NH2	79:B5:79:C:OP1	2.41	0.50
57:BM:60:VAL:HG22	57:BM:122:VAL:HG12	1.93	0.50
4:AA:177:LYS:NZ	44:Ap:33:GLN:OE1	2.44	0.50
45:BA:125:ASP:O	45:BA:129:ASP:HB2	2.11	0.50
54:BJ:113:VAL:HG12	54:BJ:119:ALA:HB2	1.93	0.50
55:BK:86:ILE:HG23	55:BK:87:VAL:HG23	1.94	0.50
61:BQ:94:GLN:HB2	61:BQ:102:LYS:HD3	1.93	0.50
64:BT:65:ILE:HD13	64:BT:71:VAL:HB	1.93	0.50
65:BU:100:VAL:HA	65:BU:103:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:BY:34:ASN:O	79:B5:521:A:O2'	2.24	0.50
79:B5:1525:A:N3	79:B5:1589:C:O2'	2.44	0.50
12:AI:76:MET:HE2	12:AI:148:VAL:HG22	1.92	0.50
1:A1:114:A:OP1	16:AN:54:LYS:NZ	2.41	0.50
1:A1:591:G:O2'	8:AE:17:ALA:O	2.27	0.50
1:A1:664:U:H5'	6:AC:107:ARG:HA	1.94	0.50
1:A1:2209:U:H3	1:A1:2230:C:H5''	1.76	0.50
4:AA:113:VAL:HG12	4:AA:166:ILE:HD13	1.93	0.50
20:AR:13:SER:OG	20:AR:38:ARG:NH2	2.40	0.50
66:BV:15:ARG:NH1	66:BV:33:GLN:OE1	2.44	0.50
79:B5:514:G:H1	79:B5:543:C:H5	1.58	0.50
79:B5:1687:U:OP1	79:B5:1707:A:O2'	2.29	0.50
1:A1:775:A:OP1	30:Ab:44:LYS:NZ	2.44	0.50
28:AZ:50:PRO:HD3	28:AZ:68:ILE:HG12	1.94	0.50
46:BB:118:GLN:OE1	46:BB:208:GLN:NE2	2.44	0.50
49:BE:100:ARG:HB2	49:BE:114:ILE:HD13	1.93	0.50
77:Bg:116:ASP:OD1	77:Bg:116:ASP:N	2.44	0.50
77:Bg:200:ASN:H	77:Bg:215:GLY:HA2	1.76	0.50
1:A1:520:U:OP2	9:AF:70:LYS:NZ	2.44	0.50
1:A1:2799:A:O2'	29:Aa:42:ARG:NH1	2.45	0.50
14:AL:57:VAL:HG22	14:AL:147:ILE:HG23	1.93	0.50
1:A1:1873:U:OP1	20:AR:21:LYS:NZ	2.34	0.50
4:AA:117:GLU:HB2	4:AA:162:ALA:HB1	1.94	0.50
6:AC:315:LYS:HB3	6:AC:320:ASN:HD22	1.76	0.50
10:AG:74:THR:HG22	10:AG:164:VAL:HG22	1.93	0.50
31:Ac:30:THR:HG23	31:Ac:91:SER:HB2	1.92	0.50
48:BD:105:MET:HE1	48:BD:136:VAL:HG11	1.92	0.50
55:BK:5:LYS:NZ	55:BK:79:TYR:OH	2.44	0.50
65:BU:68:ARG:HH22	65:BU:77:LYS:HG3	1.76	0.50
75:Be:55:ARG:NH2	79:B5:558:U:OP2	2.40	0.50
1:A1:996:A:N3	2:A3:80:G:O2'	2.45	0.50
4:AA:45:VAL:HG22	4:AA:61:VAL:HG22	1.93	0.50
11:AH:101:VAL:HG22	11:AH:114:VAL:HG22	1.92	0.50
32:Ad:20:LEU:HD11	32:Ad:32:ALA:HB2	1.94	0.50
52:BH:49:ILE:HB	52:BH:57:ALA:HB3	1.94	0.50
58:BN:124:ARG:NH2	79:B5:967:A:OP2	2.44	0.50
79:B5:192:U:H4'	79:B5:195:G:H1	1.75	0.50
79:B5:1235:C:H2'	79:B5:1236:A:C8	2.47	0.50
1:A1:718:G:OP1	29:Aa:117:ARG:NH2	2.45	0.49
1:A1:1613:A:OP1	39:Ak:2:ALA:N	2.45	0.49
1:A1:1825:G:H5''	39:Ak:48:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AB:122:TRP:O	5:AB:127:LYS:NZ	2.45	0.49
79:B5:319:U:H4'	79:B5:323:A:C8	2.46	0.49
46:BB:154:SER:O	46:BB:154:SER:OG	2.26	0.49
53:BI:10:LYS:NZ	79:B5:322:G:O2'	2.45	0.49
65:BU:97:VAL:HG13	65:BU:98:GLN:HG2	1.93	0.49
69:BY:55:VAL:HG22	69:BY:75:VAL:HG22	1.93	0.49
79:B5:869:A:H61	79:B5:958:U:H3	1.60	0.49
1:A1:815:G:OP2	38:Aj:31:LYS:NZ	2.40	0.49
1:A1:1795:U:OP2	4:AA:50:HIS:NE2	2.45	0.49
60:BP:81:ARG:NH2	60:BP:117:GLY:O	2.45	0.49
79:B5:1591:C:H2'	79:B5:1592:A:H8	1.77	0.49
3:A4:29:U:H5''	14:AL:27:ASP:HB3	1.95	0.49
7:AD:119:TYR:OH	7:AD:139:PRO:O	2.28	0.49
8:AE:62:THR:HG21	8:AE:78:ARG:HD2	1.93	0.49
9:AF:116:PHE:O	9:AF:199:ASN:ND2	2.37	0.49
45:BA:118:PRO:HG2	45:BA:141:ILE:HD13	1.95	0.49
58:BN:3:ARG:HB3	58:BN:6:SER:HB3	1.94	0.49
68:BX:30:LYS:NZ	79:B5:1132:A:OP1	2.38	0.49
75:Be:54:ARG:HE	75:Be:56:MET:HE2	1.77	0.49
1:A1:847:A:OP1	58:BN:140:LYS:NZ	2.40	0.49
5:AB:77:THR:OG1	5:AB:326:GLY:O	2.29	0.49
39:Ak:8:ILE:HD12	39:Ak:65:LEU:HD11	1.94	0.49
49:BE:200:ARG:NH2	79:B5:737:A:OP1	2.46	0.49
50:BF:63:GLN:HB3	50:BF:88:PRO:HA	1.95	0.49
79:B5:162:A:H3'	79:B5:163:G:H21	1.77	0.49
79:B5:1164:G:O2'	79:B5:1612:U:O2	2.29	0.49
1:A1:874:U:N3	1:A1:2978:U:OP1	2.38	0.49
1:A1:2618:G:O2'	1:A1:2865:U:OP1	2.30	0.49
50:BF:166:ARG:NH2	79:B5:1163:A:O3'	2.45	0.49
58:BN:64:ARG:O	58:BN:64:ARG:NH1	2.40	0.49
61:BQ:143:ARG:NH2	79:B5:1464:G:OP1	2.46	0.49
18:AP:47:TYR:OH	18:AP:57:ALA:O	2.28	0.49
46:BB:138:PHE:O	46:BB:212:VAL:O	2.30	0.49
48:BD:124:ARG:NH2	78:Bh:124:GLN:OE1	2.46	0.49
52:BH:150:GLN:HB3	52:BH:181:ILE:HG13	1.95	0.49
73:Bc:19:THR:HG21	73:Bc:66:LEU:HA	1.95	0.49
1:A1:3094:A:OP1	24:AV:14:SER:OG	2.31	0.49
1:A1:3275:U:O2'	34:Af:99:ARG:NH1	2.46	0.49
3:A4:97:A:OP1	36:Ah:67:ARG:NH2	2.42	0.49
4:AA:180:LEU:HD22	44:Ap:18:TYR:HB3	1.95	0.49
18:AP:29:THR:HA	18:AP:32:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BK:1:MET:HE3	79:B5:1219:A:H4'	1.95	0.49
58:BN:119:GLU:HG2	58:BN:141:TYR:HE2	1.78	0.49
59:BO:132:ARG:NH2	79:B5:1789:G:OP2	2.43	0.49
1:A1:1746:U:O2'	39:Ak:4:GLU:OE2	2.24	0.49
13:AJ:32:ARG:HD2	13:AJ:120:ILE:HG12	1.95	0.49
26:AX:108:LEU:HD23	26:AX:125:ARG:HD3	1.95	0.49
29:Aa:112:ILE:HB	29:Aa:130:VAL:HG12	1.95	0.49
64:BT:106:GLN:NE2	79:B5:1500:C:OP1	2.46	0.49
70:BZ:61:SER:OG	70:BZ:62:VAL:N	2.46	0.49
71:Ba:57:SER:OG	71:Ba:58:VAL:O	2.29	0.49
79:B5:647:G:H21	79:B5:687:G:H1	1.61	0.49
1:A1:2697:A:H2'	1:A1:2698:G:C8	2.48	0.49
4:AA:33:ASP:OD1	4:AA:33:ASP:N	2.46	0.49
22:AT:136:ARG:HD2	22:AT:139:ARG:HH12	1.77	0.49
24:AV:59:MET:HE1	24:AV:75:PRO:HG3	1.94	0.49
49:BE:181:VAL:HG13	49:BE:225:VAL:HG13	1.95	0.49
61:BQ:15:SER:O	61:BQ:15:SER:OG	2.31	0.49
63:BS:26:ILE:HG23	63:BS:31:ALA:HB2	1.94	0.49
79:B5:1356:U:O4	79:B5:1367:G:O6	2.31	0.49
1:A1:879:U:O2'	18:AP:135:ARG:NH2	2.38	0.48
21:AS:77:VAL:HG11	21:AS:106:LEU:HD22	1.95	0.48
39:Ak:14:LEU:HD12	39:Ak:17:ARG:HD3	1.95	0.48
53:BI:191:PHE:O	53:BI:195:ARG:HB2	2.12	0.48
63:BS:30:TYR:HE1	63:BS:40:ARG:HD3	1.77	0.48
79:B5:1297:G:N2	79:B5:1300:A:OP2	2.36	0.48
79:B5:1533:C:H4'	79:B5:1539:G:C6	2.48	0.48
34:Af:37:THR:HG22	34:Af:39:GLN:H	1.78	0.48
64:BT:39:THR:HA	64:BT:100:ILE:HD12	1.95	0.48
71:Ba:88:SER:HA	79:B5:1628:U:H5'	1.95	0.48
74:Bd:30:LEU:O	79:B5:1199:G:N2	2.46	0.48
77:Bg:12:THR:HG22	77:Bg:311:ARG:HG3	1.94	0.48
77:Bg:89:LEU:HB2	77:Bg:103:PHE:HB2	1.95	0.48
1:A1:1805:C:H2'	1:A1:1806:A:H8	1.77	0.48
1:A1:2940:A:OP2	5:AB:2:SER:N	2.47	0.48
48:BD:54:ARG:HB3	48:BD:57:ASP:HB2	1.95	0.48
49:BE:122:LYS:HD2	49:BE:164:LEU:HD21	1.95	0.48
65:BU:66:SER:HA	65:BU:80:GLU:O	2.14	0.48
67:BW:41:MET:HG2	67:BW:129:VAL:HG21	1.94	0.48
1:A1:2176:U:OP1	4:AA:54:ARG:NH2	2.38	0.48
1:A1:2947:G:N3	5:AB:250:ALA:HB1	2.29	0.48
12:AI:19:LYS:HD2	12:AI:26:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Ao:61:LYS:NZ	43:Ao:63:LYS:O	2.45	0.48
57:BM:33:ARG:HH21	57:BM:36:LEU:HD22	1.78	0.48
1:A1:907:G:H4'	1:A1:908:OMG:H5'	1.96	0.48
4:AA:116:VAL:HG13	4:AA:126:LEU:HB2	1.96	0.48
29:Aa:101:VAL:HA	29:Aa:124:ILE:HB	1.94	0.48
47:BC:81:MET:HB2	47:BC:101:VAL:HG23	1.94	0.48
53:BI:166:TYR:HB3	53:BI:184:LEU:HD12	1.95	0.48
64:BT:89:ARG:NH1	79:B5:1562:G:OP1	2.44	0.48
64:BT:97:SER:OG	79:B5:1504:G:OP1	2.31	0.48
1:A1:1334:U:HO2'	9:AF:151:ARG:HH12	1.59	0.48
1:A1:3050:U:O2'	25:AW:16:GLY:O	2.29	0.48
5:AB:85:VAL:HG22	5:AB:202:THR:HG22	1.95	0.48
12:AI:153:ARG:HA	12:AI:156:ARG:HD2	1.94	0.48
39:Ak:7:ASP:HB3	39:Ak:10:GLN:HB3	1.95	0.48
1:A1:1863:G:N1	1:A1:1866:C:OP2	2.38	0.48
4:AA:47:GLN:HB3	4:AA:49:VAL:HG13	1.95	0.48
13:AJ:23:VAL:HG11	13:AJ:29:ARG:HG2	1.95	0.48
28:AZ:97:SER:O	28:AZ:100:THR:OG1	2.29	0.48
52:BH:97:ARG:NH1	79:B5:856:A:OP1	2.46	0.48
59:BO:125:SER:HB3	79:B5:926:A:H2	1.78	0.48
77:Bg:69:GLN:OE1	77:Bg:85:TRP:NE1	2.38	0.48
79:B5:1290:U:H2'	79:B5:1291:G:C8	2.49	0.48
79:B5:1682:U:O4	79:B5:1720:G:N2	2.47	0.48
1:A1:2185:G:O2'	1:A1:2314:U:OP2	2.31	0.48
1:A1:2767:U:O2'	43:Ao:30:ALA:O	2.30	0.48
9:AF:86:VAL:O	9:AF:114:GLY:HA2	2.13	0.48
25:AW:6:ASP:HB3	25:AW:11:ALA:H	1.78	0.48
64:BT:48:GLN:OE1	79:B5:1531:G:N2	2.41	0.48
64:BT:71:VAL:HG13	64:BT:75:LYS:HB2	1.96	0.48
79:B5:1280:4AC:H2'	79:B5:1281:G:C8	2.49	0.48
1:A1:339:C:OP1	1:A1:1380:G:O2'	2.32	0.48
12:AI:5:PRO:HB2	12:AI:7:ARG:HG2	1.96	0.48
13:AJ:49:LYS:HB3	13:AJ:62:ASN:HA	1.96	0.48
14:AL:46:ILE:HD11	14:AL:51:LEU:HA	1.95	0.48
38:Aj:54:LYS:O	38:Aj:58:THR:HB	2.14	0.48
46:BB:27:LYS:NZ	46:BB:49:ASN:OD1	2.41	0.48
55:BK:64:TYR:OH	79:B5:1435:G:O6	2.31	0.48
58:BN:109:LYS:HD2	79:B5:975:C:H5''	1.95	0.48
62:BR:34:LEU:HB3	77:Bg:150:TRP:HH2	1.78	0.48
71:Ba:32:LYS:O	71:Ba:37:LYS:NZ	2.37	0.48
1:A1:1352:A:H1'	1:A1:1353:U:H4'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AZ:46:ILE:HG23	28:AZ:68:ILE:HG23	1.96	0.48
70:BZ:74:SER:OG	79:B5:1534:G:OP2	2.32	0.48
77:Bg:211:ILE:HB	77:Bg:223:TRP:HB2	1.96	0.48
79:B5:1474:G:H2'	79:B5:1475:A:C8	2.48	0.48
8:AE:40:LEU:HD11	8:AE:54:TYR:HB2	1.95	0.47
36:Ah:12:LYS:NZ	36:Ah:20:GLN:OE1	2.38	0.47
45:BA:73:VAL:HG13	45:BA:120:LEU:HD23	1.96	0.47
46:BB:138:PHE:C	46:BB:212:VAL:O	2.57	0.47
64:BT:57:ARG:NH1	64:BT:101:ASN:OD1	2.47	0.47
68:BX:19:ARG:O	68:BX:23:ARG:HB2	2.14	0.47
71:Ba:44:ILE:HG23	71:Ba:45:VAL:HG13	1.96	0.47
79:B5:1483:A:OP2	79:B5:1521:G:N2	2.47	0.47
1:A1:2559:U:OP1	10:AG:32:LYS:NZ	2.47	0.47
1:A1:3140:G:N7	5:AB:28:ARG:NH2	2.55	0.47
7:AD:163:LEU:HD11	7:AD:175:HIS:HB3	1.96	0.47
51:BG:74:LYS:HA	51:BG:96:SER:HA	1.96	0.47
52:BH:96:ARG:NH1	52:BH:128:ASP:OD2	2.46	0.47
1:A1:490:C:O2'	1:A1:491:A:N7	2.43	0.47
1:A1:1157:G:O2'	1:A1:1169:A:N3	2.46	0.47
10:AG:133:LYS:HD2	10:AG:138:HIS:HE1	1.79	0.47
17:AO:177[A]:LYS:HE2	17:AO:177[A]:LYS:HB3	1.70	0.47
46:BB:125:VAL:O	46:BB:136:ARG:HA	2.14	0.47
49:BE:104:ASP:HB3	49:BE:110:ALA:HB2	1.97	0.47
53:BI:49:ARG:O	53:BI:52:ASN:ND2	2.46	0.47
57:BM:46:ARG:HD3	76:Bf:99:LYS:HD3	1.96	0.47
64:BT:131:ASP:OD1	64:BT:134:ARG:NH2	2.48	0.47
1:A1:1347:U:H5''	6:AC:303:GLY:H	1.79	0.47
1:A1:2880:U:OP1	24:AV:47:ASN:ND2	2.38	0.47
5:AB:41:VAL:HA	5:AB:185:GLY:HA3	1.97	0.47
27:AY:11:ASP:HB3	27:AY:14:LYS:HB2	1.95	0.47
47:BC:156:THR:HG23	67:BW:95:PRO:HB2	1.96	0.47
48:BD:195:SER:OG	48:BD:196:ARG:N	2.47	0.47
60:BP:59:LYS:HB3	60:BP:76:VAL:HG21	1.95	0.47
1:A1:874:U:OP2	5:AB:240:ARG:NH2	2.47	0.47
7:AD:182:GLY:HA2	7:AD:194:LEU:HD23	1.97	0.47
51:BG:126:ASP:OD1	51:BG:126:ASP:N	2.47	0.47
53:BI:22:ARG:HG3	79:B5:385:A:H5''	1.97	0.47
59:BO:121:VAL:O	79:B5:886:U:O2'	2.33	0.47
68:BX:30:LYS:HE2	68:BX:34:LEU:HD11	1.97	0.47
5:AB:211:GLN:NE2	5:AB:283:TYR:O	2.48	0.47
6:AC:92:ASN:OD1	6:AC:92:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AF:155:LYS:HG3	9:AF:158:LYS:HA	1.96	0.47
19:AQ:147:ARG:HB3	19:AQ:150:VAL:HG23	1.96	0.47
48:BD:192:PRO:HB2	48:BD:201:ALA:HA	1.97	0.47
51:BG:120:GLU:HG3	51:BG:125:THR:HB	1.97	0.47
67:BW:31:SER:HB2	79:B5:636:A:H5''	1.96	0.47
79:B5:31:C:O2'	79:B5:547:U:OP1	2.32	0.47
79:B5:580:A:O2'	79:B5:582:U:OP1	2.33	0.47
79:B5:1114:G:O2'	79:B5:1130:G:O6	2.31	0.47
79:B5:1785:U:H2'	79:B5:1786:G:H8	1.80	0.47
1:A1:655:C:H2'	1:A1:656:A:C8	2.49	0.47
1:A1:1686:U:O4	23:AU:82:LYS:NZ	2.43	0.47
1:A1:1721:U:OP2	20:AR:124:TYR:OH	2.27	0.47
1:A1:2617:U:H3'	30:Ab:3:LYS:HD3	1.97	0.47
1:A1:3003:G:HO2'	5:AB:92:TYR:HH	1.57	0.47
3:A4:58:G:O6	38:Aj:63:ARG:NH2	2.47	0.47
7:AD:277:LEU:HD22	7:AD:281:GLU:HG3	1.96	0.47
16:AN:80:THR:HB	16:AN:87:GLN:HG2	1.96	0.47
21:AS:81:TYR:CE1	21:AS:90:MET:HE3	2.50	0.47
45:BA:197:ILE:HG23	45:BA:201:LEU:HD21	1.96	0.47
49:BE:22:LYS:N	79:B5:773:C:OP1	2.44	0.47
58:BN:49:GLN:HA	58:BN:52:VAL:HG12	1.95	0.47
63:BS:140:THR:O	63:BS:143:ARG:NH1	2.47	0.47
68:BX:126:LYS:HE2	68:BX:129:GLY:HA2	1.96	0.47
1:A1:908:OMG:HN1	1:A1:2414:G:H5''	1.80	0.47
1:A1:1809:A:OP2	28:AZ:65:ARG:NH1	2.47	0.47
1:A1:2588:U:OP1	10:AG:241:LYS:NZ	2.47	0.47
1:A1:3086:A:H4'	5:AB:366:GLY:HA2	1.95	0.47
1:A1:3164:C:O2'	1:A1:3165:A:O4'	2.33	0.47
11:AH:186:PHE:HB2	11:AH:189:GLU:HB2	1.97	0.47
49:BE:131:LEU:HD12	79:B5:251:A:H2	1.80	0.47
57:BM:86:VAL:HG13	57:BM:140:PHE:HE1	1.80	0.47
76:Bf:120:GLU:HB3	76:Bf:129:GLY:HA2	1.97	0.47
79:B5:1553:G:N1	79:B5:1556:A:OP2	2.46	0.47
1:A1:269:G:H5''	16:AN:14:LYS:HE2	1.97	0.47
1:A1:896:A:H5''	4:AA:183:GLY:HA2	1.97	0.47
1:A1:1324:U:H4'	21:AS:2:ALA:HB2	1.95	0.47
6:AC:208:VAL:HA	6:AC:228:ALA:O	2.14	0.47
16:AN:18:VAL:HG13	16:AN:19:LEU:HD12	1.97	0.47
31:Ac:9:SER:OG	31:Ac:10:ILE:N	2.45	0.47
49:BE:30:ARG:NH2	79:B5:298:C:O3'	2.48	0.47
79:B5:34:G:O2'	79:B5:515:A:O2'	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1312:C:O2'	17:AO:83[A]:ALA:O	2.32	0.47
1:A1:1386:A:O4'	6:AC:141:ARG:NH2	2.48	0.47
10:AG:25:PRO:HB2	28:AZ:125:GLY:H	1.80	0.47
12:AI:30:LYS:HD3	12:AI:63:GLU:HG3	1.97	0.47
27:AY:23:PRO:HG2	27:AY:26:GLN:HG3	1.97	0.47
34:Af:6:ARG:NH1	34:Af:8:TYR:O	2.48	0.47
45:BA:20:ALA:HB2	62:BR:91:LEU:HD21	1.96	0.47
48:BD:109:LEU:HD22	48:BD:115:ILE:HD13	1.97	0.47
1:A1:950:G:N1	1:A1:1368:U:OP2	2.39	0.46
1:A1:2896:A:OP1	41:Am:124:LYS:NZ	2.45	0.46
1:A1:3352:U:O2'	53:BI:162:ALA:O	2.29	0.46
25:AW:18:GLY:HA3	25:AW:31:PHE:O	2.15	0.46
45:BA:156:VAL:O	66:BV:65:SER:OG	2.31	0.46
48:BD:23:GLU:OE1	55:BK:61:TRP:NE1	2.33	0.46
67:BW:81:VAL:O	67:BW:122:SER:OG	2.29	0.46
1:A1:911:C:OP1	4:AA:14:SER:OG	2.33	0.46
1:A1:1864:A:OP1	20:AR:88:ARG:NH1	2.46	0.46
1:A1:3016:A:H2'	1:A1:3017:A:C8	2.50	0.46
6:AC:138:ARG:HE	6:AC:240:PRO:HD2	1.79	0.46
7:AD:211:LEU:HD12	7:AD:223:PHE:HE2	1.80	0.46
45:BA:31:VAL:HA	45:BA:34:GLU:HG3	1.96	0.46
45:BA:123:VAL:HG21	45:BA:133:ILE:HD11	1.97	0.46
63:BS:138:THR:N	79:B5:1458:G:OP1	2.47	0.46
78:Bh:55:SER:HA	78:Bh:59:GLY:HA3	1.97	0.46
79:B5:816:G:H2'	79:B5:817:A:H8	1.81	0.46
79:B5:1716:C:O2'	79:B5:1717:G:O4'	2.28	0.46
1:A1:1724:U:H1'	1:A1:1725:C:C6	2.50	0.46
3:A4:27:U:H4'	6:AC:51:ALA:HB3	1.97	0.46
5:AB:219:ALA:HB2	5:AB:336:VAL:HG23	1.98	0.46
6:AC:31:ARG:HG3	6:AC:120:TYR:HE2	1.80	0.46
6:AC:361:HIS:O	21:AS:28:ARG:NH2	2.47	0.46
15:AM:121:MET:HB3	15:AM:121:MET:HE2	1.78	0.46
20:AR:21:LYS:HE2	20:AR:55:VAL:HA	1.98	0.46
47:BC:67:GLN:HA	47:BC:70:ASP:HB2	1.96	0.46
60:BP:49:MET:SD	60:BP:49:MET:N	2.89	0.46
65:BU:87:HIS:ND1	79:B5:1383:G:OP1	2.48	0.46
74:Bd:32:ARG:NH1	79:B5:1597:A:OP2	2.46	0.46
77:Bg:70:ASP:HB3	77:Bg:113:VAL:HG12	1.97	0.46
1:A1:1497:C:O2'	1:A1:1602:A:N3	2.43	0.46
1:A1:1915:A:H5''	20:AR:84:THR:HG22	1.98	0.46
1:A1:2768:U:H2'	1:A1:2769:A:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:3109:G:N2	11:AH:156:GLN:OE1	2.47	0.46
12:AI:145:LYS:HD2	12:AI:167:LEU:HD11	1.96	0.46
24:AV:101:VAL:HG11	24:AV:114:ILE:HG12	1.97	0.46
46:BB:137:ILE:HG21	46:BB:172:LEU:HD22	1.96	0.46
47:BC:116:LYS:HG2	47:BC:127:ALA:HB3	1.97	0.46
51:BG:12:SER:OG	51:BG:124:LEU:O	2.33	0.46
63:BS:82:PRO:HD3	64:BT:36:ILE:HD11	1.98	0.46
65:BU:60:THR:HG23	79:B5:1382:A:H5''	1.97	0.46
79:B5:392:G:O2'	79:B5:1673:G:N3	2.47	0.46
1:A1:3068:U:OP2	20:AR:62:ARG:NH1	2.38	0.46
13:AJ:108:GLU:HA	13:AJ:122:ILE:HG13	1.98	0.46
16:AN:11:GLN:HA	16:AN:19:LEU:HD21	1.97	0.46
20:AR:105:LEU:HD13	20:AR:135:LYS:HE3	1.98	0.46
24:AV:87:ARG:HH22	24:AV:137:VAL:HG21	1.80	0.46
41:Am:99:CYS:HB2	41:Am:114:LYS:HE3	1.97	0.46
52:BH:49:ILE:HG13	52:BH:172:VAL:HG23	1.97	0.46
79:B5:1688:U:H1'	79:B5:1713:G:H22	1.80	0.46
1:A1:860:G:C5	4:AA:181:LYS:HB2	2.50	0.46
1:A1:1446:A:H5''	18:AP:65:SER:HB2	1.97	0.46
2:A3:7:G:OP1	7:AD:33:ARG:NH1	2.48	0.46
5:AB:346:THR:HG22	5:AB:351:LEU:HD11	1.98	0.46
11:AH:23:ARG:HE	11:AH:39:LYS:HA	1.80	0.46
15:AM:17:VAL:HG11	15:AM:74:ARG:HA	1.96	0.46
24:AV:28:ASN:HD21	24:AV:112:SER:HB2	1.80	0.46
29:Aa:74:ASN:HB3	29:Aa:115:LYS:HB3	1.98	0.46
57:BM:52:LEU:HG	57:BM:122:VAL:HG13	1.97	0.46
58:BN:61:THR:OG1	58:BN:62:GLN:N	2.49	0.46
63:BS:123:ARG:HG3	63:BS:133:VAL:HB	1.98	0.46
1:A1:67:A:O2'	1:A1:315:C:O2	2.30	0.46
1:A1:448:U:O2'	1:A1:489:U:OP1	2.30	0.46
1:A1:1412:G:OP1	33:Ae:105:ARG:NH1	2.48	0.46
1:A1:2512:C:H5''	10:AG:249:ARG:HH22	1.80	0.46
1:A1:3058:U:O4	32:Ad:65:LYS:NZ	2.41	0.46
38:Aj:72:ARG:HA	38:Aj:75:LYS:HE2	1.97	0.46
45:BA:111:ILE:HD11	79:B5:1292:G:H21	1.80	0.46
47:BC:188:LEU:HD13	47:BC:196:VAL:HG11	1.98	0.46
48:BD:75:LYS:NZ	55:BK:18:GLU:OE2	2.48	0.46
79:B5:217:A:N1	79:B5:844:A:O2'	2.47	0.46
79:B5:513:U:H2'	79:B5:514:G:C8	2.50	0.46
79:B5:1591:C:H2'	79:B5:1592:A:C8	2.50	0.46
1:A1:115:A:OP2	16:AN:49:ARG:NE	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:651:G:O2'	1:A1:1435:A:OP1	2.26	0.46
1:A1:1813:A:H4'	1:A1:1817:G:H1'	1.98	0.46
1:A1:1914:G:O2'	20:AR:82:LYS:O	2.30	0.46
1:A1:2357:A:H2'	1:A1:2358:A:C8	2.51	0.46
8:AE:66:SER:HB2	8:AE:76:LEU:HD23	1.97	0.46
45:BA:79:ARG:HH12	45:BA:164:ASN:HB3	1.81	0.46
45:BA:83:GLN:HE22	45:BA:100:GLY:HA2	1.81	0.46
48:BD:163:PRO:HA	48:BD:166:ASP:HB2	1.98	0.46
79:B5:800:U:H2'	79:B5:801:G:C8	2.51	0.46
1:A1:683:U:H5'	16:AN:204:LYS:HE3	1.97	0.46
12:AI:49:CYS:HB3	12:AI:168:SER:HB3	1.97	0.46
46:BB:100:PHE:HB3	46:BB:181:LEU:HD21	1.97	0.46
71:Ba:12:LYS:HZ2	71:Ba:16:GLY:H	1.64	0.46
79:B5:65:A:H2	79:B5:84:A:H62	1.63	0.46
1:A1:1795:U:C2	44:Ap:51:ALA:HB2	2.51	0.46
3:A4:110:C:O2'	3:A4:112:U:OP2	2.28	0.46
29:Aa:24:LYS:O	29:Aa:26:ARG:HG2	2.16	0.46
59:BO:72:LYS:HA	59:BO:72:LYS:HD3	1.80	0.46
77:Bg:159:ASN:ND2	77:Bg:163:ASP:OD1	2.42	0.46
79:B5:1592:A:H2'	79:B5:1593:A:C8	2.52	0.46
1:A1:1019:G:N2	1:A1:1034:U:OP1	2.49	0.45
1:A1:2253:G:H22	1:A1:2264:U:H5	1.62	0.45
5:AB:292:ALA:HB1	5:AB:295:ALA:HB3	1.98	0.45
11:AH:90:MET:HB2	11:AH:144:ILE:HG23	1.97	0.45
46:BB:88:VAL:HG11	46:BB:96:LEU:HD13	1.99	0.45
46:BB:117:TRP:HE1	79:B5:1799:U:H5'	1.81	0.45
49:BE:72:VAL:HG22	49:BE:90:ILE:HG12	1.98	0.45
49:BE:148:ARG:HD2	79:B5:125:U:H5'	1.97	0.45
52:BH:14:THR:OG1	52:BH:15:GLU:N	2.38	0.45
54:BJ:134:ILE:HD12	54:BJ:134:ILE:H	1.80	0.45
63:BS:86:LEU:HD22	63:BS:99:HIS:HB2	1.98	0.45
1:A1:1522:U:OP1	26:AX:123:TYR:OH	2.31	0.45
1:A1:1696:A:H2'	1:A1:1697:A:C8	2.51	0.45
1:A1:2827:U:O2'	1:A1:2829:U:O4	2.31	0.45
1:A1:3016:A:H2'	1:A1:3017:A:H8	1.81	0.45
58:BN:5:HIS:HD2	79:B5:627:C:H5''	1.80	0.45
64:BT:117:SER:HB2	64:BT:123:ARG:HG3	1.97	0.45
67:BW:24:GLN:HA	67:BW:63:VAL:O	2.15	0.45
79:B5:906:A:H2	79:B5:998:A:H1'	1.81	0.45
1:A1:571:U:H2'	1:A1:572:A:H8	1.82	0.45
1:A1:2815:OMG:N2	1:A1:2818:U:O2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ae:9:ILE:HG12	33:Ae:63:THR:HB	1.98	0.45
48:BD:113:LEU:HD22	48:BD:118:ALA:HB2	1.99	0.45
65:BU:53:LYS:HB2	65:BU:92:ASP:HB2	1.98	0.45
1:A1:26:A:N3	1:A1:328:U:O2'	2.44	0.45
1:A1:1836:C:O2'	1:A1:1842:A:N1	2.43	0.45
3:A4:26:U:O2'	6:AC:51:ALA:O	2.33	0.45
16:AN:45:PRO:O	16:AN:49:ARG:HG3	2.17	0.45
17:AO:115[A]:LYS:O	17:AO:117[A]:ARG:NH1	2.46	0.45
48:BD:196:ARG:HH11	48:BD:200:LYS:HD3	1.81	0.45
49:BE:79:ASP:HB3	49:BE:82:TYR:HB2	1.98	0.45
50:BF:103:ASN:HA	50:BF:106:LYS:HD2	1.98	0.45
74:Bd:34:TYR:OH	79:B5:1487:A:OP1	2.31	0.45
79:B5:781:U:O2'	79:B5:782:U:O4'	2.31	0.45
1:A1:1778:G:O2'	1:A1:1780:G:OP2	2.31	0.45
16:AN:84:PRO:HA	16:AN:87:GLN:HG3	1.99	0.45
17:AO:126[A]:VAL:O	21:AS:154:HIS:NE2	2.48	0.45
34:Af:16:TYR:OH	34:Af:89:LEU:O	2.28	0.45
47:BC:39:THR:O	47:BC:42:GLY:N	2.44	0.45
56:BL:46:LYS:HB2	56:BL:46:LYS:HE2	1.84	0.45
74:Bd:20:GLN:HB2	74:Bd:25:SER:HA	1.98	0.45
74:Bd:42:CYS:SG	79:B5:1433:G:N2	2.80	0.45
79:B5:1171:A:H2'	79:B5:1172:G:H8	1.82	0.45
1:A1:52:A:N3	1:A1:811:U:O2'	2.50	0.45
1:A1:2555:G:O6	35:Ag:99:LYS:NZ	2.42	0.45
4:AA:80:GLU:HG3	44:Ap:66:GLY:HA2	1.99	0.45
6:AC:156:LEU:HD12	6:AC:159:ILE:HD12	1.98	0.45
10:AG:91:PHE:O	10:AG:95:ASN:ND2	2.49	0.45
10:AG:162:LEU:HD21	16:AN:45:PRO:HG2	1.98	0.45
22:AT:46:GLY:O	22:AT:49:GLN:NE2	2.50	0.45
27:AY:116:LYS:HG2	27:AY:126:LEU:HD11	1.99	0.45
56:BL:101:GLU:OE1	68:BX:16:ARG:NH1	2.46	0.45
63:BS:65:GLU:HG2	63:BS:68:ARG:HH21	1.81	0.45
68:BX:92:CYS:HA	68:BX:95:PHE:HD2	1.81	0.45
68:BX:96:VAL:HA	68:BX:127:VAL:HG21	1.99	0.45
72:Bb:15:GLU:OE1	72:Bb:18:LYS:NZ	2.47	0.45
79:B5:1592:A:H2'	79:B5:1593:A:H8	1.82	0.45
79:B5:1672:G:H2'	79:B5:1673:G:C8	2.52	0.45
79:B5:1717:G:H2'	79:B5:1718:G:C8	2.51	0.45
1:A1:957:C:H1'	29:Aa:43:ILE:HD11	1.99	0.45
1:A1:2814:G:OP1	6:AC:73:ARG:NH1	2.45	0.45
46:BB:166:LYS:HB2	46:BB:166:LYS:HE2	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BG:74:LYS:HG2	51:BG:96:SER:HB3	1.99	0.45
60:BP:97:TYR:OH	79:B5:1211:A:N3	2.41	0.45
1:A1:505:G:H5''	6:AC:315:LYS:HA	1.99	0.45
1:A1:1686:U:OP1	23:AU:42:LYS:NZ	2.38	0.45
11:AH:21:LYS:HG3	11:AH:22:SER:H	1.82	0.45
23:AU:49:ASN:HD22	23:AU:49:ASN:C	2.23	0.45
45:BA:90:ALA:HA	45:BA:95:ALA:HB3	1.99	0.45
53:BI:169:ILE:HD12	53:BI:179:CYS:HB3	1.99	0.45
63:BS:37:GLY:O	63:BS:99:HIS:NE2	2.45	0.45
77:Bg:74:THR:HA	77:Bg:115:ILE:HD11	1.98	0.45
77:Bg:112:SER:HB3	77:Bg:154:VAL:HG22	1.99	0.45
79:B5:1240:U:H3	79:B5:1242:A:HO2'	1.65	0.45
1:A1:1333:C:OP1	19:AQ:2:GLY:N	2.49	0.45
1:A1:1378:U:H2'	1:A1:1379:G:H8	1.82	0.45
1:A1:2809:C:H5''	1:A1:2956:A:H5''	1.99	0.45
1:A1:2989:U:O2'	5:AB:267:ALA:O	2.26	0.45
27:AY:51:ARG:HG2	27:AY:52:ARG:H	1.81	0.45
47:BC:139:ILE:HD13	47:BC:191:ALA:HB1	1.99	0.45
52:BH:64:VAL:HG22	52:BH:94:ALA:HB1	1.98	0.45
53:BI:3:ILE:O	53:BI:30:GLY:N	2.50	0.45
59:BO:20:TYR:HB3	59:BO:27:PHE:HB2	1.99	0.45
59:BO:21:ALA:HB2	59:BO:98:GLY:HA3	1.99	0.45
68:BX:130:VAL:HG11	68:BX:142:LYS:HA	1.99	0.45
75:Be:13:LYS:NZ	75:Be:17:GLN:OE1	2.49	0.45
1:A1:2402:A:H2'	6:AC:67:THR:HG21	1.99	0.45
1:A1:2880:U:H5''	5:AB:236:LYS:HD3	1.99	0.45
6:AC:42:VAL:HG12	6:AC:236:LEU:HD21	1.99	0.45
46:BB:53:GLY:HA2	46:BB:54:LEU:HA	1.58	0.45
52:BH:78:THR:HG23	52:BH:90:VAL:HG13	1.99	0.45
55:BK:60:SER:HB3	55:BK:65:TYR:HE2	1.82	0.45
57:BM:65:SER:HB3	57:BM:91:VAL:HB	1.99	0.45
79:B5:1466:G:O2'	79:B5:1602:C:OP1	2.31	0.45
1:A1:1175:C:H1'	17:AO:87[A]:MET:HG2	1.99	0.44
1:A1:1661:G:H2'	1:A1:1662:G:C8	2.52	0.44
9:AF:54:GLU:OE2	9:AF:186:HIS:NE2	2.48	0.44
18:AP:33:ALA:HB1	18:AP:117:ILE:HG12	1.98	0.44
27:AY:3:LYS:HD2	27:AY:8:VAL:HG13	1.98	0.44
48:BD:141:LYS:O	48:BD:179:GLN:NE2	2.43	0.44
49:BE:141:THR:OG1	49:BE:143:ASP:OD1	2.35	0.44
51:BG:2:LYS:HG2	51:BG:17:GLU:HG3	1.99	0.44
54:BJ:114:TYR:HA	54:BJ:119:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BM:44:GLY:HA2	79:B5:1227:A:C2	2.51	0.44
58:BN:6:SER:OG	58:BN:7:ALA:N	2.50	0.44
64:BT:86:ARG:NH1	64:BT:90:PRO:O	2.45	0.44
67:BW:14:ILE:HA	67:BW:25:VAL:HG11	1.98	0.44
71:Ba:46:GLU:HB3	71:Ba:48:ALA:H	1.81	0.44
79:B5:1717:G:H2'	79:B5:1718:G:H8	1.82	0.44
1:A1:664:U:H2'	1:A1:665:A:C8	2.53	0.44
1:A1:1747:G:OP1	39:Ak:42:LYS:NZ	2.43	0.44
27:AY:5:SER:HB3	27:AY:8:VAL:HG12	1.99	0.44
49:BE:54:TYR:O	69:BY:15:ASN:ND2	2.51	0.44
53:BI:76:THR:HG21	53:BI:104:ILE:HD12	1.98	0.44
71:Ba:70:LYS:NZ	79:B5:933:A:OP1	2.35	0.44
79:B5:1294:G:O2'	79:B5:1321:A:N1	2.50	0.44
1:A1:904:A:OP2	38:Aj:30:GLN:NE2	2.45	0.44
1:A1:1739:U:O2'	35:Ag:56:THR:OG1	2.32	0.44
51:BG:27:PHE:HE1	51:BG:36:VAL:HG21	1.82	0.44
57:BM:141:SER:OG	57:BM:142:GLN:OE1	2.35	0.44
79:B5:924:A:H2'	79:B5:925:G:C8	2.53	0.44
1:A1:715:A:C8	29:Aa:115:LYS:HD3	2.52	0.44
1:A1:1129:A:N3	1:A1:2826:U:O2'	2.44	0.44
1:A1:2768:U:H2'	1:A1:2769:A:C8	2.53	0.44
1:A1:3275:U:H5'	34:Af:68:TRP:HZ2	1.82	0.44
2:A3:121:U:H5''	7:AD:265:TYR:HE1	1.83	0.44
21:AS:26:ARG:H	22:AT:150:THR:HB	1.83	0.44
31:Ac:24:THR:HG22	31:Ac:91:SER:HB3	1.99	0.44
44:Ap:36:ARG:HB3	44:Ap:45:LYS:HG2	1.98	0.44
51:BG:92:ARG:O	79:B5:405:C:O2'	2.27	0.44
69:BY:112:LYS:NZ	79:B5:55:A:OP1	2.42	0.44
77:Bg:266:ASP:OD1	77:Bg:267:PRO:HD3	2.18	0.44
79:B5:1175:U:H2'	79:B5:1176:G:C8	2.52	0.44
5:AB:385:LYS:O	5:AB:387:LEU:N	2.50	0.44
9:AF:92:ILE:HD12	19:AQ:4:ASP:HB2	1.99	0.44
9:AF:156:ILE:HD12	9:AF:161:VAL:HB	1.99	0.44
52:BH:13:PRO:HA	52:BH:14:THR:HA	1.81	0.44
53:BI:138:ASN:OD1	79:B5:197:A:N6	2.51	0.44
54:BJ:143:ILE:HG21	79:B5:768:C:H1'	1.99	0.44
69:BY:44:LEU:HA	69:BY:47:VAL:HG12	2.00	0.44
76:Bf:119:ARG:HH22	76:Bf:152:ALA:HA	1.81	0.44
77:Bg:275:ARG:HA	77:Bg:275:ARG:HD3	1.81	0.44
1:A1:1203:A:H2'	1:A1:1204:A:C8	2.53	0.44
1:A1:2592:G:H4'	1:A1:2594:C:C2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AD:68:THR:OG1	7:AD:71:GLY:O	2.30	0.44
9:AF:120:THR:HB	22:AT:132:PRO:HB2	1.99	0.44
17:AO:155[A]:LYS:HB3	17:AO:155[A]:LYS:HE3	1.78	0.44
47:BC:101:VAL:HG12	47:BC:115:ILE:HG12	1.99	0.44
50:BF:93:LEU:HD12	50:BF:172:ILE:HG23	2.00	0.44
54:BJ:39:LYS:HA	54:BJ:42:ILE:HD12	2.00	0.44
69:BY:37:LYS:HG3	79:B5:522:U:H5''	1.99	0.44
77:Bg:124:SER:OG	77:Bg:134:TRP:NE1	2.43	0.44
79:B5:1174:C:O2'	79:B5:1196:A:N6	2.51	0.44
79:B5:1201:G:H21	79:B5:1600:A:H5'	1.83	0.44
79:B5:1687:U:N3	79:B5:1709:C:OP1	2.51	0.44
1:A1:655:C:H2'	1:A1:656:A:H8	1.82	0.44
1:A1:715:A:H8	29:Aa:115:LYS:HD3	1.82	0.44
1:A1:1003:A:N1	1:A1:1049:C:O2'	2.50	0.44
1:A1:1604:G:H4'	1:A1:1835:A:H4'	1.99	0.44
1:A1:2261:G:H1'	1:A1:2262:A:H2	1.82	0.44
1:A1:3258:U:O2'	1:A1:3260:G:OP1	2.31	0.44
5:AB:73:VAL:O	24:AV:86:ARG:NH2	2.51	0.44
12:AI:51:HIS:CD2	12:AI:168:SER:HB2	2.52	0.44
31:Ac:92:ILE:HG21	31:Ac:100:ILE:HD11	1.99	0.44
44:Ap:23:ARG:HA	44:Ap:26:VAL:HG12	1.99	0.44
50:BF:95:ASN:O	79:B5:1611:A:O2'	2.35	0.44
79:B5:800:U:H2'	79:B5:801:G:H8	1.82	0.44
1:A1:76:G:N7	14:AL:101:ARG:HB3	2.33	0.44
1:A1:1376:C:O2'	1:A1:1408:G:O2'	2.29	0.44
1:A1:1831:U:O2'	3:A4:114:G:OP1	2.27	0.44
1:A1:2955:U:H2'	1:A1:2956:A:C8	2.53	0.44
5:AB:287:LYS:HB3	5:AB:287:LYS:HE3	1.76	0.44
7:AD:60:ILE:HB	7:AD:80:SER:HB3	2.00	0.44
13:AJ:20:ASN:HB2	13:AJ:126:ASP:HB2	1.99	0.44
21:AS:132:THR:HG23	21:AS:144:LEU:HD13	2.00	0.44
22:AT:101:CYS:SG	22:AT:102:ARG:N	2.90	0.44
45:BA:126:PRO:HG3	45:BA:147:THR:HG22	1.98	0.44
46:BB:187:LYS:HB3	46:BB:193:ILE:HD11	2.00	0.44
52:BH:114:ARG:NH1	79:B5:637:C:O2	2.45	0.44
53:BI:48:THR:OG1	53:BI:52:ASN:O	2.35	0.44
62:BR:23:LYS:HD3	62:BR:23:LYS:HA	1.78	0.44
68:BX:107:PHE:CE2	68:BX:114:LYS:HB3	2.53	0.44
79:B5:1354:G:N1	79:B5:1369:U:N3	2.64	0.44
1:A1:63:A:H5''	16:AN:174:ILE:HG21	1.98	0.44
1:A1:1315:U:H4'	1:A1:1317:A:H1'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:2218:G:H2'	1:A1:2219:A:C8	2.53	0.44
4:AA:127:ALA:HB2	4:AA:134:VAL:HG23	1.98	0.44
9:AF:178:ILE:HG23	9:AF:183:ASP:HB2	1.99	0.44
12:AI:43:VAL:HG21	12:AI:197:VAL:HB	1.99	0.44
13:AJ:92:ARG:HA	13:AJ:172:LEU:H	1.82	0.44
16:AN:149:ASN:HB2	36:Ah:92:LEU:HD11	2.00	0.44
45:BA:74:VAL:HA	45:BA:96:THR:O	2.18	0.44
46:BB:130:SER:HB2	46:BB:180:THR:HG22	2.00	0.44
48:BD:204:ASP:OD1	48:BD:204:ASP:N	2.50	0.44
53:BI:84:HIS:NE2	53:BI:97:THR:OG1	2.34	0.44
60:BP:111:MET:HA	63:BS:119:ILE:HD11	2.00	0.44
79:B5:1681:A:N6	79:B5:1720:G:O2'	2.51	0.44
1:A1:307:A:H2'	1:A1:308:A:C8	2.53	0.43
1:A1:417:A:H2'	1:A1:418:A:C8	2.53	0.43
8:AE:14:ASP:OD1	8:AE:14:ASP:N	2.48	0.43
10:AG:98:ARG:NH2	10:AG:188:THR:O	2.51	0.43
52:BH:9:LEU:HD21	52:BH:17:GLU:HG3	2.00	0.43
1:A1:860:G:H5'	1:A1:861:C:H5''	2.00	0.43
1:A1:1222:G:H21	1:A1:1286:A:H62	1.67	0.43
2:A3:81:U:H2'	2:A3:82:G:H8	1.82	0.43
4:AA:80:GLU:HB2	4:AA:170:ALA:HA	2.01	0.43
17:AO:21[A]:SER:OG	17:AO:87[A]:MET:SD	2.75	0.43
22:AT:77:ASN:HB3	22:AT:84:TYR:HD2	1.83	0.43
29:Aa:34:MET:HB3	29:Aa:34:MET:HE3	1.81	0.43
43:Ao:26:THR:HA	43:Ao:93:LEU:HD21	2.00	0.43
48:BD:117:ARG:HA	78:Bh:123:ALA:HB2	2.00	0.43
49:BE:45:ILE:HG13	49:BE:61:VAL:HG21	1.99	0.43
51:BG:188:ARG:HD3	79:B5:283:U:H5''	1.99	0.43
54:BJ:83:VAL:HA	54:BJ:149:ARG:HA	2.00	0.43
77:Bg:10:ARG:HA	77:Bg:10:ARG:HD3	1.79	0.43
79:B5:209:U:H2'	79:B5:210:A:C8	2.53	0.43
79:B5:497:G:OP2	79:B5:498:G:N2	2.48	0.43
79:B5:1511:U:H2'	79:B5:1512:G:C8	2.54	0.43
1:A1:3319:U:H5'	1:A1:3320:A:H5'	2.00	0.43
5:AB:187:SER:HB3	5:AB:190:GLU:HB2	2.01	0.43
7:AD:33:ARG:HH12	7:AD:50:ARG:NH2	2.16	0.43
7:AD:65:ILE:HG12	7:AD:74:VAL:HG22	2.00	0.43
46:BB:134:VAL:HB	46:BB:219:LYS:HB2	2.00	0.43
48:BD:115:ILE:HG13	48:BD:142:LEU:HD11	1.99	0.43
49:BE:160:VAL:HB	49:BE:169:ILE:HD12	2.00	0.43
68:BX:73:ARG:NH1	68:BX:84:THR:OG1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:B5:1496:U:O2'	79:B5:1519:U:O2'	2.31	0.43
1:A1:1247:U:O4	1:A1:1270:A:O2'	2.29	0.43
1:A1:3182:G:H4'	17:AO:161[A]:LYS:HG2	2.01	0.43
4:AA:111:THR:HB	4:AA:136:ILE:HD12	1.99	0.43
6:AC:22:LEU:HA	6:AC:23:PRO:HD3	1.84	0.43
14:AL:76:THR:OG1	14:AL:101:ARG:NH1	2.51	0.43
45:BA:56:LYS:HE3	45:BA:56:LYS:HB3	1.86	0.43
53:BI:25:ARG:HA	79:B5:400:A:H5''	1.99	0.43
77:Bg:83:ALA:HB2	77:Bg:113:VAL:HB	2.00	0.43
79:B5:92:A:H5''	79:B5:93:A:H5''	2.01	0.43
1:A1:19:U:H2'	1:A1:20:A:C8	2.53	0.43
1:A1:737:G:H2'	1:A1:738:A:H8	1.84	0.43
1:A1:1596:C:H2'	1:A1:1597:C:C6	2.53	0.43
1:A1:3121:U:H1'	1:A1:3122:A:H5''	2.00	0.43
14:AL:76:THR:O	14:AL:79:GLU:N	2.42	0.43
17:AO:37[A]:ARG:HG3	17:AO:108[A]:ILE:HG13	2.01	0.43
22:AT:100:LYS:O	22:AT:104:GLU:HG2	2.18	0.43
49:BE:88:ASP:OD1	49:BE:122:LYS:NZ	2.51	0.43
53:BI:104:ILE:HG13	53:BI:105:ASP:H	1.83	0.43
54:BJ:147:MET:HE2	54:BJ:147:MET:HB2	1.80	0.43
60:BP:22:LEU:HA	60:BP:25:LEU:HG	1.99	0.43
61:BQ:46:PHE:HA	61:BQ:49:TYR:HB2	1.99	0.43
61:BQ:48:VAL:HG13	61:BQ:78:VAL:HG13	2.00	0.43
68:BX:41:SER:O	68:BX:41:SER:OG	2.28	0.43
71:Ba:2:PRO:HB3	79:B5:1142:A:H5''	1.99	0.43
74:Bd:7:TRP:O	79:B5:1450:U:O2'	2.24	0.43
1:A1:3092:C:O2'	1:A1:3094:A:OP2	2.26	0.43
5:AB:106:TRP:O	5:AB:137:TYR:OH	2.33	0.43
5:AB:257:PRO:HG2	5:AB:261:MET:HE2	1.99	0.43
44:Ap:53:GLY:O	44:Ap:65:ALA:HA	2.19	0.43
46:BB:27:LYS:HD3	46:BB:47:LEU:HB3	2.01	0.43
53:BI:86:SER:OG	79:B5:328:A:N3	2.49	0.43
54:BJ:37:LYS:NZ	79:B5:594:A:OP2	2.49	0.43
58:BN:4:MET:HE3	58:BN:4:MET:HB2	1.87	0.43
1:A1:727:G:OP2	1:A1:742:G:N2	2.46	0.43
1:A1:2160:G:H2'	1:A1:2161:G:C8	2.54	0.43
4:AA:52:SER:HB3	4:AA:191:LEU:HD23	2.01	0.43
8:AE:150:LYS:HE3	8:AE:150:LYS:HB3	1.85	0.43
31:Ac:103:THR:HG22	31:Ac:105:ALA:H	1.84	0.43
49:BE:92:LEU:HD13	69:BY:17:LEU:HD11	2.00	0.43
57:BM:60:VAL:HG23	57:BM:86:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BN:46:THR:HB	58:BN:49:GLN:HG3	2.01	0.43
61:BQ:44:LEU:HB3	61:BQ:78:VAL:HG11	2.01	0.43
69:BY:109:LYS:NZ	79:B5:459:G:OP1	2.51	0.43
79:B5:1291:G:H22	79:B5:1324:G:N2	2.17	0.43
1:A1:158:G:H2'	1:A1:159:A:H8	1.84	0.43
1:A1:2666:C:OP2	1:A1:2687:G:N1	2.42	0.43
1:A1:2714:G:OP1	43:Ao:20:HIS:NE2	2.50	0.43
3:A4:103:G:OP2	3:A4:105:A:O2'	2.28	0.43
19:AQ:158:HIS:H	19:AQ:186:VAL:HG12	1.83	0.43
19:AQ:176:ARG:NH1	29:Aa:46:ASP:OD2	2.46	0.43
20:AR:159:ALA:HB1	20:AR:163:ARG:HH11	1.84	0.43
27:AY:73:VAL:HG13	27:AY:80:VAL:HG12	2.00	0.43
29:Aa:77:LYS:O	29:Aa:79:TRP:N	2.42	0.43
47:BC:119:LYS:HE3	79:B5:1291:G:H5'	1.99	0.43
48:BD:141:LYS:HA	78:Bh:110:TRP:HE1	1.84	0.43
51:BG:74:LYS:HE3	51:BG:94:ARG:HG3	2.00	0.43
58:BN:22:ALA:HB3	58:BN:65:VAL:HG11	2.00	0.43
1:A1:29:C:H4'	1:A1:62:A:H4'	2.01	0.43
1:A1:1144:U:OP1	1:A1:1367:G:O2'	2.29	0.43
1:A1:2681:U:H2'	1:A1:2682:C:H6	1.84	0.43
1:A1:3008:A:OP2	17:AO:74[A]:ARG:NH1	2.52	0.43
1:A1:3116:G:N2	1:A1:3116:G:OP1	2.51	0.43
2:A3:81:U:H2'	2:A3:82:G:C8	2.54	0.43
12:AI:48:LEU:HD11	12:AI:167:LEU:HD12	2.01	0.43
19:AQ:20:LYS:HE3	19:AQ:20:LYS:HB3	1.90	0.43
31:Ac:99:ASP:OD1	31:Ac:99:ASP:N	2.52	0.43
35:Ag:19:LYS:HA	35:Ag:19:LYS:HD3	1.83	0.43
43:Ao:25:VAL:HG12	43:Ao:93:LEU:HD11	2.00	0.43
54:BJ:105:LEU:HD13	54:BJ:108:ARG:HD2	2.01	0.43
57:BM:42:ALA:HB1	57:BM:51:ALA:HB1	2.01	0.43
79:B5:980:G:H4'	79:B5:1776:A:H4'	2.00	0.43
1:A1:1145:G:O2'	33:Ae:45:ARG:O	2.34	0.43
1:A1:2557:A:OP1	4:AA:69:TYR:OH	2.27	0.43
1:A1:3002:C:OP1	5:AB:26:ARG:NH2	2.49	0.43
1:A1:3252:G:H2'	1:A1:3253:G:C8	2.54	0.43
13:AJ:80:LEU:HD21	13:AJ:129:VAL:HG21	2.01	0.43
43:Ao:2:VAL:N	43:Ao:90:HIS:O	2.52	0.43
45:BA:201:LEU:HB3	62:BR:85:VAL:HG22	2.00	0.43
49:BE:107:GLY:HA2	49:BE:189:LEU:HG	2.01	0.43
52:BH:177:THR:HG22	52:BH:179:LYS:HG3	2.01	0.43
56:BL:99:ARG:HG2	68:BX:9:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BQ:68:ARG:HD3	61:BQ:68:ARG:HA	1.93	0.43
63:BS:35:ILE:H	63:BS:35:ILE:HG13	1.68	0.43
66:BV:44:ARG:HA	66:BV:44:ARG:HD3	1.85	0.43
71:Ba:35:ALA:O	71:Ba:73:TYR:O	2.36	0.43
73:Bc:41:VAL:HG12	73:Bc:63:ALA:HB3	2.01	0.43
79:B5:1279:C:H2'	79:B5:1280:4AC:H6	2.01	0.43
1:A1:911:C:H42	4:AA:3:ARG:HD3	1.84	0.42
3:A4:8:C:H2'	3:A4:9:A:C8	2.54	0.42
5:AB:228:GLY:O	5:AB:232:ARG:HB2	2.19	0.42
7:AD:34:LYS:HA	22:AT:27:LEU:HD11	2.00	0.42
16:AN:80:THR:HG22	16:AN:82:GLY:N	2.33	0.42
31:Ac:17:VAL:HG21	31:Ac:100:ILE:HD13	2.00	0.42
46:BB:207:LEU:HD23	46:BB:207:LEU:HA	1.87	0.42
49:BE:127:LYS:HD2	49:BE:127:LYS:HA	1.79	0.42
51:BG:15:THR:OG1	79:B5:153:G:OP1	2.31	0.42
52:BH:23:ALA:HB1	52:BH:84:LYS:HD2	2.01	0.42
53:BI:7:SER:O	53:BI:18:ARG:NH1	2.52	0.42
54:BJ:115:LYS:HD3	54:BJ:115:LYS:HA	1.85	0.42
55:BK:59:PHE:CZ	55:BK:62:GLN:HA	2.54	0.42
68:BX:43:PHE:O	68:BX:45:GLY:N	2.51	0.42
77:Bg:37:SER:OG	77:Bg:38:ARG:N	2.50	0.42
1:A1:148:G:OP2	16:AN:4:TYR:OH	2.28	0.42
1:A1:155:G:N1	1:A1:265:A:OP2	2.40	0.42
1:A1:422:A:C2	1:A1:2363:A:H4'	2.54	0.42
1:A1:2183:A:H5''	4:AA:7:ASN:HB2	2.00	0.42
1:A1:2727:A:C2	29:Aa:43:ILE:HG23	2.54	0.42
1:A1:3309:G:O6	5:AB:21:ARG:NH2	2.52	0.42
12:AI:48:LEU:O	12:AI:139:ARG:HA	2.19	0.42
32:Ad:84:ASP:OD1	32:Ad:84:ASP:N	2.51	0.42
51:BG:7:TYR:HE2	51:BG:10:ASN:ND2	2.17	0.42
77:Bg:109:ASP:OD2	77:Bg:127:ARG:NH1	2.46	0.42
77:Bg:260:ILE:O	77:Bg:274:LEU:N	2.52	0.42
1:A1:737:G:H2'	1:A1:738:A:C8	2.54	0.42
1:A1:1786:G:H2'	1:A1:1787:A:C8	2.54	0.42
13:AJ:93:ASP:HB3	13:AJ:172:LEU:HD22	2.02	0.42
21:AS:10:ILE:HD12	21:AS:60:SER:HB3	1.99	0.42
34:Af:42:GLN:HA	34:Af:45:LEU:HG	2.00	0.42
41:Am:110:CYS:SG	41:Am:111:ARG:N	2.91	0.42
46:BB:142:PHE:HB2	46:BB:208:GLN:HG3	2.01	0.42
49:BE:105:VAL:HG21	49:BE:245:LYS:H	1.84	0.42
52:BH:81:LEU:O	52:BH:85:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BK:56:LYS:HE2	55:BK:69:THR:HG22	2.00	0.42
59:BO:17:ALA:HB3	59:BO:81:VAL:HA	2.00	0.42
61:BQ:13:LYS:HD2	61:BQ:13:LYS:HA	1.92	0.42
71:Ba:35:ALA:C	71:Ba:73:TYR:O	2.62	0.42
72:Bb:50:ALA:O	72:Bb:52:THR:N	2.52	0.42
77:Bg:20:VAL:HB	77:Bg:304:GLY:HA3	2.01	0.42
77:Bg:88:THR:HG22	77:Bg:104:VAL:HG12	2.01	0.42
79:B5:436:A2M:O5'	79:B5:436:A2M:H8	2.19	0.42
79:B5:591:A:H2'	79:B5:592:A:C8	2.54	0.42
1:A1:114:A:N1	1:A1:266:A:O2'	2.44	0.42
1:A1:1456:A:N1	1:A1:1476:G:O2'	2.44	0.42
1:A1:2129:U:H2'	1:A1:2130:G:C8	2.54	0.42
1:A1:2895:G:O2'	41:Am:100:TYR:O	2.30	0.42
1:A1:3295:A:H2'	1:A1:3296:A:C8	2.54	0.42
4:AA:20:THR:HG22	4:AA:23:ARG:HD2	2.01	0.42
23:AU:33:TYR:HD2	23:AU:63:VAL:HG21	1.84	0.42
28:AZ:90:GLU:HG3	28:AZ:93:LYS:HE3	2.01	0.42
45:BA:70:PRO:HB2	45:BA:94:GLY:HA3	2.01	0.42
45:BA:120:LEU:HD12	45:BA:142:PRO:HB2	2.01	0.42
53:BI:38:ILE:HG12	53:BI:96:LEU:HD11	2.01	0.42
59:BO:40:ALA:HB2	59:BO:70:LYS:HD3	2.01	0.42
64:BT:77:ASN:HB3	64:BT:95:ASP:HB3	2.00	0.42
77:Bg:211:ILE:HD11	77:Bg:225:LEU:HD22	2.01	0.42
79:B5:505:A:H2'	79:B5:507:U:C2	2.55	0.42
79:B5:753:A:H2	79:B5:796:A2M:H62	1.67	0.42
1:A1:528:U:H2'	1:A1:529:A:C8	2.54	0.42
1:A1:2728:G:N7	22:AT:87:LYS:NZ	2.46	0.42
28:AZ:81:LEU:HD22	35:Ag:90:ILE:HG12	2.01	0.42
39:Ak:8:ILE:HG23	39:Ak:65:LEU:HD11	2.02	0.42
51:BG:187:LYS:NZ	79:B5:139:C:O2'	2.52	0.42
57:BM:50:LYS:HZ2	79:B5:1254:U:H3	1.67	0.42
65:BU:103:ILE:HA	65:BU:106:ILE:HG12	2.02	0.42
73:Bc:10:ALA:HB1	73:Bc:30:VAL:HB	2.02	0.42
77:Bg:48:THR:OG1	77:Bg:50:ASP:OD2	2.25	0.42
79:B5:871:G:H2'	79:B5:872:G:C8	2.54	0.42
1:A1:2115:G:H22	1:A1:2120:A:H1'	1.85	0.42
7:AD:38:THR:HG23	22:AT:30:TYR:HB3	2.00	0.42
14:AL:75:PHE:H	14:AL:97:VAL:HA	1.83	0.42
22:AT:143:THR:HG23	22:AT:148:PRO:HD3	2.02	0.42
23:AU:80:THR:HG21	23:AU:95:PHE:CD1	2.54	0.42
27:AY:70:ILE:HA	27:AY:82:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ad:77:ARG:HD2	32:Ad:89:LEU:HD13	2.00	0.42
38:Aj:27:PHE:HA	38:Aj:34:CYS:HA	2.01	0.42
57:BM:31:VAL:HG11	57:BM:136:ILE:HG21	2.02	0.42
63:BS:83:ALA:HA	63:BS:86:LEU:HG	2.00	0.42
76:Bf:99:LYS:NZ	79:B5:1229:G:N7	2.63	0.42
78:Bh:83:LYS:HD3	78:Bh:83:LYS:HA	1.88	0.42
79:B5:209:U:H2'	79:B5:210:A:H8	1.85	0.42
1:A1:2228:A:H2'	1:A1:2229:A:C8	2.55	0.42
1:A1:2423:U:H2'	1:A1:2424:A:C8	2.55	0.42
4:AA:41:ILE:HG12	4:AA:63:PHE:HD2	1.85	0.42
9:AF:239:LEU:HG	9:AF:243:MET:HE2	2.01	0.42
11:AH:150:SER:HB3	11:AH:153:ASP:HB2	2.01	0.42
32:Ad:55:LEU:HB2	32:Ad:95:PRO:HD3	2.01	0.42
45:BA:84:ARG:NH2	62:BR:84:TYR:O	2.43	0.42
52:BH:91:ILE:HG12	52:BH:169:PHE:HE1	1.84	0.42
58:BN:102:LEU:HD23	58:BN:102:LEU:HA	1.92	0.42
59:BO:136:ARG:O	79:B5:1006:C:O2'	2.33	0.42
63:BS:127:HIS:CD2	63:BS:133:VAL:HG11	2.55	0.42
79:B5:58:U:O2'	79:B5:451:A:N3	2.52	0.42
79:B5:884:A:H2'	79:B5:885:G:C8	2.54	0.42
5:AB:53:MET:HE2	5:AB:53:MET:HB3	1.96	0.42
5:AB:113:GLU:OE2	5:AB:167:ARG:HG2	2.20	0.42
9:AF:84:VAL:HG23	9:AF:117:VAL:HB	2.01	0.42
9:AF:216:VAL:HA	9:AF:217:PRO:HD2	1.89	0.42
12:AI:53:VAL:HG21	12:AI:166:ILE:HD12	2.02	0.42
19:AQ:161:LYS:HD2	19:AQ:161:LYS:HA	1.82	0.42
47:BC:233:GLN:HA	47:BC:234:PRO:HD3	1.91	0.42
49:BE:141:THR:HG21	49:BE:162:ILE:HD11	2.02	0.42
77:Bg:82:SER:HB3	77:Bg:92:TRP:HE1	1.85	0.42
79:B5:29:U:H2'	79:B5:30:G:H8	1.83	0.42
79:B5:1397:U:O2'	79:B5:1400:A:N6	2.53	0.42
79:B5:1650:U:H2'	79:B5:1651:A:C8	2.54	0.42
1:A1:710:A:H2'	1:A1:711:A:C8	2.55	0.42
1:A1:1724:U:O4	20:AR:125:LYS:NZ	2.52	0.42
1:A1:2960:C:H2'	1:A1:2961:G:C8	2.55	0.42
1:A1:3139:A:OP2	5:AB:30:LYS:NZ	2.36	0.42
5:AB:83:PRO:O	5:AB:165:GLN:NE2	2.50	0.42
6:AC:26:PHE:HA	6:AC:127:ALA:HA	2.01	0.42
10:AG:82:LEU:HG	10:AG:86:THR:HG23	2.02	0.42
14:AL:62:THR:O	14:AL:64:LYS:N	2.53	0.42
14:AL:171:ARG:HA	14:AL:171:ARG:HD2	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AS:27:MET:HE2	21:AS:27:MET:HB3	1.90	0.42
27:AY:42:GLN:NE2	27:AY:127:GLU:O	2.47	0.42
32:Ad:46:THR:HA	32:Ad:87:ASN:HD21	1.84	0.42
48:BD:21:LEU:HD12	48:BD:21:LEU:HA	1.91	0.42
61:BQ:47:LYS:HB3	61:BQ:82:ARG:HD2	2.02	0.42
64:BT:31:PRO:HD2	64:BT:34:VAL:HG13	2.02	0.42
69:BY:60:PHE:O	79:B5:522:U:O2'	2.37	0.42
72:Bb:18:LYS:O	72:Bb:29:ARG:NH2	2.43	0.42
79:B5:538:A:H5'	79:B5:543:C:H42	1.84	0.42
79:B5:1359:C:H2'	79:B5:1360:A:C8	2.55	0.42
79:B5:1561:U:H4'	79:B5:1599:C:H4'	2.02	0.42
1:A1:87:U:H2'	1:A1:88:A:C8	2.54	0.42
1:A1:302:U:H5''	16:AN:179:LYS:HE3	2.01	0.42
1:A1:2423:U:H2'	1:A1:2424:A:H8	1.84	0.42
1:A1:2683:U:H2'	1:A1:2684:C:C6	2.55	0.42
6:AC:181:VAL:HG22	6:AC:202:ARG:HB2	2.01	0.42
14:AL:5:LYS:H	14:AL:5:LYS:HG3	1.68	0.42
29:Aa:36:GLY:HA3	29:Aa:40:HIS:CE1	2.54	0.42
33:Ae:126:LEU:HD23	33:Ae:126:LEU:HA	1.87	0.42
35:Ag:57:LEU:HB3	35:Ag:61:GLN:HB2	2.02	0.42
46:BB:174:LYS:HB3	46:BB:174:LYS:HE2	1.83	0.42
48:BD:136:VAL:HG22	48:BD:186:VAL:HG22	2.00	0.42
70:BZ:55:PRO:HD3	70:BZ:88:ILE:HD12	2.01	0.42
79:B5:1760:G:H1'	79:B5:1781:MA6:H2	2.02	0.42
1:A1:848:A:C8	79:B5:973:A:H4'	2.55	0.41
1:A1:1794:G:O2'	1:A1:1796:G:N2	2.53	0.41
1:A1:1886:A:O2'	5:AB:226:PHE:O	2.29	0.41
1:A1:2218:G:H2'	1:A1:2219:A:H8	1.85	0.41
1:A1:2759:U:H5''	1:A1:2760:C:H5'	2.02	0.41
5:AB:27:ALA:HB2	5:AB:220:VAL:HG23	2.01	0.41
9:AF:208:SER:OG	9:AF:209:ASN:N	2.51	0.41
10:AG:189:LEU:HD12	10:AG:190:VAL:HG13	2.02	0.41
13:AJ:80:LEU:HA	13:AJ:80:LEU:HD23	1.82	0.41
14:AL:116:LEU:HD23	14:AL:116:LEU:HA	1.85	0.41
38:Aj:29:VAL:O	38:Aj:32:LYS:NZ	2.51	0.41
52:BH:113:PRO:HG2	52:BH:116:ARG:HD3	2.02	0.41
66:BV:64:GLU:HG2	72:Bb:3:LEU:HB2	2.00	0.41
79:B5:565:C:H4'	79:B5:566:C:H5''	2.02	0.41
1:A1:40:A:H5''	29:Aa:35:ALA:HB1	2.02	0.41
1:A1:627:U:H4'	1:A1:1399:A:H1'	2.01	0.41
1:A1:629:U:H2'	1:A1:630:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1497:C:H2'	1:A1:1498:A:C8	2.54	0.41
2:A3:112:G:H2'	2:A3:113:C:C6	2.55	0.41
15:AM:23:ILE:O	15:AM:30:GLY:N	2.52	0.41
27:AY:63:LYS:HD2	27:AY:85:VAL:HG13	2.02	0.41
28:AZ:26:VAL:HG11	28:AZ:96:VAL:HB	2.01	0.41
29:Aa:56:VAL:HG12	29:Aa:57:GLY:H	1.84	0.41
34:Af:49:ILE:HD11	34:Af:71:VAL:HG22	2.02	0.41
35:Ag:58:ARG:HD2	35:Ag:58:ARG:HA	1.86	0.41
38:Aj:21:ARG:NH2	38:Aj:41:ALA:O	2.28	0.41
44:Ap:36:ARG:HG3	44:Ap:48:LYS:HD3	2.01	0.41
50:BF:166:ARG:HB2	73:Bc:46:GLY:HA3	2.02	0.41
53:BI:121:LEU:HD22	53:BI:157:GLU:HG3	2.01	0.41
69:BY:60:PHE:HA	69:BY:70:VAL:O	2.20	0.41
79:B5:273:G:O6	79:B5:283:U:O2	2.37	0.41
1:A1:345:G:O2'	3:A4:25:G:N3	2.52	0.41
1:A1:532:A:H2'	1:A1:533:A:C8	2.56	0.41
1:A1:675:C:O2'	1:A1:679:U:OP1	2.32	0.41
1:A1:900:G:H1'	1:A1:1589:A:N6	2.35	0.41
1:A1:911:C:N4	4:AA:3:ARG:HD3	2.35	0.41
1:A1:943:U:H3'	29:Aa:13:GLY:HA2	2.01	0.41
1:A1:1646:G:O2'	1:A1:1808:G:N2	2.37	0.41
4:AA:3:ARG:HB2	4:AA:207:VAL:HG22	2.02	0.41
9:AF:92:ILE:HD11	9:AF:110:ARG:HA	2.02	0.41
49:BE:171:ASP:OD2	49:BE:171:ASP:N	2.52	0.41
54:BJ:108:ARG:NH1	54:BJ:110:GLN:OE1	2.51	0.41
62:BR:34:LEU:HB3	77:Bg:150:TRP:CH2	2.54	0.41
62:BR:116:LYS:HA	62:BR:116:LYS:HD2	1.82	0.41
67:BW:56:HIS:O	79:B5:861:U:O2'	2.29	0.41
79:B5:1188:G:O2'	79:B5:1430:U:OP1	2.31	0.41
1:A1:49:A:OP1	14:AL:16:LYS:NZ	2.38	0.41
1:A1:1095:U:H4'	1:A1:1096:U:H5''	2.02	0.41
1:A1:1497:C:H2'	1:A1:1498:A:H8	1.86	0.41
1:A1:1621:A:H2'	1:A1:1622:U:C6	2.55	0.41
1:A1:2213:A:H2'	1:A1:2214:A:C8	2.55	0.41
6:AC:120:TYR:CE1	6:AC:277:PRO:HB3	2.55	0.41
13:AJ:16:LYS:HE3	13:AJ:130:VAL:HG21	2.03	0.41
17:AO:64[A]:PHE:HE2	17:AO:68[A]:ARG:HH11	1.68	0.41
26:AX:73:MET:HE2	26:AX:142:ILE:HB	2.02	0.41
28:AZ:72:ILE:HG22	28:AZ:101:PHE:CZ	2.55	0.41
29:Aa:75:LEU:HD11	29:Aa:134:ALA:HA	2.03	0.41
35:Ag:3:GLN:HE22	35:Ag:29:ILE:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BB:219:LYS:HB3	46:BB:219:LYS:HE3	1.76	0.41
61:BQ:50:GLU:OE1	61:BQ:82:ARG:NH2	2.53	0.41
79:B5:968:U:O3'	79:B5:1032:G:N2	2.53	0.41
3:A4:74:U:O2'	3:A4:76:C:OP2	2.37	0.41
15:AM:19:ARG:NH1	15:AM:66:THR:O	2.46	0.41
20:AR:15:VAL:HG23	20:AR:17:VAL:HG22	2.00	0.41
43:Ao:100:LYS:HE3	43:Ao:100:LYS:HB2	1.82	0.41
48:BD:64:ARG:NH1	55:BK:91:TYR:HB2	2.35	0.41
50:BF:80:LYS:HB2	50:BF:83:ARG:HG3	2.03	0.41
50:BF:136:ALA:O	50:BF:140:THR:HG22	2.21	0.41
53:BI:83:TYR:HB3	53:BI:101:ILE:HB	2.02	0.41
53:BI:112:TRP:O	53:BI:116:HIS:HB2	2.21	0.41
61:BQ:22:VAL:HG22	61:BQ:65:ILE:HG23	2.02	0.41
61:BQ:136:SER:HA	79:B5:1581:C:H5'	2.03	0.41
63:BS:101:LEU:HB3	63:BS:102:ALA:H	1.80	0.41
65:BU:69:LYS:HG2	79:B5:1280:4AC:H5''	2.02	0.41
67:BW:51:GLU:HG2	72:Bb:8:LEU:HD11	2.03	0.41
77:Bg:292:LEU:HD12	77:Bg:301:LEU:HD11	2.02	0.41
79:B5:17:C:H2'	79:B5:18:C:C6	2.56	0.41
1:A1:411:U:H2'	1:A1:412:G:H8	1.84	0.41
1:A1:2941:A:OP1	1:A1:2943:G:O2'	2.35	0.41
1:A1:3113:A:H4'	11:AH:69:ARG:HG3	2.02	0.41
1:A1:3280:U:O2'	1:A1:3281:U:O5'	2.34	0.41
1:A1:3348:G:O6	1:A1:3357:U:O4	2.38	0.41
14:AL:59:ARG:HA	14:AL:59:ARG:HD3	1.93	0.41
17:AO:189[A]:ASP:OD1	17:AO:189[A]:ASP:N	2.52	0.41
28:AZ:25:ILE:HG23	28:AZ:41:ALA:HB1	2.03	0.41
46:BB:33:LYS:O	46:BB:98:THR:OG1	2.29	0.41
49:BE:3:ARG:HG3	79:B5:399:A:H4'	2.01	0.41
49:BE:27:TYR:O	79:B5:447:U:O2'	2.30	0.41
64:BT:36:ILE:HG23	64:BT:37:VAL:HG23	2.02	0.41
64:BT:68:ARG:NE	79:B5:1521:G:O6	2.51	0.41
75:Be:31:LYS:HD2	79:B5:545:A:H2'	2.03	0.41
79:B5:97:C:O2	79:B5:425:A:O2'	2.37	0.41
1:A1:76:G:O2'	14:AL:100:ARG:NH1	2.44	0.41
1:A1:662:U:H2'	1:A1:663:OMC:C6	2.56	0.41
1:A1:673:U:H2'	1:A1:674:G:C8	2.56	0.41
1:A1:804:C:OP1	6:AC:98:ARG:NH2	2.32	0.41
1:A1:1750:A:OP1	39:Ak:44:LYS:NZ	2.36	0.41
7:AD:52:VAL:HG21	7:AD:65:ILE:HD12	2.03	0.41
27:AY:74:TYR:HD2	27:AY:77:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:52:LYS:HE3	66:BV:82:VAL:HA	2.01	0.41
60:BP:51:SER:O	60:BP:51:SER:OG	2.31	0.41
69:BY:35:VAL:HG23	69:BY:36:SER:H	1.85	0.41
79:B5:139:C:N4	79:B5:175:G:O2'	2.53	0.41
79:B5:702:G:O6	79:B5:737:A:N6	2.52	0.41
79:B5:1175:U:H2'	79:B5:1176:G:H8	1.85	0.41
1:A1:746:A:OP1	19:AQ:145:ASN:ND2	2.53	0.41
1:A1:1119:C:H2'	1:A1:1120:A:C8	2.56	0.41
1:A1:2413:A:H2'	1:A1:2414:G:H8	1.86	0.41
1:A1:2683:U:H5'	13:AJ:18:VAL:HG11	2.02	0.41
1:A1:3322:A:H2'	1:A1:3323:A:C8	2.56	0.41
5:AB:380:MET:HE2	5:AB:383:LEU:HD21	2.03	0.41
10:AG:82:LEU:HD13	10:AG:222:PHE:HE2	1.86	0.41
10:AG:140:VAL:HG22	10:AG:166:LEU:HD21	2.03	0.41
60:BP:103:ASN:OD1	60:BP:120:SER:OG	2.39	0.41
67:BW:85:ASP:OD2	67:BW:85:ASP:N	2.53	0.41
69:BY:62:THR:HA	69:BY:69:SER:HA	2.03	0.41
71:Ba:13:LYS:O	71:Ba:15:ARG:NH2	2.54	0.41
74:Bd:15:GLY:O	74:Bd:19:ARG:NH1	2.54	0.41
79:B5:818:C:O2'	79:B5:819:G:O5'	2.34	0.41
79:B5:1241:G:OP1	79:B5:1241:G:N2	2.45	0.41
1:A1:107:A:O2'	1:A1:324:A:N3	2.50	0.41
1:A1:609:G:O6	6:AC:308:LYS:NZ	2.48	0.41
1:A1:656:A:H2'	1:A1:657:A:C8	2.56	0.41
1:A1:985:U:H2'	1:A1:986:U:H6	1.85	0.41
1:A1:1190:A:H4'	41:Am:113:ARG:NH2	2.35	0.41
1:A1:1351:U:O2	1:A1:1355:A:N7	2.54	0.41
1:A1:1466:G:N2	1:A1:1510:G:H5''	2.36	0.41
1:A1:2284:C:N4	1:A1:2308:C:OP2	2.52	0.41
1:A1:2618:G:H5''	12:AI:116:ARG:HB2	2.02	0.41
1:A1:2632:G:H5''	22:AT:12:ARG:HB2	2.01	0.41
1:A1:3214:U:C4	15:AM:121:MET:HG3	2.56	0.41
1:A1:3294:A:H2'	1:A1:3295:A:O4'	2.21	0.41
2:A3:64:A:N7	12:AI:209:ASN:ND2	2.67	0.41
5:AB:331:ASN:OD1	5:AB:331:ASN:N	2.50	0.41
34:Af:89:LEU:HD23	34:Af:89:LEU:HA	1.87	0.41
37:Ai:66:GLU:O	37:Ai:70:ARG:HB2	2.21	0.41
45:BA:206:ASP:HA	45:BA:207:PRO:HA	1.88	0.41
48:BD:151:LYS:NZ	79:B5:1423:U:OP1	2.45	0.41
51:BG:177:ARG:NH2	79:B5:143:G:O6	2.44	0.41
52:BH:91:ILE:HG21	52:BH:129:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BL:124:THR:HB	56:BL:141:LYS:HB3	2.03	0.41
57:BM:106:ILE:HG22	57:BM:115:VAL:HG21	2.02	0.41
59:BO:17:ALA:HA	59:BO:30:VAL:HG22	2.02	0.41
59:BO:114:ARG:HD3	59:BO:114:ARG:HA	1.87	0.41
65:BU:63:LEU:O	65:BU:83:GLU:HA	2.20	0.41
71:Ba:17:HIS:NE2	79:B5:1789:G:OP1	2.41	0.41
76:Bf:98:VAL:HG23	76:Bf:100:LEU:HD23	2.01	0.41
77:Bg:302:PHE:HD1	77:Bg:312:VAL:HG22	1.86	0.41
79:B5:1041:G:H2'	79:B5:1042:G:C8	2.56	0.41
79:B5:1354:G:C6	79:B5:1369:U:N3	2.89	0.41
1:A1:268:A:N1	1:A1:295:A:H5'	2.36	0.41
1:A1:1432:C:O2'	1:A1:1434:G:OP2	2.39	0.41
1:A1:2819:A:OP1	1:A1:2866:U:O2'	2.34	0.41
2:A3:84:A:H2'	2:A3:85:G:C8	2.55	0.41
8:AE:72:ASN:HB3	8:AE:160:SER:HA	2.03	0.41
16:AN:138:GLN:HA	16:AN:143:ARG:HH11	1.86	0.41
37:Ai:56:ARG:HH12	37:Ai:76:ARG:HD2	1.86	0.41
46:BB:119:THR:HG21	46:BB:161:ILE:HD11	2.03	0.41
48:BD:142:LEU:HB2	78:Bh:110:TRP:CD1	2.56	0.41
52:BH:67:LEU:HD11	52:BH:94:ALA:HB2	2.02	0.41
53:BI:4:SER:OG	53:BI:6:ASP:OD1	2.38	0.41
55:BK:31:LYS:HD3	55:BK:31:LYS:HA	1.96	0.41
58:BN:16:ILE:O	67:BW:57:ARG:NH2	2.50	0.41
64:BT:5:SER:OG	64:BT:6:VAL:N	2.53	0.41
65:BU:57:ARG:HG2	65:BU:89:ARG:HG2	2.03	0.41
67:BW:42:GLN:NE2	67:BW:48:GLY:O	2.50	0.41
69:BY:82:ALA:O	69:BY:86:GLU:HB2	2.20	0.41
71:Ba:53:LEU:O	71:Ba:57:SER:CB	2.68	0.41
73:Bc:27:GLN:OE1	73:Bc:65:ARG:O	2.39	0.41
1:A1:1490:A:O2'	38:Aj:12:HIS:O	2.34	0.40
1:A1:1899:G:O2'	1:A1:2334:U:O4	2.30	0.40
11:AH:99:ILE:HG22	11:AH:101:VAL:HG23	2.02	0.40
13:Aj:110:ILE:HG13	13:Aj:111:ASP:H	1.86	0.40
15:AM:46:ILE:HD11	15:AM:56:GLN:HE21	1.86	0.40
18:AP:116:HIS:HB3	18:AP:149:VAL:HB	2.04	0.40
27:AY:106:ILE:HG21	27:AY:109:LEU:HD23	2.03	0.40
28:AZ:61:LYS:O	28:AZ:65:ARG:HG2	2.21	0.40
36:Ah:100:VAL:HG22	36:Ah:104:GLN:HB3	2.03	0.40
47:BC:121:VAL:O	47:BC:125:ILE:HG12	2.21	0.40
49:BE:31:PRO:HD2	49:BE:38:LEU:HG	2.03	0.40
52:BH:30:SER:OG	52:BH:33:GLU:OE2	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BI:56:ARG:HH22	79:B5:332:U:P	2.44	0.40
58:BN:127:ARG:O	58:BN:131:THR:HG23	2.21	0.40
63:BS:80:LYS:HA	63:BS:80:LYS:HD3	1.84	0.40
70:BZ:60:VAL:HB	70:BZ:101:TYR:HB2	2.03	0.40
71:Ba:7:SER:O	71:Ba:7:SER:OG	2.36	0.40
79:B5:5:U:H2'	79:B5:6:G:H8	1.86	0.40
79:B5:509:G:H2'	79:B5:510:G:C8	2.57	0.40
79:B5:1344:A:O2'	79:B5:1345:A:O4'	2.39	0.40
79:B5:1515:A:O2'	79:B5:1517:U:OP2	2.28	0.40
1:A1:75:G:H1'	14:AL:61:PRO:HG3	2.03	0.40
1:A1:282:G:O2'	1:A1:283:G:OP2	2.37	0.40
1:A1:963:G:O2'	29:Aa:29:PRO:O	2.36	0.40
1:A1:1389:G:OP1	33:Ae:104:ASN:ND2	2.49	0.40
1:A1:1495:U:H5	1:A1:1835:A:N1	2.19	0.40
6:AC:178:LEU:HD23	6:AC:178:LEU:HA	1.90	0.40
7:AD:164:LYS:NZ	7:AD:168:ASP:OD1	2.54	0.40
50:BF:29:ILE:O	50:BF:34:GLN:NE2	2.49	0.40
51:BG:136:LYS:HD3	79:B5:168:A:H4'	2.03	0.40
51:BG:216:LEU:HG	51:BG:220:LYS:HE3	2.03	0.40
69:BY:15:ASN:OD1	69:BY:18:LEU:N	2.43	0.40
79:B5:891:A:H2'	79:B5:892:A:C8	2.56	0.40
79:B5:1216:C:O2'	79:B5:1444:A:N1	2.47	0.40
1:A1:1447:G:N7	18:AP:25:SER:OG	2.47	0.40
1:A1:2219:A:H2'	1:A1:2220:A2M:C8	2.51	0.40
1:A1:2697:A:H2'	1:A1:2698:G:H8	1.87	0.40
1:A1:2948:OMC:H5'	5:AB:243:HIC:HB2	2.03	0.40
5:AB:232:ARG:HD3	5:AB:233:TRP:NE1	2.36	0.40
9:AF:77:VAL:HB	22:AT:139:ARG:HB2	2.02	0.40
11:AH:93:VAL:HG22	41:Am:82:LEU:HB3	2.03	0.40
12:AI:146:ASP:HA	12:AI:149:VAL:HG22	2.04	0.40
14:AL:36:ARG:HG2	14:AL:39:ARG:HH21	1.87	0.40
55:BK:40:LEU:HD11	79:B5:1217:A:C5	2.57	0.40
61:BQ:77:GLN:O	61:BQ:81:ILE:HG12	2.21	0.40
63:BS:108:LYS:HA	63:BS:108:LYS:HD2	1.88	0.40
64:BT:22:LEU:HD13	64:BT:28:LEU:HD22	2.03	0.40
68:BX:87:VAL:HA	68:BX:88:PRO:HD3	1.97	0.40
78:Bh:88:ARG:HH22	78:Bh:91:THR:HG1	1.61	0.40
79:B5:1171:A:O2'	79:B5:1570:A:N3	2.49	0.40
79:B5:1561:U:H2'	79:B5:1562:G:C8	2.54	0.40
79:B5:1585:U:N3	79:B5:1611:A:H2	2.18	0.40
1:A1:965:A:H2	29:Aa:43:ILE:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1127:G:H5'	12:AI:118:ALA:O	2.21	0.40
1:A1:2424:A:OP1	16:AN:90:ASN:ND2	2.40	0.40
2:A3:9:C:OP1	22:AT:26:HIS:ND1	2.54	0.40
4:AA:195:SER:O	4:AA:198:LYS:NZ	2.43	0.40
6:AC:2:SER:OG	6:AC:3:ARG:N	2.54	0.40
12:AI:54:SER:HB2	12:AI:135:ILE:HD11	2.02	0.40
12:AI:76:MET:O	12:AI:80:SER:OG	2.36	0.40
18:AP:16:SER:O	18:AP:101:ASN:ND2	2.51	0.40
18:AP:25:SER:O	18:AP:29:THR:OG1	2.30	0.40
19:AQ:67:ILE:HG12	19:AQ:81:VAL:HG11	2.02	0.40
25:AW:12:LYS:HB2	25:AW:12:LYS:HE2	1.85	0.40
29:Aa:94:ALA:HA	29:Aa:121:VAL:HG13	2.02	0.40
36:Ah:31:LEU:HB3	36:Ah:44:ILE:HD13	2.04	0.40
45:BA:122:ILE:HA	45:BA:144:ILE:O	2.22	0.40
48:BD:45:LYS:HA	48:BD:83:THR:O	2.21	0.40
56:BL:26:LYS:HE3	56:BL:26:LYS:HB3	1.91	0.40
57:BM:28:LEU:HD23	57:BM:28:LEU:HA	1.97	0.40
67:BW:79:PHE:O	67:BW:124:LYS:HA	2.22	0.40
73:Bc:30:VAL:O	73:Bc:39:THR:HA	2.22	0.40
79:B5:874:C:H2'	79:B5:875:G:C8	2.57	0.40
1:A1:66:A:H3'	1:A1:316:U:H5''	2.03	0.40
1:A1:187:A:N3	1:A1:208:C:O2'	2.43	0.40
1:A1:267:G:OP2	1:A1:318:A:N6	2.54	0.40
1:A1:816:A:H5'	1:A1:906:A:N6	2.35	0.40
1:A1:1643:A:H2'	1:A1:1644:C:C2	2.55	0.40
1:A1:1793:C:OP2	44:Ap:49:ARG:NH2	2.36	0.40
1:A1:2216:G:H22	1:A1:2229:A:H2	1.69	0.40
4:AA:248:GLY:O	79:B5:1011:G:O2'	2.40	0.40
8:AE:40:LEU:O	8:AE:51:ARG:HA	2.21	0.40
9:AF:88:ARG:HA	9:AF:134:VAL:HG12	2.04	0.40
10:AG:148:ALA:HA	10:AG:201:THR:HG22	2.03	0.40
12:AI:206:LEU:HD23	12:AI:206:LEU:HA	1.93	0.40
16:AN:73:ARG:HB2	16:AN:92:LEU:HD12	2.03	0.40
21:AS:71:LYS:NZ	21:AS:128:GLU:OE2	2.55	0.40
47:BC:178:ILE:HG21	47:BC:185:LYS:HA	2.03	0.40
50:BF:212:LYS:HE3	50:BF:212:LYS:HB2	1.89	0.40
51:BG:187:LYS:O	51:BG:191:ARG:HG3	2.22	0.40
56:BL:109:VAL:HG21	56:BL:125:VAL:HG11	2.02	0.40
58:BN:132:VAL:HG13	58:BN:134:VAL:HG23	2.03	0.40
60:BP:98:ASN:ND2	60:BP:121:ILE:O	2.32	0.40
67:BW:16:ASN:ND2	79:B5:1037:C:O2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Ba:13:LYS:O	79:B5:1075:C:O2'	2.34	0.40
77:Bg:84:SER:OG	77:Bg:85:TRP:N	2.53	0.40
77:Bg:221:MET:HG2	77:Bg:233:THR:HG23	2.04	0.40
79:B5:1645:G:H2'	79:B5:1646:C:H6	1.86	0.40
79:B5:1688:U:H3	79:B5:1712:A:N6	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AA	245/247 (99%)	232 (95%)	13 (5%)	0	100	100
5	AB	383/386 (99%)	363 (95%)	20 (5%)	0	100	100
6	AC	359/361 (99%)	326 (91%)	31 (9%)	2 (1%)	22	49
7	AD	290/292 (99%)	272 (94%)	17 (6%)	1 (0%)	37	64
8	AE	152/156 (97%)	139 (91%)	13 (9%)	0	100	100
9	AF	220/222 (99%)	207 (94%)	11 (5%)	2 (1%)	14	40
10	AG	228/230 (99%)	216 (95%)	12 (5%)	0	100	100
11	AH	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
12	AI	201/205 (98%)	187 (93%)	14 (7%)	0	100	100
13	AJ	167/169 (99%)	147 (88%)	20 (12%)	0	100	100
14	AL	191/193 (99%)	165 (86%)	22 (12%)	4 (2%)	5	21
15	AM	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
16	AN	201/203 (99%)	186 (92%)	14 (7%)	1 (0%)	25	54
17	AO	195/197 (99%)	191 (98%)	2 (1%)	2 (1%)	13	38
18	AP	171/175 (98%)	163 (95%)	8 (5%)	0	100	100
19	AQ	183/185 (99%)	177 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AR	186/188 (99%)	176 (95%)	10 (5%)	0	100	100
21	AS	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	AT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
23	AU	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
24	AV	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
25	AW	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
26	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
27	AY	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
28	AZ	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	16	43
29	Aa	146/148 (99%)	126 (86%)	18 (12%)	2 (1%)	9	30
30	Ab	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
31	Ac	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
32	Ad	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
33	Ae	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
34	Af	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
35	Ag	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
36	Ah	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	14	40
37	Ai	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
38	Aj	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
39	Ak	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
40	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	Am	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
42	An	23/25 (92%)	23 (100%)	0	0	100	100
43	Ao	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
44	Ap	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	12	35
45	BA	204/206 (99%)	185 (91%)	18 (9%)	1 (0%)	25	54
46	BB	212/214 (99%)	186 (88%)	24 (11%)	2 (1%)	14	40
47	BC	215/217 (99%)	197 (92%)	17 (8%)	1 (0%)	25	54
48	BD	221/223 (99%)	207 (94%)	14 (6%)	0	100	100
49	BE	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
50	BF	204/206 (99%)	185 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BG	224/226 (99%)	209 (93%)	13 (6%)	2 (1%)	14	40
52	BH	182/184 (99%)	166 (91%)	14 (8%)	2 (1%)	12	35
53	BI	184/188 (98%)	156 (85%)	28 (15%)	0	100	100
54	BJ	183/185 (99%)	168 (92%)	14 (8%)	1 (0%)	25	54
55	BK	94/96 (98%)	77 (82%)	17 (18%)	0	100	100
56	BL	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
57	BM	119/121 (98%)	93 (78%)	26 (22%)	0	100	100
58	BN	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
59	BO	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
60	BP	122/124 (98%)	101 (83%)	19 (16%)	2 (2%)	8	27
61	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	46
62	BR	117/121 (97%)	106 (91%)	10 (8%)	1 (1%)	14	40
63	BS	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	9	30
64	BT	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
65	BU	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
66	BV	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
67	BW	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	43
68	BX	142/144 (99%)	120 (84%)	20 (14%)	2 (1%)	9	30
69	BY	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
70	BZ	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
71	Ba	95/97 (98%)	76 (80%)	16 (17%)	3 (3%)	3	14
72	Bb	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
73	Bc	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
74	Bd	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
75	Be	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
76	Bf	53/57 (93%)	39 (74%)	14 (26%)	0	100	100
77	Bg	310/312 (99%)	275 (89%)	35 (11%)	0	100	100
78	Bh	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
All	All	10956/11121 (98%)	10091 (92%)	827 (8%)	38 (0%)	38	64

All (38) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
6	AC	339	LEU
9	AF	159	GLN
14	AL	48	PRO
14	AL	63	VAL
16	AN	81	TYR
17	AO	111[A]	PRO
29	Aa	78	LEU
51	BG	68	LEU
68	BX	97	ASP
46	BB	206	PRO
46	BB	207	LEU
47	BC	40	LYS
51	BG	173	PRO
52	BH	111	LYS
54	BJ	134	ILE
63	BS	91	ASP
71	Ba	36	ILE
7	AD	20	PHE
14	AL	76	THR
14	AL	77	LEU
45	BA	4	PRO
60	BP	125	PRO
62	BR	24	LEU
71	Ba	35	ALA
71	Ba	62	TYR
36	Ah	91	ALA
44	Ap	52	ALA
6	AC	268	ALA
68	BX	96	VAL
28	AZ	17	ARG
29	Aa	47	LYS
61	BQ	33	GLY
60	BP	107	ILE
9	AF	216	VAL
63	BS	92	ILE
52	BH	65	PRO
17	AO	110[A]	PRO
67	BW	67	GLY

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AA	189/189 (100%)	189 (100%)	0	100	100
5	AB	321/321 (100%)	321 (100%)	0	100	100
6	AC	288/288 (100%)	288 (100%)	0	100	100
7	AD	241/241 (100%)	241 (100%)	0	100	100
8	AE	134/134 (100%)	134 (100%)	0	100	100
9	AF	186/186 (100%)	186 (100%)	0	100	100
10	AG	189/189 (100%)	189 (100%)	0	100	100
11	AH	170/170 (100%)	170 (100%)	0	100	100
12	AI	176/176 (100%)	176 (100%)	0	100	100
13	AJ	147/147 (100%)	147 (100%)	0	100	100
14	AL	154/154 (100%)	154 (100%)	0	100	100
15	AM	107/107 (100%)	107 (100%)	0	100	100
16	AN	175/175 (100%)	175 (100%)	0	100	100
17	AO	160/160 (100%)	160 (100%)	0	100	100
18	AP	141/141 (100%)	141 (100%)	0	100	100
19	AQ	150/150 (100%)	150 (100%)	0	100	100
20	AR	153/153 (100%)	153 (100%)	0	100	100
21	AS	156/156 (100%)	156 (100%)	0	100	100
22	AT	136/136 (100%)	136 (100%)	0	100	100
23	AU	87/87 (100%)	86 (99%)	1 (1%)	70	83
24	AV	104/104 (100%)	104 (100%)	0	100	100
25	AW	55/55 (100%)	55 (100%)	0	100	100
26	AX	105/105 (100%)	105 (100%)	0	100	100
27	AY	109/109 (100%)	109 (100%)	0	100	100
28	AZ	115/115 (100%)	115 (100%)	0	100	100
29	Aa	118/118 (100%)	118 (100%)	0	100	100
30	Ab	46/46 (100%)	46 (100%)	0	100	100
31	Ac	81/81 (100%)	81 (100%)	0	100	100
32	Ad	96/96 (100%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Ae	109/109 (100%)	109 (100%)	0	100	100
34	Af	90/90 (100%)	90 (100%)	0	100	100
35	Ag	95/95 (100%)	95 (100%)	0	100	100
36	Ah	104/104 (100%)	104 (100%)	0	100	100
37	Ai	81/81 (100%)	81 (100%)	0	100	100
38	Aj	70/70 (100%)	70 (100%)	0	100	100
39	Ak	68/68 (100%)	68 (100%)	0	100	100
40	Al	45/45 (100%)	45 (100%)	0	100	100
41	Am	47/47 (100%)	47 (100%)	0	100	100
42	An	23/23 (100%)	23 (100%)	0	100	100
43	Ao	90/90 (100%)	90 (100%)	0	100	100
44	Ap	71/71 (100%)	71 (100%)	0	100	100
45	BA	173/173 (100%)	173 (100%)	0	100	100
46	BB	191/191 (100%)	190 (100%)	1 (0%)	86	91
47	BC	176/176 (100%)	176 (100%)	0	100	100
48	BD	182/182 (100%)	182 (100%)	0	100	100
49	BE	221/221 (100%)	221 (100%)	0	100	100
50	BF	173/173 (100%)	173 (100%)	0	100	100
51	BG	193/193 (100%)	193 (100%)	0	100	100
52	BH	165/165 (100%)	165 (100%)	0	100	100
53	BI	150/150 (100%)	150 (100%)	0	100	100
54	BJ	158/158 (100%)	158 (100%)	0	100	100
55	BK	89/89 (100%)	89 (100%)	0	100	100
56	BL	136/136 (100%)	136 (100%)	0	100	100
57	BM	98/98 (100%)	98 (100%)	0	100	100
58	BN	127/127 (100%)	127 (100%)	0	100	100
59	BO	96/96 (100%)	96 (100%)	0	100	100
60	BP	104/104 (100%)	104 (100%)	0	100	100
61	BQ	117/117 (100%)	117 (100%)	0	100	100
62	BR	110/110 (100%)	110 (100%)	0	100	100
63	BS	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	BT	113/113 (100%)	113 (100%)	0	100	100
65	BU	100/100 (100%)	100 (100%)	0	100	100
66	BV	74/74 (100%)	74 (100%)	0	100	100
67	BW	110/110 (100%)	110 (100%)	0	100	100
68	BX	119/119 (100%)	119 (100%)	0	100	100
69	BY	112/112 (100%)	112 (100%)	0	100	100
70	BZ	61/61 (100%)	61 (100%)	0	100	100
71	Ba	83/83 (100%)	83 (100%)	0	100	100
72	Bb	70/70 (100%)	69 (99%)	1 (1%)	62	79
73	Bc	56/56 (100%)	56 (100%)	0	100	100
74	Bd	47/47 (100%)	46 (98%)	1 (2%)	48	69
75	Be	51/51 (100%)	51 (100%)	0	100	100
76	Bf	49/49 (100%)	49 (100%)	0	100	100
77	Bg	256/257 (100%)	256 (100%)	0	100	100
78	Bh	68/68 (100%)	68 (100%)	0	100	100
All	All	9338/9339 (100%)	9334 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	AU	49	ASN
46	BB	146	GLN
72	Bb	42	ASN
74	Bd	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
4	AA	97	ASN
4	AA	132	ASN
5	AB	68	HIS
5	AB	121	ASN
6	AC	213	ASN
6	AC	260	GLN
7	AD	90	HIS
9	AF	194	HIS

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Mol	Chain	Res	Type
10	AG	95	ASN
11	AH	96	HIS
11	AH	163	GLN
14	AL	105	ASN
14	AL	120	GLN
14	AL	137	GLN
15	AM	56	GLN
16	AN	95	GLN
17	AO	26[A]	GLN
17	AO	31[A]	GLN
18	AP	54	HIS
19	AQ	23	ASN
20	AR	66	HIS
22	AT	49	GLN
22	AT	98	HIS
23	AU	49	ASN
27	AY	110	HIS
28	AZ	78	ASN
28	AZ	122	HIS
29	Aa	120	ASN
31	Ac	11	ASN
35	Ag	3	GLN
36	Ah	16	GLN
36	Ah	76	GLN
36	Ah	113	GLN
38	Aj	69	HIS
40	Al	32	ASN
40	Al	33	ASN
41	Am	90	ASN
46	BB	146	GLN
46	BB	183	GLN
46	BB	194	ASN
46	BB	208	GLN
46	BB	209	ASN
47	BC	201	ASN
48	BD	165	ASN
49	BE	17	HIS
49	BE	50	ASN
49	BE	157	ASN
50	BF	63	GLN
51	BG	190	GLN
51	BG	197	ASN

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Mol	Chain	Res	Type
52	BH	11	GLN
52	BH	22	GLN
52	BH	42	GLN
52	BH	161	GLN
53	BI	103	GLN
55	BK	93	GLN
56	BL	14	GLN
56	BL	21	ASN
56	BL	92	HIS
57	BM	84	ASN
58	BN	78	ASN
62	BR	62	GLN
63	BS	8	GLN
63	BS	25	ASN
63	BS	75	ASN
65	BU	17	GLN
65	BU	105	GLN
67	BW	39	GLN
67	BW	70	ASN
72	Bb	5	GLN
72	Bb	9	HIS
74	Bd	48	ASN
77	Bg	237	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	3150/3156 (99%)	695 (22%)	13 (0%)
2	A3	120/121 (99%)	15 (12%)	0
3	A4	156/158 (98%)	34 (21%)	2 (1%)
79	B5	1781/1783 (99%)	459 (25%)	14 (0%)
All	All	5207/5218 (99%)	1203 (23%)	29 (0%)

All (1203) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	14	U
1	A1	18	G
1	A1	21	G
1	A1	26	A
1	A1	34	A

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Mol	Chain	Res	Type
1	A1	40	A
1	A1	43	A
1	A1	49	A
1	A1	57	A
1	A1	59	G
1	A1	60	A
1	A1	65	A
1	A1	66	A
1	A1	72	C
1	A1	75	G
1	A1	76	G
1	A1	85	A
1	A1	92	G
1	A1	109	A
1	A1	110	G
1	A1	111	C
1	A1	115	A
1	A1	116	A
1	A1	117	U
1	A1	120	G
1	A1	121	A
1	A1	122	A
1	A1	134	U
1	A1	135	C
1	A1	136	G
1	A1	143	G
1	A1	148	G
1	A1	150	A
1	A1	154	U
1	A1	156	G
1	A1	157	A
1	A1	164	A
1	A1	165	A
1	A1	166	C
1	A1	170	G
1	A1	187	A
1	A1	190	U
1	A1	191	U
1	A1	200	C
1	A1	206	G
1	A1	210	U
1	A1	211	A

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Mol	Chain	Res	Type
1	A1	219	A
1	A1	220	G
1	A1	231	G
1	A1	239	G
1	A1	240	U
1	A1	242	C
1	A1	243	G
1	A1	244	G
1	A1	249	U
1	A1	250	U
1	A1	251	G
1	A1	252	U
1	A1	266	A
1	A1	267	G
1	A1	268	A
1	A1	269	G
1	A1	281	G
1	A1	283	G
1	A1	285	A
1	A1	286	U
1	A1	295	A
1	A1	297	G
1	A1	299	G
1	A1	305	U
1	A1	315	C
1	A1	316	U
1	A1	329	U
1	A1	337	G
1	A1	339	C
1	A1	352	A
1	A1	359	U
1	A1	371	G
1	A1	372	A
1	A1	374	A
1	A1	375	A
1	A1	376	G
1	A1	384	A
1	A1	387	A
1	A1	398	A
1	A1	399	A
1	A1	400	G
1	A1	401	U

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Mol	Chain	Res	Type
1	A1	402	A
1	A1	403	C
1	A1	420	G
1	A1	421	G
1	A1	422	A
1	A1	429	U
1	A1	439	C
1	A1	440	A
1	A1	441	U
1	A1	442	G
1	A1	443	G
1	A1	446	U
1	A1	447	U
1	A1	448	U
1	A1	450	G
1	A1	451	U
1	A1	487	U
1	A1	488	U
1	A1	489	U
1	A1	491	A
1	A1	493	U
1	A1	494	G
1	A1	498	A
1	A1	520	U
1	A1	521	A
1	A1	523	A
1	A1	535	G
1	A1	542	G
1	A1	543	C
1	A1	545	U
1	A1	546	C
1	A1	547	G
1	A1	548	G
1	A1	550	A
1	A1	551	A
1	A1	552	G
1	A1	555	U
1	A1	557	A
1	A1	558	U
1	A1	559	A
1	A1	560	G
1	A1	569	A

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Mol	Chain	Res	Type
1	A1	578	A
1	A1	579	G
1	A1	588	G
1	A1	589	A
1	A1	592	A
1	A1	602	A
1	A1	604	G
1	A1	611	A
1	A1	620	U
1	A1	621	A
1	A1	637	C
1	A1	647	A
1	A1	649	A2M
1	A1	660	A
1	A1	677	A
1	A1	681	U
1	A1	690	A
1	A1	691	A
1	A1	705	A
1	A1	719	U
1	A1	725	G
1	A1	736	A
1	A1	765	C
1	A1	766	U
1	A1	767	U
1	A1	774	G
1	A1	775	A
1	A1	780	A
1	A1	781	G
1	A1	784	A
1	A1	785	G
1	A1	786	A
1	A1	799	G
1	A1	801	A
1	A1	806	A
1	A1	813	G
1	A1	817	A2M
1	A1	826	G
1	A1	830	A
1	A1	844	G
1	A1	845	G
1	A1	849	C

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Mol	Chain	Res	Type
1	A1	861	C
1	A1	862	U
1	A1	871	U
1	A1	874	U
1	A1	879	U
1	A1	896	A
1	A1	897	U
1	A1	907	G
1	A1	914	A
1	A1	916	G
1	A1	917	A
1	A1	921	A
1	A1	923	C
1	A1	924	G
1	A1	925	A
1	A1	934	G
1	A1	937	G
1	A1	944	C
1	A1	959	C
1	A1	960	U
1	A1	963	G
1	A1	970	A
1	A1	974	G
1	A1	979	U
1	A1	981	U
1	A1	994	G
1	A1	1000	C
1	A1	1002	A
1	A1	1006	A
1	A1	1010	G
1	A1	1014	U
1	A1	1016	C
1	A1	1017	C
1	A1	1018	G
1	A1	1019	G
1	A1	1021	G
1	A1	1032	C
1	A1	1033	U
1	A1	1034	U
1	A1	1035	G
1	A1	1047	A
1	A1	1049	C

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Mol	Chain	Res	Type
1	A1	1052	U
1	A1	1064	A
1	A1	1072	G
1	A1	1075	A
1	A1	1081	U
1	A1	1087	G
1	A1	1094	U
1	A1	1095	U
1	A1	1096	U
1	A1	1097	G
1	A1	1098	A
1	A1	1103	A
1	A1	1104	G
1	A1	1117	G
1	A1	1131	G
1	A1	1132	C
1	A1	1143	A
1	A1	1144	U
1	A1	1153	A
1	A1	1155	C
1	A1	1156	C
1	A1	1159	A
1	A1	1160	C
1	A1	1177	G
1	A1	1179	A
1	A1	1180	A
1	A1	1181	U
1	A1	1182	A
1	A1	1186	G
1	A1	1190	A
1	A1	1192	C
1	A1	1193	A
1	A1	1201	C
1	A1	1207	G
1	A1	1208	U
1	A1	1219	C
1	A1	1222	G
1	A1	1223	A
1	A1	1225	A
1	A1	1227	C
1	A1	1228	C
1	A1	1231	A

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Mol	Chain	Res	Type
1	A1	1232	C
1	A1	1233	G
1	A1	1235	U
1	A1	1236	G
1	A1	1237	G
1	A1	1239	C
1	A1	1240	A
1	A1	1241	U
1	A1	1242	G
1	A1	1243	G
1	A1	1244	A
1	A1	1246	G
1	A1	1247	U
1	A1	1248	C
1	A1	1249	G
1	A1	1250	G
1	A1	1251	A
1	A1	1252	A
1	A1	1263	A
1	A1	1264	G
1	A1	1266	G
1	A1	1268	G
1	A1	1270	A
1	A1	1271	A
1	A1	1272	C
1	A1	1276	U
1	A1	1277	C
1	A1	1278	A
1	A1	1281	G
1	A1	1283	C
1	A1	1286	A
1	A1	1287	A
1	A1	1306	G
1	A1	1307	G
1	A1	1309	U
1	A1	1315	U
1	A1	1317	A
1	A1	1318	A
1	A1	1325	U
1	A1	1330	A
1	A1	1331	U
1	A1	1345	G

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Mol	Chain	Res	Type
1	A1	1348	U
1	A1	1350	A
1	A1	1351	U
1	A1	1352	A
1	A1	1353	U
1	A1	1354	G
1	A1	1355	A
1	A1	1356	U
1	A1	1357	G
1	A1	1386	A
1	A1	1391	C
1	A1	1392	G
1	A1	1399	A
1	A1	1400	G
1	A1	1417	G
1	A1	1418	A
1	A1	1419	A
1	A1	1434	G
1	A1	1437	OMC
1	A1	1443	G
1	A1	1446	A
1	A1	1450	OMG
1	A1	1465	A
1	A1	1469	C
1	A1	1475	A
1	A1	1477	A
1	A1	1481	A
1	A1	1487	G
1	A1	1494	U
1	A1	1508	C
1	A1	1522	U
1	A1	1523	U
1	A1	1524	A
1	A1	1525	G
1	A1	1526	U
1	A1	1533	U
1	A1	1536	G
1	A1	1539	A
1	A1	1555	U
1	A1	1556	C
1	A1	1562	C
1	A1	1564	U

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Mol	Chain	Res	Type
1	A1	1565	G
1	A1	1566	A
1	A1	1567	U
1	A1	1569	U
1	A1	1570	U
1	A1	1572	U
1	A1	1574	C
1	A1	1576	G
1	A1	1583	A
1	A1	1587	A
1	A1	1589	A
1	A1	1590	G
1	A1	1593	A
1	A1	1596	C
1	A1	1605	A
1	A1	1628	C
1	A1	1629	U
1	A1	1630	U
1	A1	1642	A
1	A1	1643	A
1	A1	1657	C
1	A1	1683	A
1	A1	1717	U
1	A1	1722	U
1	A1	1724	U
1	A1	1730	G
1	A1	1736	G
1	A1	1741	A
1	A1	1742	U
1	A1	1750	A
1	A1	1751	G
1	A1	1756	C
1	A1	1761	C
1	A1	1762	C
1	A1	1763	U
1	A1	1764	U
1	A1	1765	U
1	A1	1766	G
1	A1	1775	G
1	A1	1778	G
1	A1	1780	G
1	A1	1794	G

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Mol	Chain	Res	Type
1	A1	1795	U
1	A1	1796	G
1	A1	1797	A
1	A1	1813	A
1	A1	1814	A
1	A1	1815	U
1	A1	1821	U
1	A1	1825	G
1	A1	1839	A
1	A1	1840	U
1	A1	1842	A
1	A1	1846	C
1	A1	1848	G
1	A1	1849	C
1	A1	1850	A
1	A1	1858	A
1	A1	1866	C
1	A1	1871	U
1	A1	1878	G
1	A1	1880	U
1	A1	1886	A
1	A1	1893	A
1	A1	1899	G
1	A1	1906	G
1	A1	1943	C
1	A1	1948	G
1	A1	1951	C
1	A1	1952	G
1	A1	1953	G
1	A1	1954	G
1	A1	2094	C
1	A1	2095	G
1	A1	2096	A
1	A1	2110	G
1	A1	2112	U
1	A1	2114	C
1	A1	2115	G
1	A1	2121	G
1	A1	2122	G
1	A1	2131	A
1	A1	2140	U
1	A1	2142	1MA

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Mol	Chain	Res	Type
1	A1	2144	A
1	A1	2145	A
1	A1	2158	A
1	A1	2169	G
1	A1	2176	U
1	A1	2188	A
1	A1	2194	G
1	A1	2197	OMC
1	A1	2205	U
1	A1	2207	A
1	A1	2208	A
1	A1	2209	U
1	A1	2210	G
1	A1	2244	A
1	A1	2249	G
1	A1	2253	G
1	A1	2256	A
1	A1	2257	C
1	A1	2258	U
1	A1	2260	U
1	A1	2268	U
1	A1	2269	U
1	A1	2270	A
1	A1	2272	G
1	A1	2273	G
1	A1	2281	A2M
1	A1	2288	OMG
1	A1	2298	U
1	A1	2306	C
1	A1	2307	G
1	A1	2308	C
1	A1	2310	U
1	A1	2313	A
1	A1	2314	U
1	A1	2315	G
1	A1	2334	U
1	A1	2336	U
1	A1	2340	U
1	A1	2366	C
1	A1	2373	A
1	A1	2374	C
1	A1	2375	G

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Mol	Chain	Res	Type
1	A1	2376	G
1	A1	2383	C
1	A1	2388	U
1	A1	2391	G
1	A1	2393	G
1	A1	2397	A
1	A1	2401	A
1	A1	2402	A
1	A1	2403	G
1	A1	2404	A
1	A1	2411	U
1	A1	2418	G
1	A1	2422	C
1	A1	2435	G
1	A1	2437	G
1	A1	2441	A
1	A1	2442	G
1	A1	2444	C
1	A1	2502	A
1	A1	2503	G
1	A1	2504	U
1	A1	2506	U
1	A1	2507	C
1	A1	2508	U
1	A1	2514	U
1	A1	2515	A
1	A1	2523	A
1	A1	2524	A
1	A1	2531	C
1	A1	2532	U
1	A1	2536	A
1	A1	2537	U
1	A1	2538	U
1	A1	2539	C
1	A1	2540	A
1	A1	2541	U
1	A1	2542	U
1	A1	2543	U
1	A1	2544	U
1	A1	2545	C
1	A1	2548	C
1	A1	2552	C

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Mol	Chain	Res	Type
1	A1	2553	U
1	A1	2561	A
1	A1	2568	C
1	A1	2569	A
1	A1	2570	U
1	A1	2571	U
1	A1	2572	C
1	A1	2573	G
1	A1	2580	A
1	A1	2585	G
1	A1	2586	G
1	A1	2593	A
1	A1	2606	G
1	A1	2607	G
1	A1	2614	G
1	A1	2629	U
1	A1	2635	A
1	A1	2648	G
1	A1	2651	G
1	A1	2652	U
1	A1	2656	A
1	A1	2666	C
1	A1	2672	G
1	A1	2674	A
1	A1	2676	A
1	A1	2677	G
1	A1	2678	A
1	A1	2679	A
1	A1	2681	U
1	A1	2688	U
1	A1	2689	A
1	A1	2690	G
1	A1	2691	A
1	A1	2703	A
1	A1	2704	A
1	A1	2705	A
1	A1	2712	U
1	A1	2714	G
1	A1	2723	U
1	A1	2726	C
1	A1	2727	A
1	A1	2728	G

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Mol	Chain	Res	Type
1	A1	2729	OMU
1	A1	2737	C
1	A1	2739	A
1	A1	2740	A
1	A1	2752	U
1	A1	2753	G
1	A1	2755	C
1	A1	2772	C
1	A1	2777	G
1	A1	2778	G
1	A1	2796	G
1	A1	2797	C
1	A1	2799	A
1	A1	2800	G
1	A1	2801	A
1	A1	2802	A
1	A1	2803	A
1	A1	2810	C
1	A1	2816	G
1	A1	2817	A
1	A1	2828	G
1	A1	2838	A
1	A1	2839	G
1	A1	2842	U
1	A1	2843	U
1	A1	2845	A
1	A1	2858	U
1	A1	2860	U
1	A1	2861	U
1	A1	2867	C
1	A1	2872	A
1	A1	2873	U
1	A1	2875	U
1	A1	2887	A
1	A1	2889	C
1	A1	2898	G
1	A1	2911	A
1	A1	2923	U
1	A1	2933	A
1	A1	2935	U
1	A1	2936	A
1	A1	2938	G

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Mol	Chain	Res	Type
1	A1	2941	A
1	A1	2942	C
1	A1	2947	G
1	A1	2948	OMC
1	A1	2951	G
1	A1	2955	U
1	A1	2956	A
1	A1	2983	C
1	A1	2990	G
1	A1	2992	U
1	A1	2997	G
1	A1	3011	A
1	A1	3012	A
1	A1	3021	A
1	A1	3022	G
1	A1	3032	A
1	A1	3056	U
1	A1	3057	U
1	A1	3059	G
1	A1	3078	U
1	A1	3079	U
1	A1	3080	G
1	A1	3086	A
1	A1	3087	A
1	A1	3092	C
1	A1	3095	U
1	A1	3109	G
1	A1	3116	G
1	A1	3129	A
1	A1	3130	A
1	A1	3131	U
1	A1	3142	A
1	A1	3143	C
1	A1	3153	U
1	A1	3154	C
1	A1	3155	U
1	A1	3156	U
1	A1	3157	U
1	A1	3165	A
1	A1	3170	A
1	A1	3172	A
1	A1	3173	G

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Mol	Chain	Res	Type
1	A1	3174	A
1	A1	3175	U
1	A1	3176	G
1	A1	3179	U
1	A1	3181	C
1	A1	3186	A
1	A1	3187	A
1	A1	3196	U
1	A1	3198	U
1	A1	3199	G
1	A1	3206	C
1	A1	3207	U
1	A1	3210	A
1	A1	3215	A
1	A1	3216	G
1	A1	3217	C
1	A1	3218	A
1	A1	3219	G
1	A1	3234	A
1	A1	3243	A
1	A1	3244	A
1	A1	3247	G
1	A1	3251	U
1	A1	3259	U
1	A1	3260	G
1	A1	3263	G
1	A1	3270	U
1	A1	3273	A
1	A1	3275	U
1	A1	3276	G
1	A1	3277	U
1	A1	3278	C
1	A1	3281	U
1	A1	3282	U
1	A1	3283	U
1	A1	3284	G
1	A1	3289	G
1	A1	3294	A
1	A1	3303	G
1	A1	3304	U
1	A1	3309	G
1	A1	3313	U

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Mol	Chain	Res	Type
1	A1	3316	A
1	A1	3320	A
1	A1	3342	A
1	A1	3345	G
1	A1	3351	U
1	A1	3352	U
1	A1	3353	G
1	A1	3354	U
1	A1	3355	U
1	A1	3356	G
1	A1	3363	U
1	A1	3369	G
1	A1	3375	A
1	A1	3378	C
1	A1	3382	U
1	A1	3383	G
1	A1	3389	U
1	A1	3390	G
2	A3	7	G
2	A3	10	C
2	A3	22	A
2	A3	38	U
2	A3	41	G
2	A3	43	U
2	A3	49	G
2	A3	54	U
2	A3	55	A
2	A3	65	G
2	A3	74	C
2	A3	76	A
2	A3	99	G
2	A3	102	A
2	A3	112	G
3	A4	13	A
3	A4	25	G
3	A4	34	U
3	A4	35	C
3	A4	51	G
3	A4	52	A
3	A4	59	A
3	A4	62	C
3	A4	63	G

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Mol	Chain	Res	Type
3	A4	68	G
3	A4	75	G
3	A4	76	C
3	A4	80	A
3	A4	81	U
3	A4	82	U
3	A4	84	C
3	A4	86	U
3	A4	87	G
3	A4	88	A
3	A4	90	U
3	A4	95	G
3	A4	97	A
3	A4	104	A
3	A4	105	A
3	A4	106	C
3	A4	111	A
3	A4	112	U
3	A4	113	U
3	A4	116	G
3	A4	125	U
3	A4	126	A
3	A4	152	G
3	A4	157	U
3	A4	158	U
79	B5	4	C
79	B5	25	C
79	B5	26	A
79	B5	34	G
79	B5	42	G
79	B5	46	A
79	B5	47	A
79	B5	57	G
79	B5	60	U
79	B5	67	A
79	B5	68	A
79	B5	72	A
79	B5	75	U
79	B5	76	A
79	B5	77	U
79	B5	78	A
79	B5	81	G

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Mol	Chain	Res	Type
79	B5	94	U
79	B5	104	A
79	B5	114	C
79	B5	115	G
79	B5	126	A
79	B5	127	G
79	B5	130	C
79	B5	133	U
79	B5	134	U
79	B5	135	A
79	B5	136	C
79	B5	137	U
79	B5	138	A
79	B5	141	U
79	B5	145	A
79	B5	158	U
79	B5	161	U
79	B5	166	C
79	B5	168	A
79	B5	171	A
79	B5	178	U
79	B5	179	A
79	B5	188	A
79	B5	189	C
79	B5	190	C
79	B5	191	C
79	B5	192	U
79	B5	193	U
79	B5	195	G
79	B5	196	G
79	B5	198	A
79	B5	200	A
79	B5	207	U
79	B5	217	A
79	B5	218	A
79	B5	224	C
79	B5	225	A
79	B5	227	U
79	B5	228	G
79	B5	229	U
79	B5	230	C
79	B5	232	U

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Mol	Chain	Res	Type
79	B5	233	C
79	B5	234	G
79	B5	239	C
79	B5	240	U
79	B5	241	U
79	B5	257	A
79	B5	260	U
79	B5	261	U
79	B5	265	A
79	B5	273	G
79	B5	278	U
79	B5	280	U
79	B5	299	A
79	B5	314	C
79	B5	316	A
79	B5	322	G
79	B5	333	A
79	B5	337	G
79	B5	338	C
79	B5	352	A
79	B5	359	A
79	B5	360	A
79	B5	361	C
79	B5	365	G
79	B5	369	A
79	B5	380	U
79	B5	388	G
79	B5	390	G
79	B5	393	C
79	B5	399	A
79	B5	400	A
79	B5	401	A
79	B5	402	C
79	B5	404	G
79	B5	417	A
79	B5	419	G
79	B5	423	G
79	B5	424	C
79	B5	425	A
79	B5	426	G
79	B5	434	G
79	B5	439	U

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Mol	Chain	Res	Type
79	B5	444	C
79	B5	448	C
79	B5	452	A
79	B5	459	G
79	B5	460	A
79	B5	468	A
79	B5	475	A
79	B5	477	A
79	B5	481	A
79	B5	484	C
79	B5	485	A
79	B5	486	G
79	B5	487	G
79	B5	489	C
79	B5	490	C
79	B5	491	C
79	B5	492	A
79	B5	493	U
79	B5	494	U
79	B5	495	C
79	B5	496	G
79	B5	497	G
79	B5	498	G
79	B5	499	U
79	B5	500	C
79	B5	501	U
79	B5	503	G
79	B5	505	A
79	B5	506	A
79	B5	507	U
79	B5	515	A
79	B5	519	C
79	B5	525	A
79	B5	527	A
79	B5	538	A
79	B5	539	G
79	B5	540	G
79	B5	541	A2M
79	B5	542	A
79	B5	556	A
79	B5	557	G
79	B5	558	U

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Mol	Chain	Res	Type
79	B5	559	C
79	B5	565	C
79	B5	566	C
79	B5	568	G
79	B5	577	G
79	B5	579	A
79	B5	580	A
79	B5	582	U
79	B5	594	A
79	B5	595	G
79	B5	606	A
79	B5	611	U
79	B5	613	G
79	B5	614	C
79	B5	617	U
79	B5	619	A2M
79	B5	620	A
79	B5	621	A
79	B5	622	A
79	B5	623	A
79	B5	635	A
79	B5	639	U
79	B5	650	U
79	B5	651	G
79	B5	652	G
79	B5	655	G
79	B5	656	G
79	B5	657	U
79	B5	658	C
79	B5	677	G
79	B5	678	A
79	B5	679	U
79	B5	681	U
79	B5	683	C
79	B5	694	U
79	B5	696	C
79	B5	697	C
79	B5	698	U
79	B5	700	C
79	B5	702	G
79	B5	703	G
79	B5	704	C

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Mol	Chain	Res	Type
79	B5	705	U
79	B5	706	A
79	B5	707	A
79	B5	708	C
79	B5	709	C
79	B5	710	U
79	B5	711	U
79	B5	714	G
79	B5	715	U
79	B5	716	C
79	B5	717	C
79	B5	718	U
79	B5	719	U
79	B5	720	G
79	B5	721	U
79	B5	722	G
79	B5	724	C
79	B5	725	U
79	B5	727	U
79	B5	729	G
79	B5	731	C
79	B5	732	G
79	B5	733	A
79	B5	734	A
79	B5	735	C
79	B5	736	C
79	B5	738	G
79	B5	740	A
79	B5	741	C
79	B5	742	U
79	B5	743	U
79	B5	745	U
79	B5	753	A
79	B5	755	A
79	B5	765	G
79	B5	766	U
79	B5	774	A
79	B5	775	G
79	B5	778	G
79	B5	779	U
79	B5	780	A
79	B5	781	U

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Mol	Chain	Res	Type
79	B5	782	U
79	B5	783	G
79	B5	784	C
79	B5	787	G
79	B5	789	A
79	B5	794	U
79	B5	812	A
79	B5	814	A
79	B5	815	G
79	B5	820	U
79	B5	821	U
79	B5	823	G
79	B5	829	A
79	B5	833	U
79	B5	836	U
79	B5	837	G
79	B5	838	G
79	B5	840	U
79	B5	846	G
79	B5	857	U
79	B5	859	A
79	B5	863	A
79	B5	873	U
79	B5	876	G
79	B5	886	U
79	B5	898	A
79	B5	906	A
79	B5	914	G
79	B5	932	U
79	B5	933	A
79	B5	935	U
79	B5	945	U
79	B5	951	A
79	B5	960	U
79	B5	964	U
79	B5	966	A
79	B5	973	A
79	B5	987	G
79	B5	992	A
79	B5	993	A
79	B5	1003	A
79	B5	1004	U

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Mol	Chain	Res	Type
79	B5	1005	A
79	B5	1021	C
79	B5	1025	A
79	B5	1026	A
79	B5	1028	C
79	B5	1030	A
79	B5	1032	G
79	B5	1039	A
79	B5	1052	U
79	B5	1056	U
79	B5	1058	U
79	B5	1060	U
79	B5	1061	A
79	B5	1062	A
79	B5	1076	A
79	B5	1082	C
79	B5	1083	G
79	B5	1086	A
79	B5	1092	A
79	B5	1097	U
79	B5	1098	U
79	B5	1100	G
79	B5	1101	G
79	B5	1111	G
79	B5	1113	A
79	B5	1126	OMG
79	B5	1138	A
79	B5	1150	G
79	B5	1158	C
79	B5	1166	A
79	B5	1185	U
79	B5	1194	A
79	B5	1196	A
79	B5	1199	G
79	B5	1200	G
79	B5	1201	G
79	B5	1202	A
79	B5	1203	A
79	B5	1207	C
79	B5	1214	U
79	B5	1217	A
79	B5	1218	G

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Mol	Chain	Res	Type
79	B5	1225	U
79	B5	1226	A
79	B5	1227	A
79	B5	1228	G
79	B5	1229	G
79	B5	1230	A
79	B5	1235	C
79	B5	1237	G
79	B5	1238	A
79	B5	1239	U
79	B5	1240	U
79	B5	1241	G
79	B5	1242	A
79	B5	1243	G
79	B5	1244	A
79	B5	1245	G
79	B5	1247	U
79	B5	1248	C
79	B5	1249	U
79	B5	1251	U
79	B5	1252	C
79	B5	1255	G
79	B5	1256	A
79	B5	1257	U
79	B5	1270	G
79	B5	1284	C
79	B5	1285	U
79	B5	1286	U
79	B5	1314	U
79	B5	1315	U
79	B5	1316	G
79	B5	1321	A
79	B5	1340	U
79	B5	1344	A
79	B5	1345	A
79	B5	1355	C
79	B5	1356	U
79	B5	1359	C
79	B5	1362	U
79	B5	1363	U
79	B5	1364	G
79	B5	1369	U

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Mol	Chain	Res	Type
79	B5	1371	A
79	B5	1372	U
79	B5	1373	C
79	B5	1378	U
79	B5	1382	A
79	B5	1390	U
79	B5	1399	C
79	B5	1400	A
79	B5	1413	U
79	B5	1415	U
79	B5	1418	G
79	B5	1425	A
79	B5	1427	A
79	B5	1428	OMG
79	B5	1432	U
79	B5	1435	G
79	B5	1436	A
79	B5	1445	G
79	B5	1446	A
79	B5	1447	C
79	B5	1458	G
79	B5	1459	C
79	B5	1461	C
79	B5	1471	A
79	B5	1477	G
79	B5	1486	G
79	B5	1491	U
79	B5	1492	A
79	B5	1493	A
79	B5	1496	U
79	B5	1503	A
79	B5	1506	G
79	B5	1514	U
79	B5	1516	A
79	B5	1520	U
79	B5	1521	G
79	B5	1523	G
79	B5	1524	A
79	B5	1537	C
79	B5	1542	G
79	B5	1557	U
79	B5	1559	A

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Mol	Chain	Res	Type
79	B5	1563	C
79	B5	1575	G7M
79	B5	1576	A
79	B5	1577	A
79	B5	1582	U
79	B5	1584	G
79	B5	1590	G
79	B5	1596	C
79	B5	1597	A
79	B5	1601	G
79	B5	1607	G
79	B5	1619	C
79	B5	1631	A
79	B5	1634	C
79	B5	1637	C
79	B5	1642	G
79	B5	1646	C
79	B5	1651	A
79	B5	1657	U
79	B5	1658	G
79	B5	1663	G
79	B5	1680	G
79	B5	1681	A
79	B5	1682	U
79	B5	1683	C
79	B5	1684	U
79	B5	1688	U
79	B5	1689	A
79	B5	1690	G
79	B5	1691	A
79	B5	1692	G
79	B5	1693	A
79	B5	1694	A
79	B5	1695	G
79	B5	1697	G
79	B5	1698	G
79	B5	1699	G
79	B5	1701	A
79	B5	1702	A
79	B5	1703	C
79	B5	1704	U
79	B5	1706	C

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Mol	Chain	Res	Type
79	B5	1708	U
79	B5	1709	C
79	B5	1710	U
79	B5	1711	C
79	B5	1713	G
79	B5	1714	A
79	B5	1716	C
79	B5	1717	G
79	B5	1730	A
79	B5	1750	A
79	B5	1766	A
79	B5	1767	G
79	B5	1768	G
79	B5	1769	U
79	B5	1780	G
79	B5	1782	MA6
79	B5	1792	G
79	B5	1793	G
79	B5	1794	A
79	B5	1795	U
79	B5	1796	C
79	B5	1799	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	267	G
1	A1	282	G
1	A1	588	G
1	A1	916	G
1	A1	1032	C
1	A1	1280	C
1	A1	1314	C
1	A1	1385	C
1	A1	1575	A
1	A1	2093	A
1	A1	2401	A
1	A1	2585	G
1	A1	3164	C
3	A4	67	U
3	A4	81	U
79	B5	187	G

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Mol	Chain	Res	Type
79	B5	224	C
79	B5	272	U
79	B5	488	G
79	B5	489	C
79	B5	819	G
79	B5	950	C
79	B5	1059	U
79	B5	1285	U
79	B5	1344	A
79	B5	1358	G
79	B5	1572	OMG
79	B5	1633	A
79	B5	1645	G

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

66 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	A1	2421	1	19,22,23	1.34	3 (15%)	25,31,34	1.87	4 (16%)
1	OMC	A1	2959	1	19,22,23	0.89	1 (5%)	25,31,34	0.99	1 (4%)
79	G7M	B5	1575	79	20,26,27	2.65	4 (20%)	16,39,42	1.14	1 (6%)
1	OMC	A1	2197	1	19,22,23	0.81	0	25,31,34	0.79	0
1	OMC	A1	2948	1	19,22,23	0.92	2 (10%)	25,31,34	1.01	2 (8%)
1	A2M	A1	876	1	18,25,26	0.90	0	20,36,39	1.19	2 (10%)
79	4AC	B5	1773	79	21,24,25	1.01	1 (4%)	28,34,37	1.38	6 (21%)
1	A2M	A1	817	81,1	18,25,26	0.86	0	20,36,39	1.72	3 (15%)
1	OMU	A1	898	1	19,22,23	1.42	4 (21%)	25,31,34	1.77	4 (16%)
79	OMC	B5	414	79	19,22,23	0.82	0	25,31,34	0.88	1 (4%)
1	A2M	A1	2220	1	18,25,26	0.81	0	20,36,39	1.53	3 (15%)
1	OMU	A1	2417	1	19,22,23	1.34	4 (21%)	25,31,34	1.77	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	A1	2946	81,1	18,25,26	0.90	0	20,36,39	1.46	3 (15%)
79	OMG	B5	1126	79	19,26,27	0.96	1 (5%)	21,38,41	1.05	2 (9%)
1	A2M	A1	649	1	18,25,26	0.77	0	20,36,39	1.36	2 (10%)
79	OMG	B5	1271	79	19,26,27	0.95	1 (5%)	21,38,41	1.04	2 (9%)
1	A2M	A1	1133	1	18,25,26	0.87	1 (5%)	20,36,39	1.48	4 (20%)
1	OMU	A1	2921	1	19,22,23	1.34	4 (21%)	25,31,34	1.87	5 (20%)
79	A2M	B5	28	81,79	18,25,26	0.88	0	20,36,39	1.26	2 (10%)
79	MA6	B5	1781	79	19,26,27	1.10	2 (10%)	18,38,41	2.11	3 (16%)
79	3AU	B5	1191	79	24,28,29	0.48	0	30,40,43	0.70	0
1	1MA	A1	2142	81,1	17,25,26	1.39	2 (11%)	17,37,40	1.32	3 (17%)
1	UR3	A1	2634	81,1	19,22,23	0.96	2 (10%)	26,32,35	1.92	4 (15%)
1	OMG	A1	2288	1	19,26,27	0.95	1 (5%)	21,38,41	1.08	2 (9%)
79	OMG	B5	562	79	19,26,27	0.93	1 (5%)	21,38,41	1.13	3 (14%)
1	5MC	A1	2870	81,1	19,22,23	1.07	3 (15%)	26,32,35	1.35	3 (11%)
79	OMG	B5	1428	81,79	19,26,27	0.89	1 (5%)	21,38,41	0.98	1 (4%)
1	OMC	A1	2337	1	19,22,23	0.94	2 (10%)	25,31,34	1.03	1 (4%)
1	A2M	A1	2281	1	18,25,26	0.79	0	20,36,39	2.10	4 (20%)
79	A2M	B5	974	79	18,25,26	0.83	0	20,36,39	1.22	2 (10%)
1	OMG	A1	867	81,1	19,26,27	0.92	1 (5%)	21,38,41	1.15	3 (14%)
1	OMG	A1	2619	1	19,26,27	0.87	1 (5%)	21,38,41	1.02	2 (9%)
79	OMU	B5	578	79	19,22,23	1.24	4 (21%)	25,31,34	1.85	6 (24%)
79	A2M	B5	100	81,79	18,25,26	0.85	0	20,36,39	1.21	2 (10%)
1	OMG	A1	2793	1	19,26,27	0.92	1 (5%)	21,38,41	1.13	2 (9%)
79	OMC	B5	1639	79	19,22,23	0.82	0	25,31,34	0.79	0
79	A2M	B5	420	79	18,25,26	0.82	0	20,36,39	1.43	4 (20%)
79	4AC	B5	1280	79	21,24,25	1.16	3 (14%)	28,34,37	1.71	3 (10%)
1	A2M	A1	1449	81,1	18,25,26	0.86	0	20,36,39	1.14	1 (5%)
79	A2M	B5	796	79	18,25,26	0.86	0	20,36,39	1.42	4 (20%)
1	1MA	A1	645	81,1	17,25,26	1.38	2 (11%)	17,37,40	1.24	3 (17%)
1	OMC	A1	663	1	19,22,23	0.90	2 (10%)	25,31,34	0.85	0
1	OMG	A1	2791	1	19,26,27	0.93	1 (5%)	21,38,41	1.17	2 (9%)
1	OMC	A1	650	1	19,22,23	0.87	2 (10%)	25,31,34	0.89	1 (4%)
1	5MC	A1	2278	81,1	19,22,23	1.31	3 (15%)	26,32,35	1.32	4 (15%)
79	OMC	B5	1007	79	19,22,23	0.83	1 (5%)	25,31,34	0.97	1 (4%)
79	OMU	B5	1269	81,79	19,22,23	1.40	4 (21%)	25,31,34	1.95	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	A1	2280	1	18,25,26	0.87	0	20,36,39	1.26	2 (10%)
1	OMU	A1	2729	1	19,22,23	1.40	3 (15%)	25,31,34	1.72	6 (24%)
1	A2M	A1	2640	1	18,25,26	0.83	0	20,36,39	1.09	2 (10%)
1	OMU	A1	2347	1	19,22,23	1.46	4 (21%)	25,31,34	1.92	7 (28%)
5	HIC	AB	243	5	8,11,12	1.44	1 (12%)	5,14,16	0.73	0
1	OMG	A1	805	1	19,26,27	0.96	1 (5%)	21,38,41	1.07	1 (4%)
1	OMG	A1	1450	1	19,26,27	0.96	1 (5%)	21,38,41	1.17	2 (9%)
1	OMG	A1	2815	1	19,26,27	0.96	1 (5%)	21,38,41	1.28	3 (14%)
1	A2M	A1	807	1	18,25,26	0.87	0	20,36,39	1.48	3 (15%)
1	OMU	A1	1888	1	19,22,23	1.41	4 (21%)	25,31,34	1.98	5 (20%)
1	OMG	A1	2922	1	19,26,27	0.91	1 (5%)	21,38,41	1.03	2 (9%)
1	OMG	A1	908	81,1	19,26,27	0.93	1 (5%)	21,38,41	1.41	3 (14%)
79	A2M	B5	436	79	18,25,26	0.80	0	20,36,39	1.28	3 (15%)
79	A2M	B5	541	79	18,25,26	0.80	0	20,36,39	1.32	3 (15%)
79	A2M	B5	619	81,79	18,25,26	0.85	0	20,36,39	1.48	3 (15%)
79	OMG	B5	1572	79	19,26,27	0.94	1 (5%)	21,38,41	1.08	2 (9%)
79	MA6	B5	1782	79	19,26,27	0.96	1 (5%)	18,38,41	2.04	3 (16%)
1	OMC	A1	1437	81,1	19,22,23	0.91	1 (5%)	25,31,34	1.49	5 (20%)
1	OMU	A1	2724	1	19,22,23	1.34	4 (21%)	25,31,34	1.85	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A1	2421	1	-	0/9/27/28	0/2/2/2
79	G7M	B5	1575	79	3/3/5/5	2/3/25/26	0/3/3/3
1	OMC	A1	2959	1	-	0/9/27/28	0/2/2/2
1	OMC	A1	2197	1	-	6/9/27/28	0/2/2/2
1	OMC	A1	2948	1	-	0/9/27/28	0/2/2/2
1	A2M	A1	876	1	-	0/5/27/28	0/3/3/3
79	4AC	B5	1773	79	-	2/11/29/30	0/2/2/2
1	A2M	A1	817	81,1	-	2/5/27/28	0/3/3/3
1	OMU	A1	898	1	-	0/9/27/28	0/2/2/2
79	OMC	B5	414	79	-	0/9/27/28	0/2/2/2
1	A2M	A1	2220	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A1	2417	1	-	2/9/27/28	0/2/2/2
1	A2M	A1	2946	81,1	-	0/5/27/28	0/3/3/3
79	OMG	B5	1126	79	-	2/5/27/28	0/3/3/3
1	A2M	A1	649	1	-	1/5/27/28	0/3/3/3
79	OMG	B5	1271	79	-	1/5/27/28	0/3/3/3
1	A2M	A1	1133	1	-	0/5/27/28	0/3/3/3
1	OMU	A1	2921	1	-	0/9/27/28	0/2/2/2
79	A2M	B5	28	81,79	-	0/5/27/28	0/3/3/3
79	MA6	B5	1781	79	-	1/7/29/30	0/3/3/3
79	3AU	B5	1191	79	1/1/7/7	3/16/34/35	0/2/2/2
1	1MA	A1	2142	81,1	-	2/3/25/26	0/3/3/3
1	UR3	A1	2634	81,1	-	0/7/25/26	0/2/2/2
1	OMG	A1	2288	1	-	2/5/27/28	0/3/3/3
79	OMG	B5	562	79	-	0/5/27/28	0/3/3/3
1	5MC	A1	2870	81,1	-	6/7/25/26	0/2/2/2
79	OMG	B5	1428	81,79	-	3/5/27/28	0/3/3/3
1	OMC	A1	2337	1	-	1/9/27/28	0/2/2/2
1	A2M	A1	2281	1	-	2/5/27/28	0/3/3/3
79	A2M	B5	974	79	-	0/5/27/28	0/3/3/3
1	OMG	A1	867	81,1	-	0/5/27/28	0/3/3/3
1	OMG	A1	2619	1	-	1/5/27/28	0/3/3/3
79	OMU	B5	578	79	-	0/9/27/28	0/2/2/2
79	A2M	B5	100	81,79	-	1/5/27/28	0/3/3/3
1	OMG	A1	2793	1	-	0/5/27/28	0/3/3/3
79	OMC	B5	1639	79	-	0/9/27/28	0/2/2/2
79	A2M	B5	420	79	-	0/5/27/28	0/3/3/3
79	4AC	B5	1280	79	-	4/11/29/30	0/2/2/2
1	A2M	A1	1449	81,1	-	0/5/27/28	0/3/3/3
79	A2M	B5	796	79	-	0/5/27/28	0/3/3/3
1	1MA	A1	645	81,1	-	0/3/25/26	0/3/3/3
1	OMC	A1	663	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	2791	1	-	0/5/27/28	0/3/3/3
1	OMC	A1	650	1	-	0/9/27/28	0/2/2/2
1	5MC	A1	2278	81,1	-	0/7/25/26	0/2/2/2
79	OMC	B5	1007	79	-	0/9/27/28	0/2/2/2
79	OMU	B5	1269	81,79	-	2/9/27/28	0/2/2/2
1	A2M	A1	2280	1	-	0/5/27/28	0/3/3/3
1	OMU	A1	2729	1	-	2/9/27/28	0/2/2/2
1	A2M	A1	2640	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A1	2347	1	-	2/9/27/28	0/2/2/2
5	HIC	AB	243	5	-	2/5/6/8	0/1/1/1
1	OMG	A1	805	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	1450	1	-	2/5/27/28	0/3/3/3
1	OMG	A1	2815	1	-	0/5/27/28	0/3/3/3
1	A2M	A1	807	1	-	1/5/27/28	0/3/3/3
1	OMU	A1	1888	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	2922	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	908	81,1	-	3/5/27/28	0/3/3/3
79	A2M	B5	436	79	-	0/5/27/28	0/3/3/3
79	A2M	B5	541	79	-	2/5/27/28	0/3/3/3
79	A2M	B5	619	81,79	-	2/5/27/28	0/3/3/3
79	OMG	B5	1572	79	-	0/5/27/28	0/3/3/3
79	MA6	B5	1782	79	-	4/7/29/30	0/3/3/3
1	OMC	A1	1437	81,1	-	2/9/27/28	0/2/2/2
1	OMU	A1	2724	1	-	0/9/27/28	0/2/2/2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	B5	1575	G7M	C8-N9	8.06	1.47	1.33
79	B5	1575	G7M	C8-N7	6.44	1.44	1.33
79	B5	1575	G7M	C5-C4	4.28	1.47	1.39
1	A1	2142	1MA	C2-N3	4.13	1.33	1.28
1	A1	2278	5MC	C5-C4	3.98	1.47	1.44
1	A1	645	1MA	C2-N3	3.67	1.33	1.28
5	AB	243	HIC	CD2-NE2	-3.63	1.32	1.38
1	A1	898	OMU	C4-N3	-3.45	1.32	1.38
1	A1	2347	OMU	C4-N3	-3.42	1.32	1.38
79	B5	1269	OMU	C4-N3	-3.31	1.32	1.38
1	A1	1888	OMU	C4-N3	-3.27	1.33	1.38
1	A1	2921	OMU	C4-N3	-3.26	1.33	1.38
1	A1	2729	OMU	C4-N3	-3.25	1.33	1.38
1	A1	2421	OMU	C4-N3	-3.19	1.33	1.38
79	B5	1781	MA6	C6-C5	3.18	1.49	1.44
1	A1	2815	OMG	C6-N1	-3.16	1.33	1.37
1	A1	2417	OMU	C4-N3	-3.13	1.33	1.38
1	A1	805	OMG	C6-N1	-3.10	1.33	1.37
1	A1	2347	OMU	C2-N3	-3.06	1.32	1.38
1	A1	2724	OMU	C4-N3	-3.03	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	B5	1126	OMG	C6-N1	-3.02	1.33	1.37
79	B5	1280	4AC	C4-N4	-3.02	1.35	1.39
1	A1	2729	OMU	C5-C4	-2.99	1.37	1.43
1	A1	2288	OMG	C6-N1	-2.96	1.33	1.37
1	A1	2791	OMG	C6-N1	-2.93	1.33	1.37
1	A1	2870	5MC	C5-C4	2.89	1.46	1.44
1	A1	2278	5MC	C6-N1	-2.88	1.33	1.38
79	B5	1271	OMG	C6-N1	-2.87	1.33	1.37
79	B5	562	OMG	C6-N1	-2.85	1.33	1.37
1	A1	2724	OMU	C2-N3	-2.83	1.33	1.38
1	A1	898	OMU	C5-C4	-2.83	1.37	1.43
1	A1	867	OMG	C6-N1	-2.82	1.33	1.37
1	A1	2793	OMG	C6-N1	-2.81	1.33	1.37
1	A1	2921	OMU	C2-N3	-2.81	1.33	1.38
1	A1	898	OMU	C2-N3	-2.78	1.33	1.38
1	A1	2421	OMU	C2-N3	-2.76	1.33	1.38
1	A1	2922	OMG	C6-N1	-2.76	1.33	1.37
79	B5	1572	OMG	C6-N1	-2.76	1.33	1.37
79	B5	1269	OMU	C2-N3	-2.75	1.33	1.38
1	A1	2724	OMU	C5-C4	-2.75	1.37	1.43
1	A1	1450	OMG	C6-N1	-2.75	1.33	1.37
79	B5	1575	G7M	C6-N1	-2.72	1.33	1.37
1	A1	2417	OMU	C2-N3	-2.71	1.33	1.38
1	A1	2347	OMU	C5-C4	-2.71	1.37	1.43
79	B5	578	OMU	C4-N3	-2.70	1.34	1.38
1	A1	645	1MA	C6-N6	2.67	1.34	1.27
1	A1	2729	OMU	C2-N3	-2.67	1.33	1.38
1	A1	1888	OMU	C2-N3	-2.66	1.33	1.38
1	A1	1888	OMU	C5-C4	-2.64	1.38	1.43
79	B5	1773	4AC	C4-N4	-2.61	1.36	1.39
1	A1	2948	OMC	C5-C4	-2.58	1.36	1.42
1	A1	2421	OMU	C5-C4	-2.57	1.38	1.43
79	B5	1428	OMG	C6-N1	-2.55	1.33	1.37
1	A1	1437	OMC	C5-C4	-2.54	1.37	1.42
1	A1	908	OMG	C6-N1	-2.50	1.34	1.37
1	A1	2417	OMU	C5-C4	-2.49	1.38	1.43
79	B5	1782	MA6	C6-C5	2.44	1.48	1.44
1	A1	2619	OMG	C6-N1	-2.43	1.34	1.37
1	A1	2959	OMC	C5-C4	-2.41	1.37	1.42
1	A1	663	OMC	C5-C4	-2.41	1.37	1.42
1	A1	650	OMC	C5-C4	-2.41	1.37	1.42
1	A1	2870	5MC	C6-C5	2.39	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	B5	578	OMU	C2-N3	-2.39	1.33	1.38
1	A1	2142	1MA	C6-N6	2.35	1.33	1.27
1	A1	2337	OMC	C5-C4	-2.34	1.37	1.42
1	A1	2921	OMU	C5-C4	-2.31	1.38	1.43
1	A1	2948	OMC	C6-N1	-2.28	1.32	1.38
79	B5	1269	OMU	C2-N1	2.27	1.42	1.38
79	B5	578	OMU	C5-C4	-2.26	1.38	1.43
79	B5	1280	4AC	C7-N4	-2.24	1.32	1.37
1	A1	1888	OMU	C6-N1	-2.24	1.32	1.38
1	A1	2634	UR3	C5-C4	-2.19	1.38	1.43
1	A1	2634	UR3	C6-N1	-2.19	1.32	1.38
79	B5	1280	4AC	C6-N1	-2.17	1.32	1.38
79	B5	1269	OMU	C5-C4	-2.16	1.39	1.43
1	A1	898	OMU	C6-N1	-2.15	1.33	1.38
1	A1	2278	5MC	C6-C5	2.13	1.38	1.34
79	B5	1781	MA6	C6-N1	2.12	1.35	1.32
1	A1	2870	5MC	C6-N1	-2.11	1.34	1.38
79	B5	1007	OMC	C5-C4	-2.09	1.38	1.42
1	A1	2347	OMU	C6-N1	-2.09	1.33	1.38
1	A1	663	OMC	C6-N1	-2.07	1.33	1.38
1	A1	1133	A2M	O4'-C1'	2.07	1.43	1.40
1	A1	2417	OMU	C6-N1	-2.05	1.33	1.38
1	A1	650	OMC	C6-N1	-2.04	1.33	1.38
1	A1	2337	OMC	C6-N1	-2.04	1.33	1.38
1	A1	2921	OMU	C6-N1	-2.03	1.33	1.38
1	A1	2724	OMU	C6-N1	-2.02	1.33	1.38
79	B5	578	OMU	C6-N1	-2.02	1.33	1.38

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	2634	UR3	C4-N3-C2	-7.58	118.48	124.58
79	B5	1280	4AC	N4-C4-N3	6.49	124.41	113.87
79	B5	1781	MA6	C2-N1-C6	6.26	122.98	116.84
79	B5	1782	MA6	C2-N1-C6	5.98	122.70	116.84
1	A1	2281	A2M	O4'-C1'-N9	5.66	116.25	108.75
1	A1	1888	OMU	C4-N3-C2	-5.01	120.39	126.61
1	A1	2220	A2M	N3-C2-N1	-4.87	122.06	128.67
79	B5	578	OMU	C4-N3-C2	-4.84	120.60	126.61
1	A1	2921	OMU	C4-N3-C2	-4.81	120.65	126.61
1	A1	2724	OMU	C4-N3-C2	-4.69	120.79	126.61
1	A1	2921	OMU	N3-C2-N1	4.69	120.99	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	2421	OMU	C4-N3-C2	-4.67	120.82	126.61
1	A1	817	A2M	O4'-C1'-N9	-4.56	102.70	108.75
1	A1	2417	OMU	C4-N3-C2	-4.52	121.01	126.61
1	A1	898	OMU	C4-N3-C2	-4.42	121.12	126.61
79	B5	1269	OMU	C4-N3-C2	-4.37	121.19	126.61
1	A1	2421	OMU	N3-C2-N1	4.35	120.55	114.89
1	A1	2347	OMU	C4-N3-C2	-4.34	121.22	126.61
1	A1	2724	OMU	C5-C4-N3	4.31	120.83	114.80
1	A1	1888	OMU	N3-C2-N1	4.28	120.47	114.89
1	A1	2347	OMU	N3-C2-N1	4.27	120.44	114.89
1	A1	649	A2M	N3-C2-N1	-4.25	122.91	128.67
79	B5	1269	OMU	N3-C2-N1	4.22	120.39	114.89
1	A1	1888	OMU	C5-C4-N3	4.18	120.66	114.80
1	A1	1437	OMC	O2-C2-N3	-4.15	115.79	122.33
1	A1	2946	A2M	N3-C2-N1	-4.14	123.05	128.67
1	A1	898	OMU	N3-C2-N1	4.10	120.22	114.89
1	A1	2421	OMU	C5-C4-N3	4.06	120.48	114.80
79	B5	1781	MA6	N3-C2-N1	-4.04	123.18	128.67
1	A1	2417	OMU	C5-C4-N3	4.02	120.44	114.80
1	A1	2417	OMU	N3-C2-N1	3.95	120.03	114.89
79	B5	578	OMU	C5-C4-N3	3.94	120.32	114.80
1	A1	2724	OMU	N3-C2-N1	3.93	120.01	114.89
1	A1	817	A2M	N3-C2-N1	-3.93	123.34	128.67
1	A1	2347	OMU	C5-C4-N3	3.92	120.29	114.80
1	A1	898	OMU	C5-C4-N3	3.90	120.27	114.80
79	B5	578	OMU	N3-C2-N1	3.90	119.97	114.89
79	B5	28	A2M	N3-C2-N1	-3.88	123.40	128.67
1	A1	2281	A2M	C4'-O4'-C1'	-3.88	106.37	109.92
1	A1	2921	OMU	C5-C4-N3	3.86	120.21	114.80
1	A1	1133	A2M	N3-C2-N1	-3.84	123.46	128.67
79	B5	1280	4AC	C5-C4-N4	-3.84	116.48	122.94
79	B5	541	A2M	N3-C2-N1	-3.84	123.47	128.67
79	B5	974	A2M	N3-C2-N1	-3.82	123.48	128.67
79	B5	420	A2M	N3-C2-N1	-3.82	123.49	128.67
79	B5	1781	MA6	C4-C5-N7	-3.80	105.33	109.34
79	B5	1782	MA6	N3-C2-N1	-3.79	123.53	128.67
79	B5	1269	OMU	C5-C4-N3	3.78	120.10	114.80
1	A1	2280	A2M	N3-C2-N1	-3.78	123.55	128.67
1	A1	2281	A2M	N3-C2-N1	-3.74	123.59	128.67
1	A1	2347	OMU	C1'-N1-C2	3.71	124.26	117.59
1	A1	2729	OMU	C4-N3-C2	-3.71	122.01	126.61
1	A1	876	A2M	N3-C2-N1	-3.66	123.70	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	2729	OMU	N3-C2-N1	3.65	119.65	114.89
79	B5	796	A2M	N3-C2-N1	-3.62	123.76	128.67
1	A1	2729	OMU	C5-C4-N3	3.62	119.86	114.80
79	B5	100	A2M	N3-C2-N1	-3.59	123.80	128.67
1	A1	807	A2M	O4'-C1'-N9	3.54	113.44	108.75
1	A1	1449	A2M	N3-C2-N1	-3.54	123.87	128.67
79	B5	1269	OMU	C1'-N1-C2	3.50	123.89	117.59
1	A1	2634	UR3	C5-C4-N3	3.48	119.63	115.04
1	A1	2640	A2M	N3-C2-N1	-3.41	124.04	128.67
1	A1	2421	OMU	O4-C4-C5	-3.38	119.33	125.16
79	B5	436	A2M	N3-C2-N1	-3.38	124.08	128.67
1	A1	2870	5MC	O2-C2-N3	-3.37	117.01	122.33
1	A1	2724	OMU	O4-C4-C5	-3.36	119.36	125.16
79	B5	1782	MA6	C4-C5-N7	-3.31	105.84	109.34
79	B5	578	OMU	O4-C4-C5	-3.27	119.52	125.16
79	B5	1773	4AC	O2-C2-N3	-3.27	117.17	122.33
1	A1	2278	5MC	O2-C2-N3	-3.24	117.22	122.33
1	A1	1437	OMC	C1'-N1-C2	3.24	125.59	118.44
1	A1	2870	5MC	C5-C6-N1	-3.21	119.83	123.31
1	A1	2278	5MC	C5-C4-N3	-3.20	118.48	121.75
1	A1	898	OMU	O4-C4-C5	-3.16	119.72	125.16
1	A1	1888	OMU	O4-C4-C5	-3.15	119.73	125.16
1	A1	2417	OMU	O4-C4-C5	-3.13	119.76	125.16
1	A1	2791	OMG	C8-N7-C5	3.11	107.84	102.55
1	A1	2729	OMU	O4-C4-C5	-3.09	119.83	125.16
1	A1	2142	1MA	C5-C6-N1	3.07	118.37	113.95
1	A1	908	OMG	O2'-C2'-C1'	3.07	114.95	109.00
1	A1	807	A2M	N3-C2-N1	-3.07	124.51	128.67
79	B5	619	A2M	N3-C2-N1	-3.05	124.53	128.67
1	A1	908	OMG	CM2-O2'-C2'	2.98	122.14	114.47
1	A1	2815	OMG	CM2-O2'-C2'	-2.98	106.83	114.47
1	A1	2870	5MC	C5-C4-N3	-2.95	118.73	121.75
79	B5	1271	OMG	C8-N7-C5	2.94	107.56	102.55
1	A1	2347	OMU	O4-C4-C5	-2.91	120.15	125.16
1	A1	2337	OMC	O2-C2-N3	-2.87	117.81	122.33
1	A1	2815	OMG	C8-N7-C5	2.86	107.41	102.55
79	B5	562	OMG	C8-N7-C5	2.85	107.40	102.55
1	A1	2793	OMG	C8-N7-C5	2.85	107.40	102.55
79	B5	1575	G7M	CN7-N7-C8	-2.83	111.82	125.43
1	A1	2948	OMC	O2-C2-N3	-2.83	117.87	122.33
1	A1	2921	OMU	O4-C4-C5	-2.82	120.30	125.16
1	A1	867	OMG	C8-N7-C5	2.81	107.33	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1437	OMC	O2-C2-N1	2.80	124.39	118.90
79	B5	1007	OMC	O2-C2-N3	-2.77	117.97	122.33
79	B5	1126	OMG	C8-N7-C5	2.75	107.23	102.55
1	A1	807	A2M	C4-C5-N7	-2.74	106.45	109.34
1	A1	2619	OMG	C8-N7-C5	2.73	107.19	102.55
79	B5	619	A2M	C4-C5-N7	-2.72	106.46	109.34
1	A1	2280	A2M	C4-C5-N7	-2.69	106.49	109.34
79	B5	619	A2M	O4'-C1'-N9	-2.69	105.18	108.75
1	A1	2288	OMG	C8-N7-C5	2.66	107.08	102.55
79	B5	1269	OMU	O2-C2-N3	-2.66	116.59	121.49
79	B5	28	A2M	C4-C5-N7	-2.65	106.54	109.34
1	A1	2922	OMG	C8-N7-C5	2.64	107.05	102.55
79	B5	1269	OMU	O4-C4-C5	-2.64	120.62	125.16
79	B5	1773	4AC	O7-C7-N4	2.64	126.05	121.90
1	A1	2959	OMC	O2-C2-N3	-2.61	118.22	122.33
1	A1	1450	OMG	C8-N7-C5	2.60	106.97	102.55
1	A1	645	1MA	C8-N7-C5	2.57	106.93	102.55
1	A1	645	1MA	N1-C2-N3	-2.55	122.70	125.90
79	B5	1773	4AC	C6-C5-C4	2.53	120.05	117.00
1	A1	2729	OMU	C1'-N1-C2	2.53	122.14	117.59
1	A1	805	OMG	C8-N7-C5	2.53	106.85	102.55
1	A1	908	OMG	C8-N7-C5	2.52	106.85	102.55
79	B5	420	A2M	C4-C5-N7	-2.52	106.68	109.34
79	B5	1428	OMG	C8-N7-C5	2.50	106.81	102.55
79	B5	796	A2M	C4-C5-N7	-2.50	106.69	109.34
79	B5	100	A2M	C4-C5-N7	-2.50	106.69	109.34
1	A1	2142	1MA	C8-N7-C5	2.50	106.80	102.55
1	A1	2281	A2M	C2'-C1'-N9	-2.49	107.03	112.56
79	B5	796	A2M	O4'-C1'-N9	2.48	112.04	108.75
79	B5	436	A2M	C4-C5-N7	-2.48	106.71	109.34
79	B5	1773	4AC	C5-C4-N3	-2.47	118.73	122.60
1	A1	2724	OMU	O2-C2-N1	-2.47	119.59	122.80
1	A1	1437	OMC	CM2-O2'-C2'	2.44	120.73	114.47
1	A1	2921	OMU	O2-C2-N1	-2.44	119.62	122.80
79	B5	541	A2M	C4-C5-N7	-2.42	106.78	109.34
1	A1	2347	OMU	O2-C2-N3	-2.40	117.07	121.49
1	A1	876	A2M	C4-C5-N7	-2.37	106.83	109.34
1	A1	645	1MA	C5-C6-N1	2.36	117.35	113.95
79	B5	1572	OMG	C8-N7-C5	2.36	106.57	102.55
1	A1	2729	OMU	C6-N1-C2	-2.35	118.13	121.00
79	B5	796	A2M	C2'-C1'-N9	-2.35	107.34	112.56
1	A1	867	OMG	C5-C6-N1	2.35	118.55	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	2640	A2M	C4-C5-N7	-2.34	106.87	109.34
1	A1	649	A2M	C4-C5-N7	-2.33	106.87	109.34
1	A1	2142	1MA	N1-C2-N3	-2.32	123.00	125.90
1	A1	2815	OMG	C5-C6-N1	2.30	118.47	114.07
79	B5	436	A2M	C4'-O4'-C1'	2.29	112.02	109.92
79	B5	1773	4AC	N4-C4-N3	2.29	117.58	113.87
1	A1	1133	A2M	O4'-C1'-N9	2.29	111.78	108.75
79	B5	974	A2M	C4-C5-N7	-2.28	106.92	109.34
79	B5	1271	OMG	C5-C6-N1	2.28	118.42	114.07
79	B5	414	OMC	O2-C2-N3	-2.28	118.74	122.33
79	B5	578	OMU	O2-C2-N1	-2.27	119.84	122.80
1	A1	2288	OMG	C5-C6-N1	2.25	118.36	114.07
1	A1	1450	OMG	C5-C6-N1	2.25	118.36	114.07
79	B5	1280	4AC	C5-C4-N3	-2.24	119.09	122.60
1	A1	2634	UR3	C1'-N1-C2	2.23	120.68	117.04
1	A1	2347	OMU	C6-N1-C2	-2.22	118.29	121.00
79	B5	541	A2M	C4'-O4'-C1'	-2.21	107.90	109.92
1	A1	2791	OMG	C5-C6-N1	2.20	118.27	114.07
1	A1	2946	A2M	O4'-C4'-C3'	-2.20	100.78	105.15
1	A1	1133	A2M	C4-C5-N7	-2.20	107.01	109.34
1	A1	2946	A2M	C4-C5-N7	-2.20	107.02	109.34
1	A1	1133	A2M	C2'-C1'-N9	-2.19	107.70	112.56
1	A1	2634	UR3	C3U-N3-C4	2.18	120.89	117.87
1	A1	2948	OMC	C1'-N1-C2	2.15	123.19	118.44
1	A1	2417	OMU	C1'-N1-C2	2.15	121.45	117.59
1	A1	2220	A2M	C2'-C1'-N9	-2.13	107.82	112.56
1	A1	2922	OMG	C5-C6-N1	2.13	118.14	114.07
1	A1	2278	5MC	C1'-N1-C6	-2.13	117.65	121.15
79	B5	1572	OMG	C5-C6-N1	2.13	118.12	114.07
1	A1	2278	5MC	C5-C6-N1	-2.12	121.01	123.31
1	A1	650	OMC	CM2-O2'-C2'	-2.12	109.02	114.47
79	B5	562	OMG	C5-C6-N1	2.10	118.08	114.07
1	A1	867	OMG	O6-C6-C5	-2.08	120.19	124.32
79	B5	420	A2M	O4'-C1'-N9	2.08	111.50	108.75
1	A1	817	A2M	O3'-C3'-C4'	-2.08	105.12	111.08
79	B5	578	OMU	C1'-N1-C2	2.07	121.32	117.59
1	A1	2619	OMG	C5-C6-N1	2.06	118.00	114.07
1	A1	1888	OMU	C2'-C1'-N1	-2.02	110.41	114.24
79	B5	1773	4AC	O2-C2-N1	2.02	122.85	118.90
1	A1	1437	OMC	C6-N1-C2	-2.01	117.06	120.46
79	B5	420	A2M	C2'-C1'-N9	-2.01	108.09	112.56
1	A1	2220	A2M	C4-C5-N7	-2.01	107.21	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	B5	562	OMG	CM2-O2'-C2'	-2.01	109.31	114.47
79	B5	1126	OMG	C5-C6-N1	2.01	117.90	114.07
1	A1	2793	OMG	C5-C6-N1	2.01	117.89	114.07

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	B5	1191	3AU	C12
79	B5	1575	G7M	C4'
79	B5	1575	G7M	C3'
79	B5	1575	G7M	C2'

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AB	243	HIC	CA-CB-CG-ND1
5	AB	243	HIC	CA-CB-CG-CD2
1	A1	908	OMG	C1'-C2'-O2'-CM2
1	A1	1437	OMC	C1'-C2'-O2'-CM2
1	A1	1450	OMG	O4'-C4'-C5'-O5'
1	A1	2197	OMC	C2'-C1'-N1-C6
1	A1	2197	OMC	O4'-C4'-C5'-O5'
1	A1	2288	OMG	O4'-C4'-C5'-O5'
1	A1	2417	OMU	C1'-C2'-O2'-CM2
1	A1	2619	OMG	C1'-C2'-O2'-CM2
1	A1	2870	5MC	C2'-C1'-N1-C2
1	A1	2870	5MC	C2'-C1'-N1-C6
79	B5	619	A2M	C3'-C4'-C5'-O5'
79	B5	1280	4AC	N3-C4-N4-C7
79	B5	1280	4AC	C5-C4-N4-C7
79	B5	1280	4AC	O7-C7-N4-C4
79	B5	1280	4AC	CM7-C7-N4-C4
79	B5	1773	4AC	N3-C4-N4-C7
79	B5	1781	MA6	C5-C6-N6-C10
79	B5	1782	MA6	O4'-C4'-C5'-O5'
79	B5	1782	MA6	C5-C6-N6-C9
1	A1	2197	OMC	C2'-C1'-N1-C2
1	A1	908	OMG	O4'-C4'-C5'-O5'
1	A1	2197	OMC	C3'-C4'-C5'-O5'
1	A1	2288	OMG	C3'-C4'-C5'-O5'
1	A1	2729	OMU	C3'-C4'-C5'-O5'
1	A1	2729	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
79	B5	1575	G7M	C3'-C4'-C5'-O5'
79	B5	1269	OMU	O4'-C1'-N1-C2
1	A1	2142	1MA	O4'-C4'-C5'-O5'
1	A1	2142	1MA	C3'-C4'-C5'-O5'
79	B5	541	A2M	O4'-C4'-C5'-O5'
79	B5	619	A2M	O4'-C4'-C5'-O5'
79	B5	1782	MA6	N1-C6-N6-C9
1	A1	1450	OMG	C3'-C4'-C5'-O5'
79	B5	1782	MA6	C3'-C4'-C5'-O5'
1	A1	2347	OMU	C3'-C4'-C5'-O5'
79	B5	541	A2M	C3'-C4'-C5'-O5'
79	B5	1428	OMG	O4'-C4'-C5'-O5'
79	B5	1191	3AU	N40-C12-C13-O31
1	A1	908	OMG	C3'-C4'-C5'-O5'
79	B5	1575	G7M	O4'-C4'-C5'-O5'
1	A1	2870	5MC	O4'-C4'-C5'-O5'
1	A1	2870	5MC	C3'-C4'-C5'-O5'
79	B5	1269	OMU	O4'-C1'-N1-C6
1	A1	2347	OMU	O4'-C4'-C5'-O5'
79	B5	1271	OMG	C1'-C2'-O2'-CM2
1	A1	2870	5MC	O4'-C1'-N1-C6
79	B5	1773	4AC	C5-C4-N4-C7
79	B5	1428	OMG	C3'-C4'-C5'-O5'
79	B5	1191	3AU	N3-C10-C11-C12
1	A1	817	A2M	C4'-C5'-O5'-P
1	A1	2281	A2M	C3'-C2'-O2'-CM'
1	A1	2870	5MC	O4'-C1'-N1-C2
79	B5	100	A2M	O4'-C4'-C5'-O5'
79	B5	1126	OMG	C4'-C5'-O5'-P
1	A1	2197	OMC	O4'-C1'-N1-C6
1	A1	2417	OMU	O4'-C4'-C5'-O5'
1	A1	2197	OMC	O4'-C1'-N1-C2
1	A1	649	A2M	C4'-C5'-O5'-P
79	B5	1428	OMG	C4'-C5'-O5'-P
1	A1	807	A2M	C3'-C2'-O2'-CM'
1	A1	817	A2M	O4'-C4'-C5'-O5'
1	A1	2337	OMC	O4'-C4'-C5'-O5'
79	B5	1126	OMG	C3'-C4'-C5'-O5'
1	A1	2281	A2M	O4'-C4'-C5'-O5'
1	A1	1437	OMC	C2'-C1'-N1-C2
79	B5	1191	3AU	N40-C12-C13-O30

There are no ring outliers.



15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	2948	OMC	1	0
1	A1	2220	A2M	2	0
79	B5	1126	OMG	2	0
1	A1	649	A2M	1	0
1	A1	1133	A2M	1	0
79	B5	1781	MA6	1	0
1	A1	2619	OMG	1	0
79	B5	1280	4AC	4	0
1	A1	1449	A2M	1	0
79	B5	796	A2M	1	0
1	A1	663	OMC	1	0
5	AB	243	HIC	1	0
1	A1	2815	OMG	1	0
1	A1	908	OMG	2	0
79	B5	436	A2M	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 377 ligands modelled in this entry, 376 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
80	3HE	A1	3401	-	21,21,21	0.43	0	23,30,30	0.76	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
80	3HE	A1	3401	-	-	0/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A1	6
79	B5	2
18	AP	1
53	BI	1
8	AE	1
12	AI	1
62	BR	1
76	Bf	1
3	A4	1
66	BV	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1253:U	O3'	1260:A	P	26.34
1	AP	155:GLU	C	164:LYS	N	24.32
1	BI	123:LYS	C	135:LYS	N	18.64
1	A1	1955:U	O3'	2093:A	P	18.09
1	B5	658:C	O3'	676:G	P	17.61
1	A1	1023:C	O3'	1030:A	P	17.20
1	AE	109:GLU	C	129:GLU	N	14.45

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	2445:A	O3'	2501:U	P	13.63
1	AI	101:LYS	C	114:GLY	N	10.06
1	A1	451:U	O3'	486:A	P	9.84
1	BR	95:ARG	C	100:LEU	N	6.89
1	Bf	125:THR	C	129:GLY	N	6.42
1	A4	73:U	O3'	74:U	P	5.20
1	BV	11:LEU	C	12:TYR	N	5.14
1	A1	444:U	O3'	445:G	P	3.94
1	B5	1798:U	O3'	1799:U	P	3.20

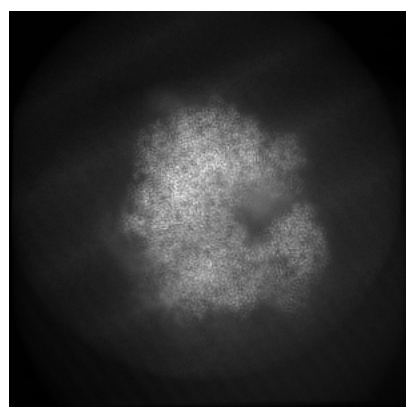
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24235. These allow visual inspection of the internal detail of the map and identification of artifacts.

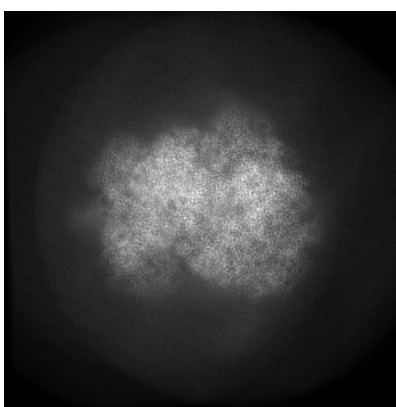
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

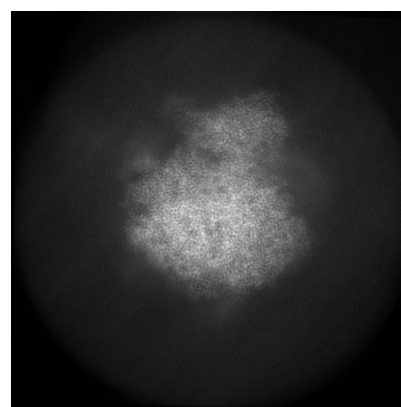
#### 6.1.1 Primary map



X



Y

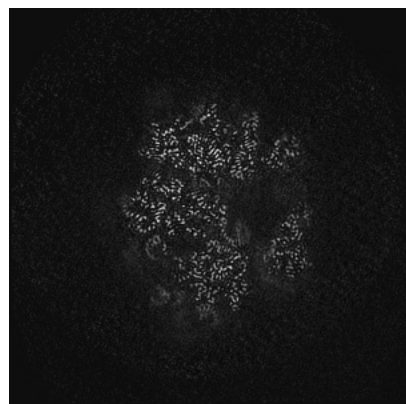


Z

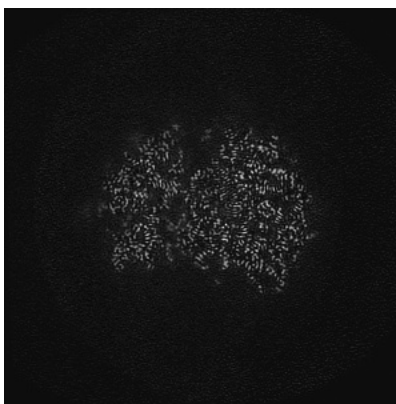
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

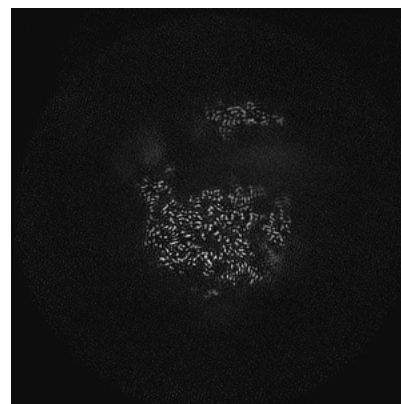
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

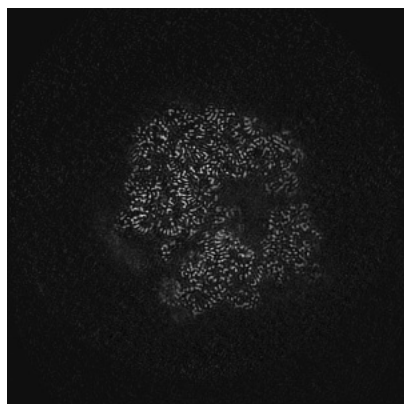


Z Index: 216

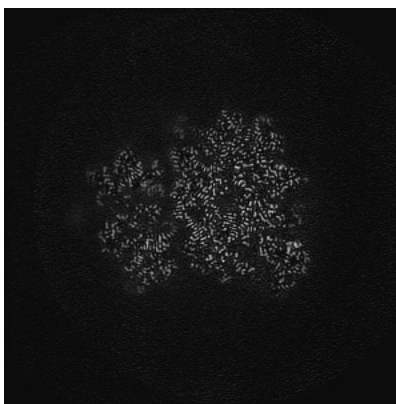
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

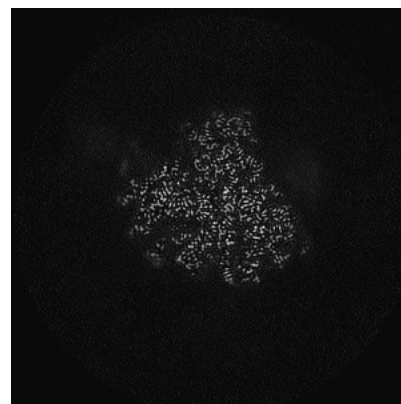
### 6.3.1 Primary map



X Index: 240



Y Index: 199

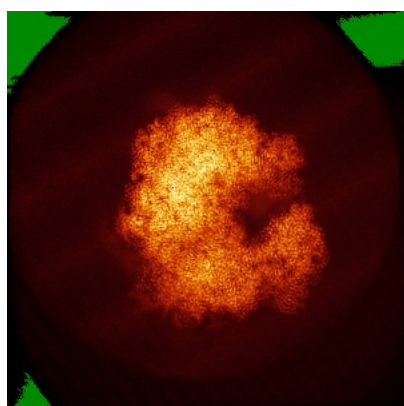


Z Index: 265

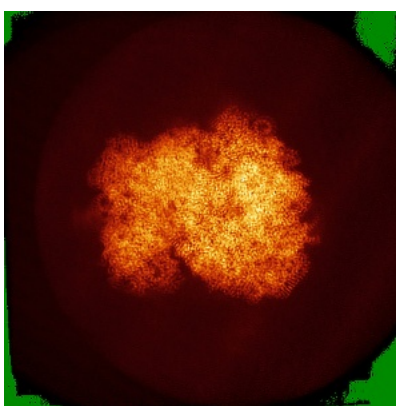
The images above show the largest variance slices of the map in three orthogonal directions.

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

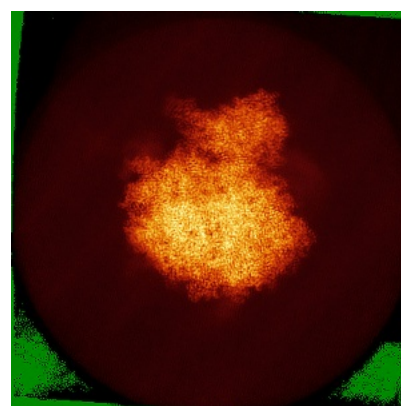
### 6.4.1 Primary map



X



Y

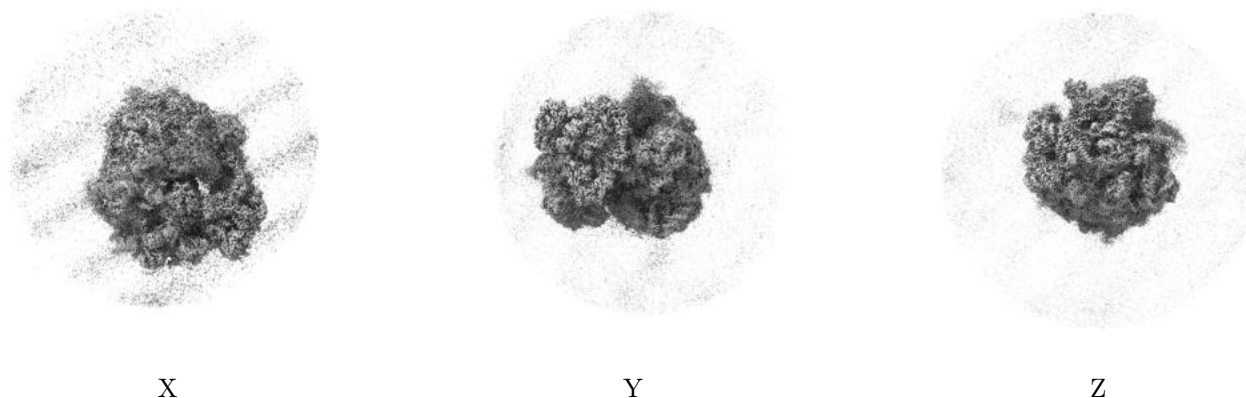


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

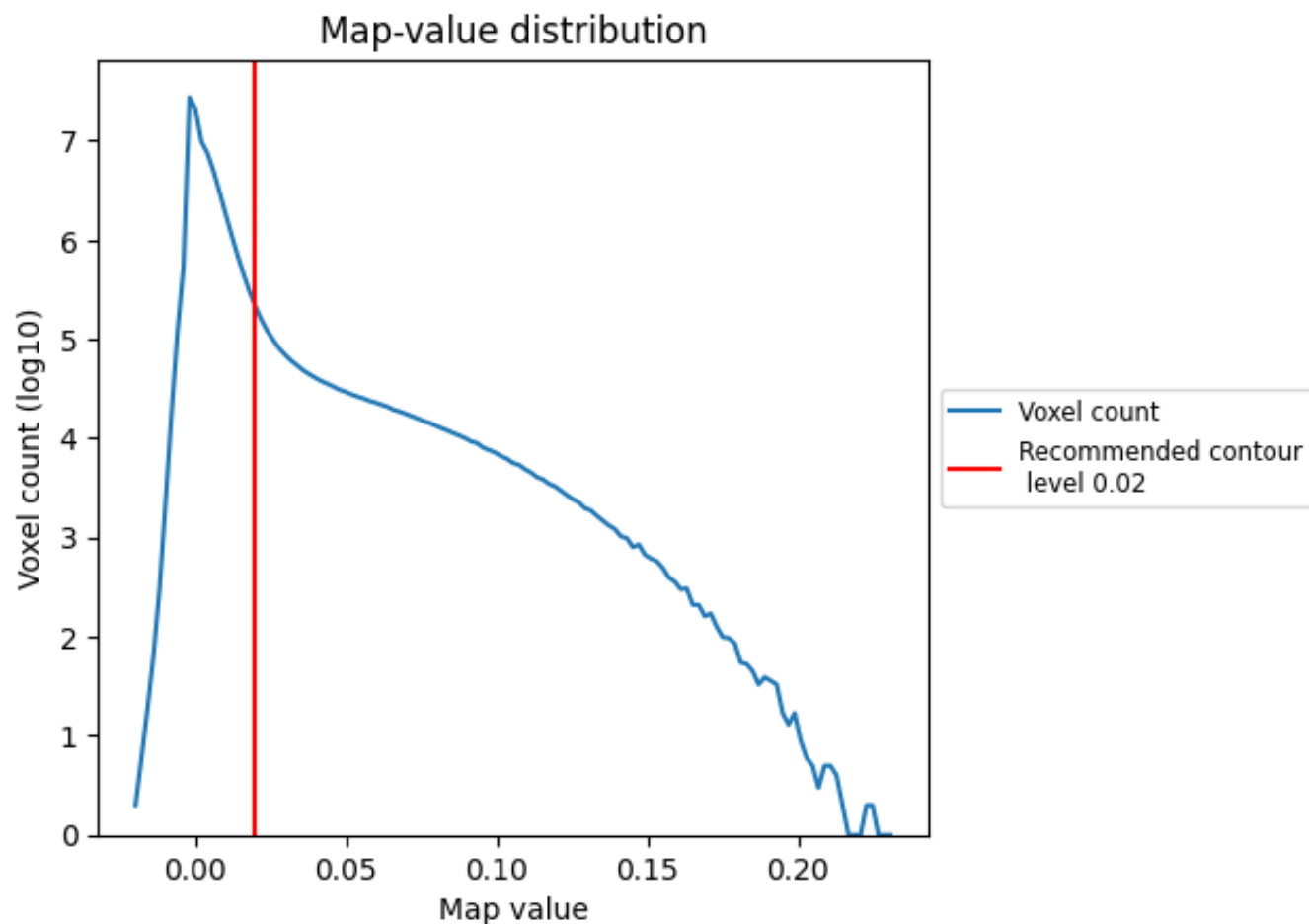
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

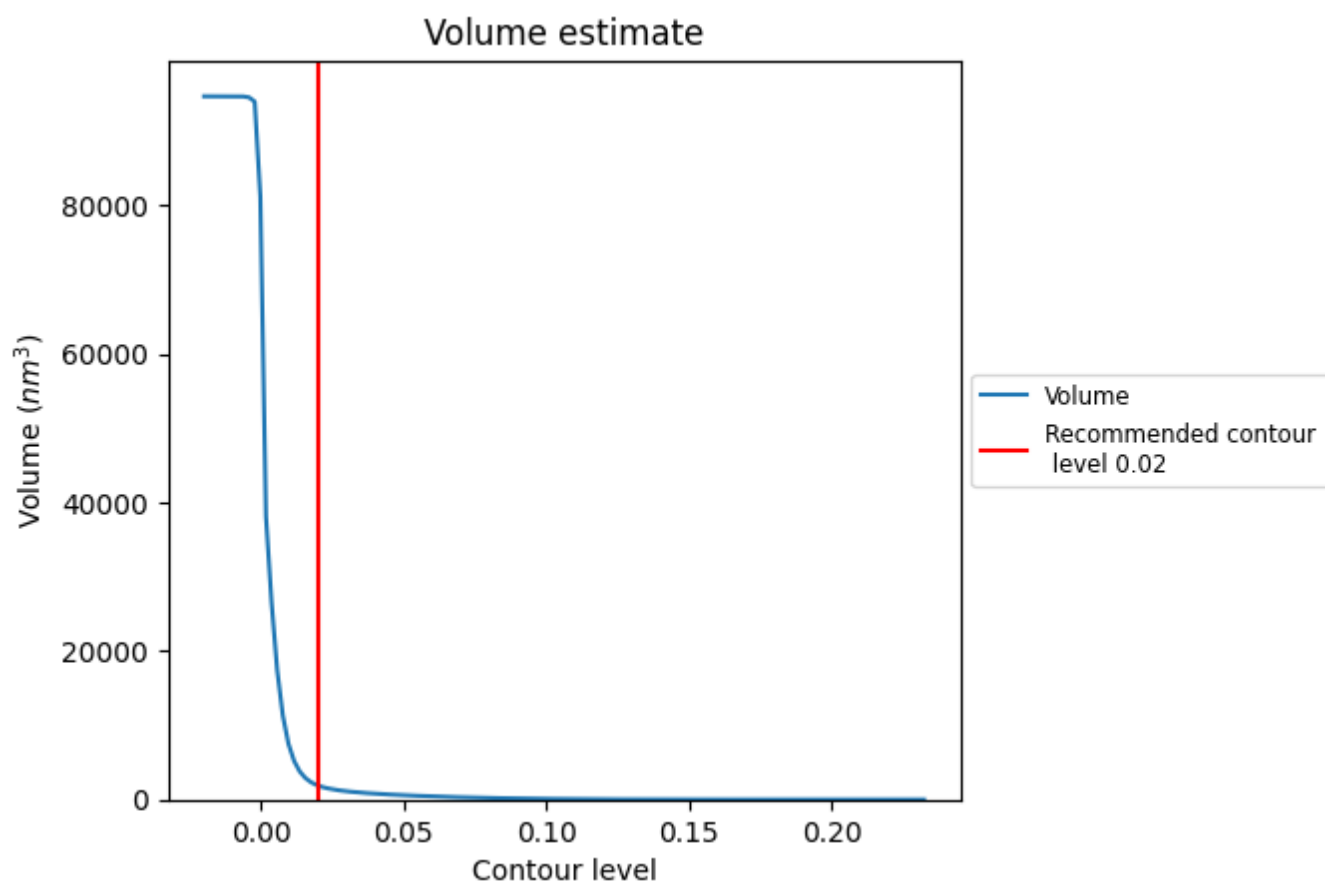
This section contains the results of statistical analysis of the map.

### 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](#)

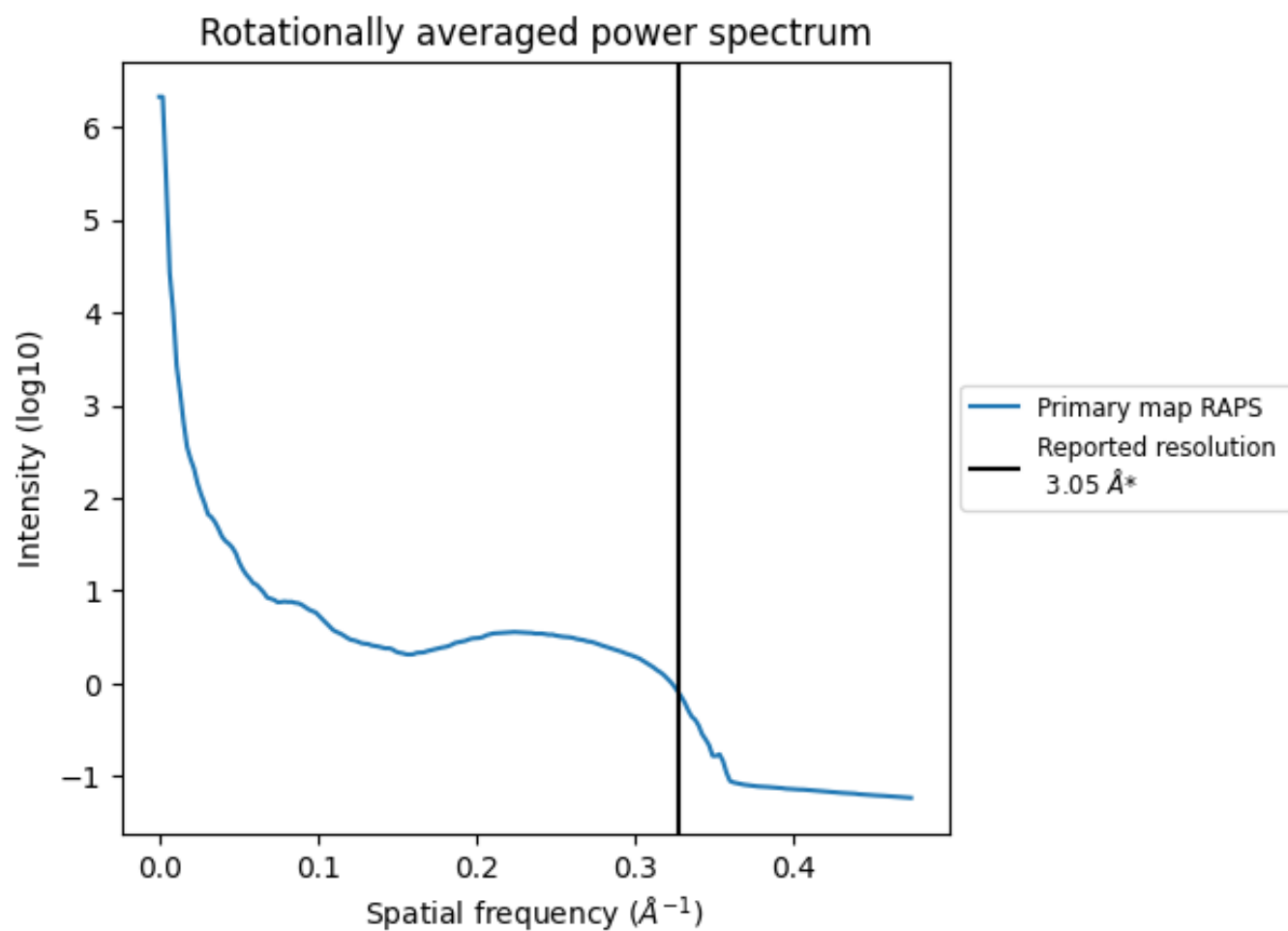


The volume at the recommended contour level is 1915  $\text{nm}^3$ ; this corresponds to an approximate mass of 1730 kDa.

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 0.328 Å<sup>-1</sup>

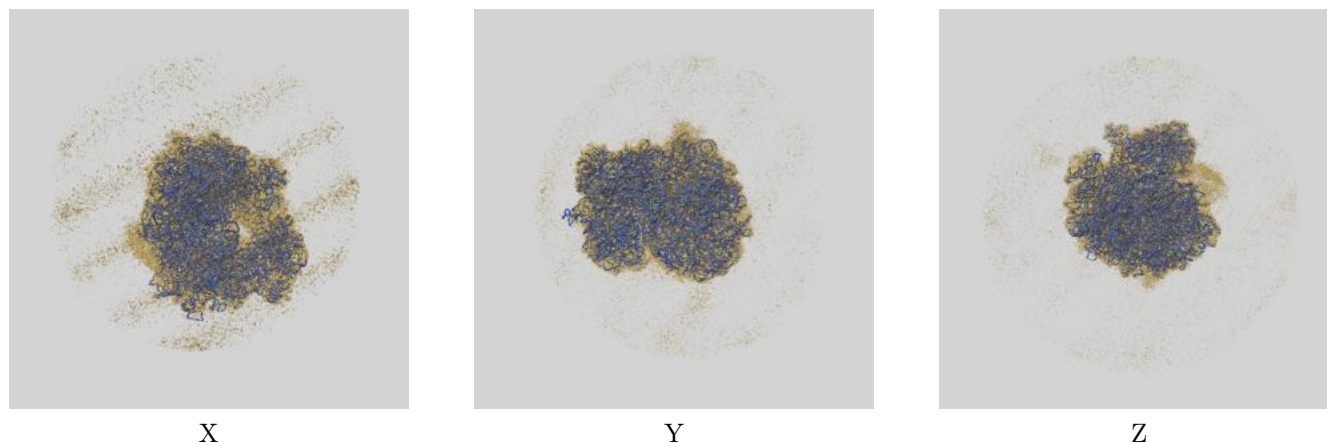
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

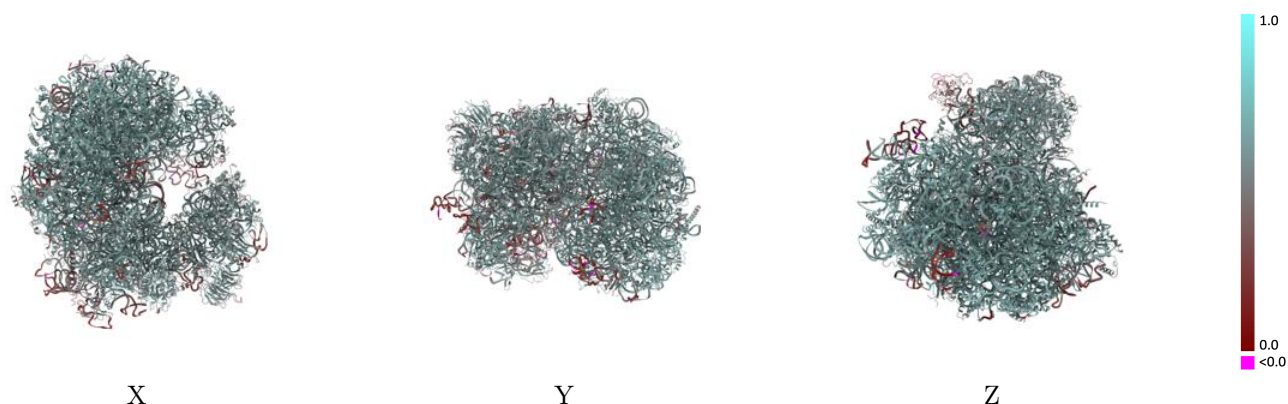
This section contains information regarding the fit between EMDB map EMD-24235 and PDB model 7N8B. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

### 9.1 Map-model overlay [i](#)



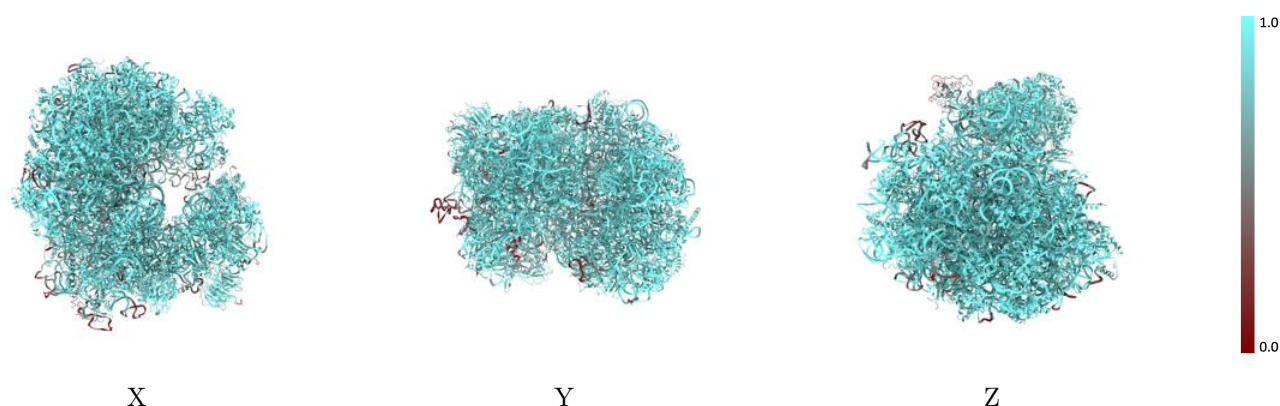
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



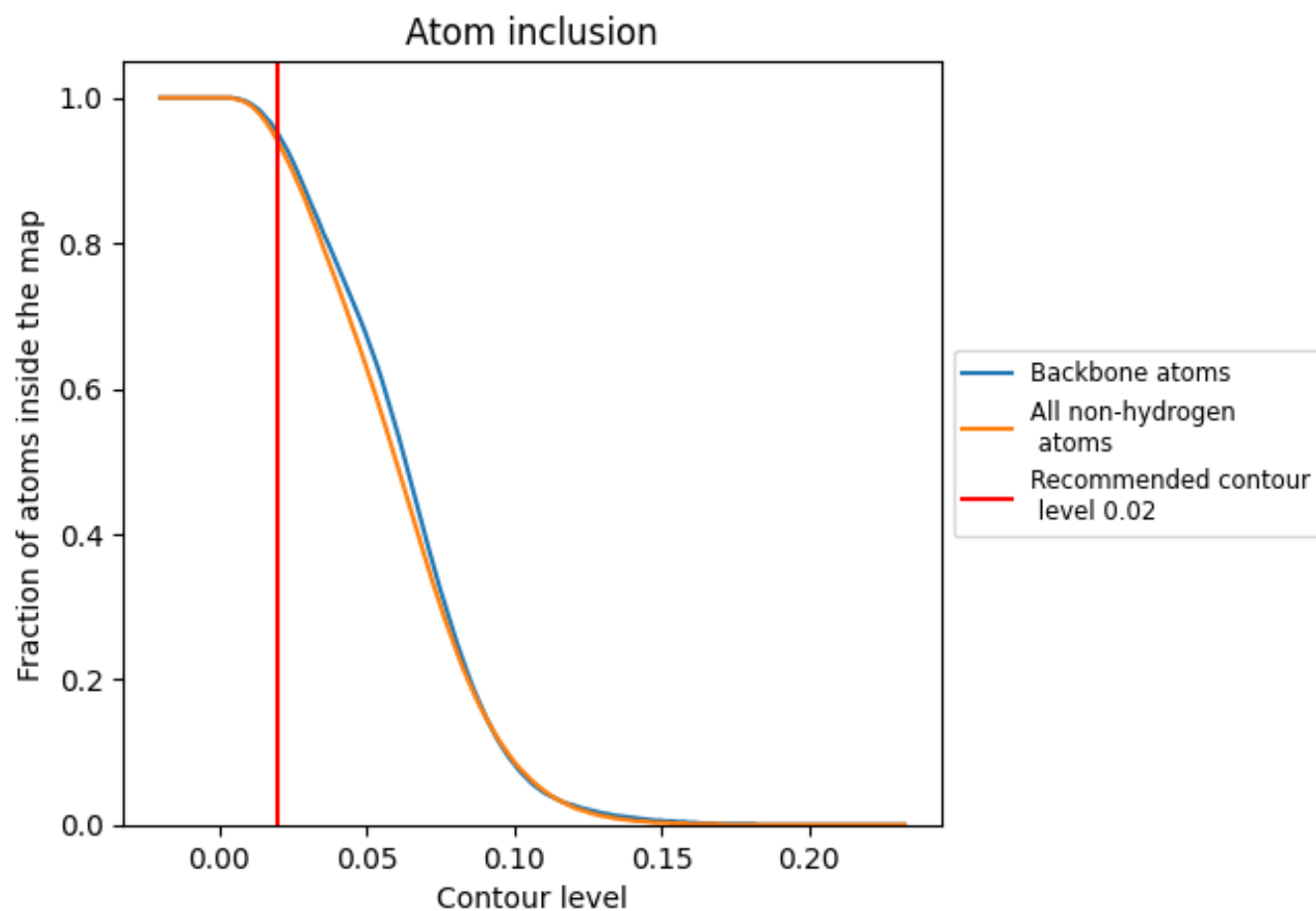
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.5700
A1	 0.9630	 0.5830
A3	 0.9940	 0.5940
A4	 0.9880	 0.6100
AA	 0.9820	 0.6150
AB	 0.9800	 0.6200
AC	 0.9750	 0.6080
AD	 0.9270	 0.5640
AE	 0.9600	 0.6000
AF	 0.9690	 0.6050
AG	 0.9430	 0.5870
AH	 0.9600	 0.5970
AI	 0.9480	 0.5810
AJ	 0.8730	 0.5080
AL	 0.9540	 0.6060
AM	 0.9710	 0.6100
AN	 0.9900	 0.6270
AO	 0.9770	 0.6120
AP	 0.9750	 0.6210
AQ	 0.9830	 0.6200
AR	 0.8830	 0.5390
AS	 0.9730	 0.6120
AT	 0.9690	 0.5970
AU	 0.9450	 0.5640
AV	 0.9740	 0.6090
AW	 0.9960	 0.6260
AX	 0.9680	 0.6080
AY	 0.9650	 0.6120
AZ	 0.9640	 0.5910
Aa	 0.9640	 0.6110
Ab	 0.9470	 0.5820
Ac	 0.9550	 0.5880
Ad	 0.9290	 0.6100
Ae	 0.9800	 0.6220
Af	 0.9940	 0.6330








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Chain	Atom inclusion	Q-score
Ag	 0.9580	 0.5980
Ah	 0.9740	 0.6150
Ai	 0.9330	 0.5620
Aj	 0.9800	 0.6190
Ak	 0.9300	 0.5730
Al	 0.9810	 0.6250
Am	 0.9400	 0.5890
An	 0.8870	 0.4910
Ao	 0.9470	 0.5910
Ap	 0.9690	 0.5960
B5	 0.9190	 0.5340
BA	 0.9460	 0.5750
BB	 0.9170	 0.5570
BC	 0.9600	 0.5870
BD	 0.9040	 0.5250
BE	 0.9540	 0.5950
BF	 0.9150	 0.5450
BG	 0.9210	 0.5630
BH	 0.8100	 0.5110
BI	 0.9430	 0.5740
BJ	 0.9280	 0.5730
BK	 0.8260	 0.4820
BL	 0.8710	 0.5500
BM	 0.3920	 0.2640
BN	 0.9490	 0.5790
BO	 0.9220	 0.5500
BP	 0.8380	 0.5160
BQ	 0.9480	 0.5790
BR	 0.8430	 0.5110
BS	 0.8920	 0.5350
BT	 0.9320	 0.5630
BU	 0.8130	 0.5050
BV	 0.9430	 0.5860
BW	 0.9730	 0.6070
BX	 0.9690	 0.5950
BY	 0.9130	 0.5750
BZ	 0.8780	 0.5410
Ba	 0.9380	 0.5700
Bb	 0.9190	 0.5710
Bc	 0.8660	 0.5190
Bd	 0.9790	 0.5790
Be	 0.9080	 0.5480

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Chain	Atom inclusion	Q-score
Bf	 0.4530	 0.2350
Bg	 0.8660	 0.5390
Bh	 0.5370	 0.3250